



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:20 AM UTC

PDB ID : 7Q57 / pdb_00007q57
EMDB ID : EMD-13828
Title : Single Particle Cryo-EM structure of photosynthetic A10B10 glyceraldehyde-3-phosphate dehydrogenase from Spinacia oleracea.
Authors : Marotta, R.; Fermani, S.; Sparla, F.; Trost, P.; Del Giudice, A.
Deposited on : 2021-11-02
Resolution : 13.00 Å (reported)
Based on initial model : 2PKQ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

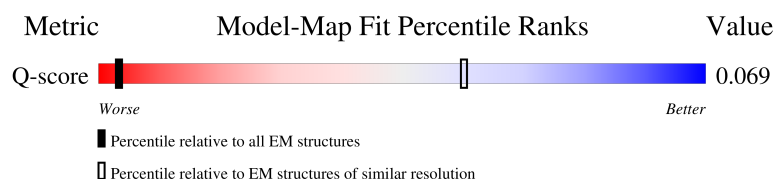
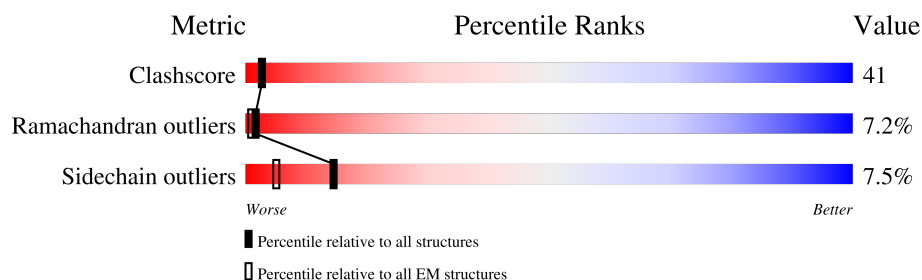
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	65 (12.50 - 13.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
1	E	451	
1	G	451	

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Mol	Chain	Length	Quality of chain
1	I	451	
1	K	451	
1	M	451	
1	O	451	
1	Q	451	
1	S	451	
2	B	337	
2	D	337	
2	F	337	
2	H	337	
2	J	337	
2	L	337	
2	N	337	
2	P	337	
2	R	337	
2	T	337	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51885 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	Q	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	A	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	C	342	Total	C	N	O	S	0	0
			2570	1629	447	485	9		
1	G	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	E	342	Total	C	N	O	S	0	0
			2570	1629	447	485	9		
1	I	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	K	342	Total	C	N	O	S	0	0
			2570	1629	447	485	9		
1	M	339	Total	C	N	O	S	0	0
			2549	1616	444	480	9		
1	S	341	Total	C	N	O	S	0	0
			2561	1624	446	482	9		

- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic.

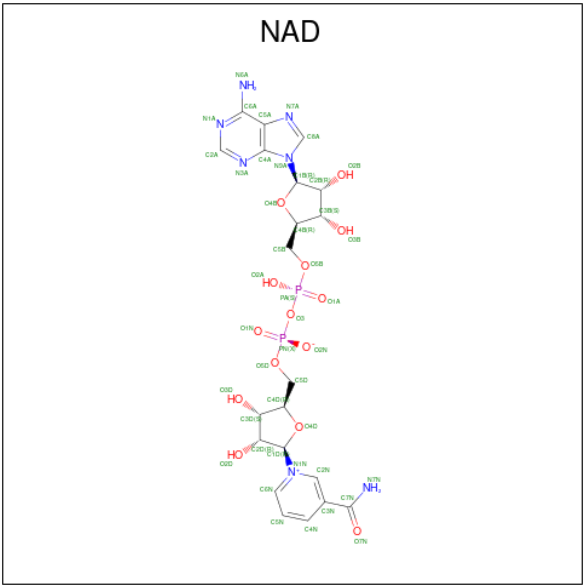
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	R	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	B	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	D	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	F	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	J	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	L	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	N	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		
2	T	337	Total	C	N	O	S	0	0
			2544	1600	445	488	11		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	O	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	P	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	Q	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	R	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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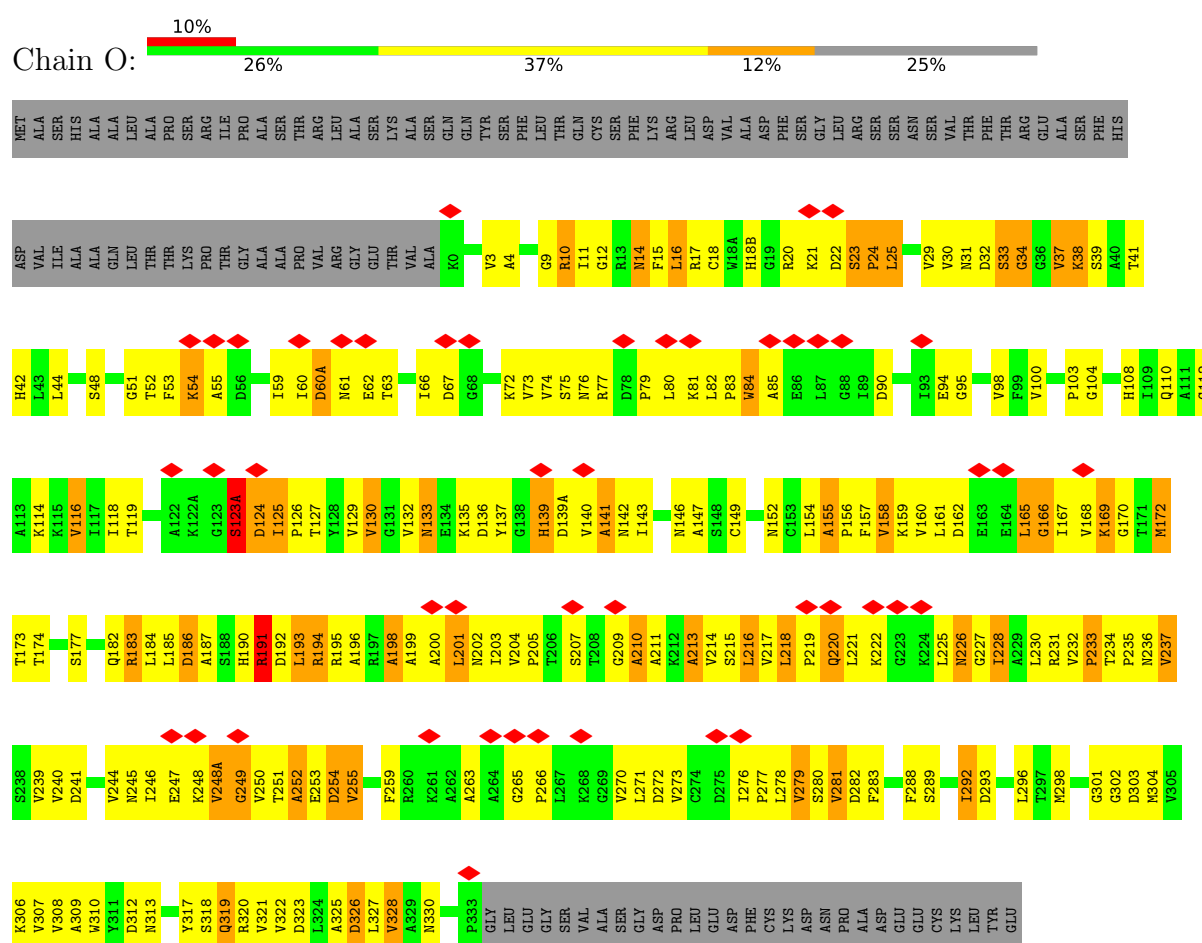
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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 44	C 21	N 7	O 14	P 2	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0
3	G	1	Total 44	C 21	N 7	O 14	P 2	0
3	H	1	Total 44	C 21	N 7	O 14	P 2	0
3	E	1	Total 44	C 21	N 7	O 14	P 2	0
3	F	1	Total 44	C 21	N 7	O 14	P 2	0
3	I	1	Total 44	C 21	N 7	O 14	P 2	0
3	J	1	Total 44	C 21	N 7	O 14	P 2	0
3	K	1	Total 44	C 21	N 7	O 14	P 2	0
3	L	1	Total 44	C 21	N 7	O 14	P 2	0
3	M	1	Total 44	C 21	N 7	O 14	P 2	0
3	N	1	Total 44	C 21	N 7	O 14	P 2	0
3	S	1	Total 44	C 21	N 7	O 14	P 2	0
3	T	1	Total 44	C 21	N 7	O 14	P 2	0

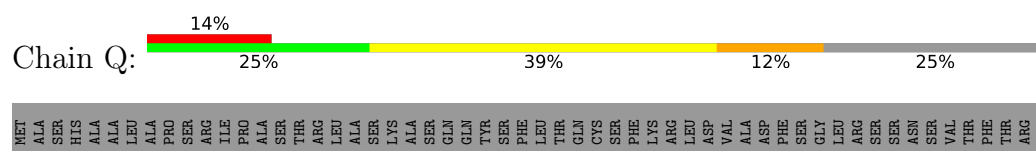
3 Residue-property plots

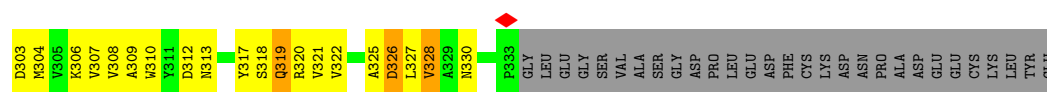
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

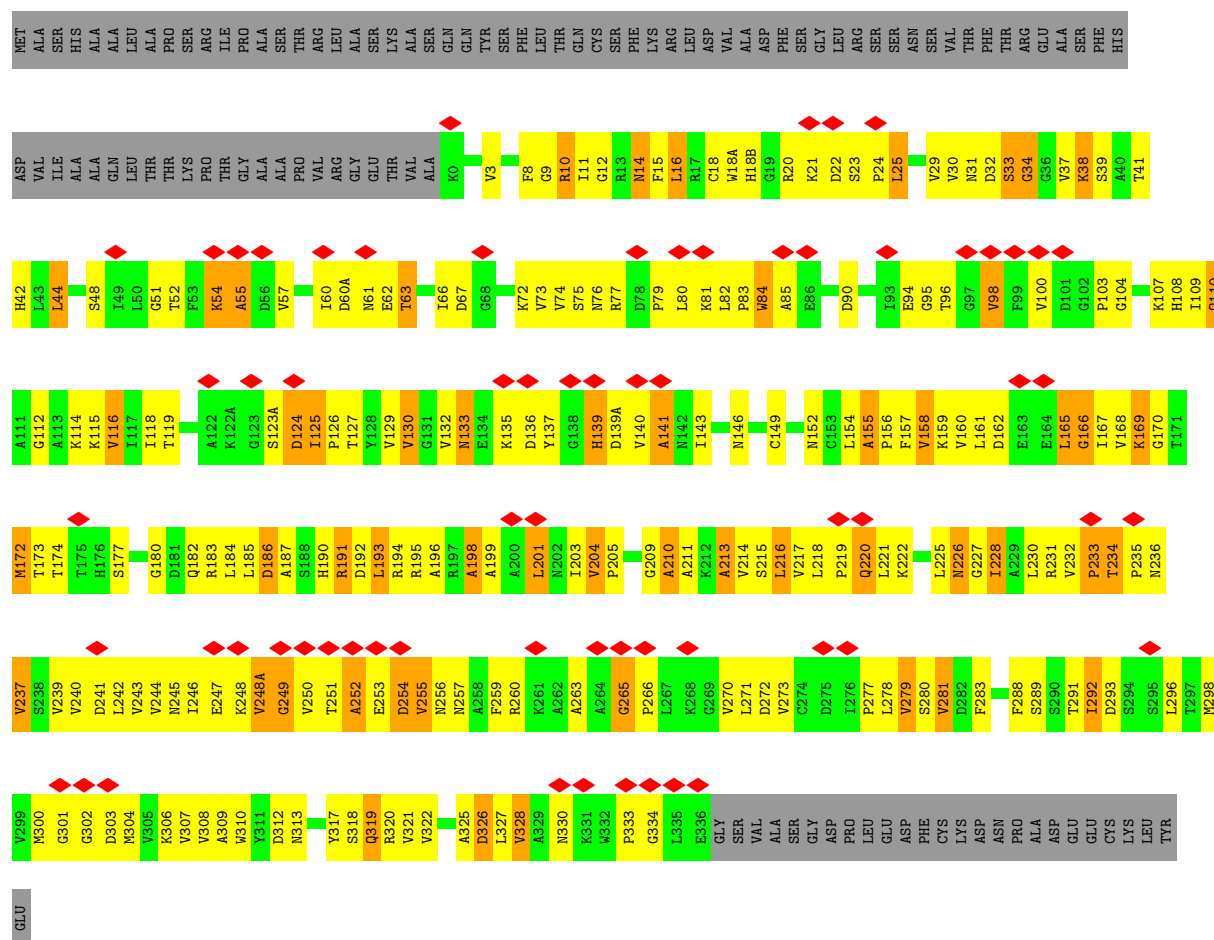
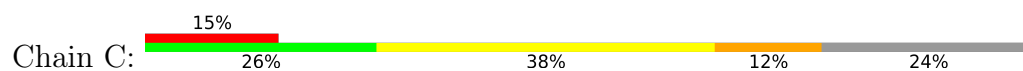


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

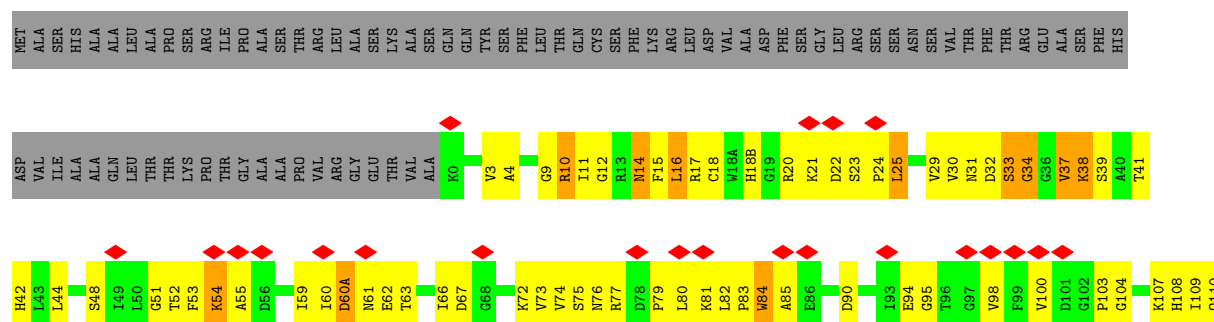
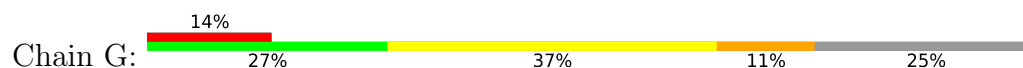


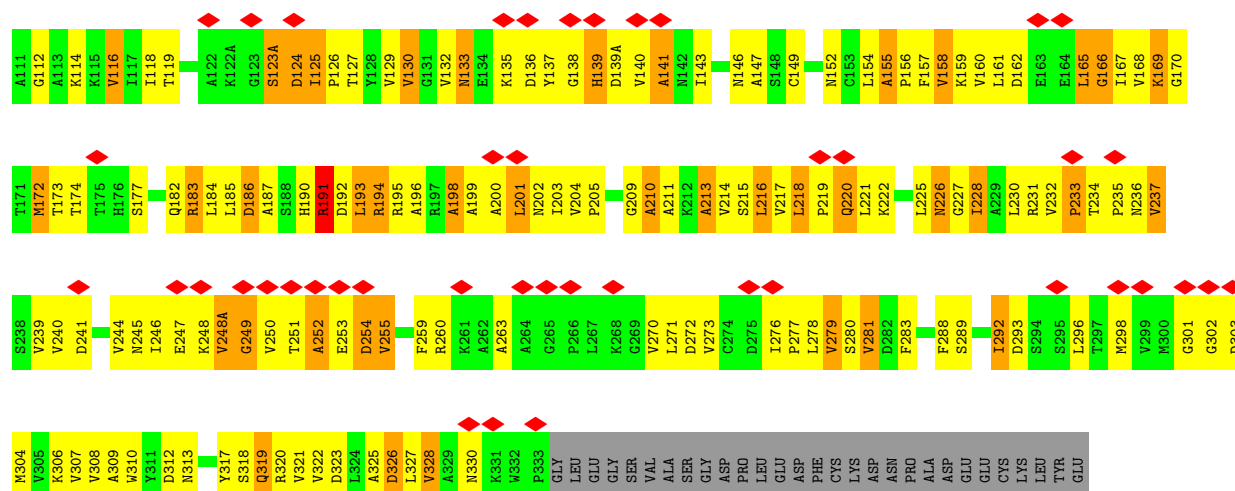


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

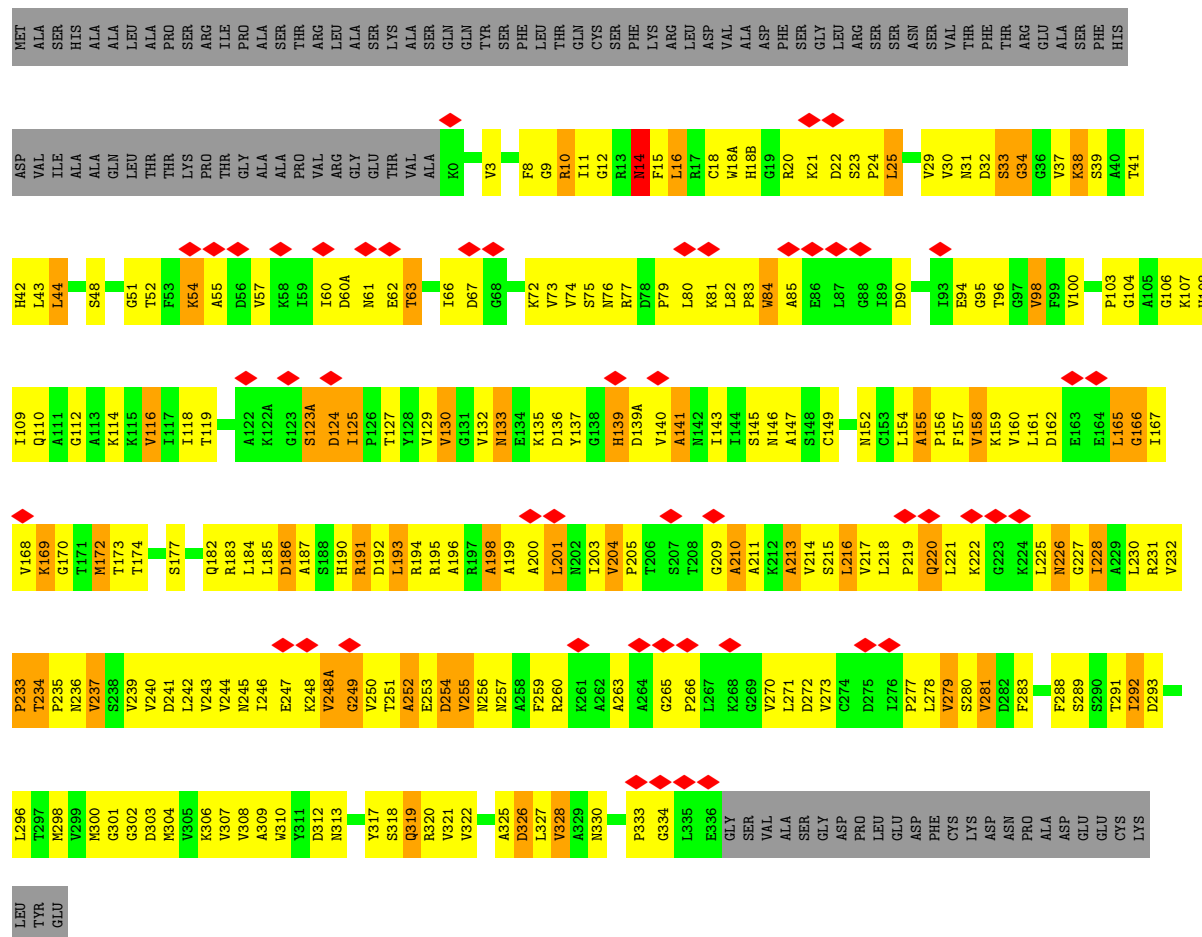
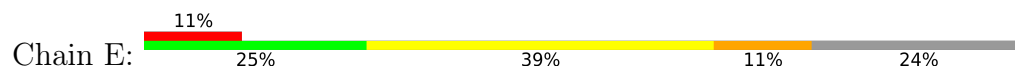


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

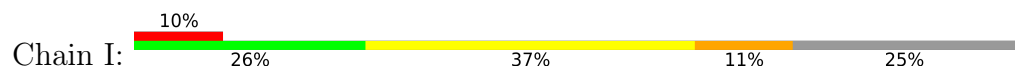


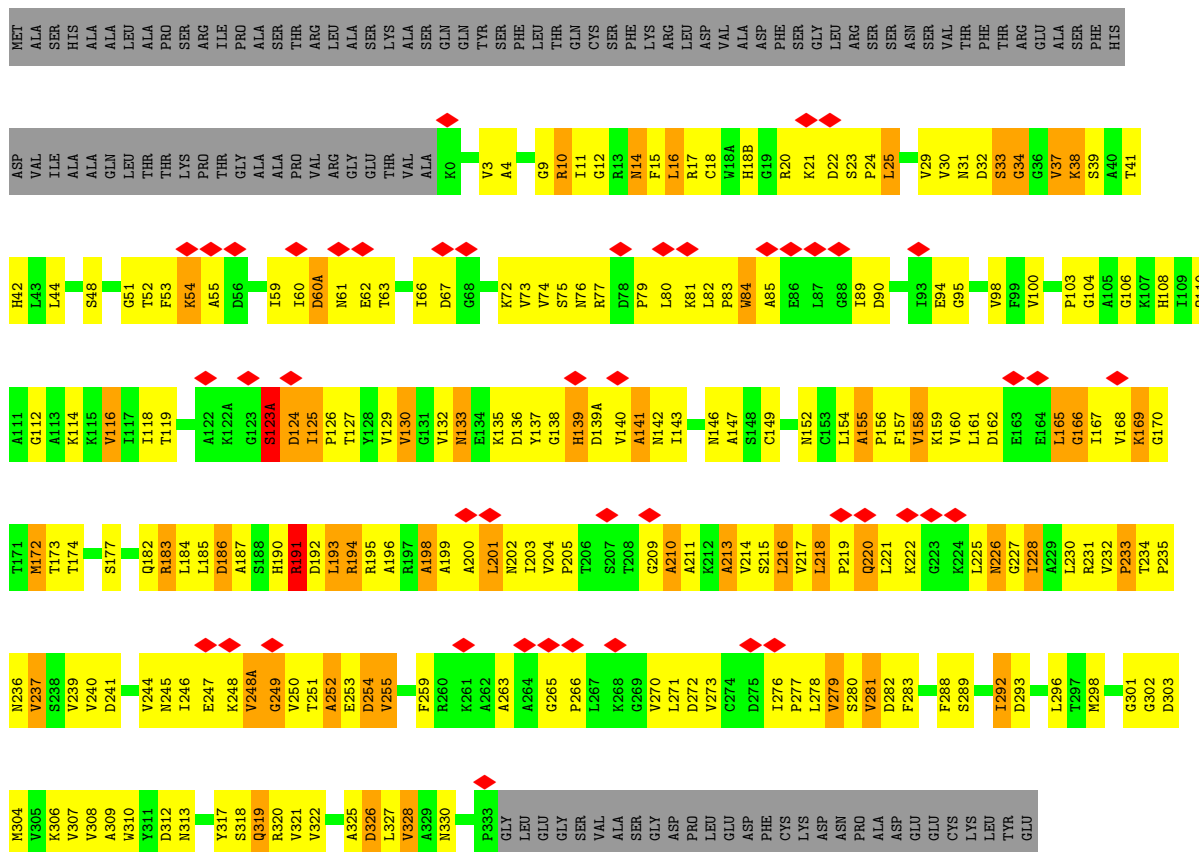


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

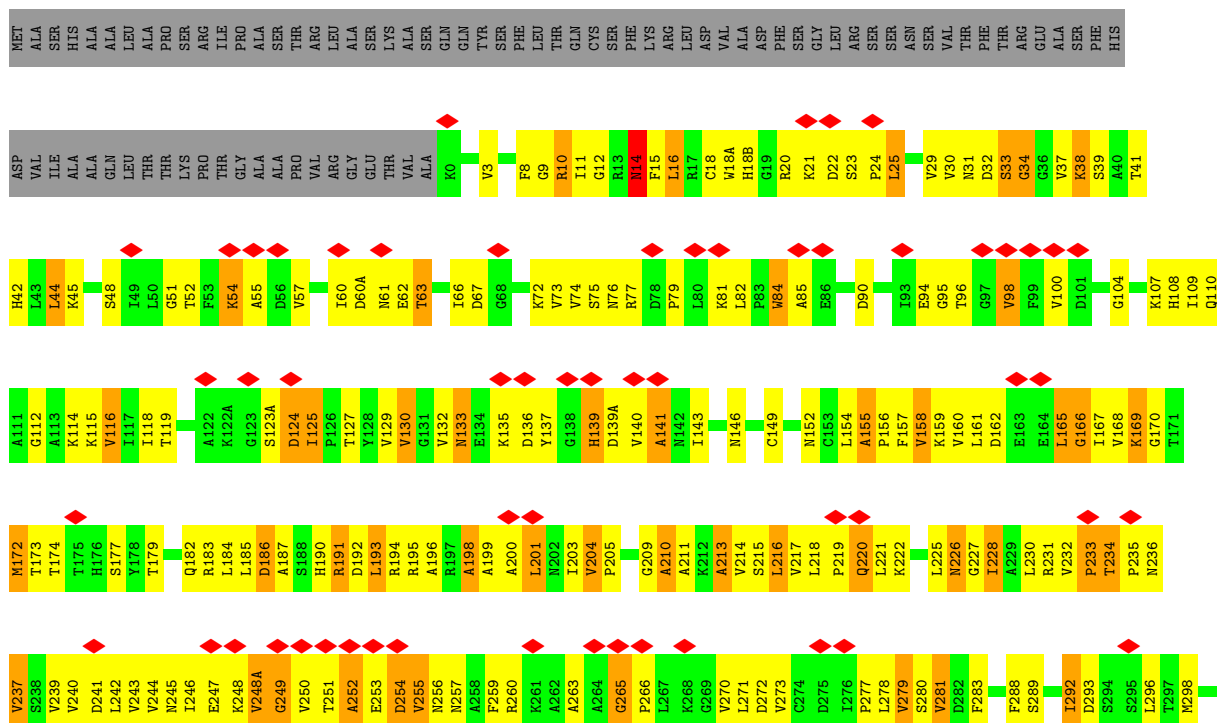
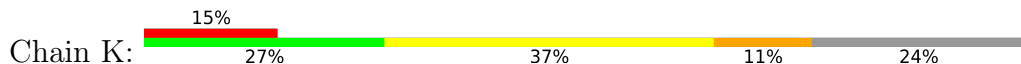


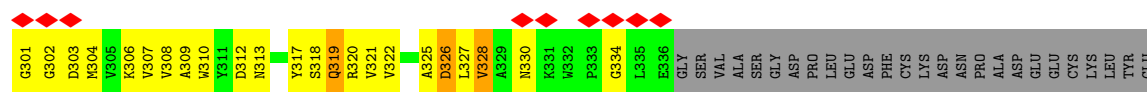
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic



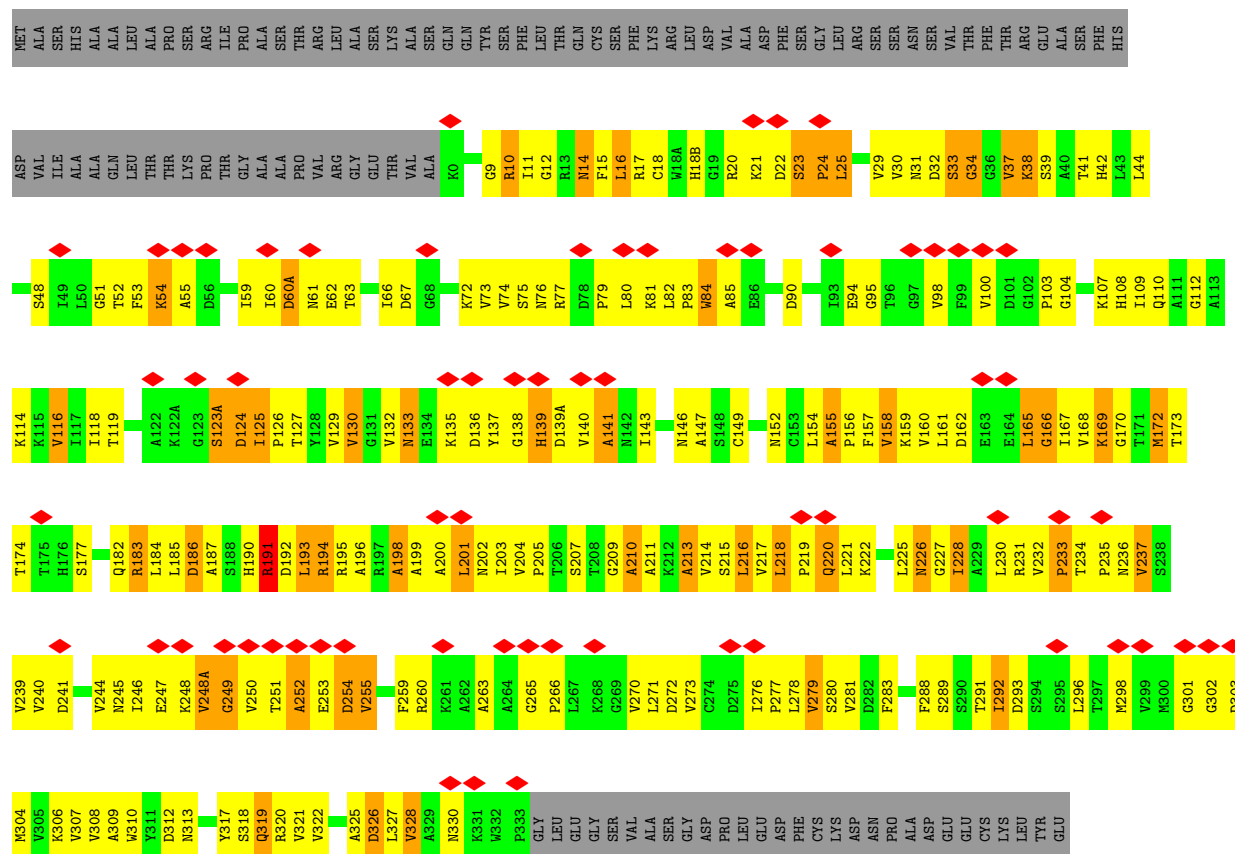
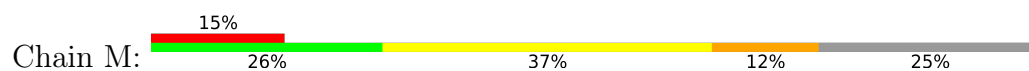


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

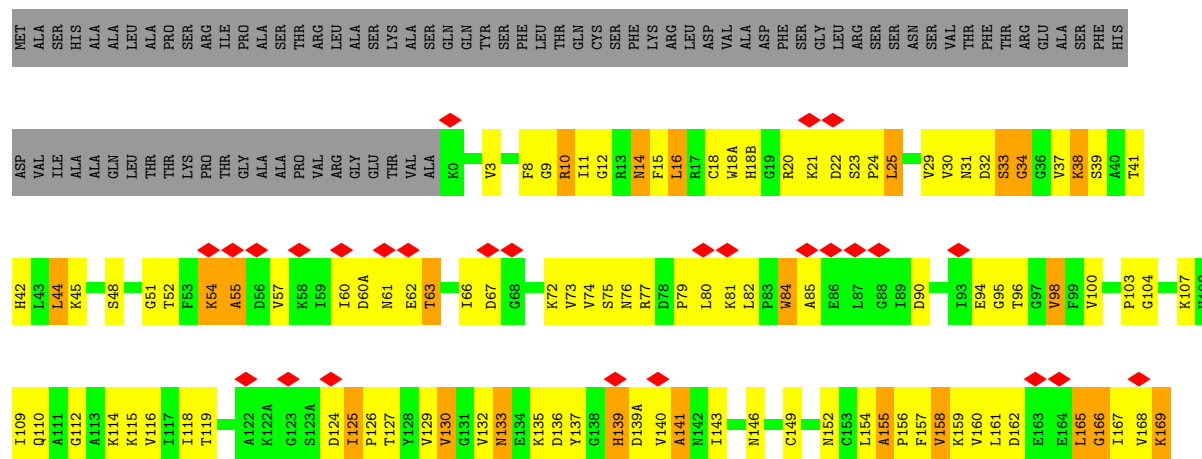
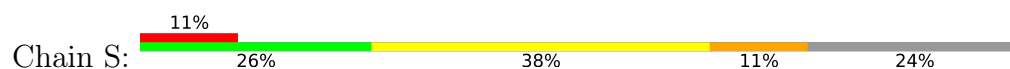


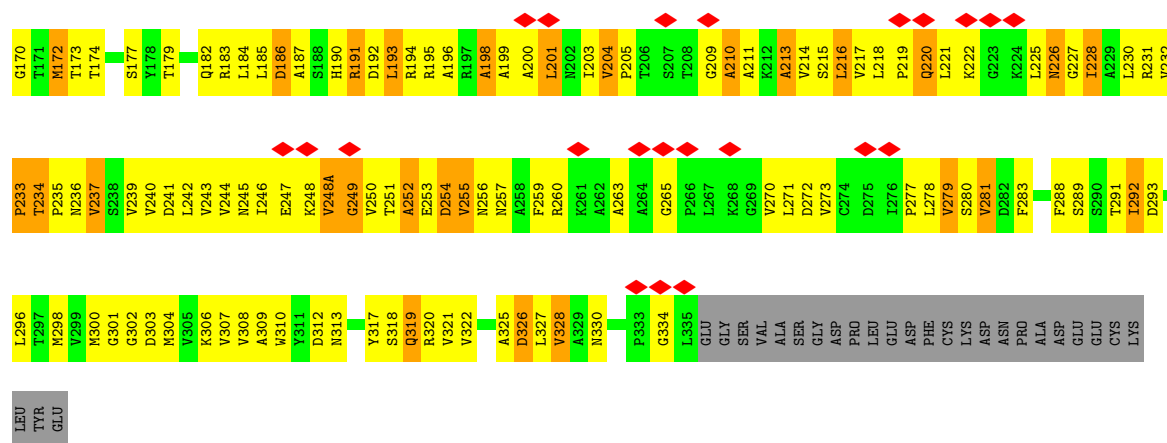


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

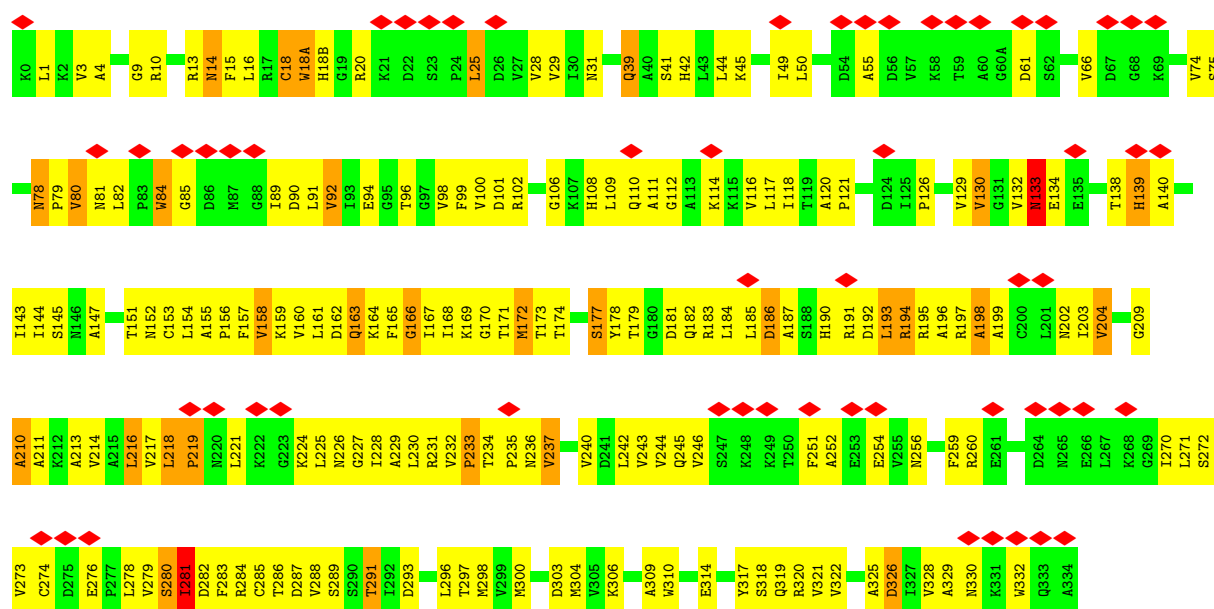


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic

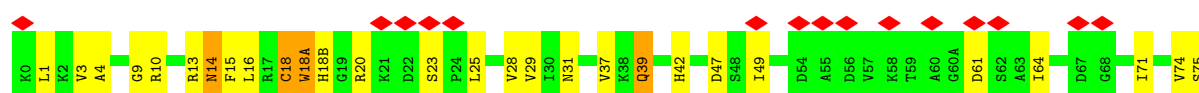


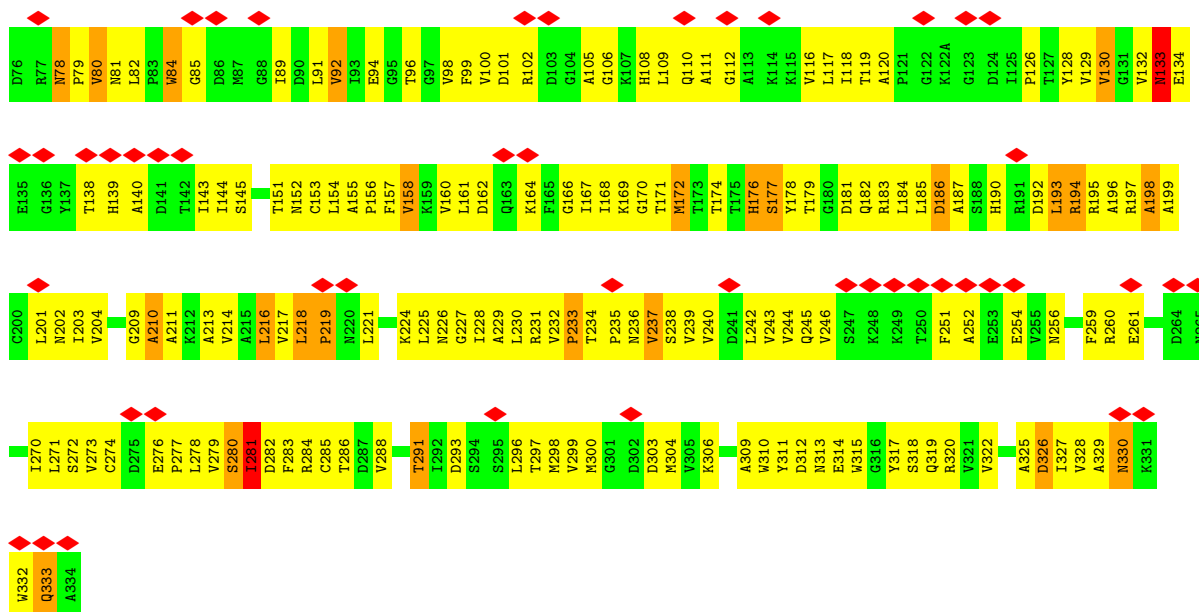


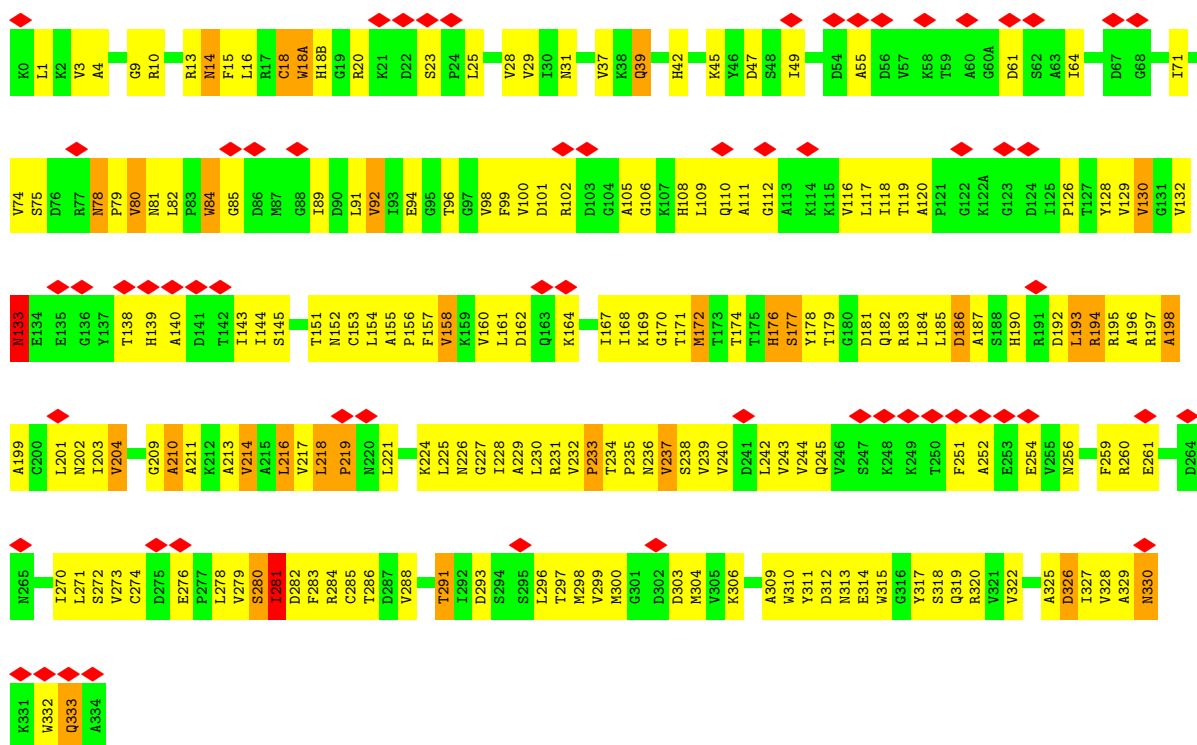
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



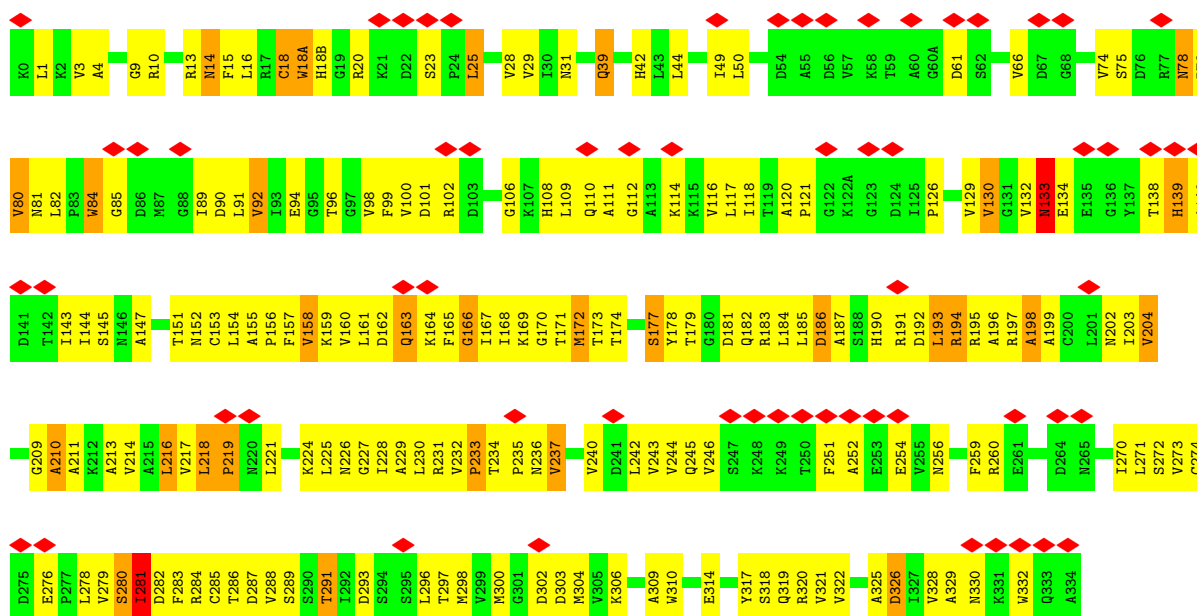
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



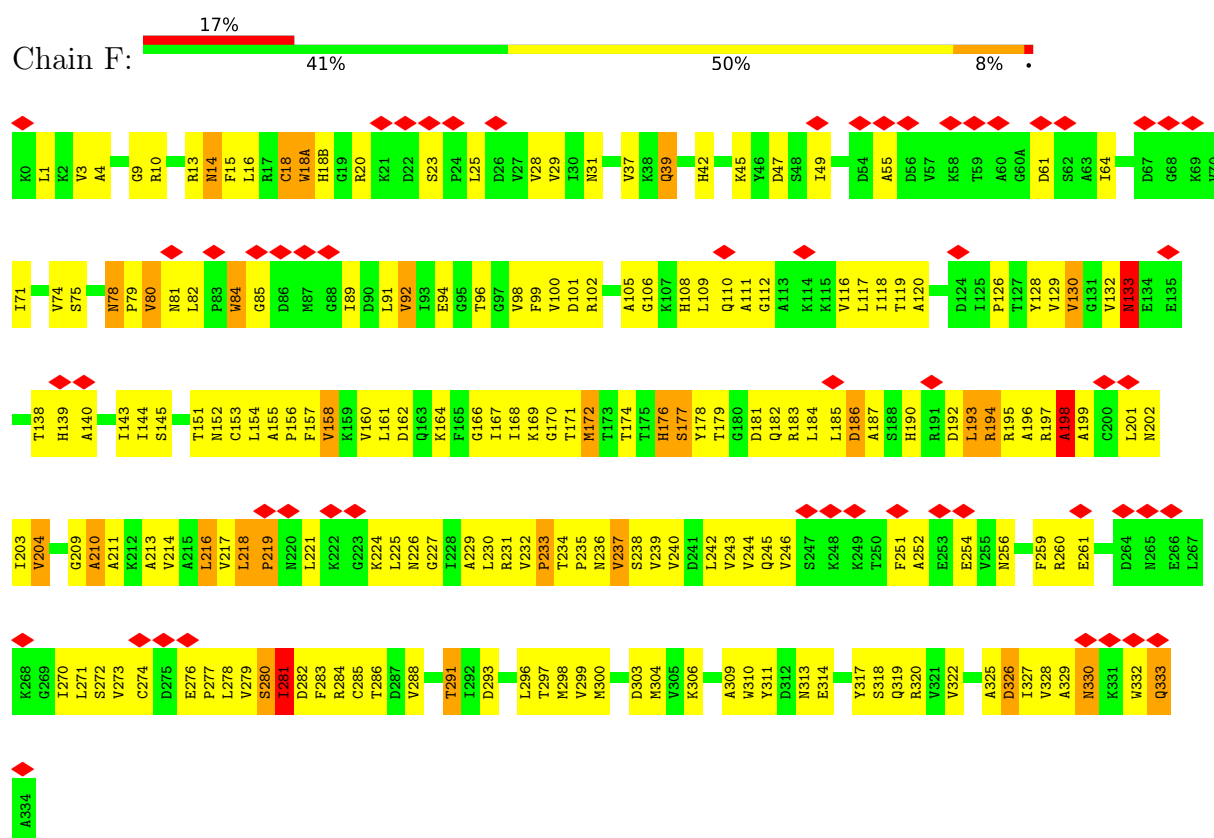




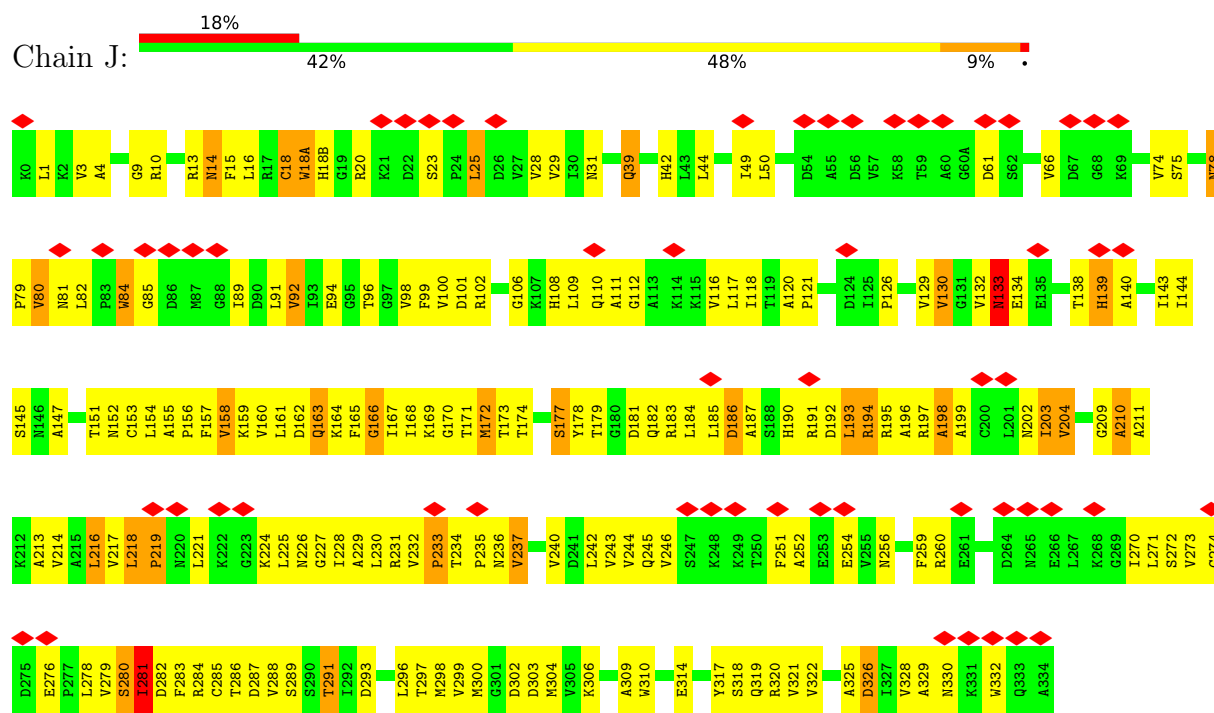
- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

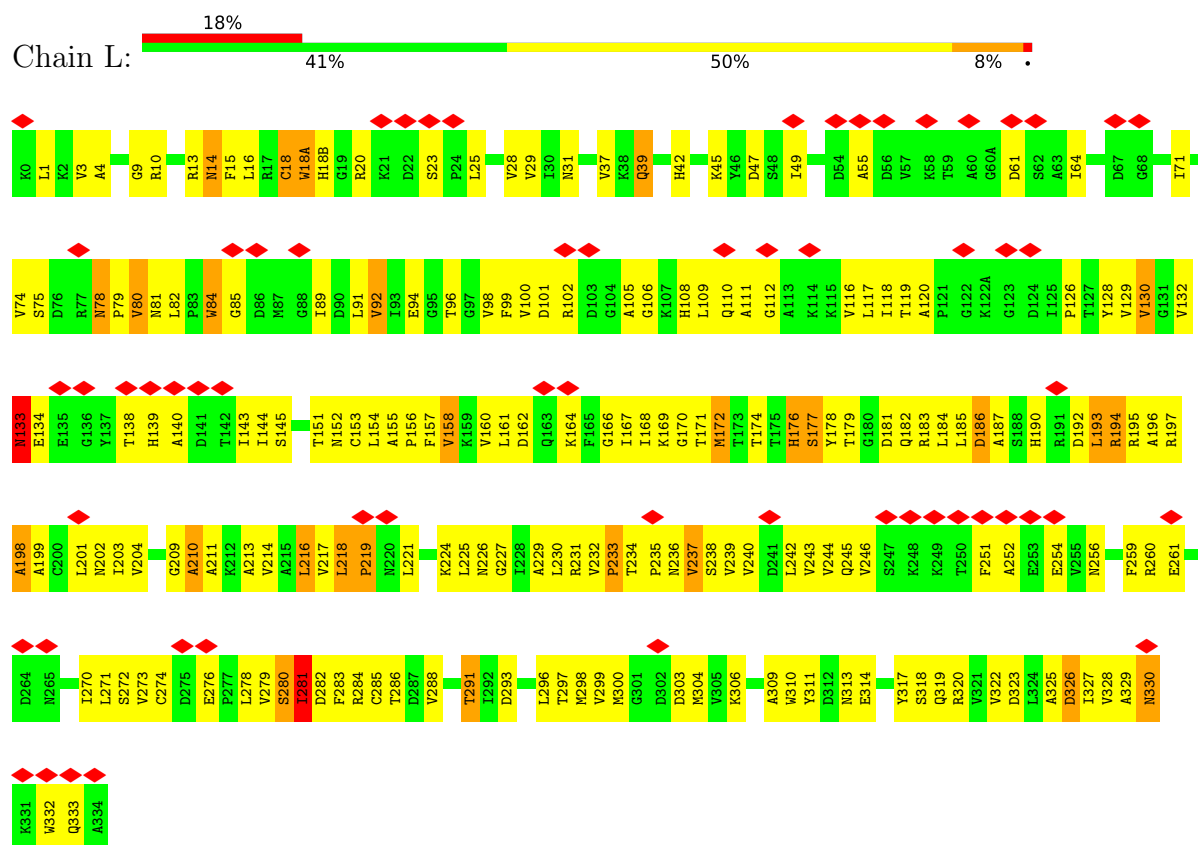


- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

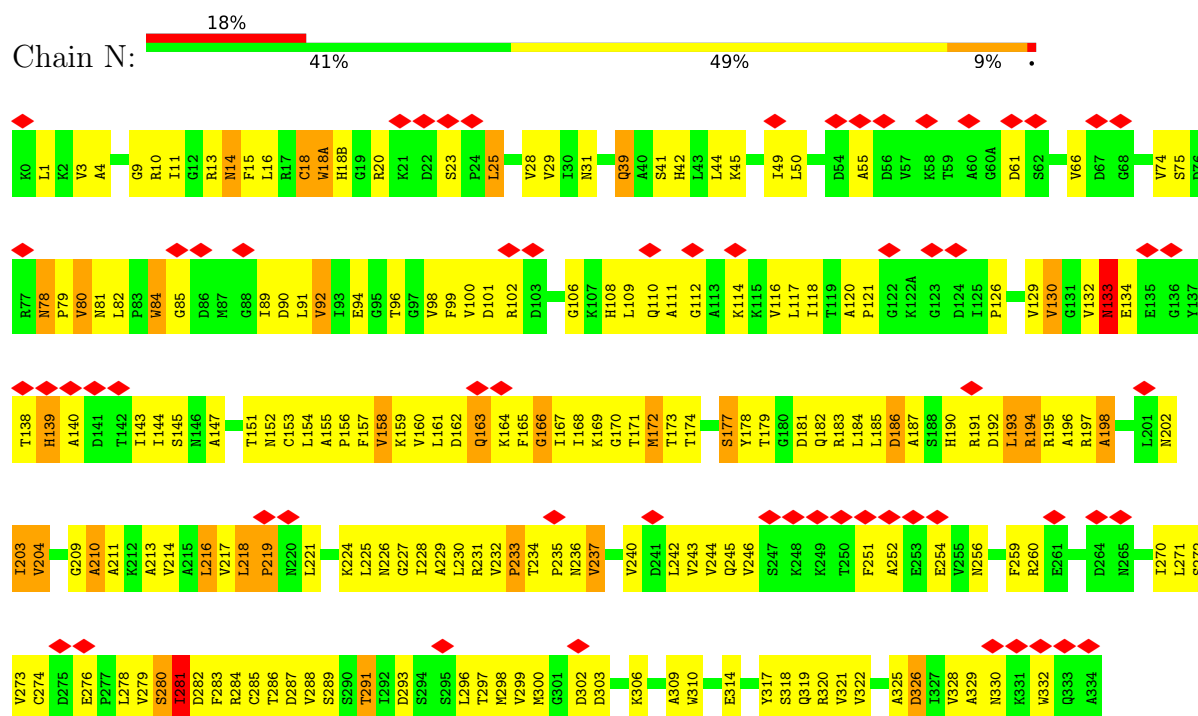


- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

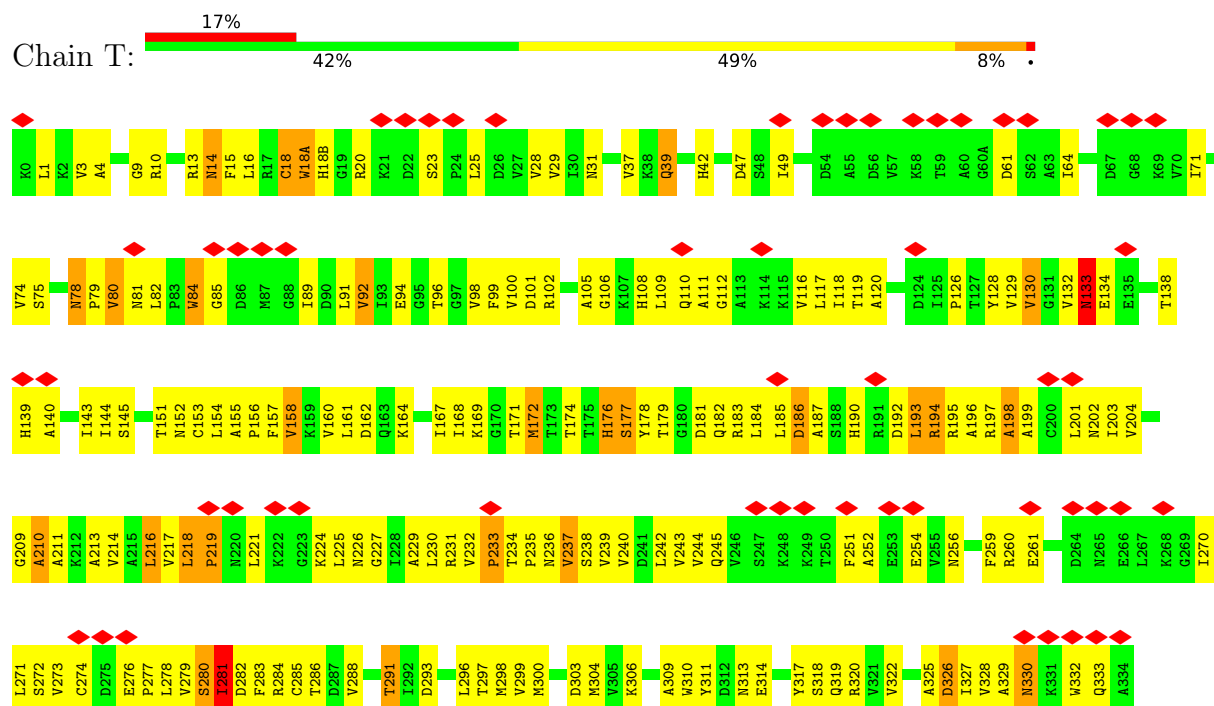
c,Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



• Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic, Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/2594 (0.0%)	1.09	18/3527 (0.5%)
1	C	0.56	2/2615 (0.1%)	1.07	21/3555 (0.6%)
1	E	0.56	2/2615 (0.1%)	1.08	20/3555 (0.6%)
1	G	0.59	1/2594 (0.0%)	1.09	19/3527 (0.5%)
1	I	0.59	1/2594 (0.0%)	1.09	18/3527 (0.5%)
1	K	0.56	2/2615 (0.1%)	1.07	23/3555 (0.6%)
1	M	0.59	1/2594 (0.0%)	1.09	18/3527 (0.5%)
1	O	0.60	1/2594 (0.0%)	1.09	19/3527 (0.5%)
1	Q	0.55	1/2594 (0.0%)	1.02	12/3527 (0.3%)
1	S	0.54	1/2606 (0.0%)	1.04	17/3543 (0.5%)
2	B	0.58	0/2585	1.02	13/3509 (0.4%)
2	D	0.55	0/2585	1.03	13/3509 (0.4%)
2	F	0.54	0/2585	1.03	13/3509 (0.4%)
2	H	0.58	0/2585	1.03	12/3509 (0.3%)
2	J	0.58	0/2585	1.03	12/3509 (0.3%)
2	L	0.54	0/2585	1.03	12/3509 (0.3%)
2	N	0.58	0/2585	1.03	12/3509 (0.3%)
2	P	0.58	0/2585	1.02	12/3509 (0.3%)
2	R	0.55	0/2585	1.03	12/3509 (0.3%)
2	T	0.54	0/2585	1.03	12/3509 (0.3%)
All	All	0.57	13/51865 (0.0%)	1.05	308/70460 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	124	ASP	CA-C	8.30	1.64	1.52
1	C	124	ASP	CA-C	8.15	1.63	1.52
1	K	124	ASP	CA-C	8.10	1.63	1.52
1	O	124	ASP	CA-C	7.83	1.63	1.52
1	I	124	ASP	CA-C	7.78	1.63	1.52
1	A	124	ASP	CA-C	7.75	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	124	ASP	CA-C	7.75	1.63	1.52
1	M	124	ASP	CA-C	7.67	1.63	1.52
1	K	234	THR	CA-CB	5.88	1.58	1.53
1	C	234	THR	CA-CB	5.69	1.58	1.53
1	E	234	THR	CA-CB	5.65	1.58	1.53
1	Q	234	THR	CA-CB	5.63	1.58	1.53
1	S	234	THR	CA-CB	5.47	1.58	1.53

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	203	ILE	N-CA-C	-10.54	92.11	108.23
1	A	203	ILE	N-CA-C	-10.50	92.17	108.23
1	G	203	ILE	N-CA-C	-10.49	92.18	108.23
1	O	203	ILE	N-CA-C	-10.47	92.20	108.23
1	I	203	ILE	N-CA-C	-10.45	92.24	108.23
1	Q	203	ILE	N-CA-C	-9.36	93.91	108.23
1	K	203	ILE	N-CA-C	-9.30	93.99	108.23
1	S	203	ILE	N-CA-C	-9.28	94.03	108.23
1	E	203	ILE	N-CA-C	-9.26	94.06	108.23
1	C	203	ILE	N-CA-C	-9.24	94.09	108.23
2	R	203	ILE	N-CA-C	-9.12	93.92	107.51
2	H	203	ILE	N-CA-C	-9.03	94.05	107.51
2	T	203	ILE	N-CA-C	-9.03	94.05	107.51
2	L	203	ILE	N-CA-C	-9.03	94.06	107.51
2	F	203	ILE	N-CA-C	-9.02	94.08	107.51
2	B	203	ILE	N-CA-C	-9.00	94.10	107.51
2	J	203	ILE	N-CA-C	-8.99	94.11	107.51
2	N	203	ILE	N-CA-C	-8.99	94.11	107.51
2	P	203	ILE	N-CA-C	-8.98	94.12	107.51
2	D	203	ILE	N-CA-C	-8.96	94.17	107.51
1	M	124	ASP	CA-C-O	8.18	129.34	120.10
1	O	124	ASP	CA-C-O	8.15	129.31	120.10
1	A	124	ASP	CA-C-O	8.11	129.26	120.10
1	G	124	ASP	CA-C-O	8.10	129.25	120.10
1	I	124	ASP	CA-C-O	8.04	129.19	120.10
1	E	124	ASP	CA-C-O	8.04	129.18	120.10
1	C	124	ASP	CA-C-O	7.97	129.11	120.10
1	K	124	ASP	CA-C-O	7.95	129.08	120.10
1	O	125	ILE	N-CA-C	7.79	125.71	108.88
1	G	125	ILE	N-CA-C	7.78	125.68	108.88
1	M	125	ILE	N-CA-C	7.76	125.65	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	ILE	N-CA-C	7.75	125.63	108.88
1	K	125	ILE	N-CA-C	7.75	125.63	108.88
1	I	125	ILE	N-CA-C	7.75	125.62	108.88
1	A	124	ASP	N-CA-C	7.75	120.62	111.71
1	A	125	ILE	N-CA-C	7.73	125.58	108.88
1	E	125	ILE	N-CA-C	7.73	125.57	108.88
1	G	124	ASP	N-CA-C	7.72	120.59	111.71
1	M	124	ASP	N-CA-C	7.70	120.57	111.71
1	O	124	ASP	N-CA-C	7.70	120.56	111.71
1	E	124	ASP	N-CA-C	7.68	120.55	111.71
1	C	124	ASP	N-CA-C	7.66	120.52	111.71
1	I	124	ASP	N-CA-C	7.65	120.50	111.71
1	K	124	ASP	N-CA-C	7.62	120.47	111.71
2	L	330	ASN	N-CA-C	-7.26	100.07	110.59
2	F	330	ASN	N-CA-C	-7.25	100.08	110.59
2	T	330	ASN	N-CA-C	-7.25	100.08	110.59
1	C	125	ILE	N-CA-CB	-7.18	101.15	111.21
2	R	330	ASN	N-CA-C	-7.18	100.18	110.59
2	D	330	ASN	N-CA-C	-7.18	100.18	110.59
1	E	125	ILE	N-CA-CB	-7.16	101.19	111.21
2	P	330	ASN	N-CA-C	-7.16	100.21	110.59
2	J	330	ASN	N-CA-C	-7.15	100.22	110.59
2	H	330	ASN	N-CA-C	-7.12	100.27	110.59
1	K	125	ILE	N-CA-CB	-7.12	101.24	111.21
2	N	330	ASN	N-CA-C	-7.11	100.29	110.59
1	I	125	ILE	N-CA-CB	-7.10	101.27	111.21
1	G	125	ILE	N-CA-CB	-7.09	101.29	111.21
2	B	330	ASN	N-CA-C	-7.07	100.33	110.59
1	M	125	ILE	N-CA-CB	-7.04	101.36	111.21
1	A	125	ILE	N-CA-CB	-7.01	101.39	111.21
1	O	125	ILE	N-CA-CB	-7.00	101.42	111.21
2	R	61	ASP	N-CA-C	-6.97	104.93	113.50
2	L	61	ASP	N-CA-C	-6.96	104.94	113.50
2	F	61	ASP	N-CA-C	-6.91	105.00	113.50
2	D	61	ASP	N-CA-C	-6.90	105.01	113.50
2	T	61	ASP	N-CA-C	-6.90	105.01	113.50
2	R	78	ASN	CA-C-N	6.90	126.41	119.24
2	R	78	ASN	C-N-CA	6.90	126.41	119.24
2	D	78	ASN	CA-C-N	6.90	126.41	119.24
2	D	78	ASN	C-N-CA	6.90	126.41	119.24
2	T	78	ASN	CA-C-N	6.88	126.40	119.24
2	T	78	ASN	C-N-CA	6.88	126.40	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	78	ASN	CA-C-N	6.82	126.33	119.24
2	L	78	ASN	C-N-CA	6.82	126.33	119.24
1	I	325	ALA	N-CA-C	-6.78	104.83	113.23
2	F	78	ASN	CA-C-N	6.75	126.26	119.24
2	F	78	ASN	C-N-CA	6.75	126.26	119.24
1	A	325	ALA	N-CA-C	-6.73	104.89	113.23
1	M	325	ALA	N-CA-C	-6.70	104.92	113.23
1	G	325	ALA	N-CA-C	-6.68	104.94	113.23
1	O	325	ALA	N-CA-C	-6.66	104.97	113.23
1	O	255	VAL	N-CA-C	-6.57	103.46	110.36
2	H	61	ASP	N-CA-C	-6.56	105.43	113.50
1	C	255	VAL	N-CA-C	-6.56	103.47	110.36
1	K	255	VAL	N-CA-C	-6.54	103.49	110.36
1	A	255	VAL	N-CA-C	-6.54	103.50	110.36
2	B	61	ASP	N-CA-C	-6.52	105.47	113.50
1	M	255	VAL	N-CA-C	-6.52	103.52	110.36
2	N	61	ASP	N-CA-C	-6.51	105.49	113.50
2	J	61	ASP	N-CA-C	-6.51	105.49	113.50
1	E	255	VAL	N-CA-C	-6.50	103.53	110.36
2	P	61	ASP	N-CA-C	-6.50	105.51	113.50
1	I	255	VAL	N-CA-C	-6.49	103.55	110.36
1	G	255	VAL	N-CA-C	-6.48	103.55	110.36
1	S	255	VAL	N-CA-C	-6.46	103.58	110.36
2	R	158	VAL	N-CA-C	-6.44	103.98	111.00
2	F	158	VAL	N-CA-C	-6.44	103.98	111.00
2	D	158	VAL	N-CA-C	-6.44	103.98	111.00
1	Q	255	VAL	N-CA-C	-6.43	103.61	110.36
1	Q	325	ALA	N-CA-C	-6.43	105.26	113.23
1	C	325	ALA	N-CA-C	-6.42	105.26	113.23
2	T	158	VAL	N-CA-C	-6.42	104.00	111.00
2	L	158	VAL	N-CA-C	-6.42	104.01	111.00
1	K	325	ALA	N-CA-C	-6.42	105.28	113.23
1	M	61	ASN	N-CA-C	-6.36	104.77	113.30
1	I	61	ASN	N-CA-C	-6.36	104.78	113.30
1	E	325	ALA	N-CA-C	-6.34	105.37	113.23
1	A	61	ASN	N-CA-C	-6.33	104.82	113.30
1	K	61	ASN	N-CA-C	-6.32	104.83	113.30
1	G	61	ASN	N-CA-C	-6.32	104.83	113.30
1	S	325	ALA	N-CA-C	-6.31	105.40	113.23
1	O	61	ASN	N-CA-C	-6.31	104.85	113.30
1	C	61	ASN	N-CA-C	-6.29	104.87	113.30
1	E	61	ASN	N-CA-C	-6.29	104.87	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	61	ASN	N-CA-C	-6.26	104.91	113.30
1	Q	61	ASN	N-CA-C	-6.25	104.92	113.30
2	N	194	ARG	N-CA-C	-6.22	102.04	111.56
2	P	194	ARG	N-CA-C	-6.22	102.05	111.56
2	B	194	ARG	N-CA-C	-6.21	102.06	111.56
2	J	194	ARG	N-CA-C	-6.19	102.09	111.56
2	H	194	ARG	N-CA-C	-6.17	102.12	111.56
1	O	123(A)	SER	N-CA-C	-6.11	97.79	110.80
1	I	123(A)	SER	N-CA-C	-6.08	97.84	110.80
1	A	123(A)	SER	N-CA-C	-6.07	97.88	110.80
1	M	123(A)	SER	N-CA-C	-6.06	97.89	110.80
1	G	123(A)	SER	N-CA-C	-6.05	97.91	110.80
1	G	125	ILE	CA-C-N	5.99	125.75	119.76
1	G	125	ILE	C-N-CA	5.99	125.75	119.76
1	I	125	ILE	CA-C-N	5.94	125.70	119.76
1	I	125	ILE	C-N-CA	5.94	125.70	119.76
1	A	125	ILE	CA-C-N	5.94	125.70	119.76
1	A	125	ILE	C-N-CA	5.94	125.70	119.76
1	O	125	ILE	CA-C-N	5.93	125.69	119.76
1	O	125	ILE	C-N-CA	5.93	125.69	119.76
2	B	158	VAL	N-CA-C	-5.93	104.53	111.00
1	M	125	ILE	CA-C-N	5.93	125.69	119.76
1	M	125	ILE	C-N-CA	5.93	125.69	119.76
2	N	158	VAL	N-CA-C	-5.92	104.55	111.00
2	L	194	ARG	N-CA-C	-5.88	102.56	111.56
2	D	194	ARG	N-CA-C	-5.88	102.57	111.56
2	F	194	ARG	N-CA-C	-5.87	102.58	111.56
2	P	158	VAL	N-CA-C	-5.86	104.61	111.00
2	H	158	VAL	N-CA-C	-5.86	104.61	111.00
2	R	194	ARG	N-CA-C	-5.85	102.61	111.56
2	T	194	ARG	N-CA-C	-5.83	102.64	111.56
2	J	158	VAL	N-CA-C	-5.83	104.65	111.00
2	H	177	SER	N-CA-C	-5.81	102.82	110.43
1	C	123(A)	SER	N-CA-C	-5.80	98.44	110.80
2	N	177	SER	N-CA-C	-5.80	102.83	110.43
1	E	123(A)	SER	N-CA-C	-5.78	98.48	110.80
2	J	177	SER	N-CA-C	-5.78	102.86	110.43
1	K	123(A)	SER	N-CA-C	-5.78	98.48	110.80
2	P	177	SER	N-CA-C	-5.78	102.86	110.43
2	B	177	SER	N-CA-C	-5.78	102.86	110.43
1	K	125	ILE	CA-C-N	5.73	125.49	119.76
1	K	125	ILE	C-N-CA	5.73	125.49	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75	SER	N-CA-C	5.70	117.25	107.28
2	N	75	SER	N-CA-C	5.70	117.25	107.28
1	C	125	ILE	CA-C-N	5.69	125.45	119.76
1	C	125	ILE	C-N-CA	5.69	125.45	119.76
1	C	54	LYS	N-CA-C	5.68	118.43	109.39
1	E	125	ILE	CA-C-N	5.68	125.44	119.76
1	E	125	ILE	C-N-CA	5.68	125.44	119.76
2	B	75	SER	N-CA-C	5.67	117.19	107.28
1	Q	54	LYS	N-CA-C	5.66	118.38	109.39
1	S	125	ILE	CA-C-N	5.65	125.41	119.76
1	S	125	ILE	C-N-CA	5.65	125.41	119.76
2	P	75	SER	N-CA-C	5.64	117.16	107.28
1	K	54	LYS	N-CA-C	5.64	118.37	109.39
1	E	54	LYS	N-CA-C	5.64	118.36	109.39
2	F	177	SER	N-CA-C	-5.64	103.04	110.43
2	J	75	SER	N-CA-C	5.62	117.12	107.28
1	S	54	LYS	N-CA-C	5.62	118.33	109.39
1	I	54	LYS	N-CA-C	5.61	118.28	108.52
1	O	194	ARG	N-CA-C	-5.61	105.22	112.68
1	I	194	ARG	N-CA-C	-5.60	105.23	112.68
1	A	194	ARG	N-CA-C	-5.60	105.23	112.68
2	D	177	SER	N-CA-C	-5.59	103.11	110.43
1	G	194	ARG	N-CA-C	-5.58	105.26	112.68
1	M	194	ARG	N-CA-C	-5.57	105.28	112.68
2	L	177	SER	N-CA-C	-5.57	103.14	110.43
1	O	54	LYS	N-CA-C	5.56	118.20	108.52
1	G	54	LYS	N-CA-C	5.56	118.19	108.52
1	A	54	LYS	N-CA-C	5.55	118.17	108.52
1	G	158	VAL	N-CA-C	-5.55	105.11	110.72
2	R	177	SER	N-CA-C	-5.54	103.17	110.43
1	M	54	LYS	N-CA-C	5.54	118.15	108.52
2	J	44	LEU	N-CA-C	-5.53	105.27	112.23
2	T	177	SER	N-CA-C	-5.53	103.19	110.43
1	A	158	VAL	N-CA-C	-5.52	105.14	110.72
2	H	44	LEU	N-CA-C	-5.52	105.28	112.23
1	M	158	VAL	N-CA-C	-5.50	105.16	110.72
2	B	44	LEU	N-CA-C	-5.48	105.32	112.23
1	O	158	VAL	N-CA-C	-5.47	105.20	110.72
1	E	158	VAL	N-CA-C	-5.46	105.05	111.00
2	R	218	LEU	CA-C-N	5.45	126.66	119.84
2	R	218	LEU	C-N-CA	5.45	126.66	119.84
1	C	334	GLY	N-CA-C	-5.45	100.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	158	VAL	N-CA-C	-5.45	105.21	110.72
2	N	44	LEU	N-CA-C	-5.45	105.36	112.23
1	K	334	GLY	N-CA-C	-5.45	100.27	113.18
2	T	218	LEU	CA-C-N	5.44	126.64	119.84
2	T	218	LEU	C-N-CA	5.44	126.64	119.84
2	P	44	LEU	N-CA-C	-5.44	105.38	112.23
1	K	158	VAL	N-CA-C	-5.43	105.08	111.00
1	S	334	GLY	N-CA-C	-5.41	100.35	113.18
2	R	75	SER	N-CA-C	5.41	116.74	107.28
2	D	218	LEU	CA-C-N	5.40	126.59	119.84
2	D	218	LEU	C-N-CA	5.40	126.59	119.84
1	E	334	GLY	N-CA-C	-5.40	100.38	113.18
1	Q	158	VAL	N-CA-C	-5.40	105.12	111.00
2	T	75	SER	N-CA-C	5.39	116.72	107.28
2	F	218	LEU	CA-C-N	5.39	126.57	119.84
2	F	218	LEU	C-N-CA	5.39	126.57	119.84
2	F	75	SER	N-CA-C	5.37	116.69	107.28
2	L	75	SER	N-CA-C	5.37	116.68	107.28
2	D	75	SER	N-CA-C	5.37	116.68	107.28
2	L	218	LEU	CA-C-N	5.36	126.54	119.84
2	L	218	LEU	C-N-CA	5.36	126.54	119.84
1	M	24	PRO	N-CA-C	-5.36	107.16	113.86
1	A	24	PRO	N-CA-C	-5.35	107.17	113.86
1	S	158	VAL	N-CA-C	-5.34	105.18	111.00
1	C	158	VAL	N-CA-C	-5.33	105.19	111.00
1	I	116	VAL	N-CA-C	5.31	115.55	108.11
2	J	218	LEU	CA-C-N	5.31	126.48	119.84
2	J	218	LEU	C-N-CA	5.31	126.48	119.84
1	M	116	VAL	N-CA-C	5.31	115.54	108.11
2	B	218	LEU	CA-C-N	5.30	126.46	119.84
2	B	218	LEU	C-N-CA	5.30	126.46	119.84
1	E	204	VAL	CA-C-N	5.30	125.46	119.90
1	E	204	VAL	C-N-CA	5.30	125.46	119.90
1	O	24	PRO	N-CA-C	-5.29	107.25	113.86
1	I	24	PRO	N-CA-C	-5.28	107.26	113.86
2	P	218	LEU	CA-C-N	5.27	126.43	119.84
2	P	218	LEU	C-N-CA	5.27	126.43	119.84
1	G	24	PRO	N-CA-C	-5.26	107.28	113.86
1	C	204	VAL	CA-C-N	5.25	125.42	119.90
1	C	204	VAL	C-N-CA	5.25	125.42	119.90
2	P	78	ASN	CA-C-N	5.25	126.41	119.84
2	P	78	ASN	C-N-CA	5.25	126.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	218	LEU	CA-C-N	5.25	126.41	119.84
2	N	218	LEU	C-N-CA	5.25	126.41	119.84
2	H	218	LEU	CA-C-N	5.25	126.40	119.84
2	H	218	LEU	C-N-CA	5.25	126.40	119.84
1	O	116	VAL	N-CA-C	5.25	115.45	108.11
1	K	204	VAL	CA-C-N	5.24	125.40	119.90
1	K	204	VAL	C-N-CA	5.24	125.40	119.90
2	J	78	ASN	CA-C-N	5.23	126.38	119.84
2	J	78	ASN	C-N-CA	5.23	126.38	119.84
2	T	176	HIS	N-CA-C	5.23	118.01	109.59
2	B	78	ASN	CA-C-N	5.22	126.36	119.84
2	B	78	ASN	C-N-CA	5.22	126.36	119.84
2	F	176	HIS	N-CA-C	5.21	117.98	109.59
1	S	116	VAL	N-CA-C	5.21	115.35	107.75
1	S	204	VAL	CA-C-N	5.20	125.36	119.90
1	S	204	VAL	C-N-CA	5.20	125.36	119.90
1	G	116	VAL	N-CA-C	5.20	115.39	108.11
1	A	116	VAL	N-CA-C	5.19	115.38	108.11
2	D	176	HIS	N-CA-C	5.19	117.95	109.59
2	R	176	HIS	N-CA-C	5.19	117.94	109.59
2	N	78	ASN	CA-C-N	5.18	126.32	119.84
2	N	78	ASN	C-N-CA	5.18	126.32	119.84
1	I	14	ASN	N-CA-C	-5.18	105.75	111.71
1	Q	204	VAL	CA-C-N	5.17	125.33	119.90
1	Q	204	VAL	C-N-CA	5.17	125.33	119.90
1	C	116	VAL	N-CA-C	5.17	115.35	108.11
2	L	176	HIS	N-CA-C	5.17	117.92	109.59
1	Q	24	PRO	N-CA-C	-5.17	107.67	114.03
1	C	24	PRO	N-CA-C	-5.17	107.67	114.03
1	K	116	VAL	N-CA-C	5.16	115.33	108.11
1	A	14	ASN	N-CA-C	-5.15	105.79	111.71
1	G	14	ASN	N-CA-C	-5.14	105.80	111.71
2	H	78	ASN	CA-C-N	5.12	126.25	119.84
2	H	78	ASN	C-N-CA	5.12	126.25	119.84
1	E	116	VAL	N-CA-C	5.12	115.27	108.11
1	M	14	ASN	N-CA-C	-5.11	105.83	111.71
1	K	24	PRO	N-CA-C	-5.11	107.75	114.03
1	O	14	ASN	N-CA-C	-5.10	105.84	111.71
1	G	147	ALA	CB-CA-C	-5.10	109.16	115.89
1	E	24	PRO	N-CA-C	-5.10	107.76	114.03
1	Q	116	VAL	N-CA-C	5.09	115.24	108.11
1	A	147	ALA	CB-CA-C	-5.09	109.17	115.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	147	ALA	CB-CA-C	-5.09	109.17	115.89
1	C	265	GLY	CA-C-N	5.09	124.59	119.19
1	C	265	GLY	C-N-CA	5.09	124.59	119.19
1	K	265	GLY	CA-C-N	5.09	124.58	119.19
1	K	265	GLY	C-N-CA	5.09	124.58	119.19
1	O	147	ALA	CB-CA-C	-5.06	109.21	115.89
1	I	147	ALA	CB-CA-C	-5.06	109.21	115.89
1	Q	265	GLY	CA-C-N	5.06	124.55	119.19
1	Q	265	GLY	C-N-CA	5.06	124.55	119.19
1	S	265	GLY	CA-C-N	5.05	124.54	119.19
1	S	265	GLY	C-N-CA	5.05	124.54	119.19
1	S	24	PRO	N-CA-C	-5.05	107.82	114.03
1	C	44	LEU	N-CA-C	-5.04	106.29	112.90
1	K	179	THR	N-CA-C	5.04	116.86	109.24
1	E	44	LEU	N-CA-C	-5.04	106.30	112.90
2	D	214	VAL	N-CA-C	-5.03	105.00	110.23
1	G	323	ASP	N-CA-C	-5.03	105.50	111.69
1	E	14	ASN	N-CA-C	-5.03	105.93	111.71
1	S	44	LEU	N-CA-C	-5.02	106.33	112.90
2	B	176	HIS	N-CA-C	5.02	117.67	109.59
1	K	14	ASN	N-CA-C	-5.02	105.94	111.71
1	O	323	ASP	N-CA-C	-5.01	105.52	111.69
1	K	44	LEU	N-CA-C	-5.01	106.34	112.90
1	S	179	THR	N-CA-C	5.01	116.80	109.24
2	F	198	ALA	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2549	0	2612	268	0
1	C	2570	0	2632	273	0
1	E	2570	0	2632	278	0
1	G	2549	0	2612	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2549	0	2612	280	0
1	K	2570	0	2632	268	0
1	M	2549	0	2612	278	0
1	O	2549	0	2612	267	0
1	Q	2549	0	2612	298	0
1	S	2561	0	2626	267	0
2	B	2544	0	2580	199	0
2	D	2544	0	2580	208	0
2	F	2544	0	2580	208	0
2	H	2544	0	2580	198	0
2	J	2544	0	2580	198	0
2	L	2544	0	2580	209	0
2	N	2544	0	2580	202	0
2	P	2544	0	2580	201	0
2	R	2544	0	2580	209	0
2	T	2544	0	2580	201	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	1	0
3	D	44	0	26	1	0
3	E	44	0	26	1	0
3	F	44	0	26	1	0
3	G	44	0	26	1	0
3	H	44	0	26	0	0
3	I	44	0	26	1	0
3	J	44	0	26	0	0
3	K	44	0	26	1	0
3	L	44	0	26	1	0
3	M	44	0	26	1	0
3	N	44	0	26	0	0
3	O	44	0	26	1	0
3	P	44	0	26	0	0
3	Q	44	0	26	1	0
3	R	44	0	26	1	0
3	S	44	0	26	1	0
3	T	44	0	26	1	0
All	All	51885	0	52514	4331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (4331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:LEU:CD2	1:E:110:GLN:OE1	1.77	1.31
1:E:80:LEU:HD21	1:E:110:GLN:OE1	1.42	1.15
1:I:124:ASP:OD1	1:I:125:ILE:HG13	1.47	1.15
1:O:124:ASP:OD1	1:O:125:ILE:HG13	1.47	1.13
1:E:124:ASP:OD1	1:E:125:ILE:HG13	1.43	1.13
1:A:124:ASP:OD1	1:A:125:ILE:HG13	1.47	1.13
1:G:107:LYS:HA	1:G:110:GLN:HE21	1.04	1.10
1:A:110:GLN:NE2	1:G:110:GLN:O	1.85	1.09
1:I:110:GLN:HB2	1:M:110:GLN:HB3	1.33	1.08
1:E:123(A):SER:O	1:K:124:ASP:HA	1.58	1.04
1:I:245:ASN:HD22	1:K:245:ASN:HD22	1.04	1.03
1:Q:125:ILE:HG23	1:Q:143:ILE:O	1.58	1.03
1:O:123(A):SER:O	1:C:124:ASP:HA	1.60	1.01
1:S:80:LEU:CD2	1:S:110:GLN:OE1	2.08	1.00
1:E:80:LEU:HD22	1:E:110:GLN:OE1	1.58	1.00
1:O:110:GLN:HB2	1:C:110:GLN:HB3	1.43	0.99
1:O:245:ASN:HD22	1:Q:245:ASN:HD22	1.04	0.99
1:Q:248:LYS:HG2	1:Q:248(A):VAL:HG12	1.45	0.99
1:M:245:ASN:HD22	1:S:245:ASN:HD22	1.04	0.98
2:N:211:ALA:HB1	2:N:226:ASN:HA	1.45	0.98
1:K:248:LYS:HG2	1:K:248(A):VAL:HG12	1.45	0.98
1:E:110:GLN:H	1:K:110:GLN:NE2	1.61	0.98
1:I:123(A):SER:O	1:M:124:ASP:HA	1.62	0.98
1:I:80:LEU:CD2	1:I:110:GLN:OE1	2.12	0.98
1:M:193:LEU:H	1:M:193:LEU:HD12	1.29	0.98
1:A:204:VAL:HG22	1:C:279:VAL:HG11	1.46	0.98
2:J:211:ALA:HB1	2:J:226:ASN:HA	1.45	0.98
1:A:123(A):SER:O	1:G:124:ASP:HA	1.63	0.98
1:I:204:VAL:HG22	1:K:279:VAL:HG11	1.46	0.97
1:A:193:LEU:H	1:A:193:LEU:HD12	1.29	0.97
2:B:211:ALA:HB1	2:B:226:ASN:HA	1.45	0.97
1:G:245:ASN:HD22	1:E:245:ASN:HD22	1.04	0.97
2:H:211:ALA:HB1	2:H:226:ASN:HA	1.45	0.97
1:I:193:LEU:H	1:I:193:LEU:HD12	1.29	0.97
1:C:248:LYS:HG2	1:C:248(A):VAL:HG12	1.45	0.97
1:G:204:VAL:HG22	1:E:279:VAL:HG11	1.46	0.97
2:N:193:LEU:H	2:N:193:LEU:HD12	1.28	0.97
2:J:193:LEU:H	2:J:193:LEU:HD12	1.28	0.97
1:G:248:LYS:HG2	1:G:248(A):VAL:HG12	1.47	0.97
1:A:248:LYS:HG2	1:A:248(A):VAL:HG12	1.47	0.97
2:P:193:LEU:H	2:P:193:LEU:HD12	1.28	0.96
1:Q:101:ASP:HB3	1:Q:122(A):LYS:HB3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:193:LEU:H	2:F:193:LEU:HD12	1.27	0.96
1:M:204:VAL:HG22	1:S:279:VAL:HG11	1.46	0.96
1:G:193:LEU:HD12	1:G:193:LEU:H	1.29	0.96
1:E:248:LYS:HG2	1:E:248(A):VAL:HG12	1.45	0.96
1:M:107:LYS:HA	1:M:110:GLN:HE21	1.30	0.96
1:A:245:ASN:HD22	1:C:245:ASN:HD22	1.04	0.96
2:H:193:LEU:H	2:H:193:LEU:HD12	1.28	0.96
1:O:248:LYS:HG2	1:O:248(A):VAL:HG12	1.47	0.96
2:D:193:LEU:HD12	2:D:193:LEU:H	1.28	0.96
1:I:248:LYS:HG2	1:I:248(A):VAL:HG12	1.47	0.96
2:D:211:ALA:HB1	2:D:226:ASN:HA	1.48	0.95
1:K:271:LEU:HD11	1:K:292:ILE:HD11	1.48	0.95
2:T:193:LEU:H	2:T:193:LEU:HD12	1.28	0.95
1:S:271:LEU:HD11	1:S:292:ILE:HD11	1.48	0.95
1:O:204:VAL:HG22	1:Q:279:VAL:HG11	1.46	0.95
1:A:110:GLN:CB	1:G:110:GLN:HB3	1.97	0.95
1:S:248:LYS:HG2	1:S:248(A):VAL:HG12	1.45	0.95
2:R:193:LEU:H	2:R:193:LEU:HD12	1.28	0.95
1:E:271:LEU:HD11	1:E:292:ILE:HD11	1.48	0.95
1:Q:271:LEU:HD11	1:Q:292:ILE:HD11	1.48	0.95
2:F:211:ALA:HB1	2:F:226:ASN:HA	1.48	0.95
2:P:211:ALA:HB1	2:P:226:ASN:HA	1.45	0.94
2:L:193:LEU:HD12	2:L:193:LEU:H	1.28	0.94
1:M:248:LYS:HG2	1:M:248(A):VAL:HG12	1.47	0.94
2:R:211:ALA:HB1	2:R:226:ASN:HA	1.48	0.94
1:O:193:LEU:HD12	1:O:193:LEU:H	1.29	0.94
2:B:193:LEU:H	2:B:193:LEU:HD12	1.28	0.94
1:C:271:LEU:HD11	1:C:292:ILE:HD11	1.49	0.94
1:S:80:LEU:HD21	1:S:110:GLN:OE1	1.68	0.93
2:T:211:ALA:HB1	2:T:226:ASN:HA	1.48	0.93
1:I:110:GLN:N	1:M:110:GLN:OE1	1.99	0.93
1:C:124:ASP:OD1	1:C:125:ILE:HG13	1.69	0.93
1:I:110:GLN:HB2	1:M:110:GLN:CB	1.99	0.93
1:O:228:ILE:HD13	1:O:228:ILE:H	1.35	0.92
2:L:211:ALA:HB1	2:L:226:ASN:HA	1.48	0.92
1:E:106:GLY:O	1:K:110:GLN:NE2	2.01	0.92
1:I:228:ILE:HD13	1:I:228:ILE:H	1.35	0.92
1:A:228:ILE:HD13	1:A:228:ILE:H	1.35	0.92
1:K:124:ASP:OD1	1:K:125:ILE:HG13	1.69	0.92
1:E:80:LEU:HD22	1:E:110:GLN:CD	1.95	0.92
1:Q:100:VAL:O	1:Q:122(A):LYS:N	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:100:VAL:C	1:Q:122(A):LYS:HB2	1.93	0.92
1:E:124:ASP:HB2	1:K:124:ASP:OD2	1.64	0.91
1:M:228:ILE:HD13	1:M:228:ILE:H	1.35	0.91
1:E:110:GLN:NE2	1:K:110:GLN:O	2.04	0.90
1:I:110:GLN:CB	1:M:110:GLN:HB3	2.01	0.90
1:O:110:GLN:CB	1:C:110:GLN:HB3	2.02	0.90
1:G:228:ILE:HD13	1:G:228:ILE:H	1.35	0.89
1:I:80:LEU:HD22	1:I:110:GLN:OE1	1.70	0.89
1:I:248(A):VAL:HG13	1:I:249:GLY:H	1.38	0.89
1:O:248(A):VAL:HG13	1:O:249:GLY:H	1.38	0.89
1:M:248(A):VAL:HG13	1:M:249:GLY:H	1.38	0.89
1:M:124:ASP:OD1	1:M:125:ILE:HG13	1.73	0.88
1:Q:110:GLN:O	1:S:110:GLN:NE2	2.07	0.88
1:C:248(A):VAL:HG13	1:C:249:GLY:H	1.38	0.88
1:O:168:VAL:HG12	1:O:169:LYS:HG3	1.55	0.88
1:Q:248(A):VAL:HG13	1:Q:249:GLY:H	1.38	0.88
1:K:248(A):VAL:HG13	1:K:249:GLY:H	1.38	0.88
1:A:110:GLN:HB2	1:G:110:GLN:HB3	1.53	0.88
1:A:248(A):VAL:HG13	1:A:249:GLY:H	1.38	0.88
1:G:124:ASP:OD1	1:G:125:ILE:HG13	1.73	0.88
1:M:168:VAL:HG12	1:M:169:LYS:HG3	1.55	0.88
1:G:248(A):VAL:HG13	1:G:249:GLY:H	1.38	0.87
1:E:248(A):VAL:HG13	1:E:249:GLY:H	1.38	0.87
1:G:107:LYS:HA	1:G:110:GLN:NE2	1.89	0.87
1:G:168:VAL:HG12	1:G:169:LYS:HG3	1.55	0.87
1:C:228:ILE:H	1:C:228:ILE:HD13	1.40	0.87
1:A:168:VAL:HG12	1:A:169:LYS:HG3	1.55	0.86
2:R:129:VAL:HG23	2:R:217:VAL:HG11	1.56	0.86
2:D:129:VAL:HG23	2:D:217:VAL:HG11	1.56	0.86
1:E:110:GLN:H	1:K:110:GLN:HE22	1.23	0.86
1:S:248(A):VAL:HG13	1:S:249:GLY:H	1.38	0.86
1:E:228:ILE:HD13	1:E:228:ILE:H	1.40	0.86
1:A:110:GLN:HB2	1:G:110:GLN:CB	2.05	0.86
1:Q:124:ASP:OD1	1:Q:125:ILE:CD1	2.24	0.86
1:I:279:VAL:HG11	1:K:204:VAL:HG22	1.58	0.86
2:T:129:VAL:HG23	2:T:217:VAL:HG11	1.56	0.85
1:E:110:GLN:N	1:K:110:GLN:HE22	1.74	0.85
1:Q:124:ASP:OD1	1:Q:125:ILE:HG13	1.74	0.85
1:I:103:PRO:HB3	1:M:109:ILE:HG21	1.59	0.85
1:I:271:LEU:HD11	1:I:292:ILE:HD11	1.58	0.85
1:I:168:VAL:HG12	1:I:169:LYS:HG3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:271:LEU:HD11	1:M:292:ILE:HD11	1.58	0.85
2:L:129:VAL:HG23	2:L:217:VAL:HG11	1.56	0.85
2:F:129:VAL:HG23	2:F:217:VAL:HG11	1.56	0.85
1:G:271:LEU:HD11	1:G:292:ILE:HD11	1.58	0.85
1:O:271:LEU:HD11	1:O:292:ILE:HD11	1.58	0.84
1:M:279:VAL:HG11	1:S:204:VAL:HG22	1.58	0.84
1:S:228:ILE:H	1:S:228:ILE:HD13	1.40	0.84
1:O:110:GLN:HB2	1:C:110:GLN:CB	2.05	0.84
1:Q:228:ILE:HD13	1:Q:228:ILE:H	1.40	0.84
1:I:110:GLN:CD	1:M:110:GLN:O	2.21	0.84
1:Q:124:ASP:HA	1:S:124:ASP:HA	1.58	0.84
1:Q:80:LEU:HD21	1:Q:110:GLN:OE1	1.78	0.83
1:A:279:VAL:HG11	1:C:204:VAL:HG22	1.58	0.83
1:G:279:VAL:HG11	1:E:204:VAL:HG22	1.58	0.83
1:A:103:PRO:HB3	1:G:109:ILE:HG21	1.59	0.83
2:H:202:ASN:ND2	2:F:281:ILE:HB	1.94	0.83
1:O:279:VAL:HG11	1:Q:204:VAL:HG22	1.58	0.83
1:K:228:ILE:H	1:K:228:ILE:HD13	1.40	0.83
1:A:271:LEU:HD11	1:A:292:ILE:HD11	1.58	0.83
2:J:202:ASN:ND2	2:L:281:ILE:HB	1.94	0.83
2:P:25:LEU:HD21	2:P:326:ASP:HA	1.61	0.83
2:B:202:ASN:ND2	2:D:281:ILE:HB	1.94	0.83
2:B:202:ASN:HD21	2:D:281:ILE:HB	1.44	0.83
2:N:202:ASN:ND2	2:T:281:ILE:HB	1.94	0.83
2:B:129:VAL:HG23	2:B:217:VAL:HG11	1.61	0.82
2:H:25:LEU:HD21	2:H:326:ASP:HA	1.61	0.82
2:T:25:LEU:HD21	2:T:326:ASP:HA	1.61	0.82
2:P:202:ASN:ND2	2:R:281:ILE:HB	1.94	0.82
1:A:106:GLY:O	1:G:110:GLN:OE1	1.97	0.82
1:A:110:GLN:N	1:G:110:GLN:OE1	2.12	0.82
2:N:202:ASN:HD21	2:T:281:ILE:HB	1.44	0.82
2:P:129:VAL:HG23	2:P:217:VAL:HG11	1.61	0.82
2:H:202:ASN:HD21	2:F:281:ILE:HB	1.44	0.82
2:J:25:LEU:HD21	2:J:326:ASP:HA	1.61	0.82
1:Q:168:VAL:HG12	1:Q:169:LYS:HG3	1.61	0.82
2:L:25:LEU:HD21	2:L:326:ASP:HA	1.61	0.82
2:H:129:VAL:HG23	2:H:217:VAL:HG11	1.61	0.82
2:N:25:LEU:HD21	2:N:326:ASP:HA	1.61	0.82
1:Q:109:ILE:HG21	1:S:103:PRO:HB3	1.60	0.82
1:Q:129:VAL:HG23	1:Q:217:VAL:HG11	1.62	0.82
2:B:25:LEU:HD21	2:B:326:ASP:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:129:VAL:HG23	2:N:217:VAL:HG11	1.61	0.82
1:E:129:VAL:HG23	1:E:217:VAL:HG11	1.63	0.81
2:J:202:ASN:HD21	2:L:281:ILE:HB	1.44	0.81
1:K:129:VAL:HG23	1:K:217:VAL:HG11	1.62	0.81
1:C:129:VAL:HG23	1:C:217:VAL:HG11	1.62	0.81
1:E:103:PRO:HB3	1:K:109:ILE:HG21	1.61	0.81
2:D:25:LEU:HD21	2:D:326:ASP:HA	1.61	0.81
2:F:25:LEU:HD21	2:F:326:ASP:HA	1.61	0.81
1:E:110:GLN:N	1:K:110:GLN:NE2	2.28	0.81
1:S:168:VAL:HG12	1:S:169:LYS:HG3	1.62	0.81
1:O:169:LYS:HZ2	1:Q:301:GLY:HA3	1.46	0.81
2:J:129:VAL:HG23	2:J:217:VAL:HG11	1.61	0.81
1:S:129:VAL:HG23	1:S:217:VAL:HG11	1.62	0.81
1:E:168:VAL:HG12	1:E:169:LYS:HG3	1.62	0.80
2:R:25:LEU:HD21	2:R:326:ASP:HA	1.61	0.80
1:Q:124:ASP:CG	1:Q:125:ILE:HG13	2.05	0.80
2:P:202:ASN:HD21	2:R:281:ILE:HB	1.44	0.80
1:K:168:VAL:HG12	1:K:169:LYS:HG3	1.62	0.80
2:B:39:GLN:HE22	1:C:190:HIS:H	1.29	0.80
1:G:249:GLY:HA2	1:G:302:GLY:O	1.82	0.80
1:M:249:GLY:HA2	1:M:302:GLY:O	1.82	0.80
1:C:168:VAL:HG12	1:C:169:LYS:HG3	1.61	0.79
2:H:39:GLN:HE22	1:E:190:HIS:H	1.29	0.79
1:I:249:GLY:HA2	1:I:302:GLY:O	1.82	0.79
1:A:249:GLY:HA2	1:A:302:GLY:O	1.82	0.79
2:N:39:GLN:HE22	1:S:190:HIS:H	1.29	0.79
1:O:249:GLY:HA2	1:O:302:GLY:O	1.82	0.79
1:S:155:ALA:HB3	1:S:156:PRO:HD3	1.63	0.79
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.64	0.79
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.63	0.79
1:S:33:SER:HA	1:S:75:SER:OG	1.83	0.79
1:M:155:ALA:HB3	1:M:156:PRO:HD3	1.65	0.79
2:J:190:HIS:HB3	2:J:196:ALA:HB2	1.64	0.78
1:K:33:SER:HA	1:K:75:SER:OG	1.83	0.78
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.63	0.78
2:B:154:LEU:HD13	2:B:240:VAL:HG21	1.66	0.78
1:M:301:GLY:HA3	1:S:169:LYS:HZ2	1.48	0.78
2:N:190:HIS:HB3	2:N:196:ALA:HB2	1.64	0.78
2:P:190:HIS:HB3	2:P:196:ALA:HB2	1.64	0.78
1:I:190:HIS:HB3	1:I:196:ALA:HB2	1.65	0.78
1:I:155:ALA:HB3	1:I:156:PRO:HD3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.64	0.78
1:E:33:SER:HA	1:E:75:SER:OG	1.83	0.78
1:I:38:LYS:HG3	1:I:39:SER:H	1.49	0.78
1:Q:124:ASP:OD1	1:Q:125:ILE:CG1	2.31	0.78
2:H:154:LEU:HD13	2:H:240:VAL:HG21	1.66	0.78
1:M:190:HIS:HB3	1:M:196:ALA:HB2	1.65	0.78
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.64	0.78
2:N:154:LEU:HD13	2:N:240:VAL:HG21	1.66	0.78
1:C:251:THR:HG22	1:C:252:ALA:H	1.49	0.78
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.64	0.78
1:Q:11:ILE:HD11	1:Q:317:TYR:HD2	1.49	0.77
1:Q:33:SER:HA	1:Q:75:SER:OG	1.83	0.77
1:G:38:LYS:HG3	1:G:39:SER:H	1.49	0.77
1:I:245:ASN:ND2	1:K:245:ASN:HD22	1.83	0.77
2:P:39:GLN:HE22	1:Q:190:HIS:H	1.29	0.77
1:K:155:ALA:HB3	1:K:156:PRO:HD3	1.63	0.77
1:A:301:GLY:HA3	1:C:169:LYS:HZ2	1.50	0.77
1:S:165:LEU:HG	1:S:246:ILE:HG12	1.66	0.77
1:O:38:LYS:HG3	1:O:39:SER:H	1.49	0.77
1:O:190:HIS:HB3	1:O:196:ALA:HB2	1.65	0.77
1:A:38:LYS:HG3	1:A:39:SER:H	1.49	0.77
2:B:190:HIS:HB3	2:B:196:ALA:HB2	1.64	0.77
2:H:190:HIS:HB3	2:H:196:ALA:HB2	1.64	0.77
1:K:165:LEU:HG	1:K:246:ILE:HG12	1.67	0.77
1:M:245:ASN:HD22	1:S:245:ASN:ND2	1.83	0.77
1:C:33:SER:HA	1:C:75:SER:OG	1.83	0.77
1:K:251:THR:HG22	1:K:252:ALA:H	1.50	0.77
1:E:251:THR:HG22	1:E:252:ALA:H	1.50	0.77
2:J:39:GLN:HE22	1:K:190:HIS:H	1.29	0.77
1:Q:251:THR:HG22	1:Q:252:ALA:H	1.50	0.77
1:S:193:LEU:H	1:S:193:LEU:HD12	1.50	0.77
1:O:251:THR:HG22	1:O:252:ALA:H	1.50	0.77
1:Q:124:ASP:OD1	1:Q:125:ILE:HD11	1.85	0.77
1:G:301:GLY:HA3	1:E:169:LYS:HZ2	1.50	0.76
1:I:251:THR:HG22	1:I:252:ALA:H	1.50	0.76
1:O:103:PRO:HB3	1:C:109:ILE:HG21	1.66	0.76
1:A:190:HIS:HB3	1:A:196:ALA:HB2	1.65	0.76
1:G:190:HIS:HB3	1:G:196:ALA:HB2	1.65	0.76
2:J:154:LEU:HD13	2:J:240:VAL:HG21	1.66	0.76
1:S:251:THR:HG22	1:S:252:ALA:H	1.49	0.76
1:O:245:ASN:ND2	1:Q:245:ASN:HD22	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:VAL:HG12	1:M:75:SER:H	1.51	0.76
2:P:154:LEU:HD13	2:P:240:VAL:HG21	1.66	0.76
1:Q:165:LEU:HG	1:Q:246:ILE:HG12	1.66	0.76
1:Q:193:LEU:H	1:Q:193:LEU:HD12	1.51	0.76
2:R:154:LEU:O	2:R:158:VAL:HG23	1.85	0.76
1:G:74:VAL:HG12	1:G:75:SER:H	1.50	0.76
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.21	0.76
1:I:301:GLY:HA3	1:K:169:LYS:HZ2	1.50	0.76
1:E:165:LEU:HG	1:E:246:ILE:HG12	1.66	0.76
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.21	0.76
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.21	0.76
1:C:11:ILE:HD11	1:C:317:TYR:HD2	1.49	0.76
2:D:190:HIS:HB3	2:D:196:ALA:HB2	1.67	0.76
2:L:154:LEU:O	2:L:158:VAL:HG23	1.85	0.76
2:T:154:LEU:O	2:T:158:VAL:HG23	1.86	0.76
1:C:165:LEU:HG	1:C:246:ILE:HG12	1.66	0.76
1:M:204:VAL:HG22	1:S:279:VAL:CG1	2.15	0.76
1:S:80:LEU:HD22	1:S:110:GLN:CD	2.10	0.76
1:I:82:LEU:HD13	1:I:84:TRP:CZ2	2.21	0.76
1:O:245:ASN:HD22	1:Q:245:ASN:ND2	1.83	0.76
2:F:154:LEU:O	2:F:158:VAL:HG23	1.85	0.76
1:K:11:ILE:HD11	1:K:317:TYR:HD2	1.49	0.76
1:G:251:THR:HG22	1:G:252:ALA:H	1.50	0.75
1:G:169:LYS:HZ2	1:E:301:GLY:HA3	1.50	0.75
1:K:193:LEU:H	1:K:193:LEU:HD12	1.50	0.75
2:D:154:LEU:O	2:D:158:VAL:HG23	1.85	0.75
1:M:38:LYS:HG3	1:M:39:SER:H	1.49	0.75
1:Q:125:ILE:CG2	1:Q:143:ILE:HG22	2.16	0.75
1:A:74:VAL:HG12	1:A:75:SER:H	1.50	0.75
1:I:204:VAL:HG22	1:K:279:VAL:CG1	2.16	0.75
1:A:204:VAL:HG22	1:C:279:VAL:CG1	2.15	0.75
2:F:190:HIS:HB3	2:F:196:ALA:HB2	1.67	0.75
1:O:74:VAL:HG12	1:O:75:SER:H	1.50	0.75
1:E:11:ILE:HD11	1:E:317:TYR:HD2	1.49	0.75
1:I:110:GLN:OE1	1:M:110:GLN:O	2.05	0.75
1:M:82:LEU:HD13	1:M:84:TRP:CZ2	2.21	0.75
1:M:251:THR:HG22	1:M:252:ALA:H	1.50	0.75
1:A:251:THR:HG22	1:A:252:ALA:H	1.50	0.75
1:G:165:LEU:HG	1:G:246:ILE:HG12	1.68	0.75
1:G:204:VAL:HG22	1:E:279:VAL:CG1	2.16	0.75
2:L:190:HIS:HB3	2:L:196:ALA:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLY:HA2	1:C:302:GLY:O	1.87	0.75
1:O:165:LEU:HG	1:O:246:ILE:HG12	1.69	0.74
1:A:169:LYS:HZ2	1:C:301:GLY:HA3	1.52	0.74
1:E:249:GLY:HA2	1:E:302:GLY:O	1.87	0.74
1:A:213:ALA:HA	1:A:216:LEU:HD23	1.69	0.74
1:I:74:VAL:HG12	1:I:75:SER:H	1.51	0.74
1:S:249:GLY:HA2	1:S:302:GLY:O	1.87	0.74
2:T:190:HIS:HB3	2:T:196:ALA:HB2	1.68	0.74
1:O:301:GLY:HA3	1:Q:169:LYS:HZ2	1.50	0.74
1:A:245:ASN:ND2	1:C:245:ASN:HD22	1.83	0.74
1:M:245:ASN:ND2	1:S:245:ASN:HD22	1.83	0.74
1:S:11:ILE:HD11	1:S:317:TYR:HD2	1.49	0.74
1:O:204:VAL:HG22	1:Q:279:VAL:CG1	2.15	0.74
1:O:213:ALA:HA	1:O:216:LEU:HD23	1.69	0.74
1:A:165:LEU:HG	1:A:246:ILE:HG12	1.68	0.74
2:R:190:HIS:HB3	2:R:196:ALA:HB2	1.67	0.74
1:C:193:LEU:H	1:C:193:LEU:HD12	1.50	0.74
1:E:193:LEU:H	1:E:193:LEU:HD12	1.51	0.74
1:S:74:VAL:HG12	1:S:75:SER:H	1.53	0.74
1:Q:74:VAL:HG12	1:Q:75:SER:H	1.53	0.74
1:G:213:ALA:HA	1:G:216:LEU:HD23	1.69	0.74
1:I:165:LEU:HG	1:I:246:ILE:HG12	1.68	0.74
1:C:245:ASN:HA	1:C:304:MET:HA	1.70	0.73
1:Q:245:ASN:HA	1:Q:304:MET:HA	1.70	0.73
1:K:245:ASN:HA	1:K:304:MET:HA	1.70	0.73
1:M:165:LEU:HG	1:M:246:ILE:HG12	1.69	0.73
1:M:292:ILE:H	1:M:292:ILE:HD12	1.52	0.73
1:S:245:ASN:HA	1:S:304:MET:HA	1.70	0.73
1:O:292:ILE:H	1:O:292:ILE:HD12	1.53	0.73
2:P:153:CYS:O	2:P:156:PRO:HD2	1.88	0.73
2:B:153:CYS:O	2:B:156:PRO:HD2	1.88	0.73
1:K:249:GLY:HA2	1:K:302:GLY:O	1.87	0.73
1:A:292:ILE:H	1:A:292:ILE:HD12	1.53	0.73
1:C:213:ALA:HA	1:C:216:LEU:HD23	1.69	0.73
1:A:301:GLY:HA3	1:C:169:LYS:NZ	2.04	0.73
1:G:301:GLY:HA3	1:E:169:LYS:NZ	2.04	0.73
1:E:245:ASN:HA	1:E:304:MET:HA	1.70	0.73
2:F:198:ALA:HB3	2:F:202:ASN:OD1	1.89	0.73
1:I:245:ASN:HD22	1:K:245:ASN:ND2	1.83	0.73
1:K:213:ALA:HA	1:K:216:LEU:HD23	1.69	0.73
2:D:155:ALA:HB3	2:D:156:PRO:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:ALA:HB3	2:D:202:ASN:OD1	1.89	0.73
1:I:213:ALA:HA	1:I:216:LEU:HD23	1.69	0.73
1:Q:249:GLY:HA2	1:Q:302:GLY:O	1.87	0.73
1:C:38:LYS:HG3	1:C:39:SER:H	1.54	0.73
1:C:154:LEU:O	1:C:158:VAL:HG23	1.89	0.73
1:K:74:VAL:HG12	1:K:75:SER:H	1.53	0.73
1:K:154:LEU:O	1:K:158:VAL:HG23	1.89	0.73
1:M:213:ALA:HA	1:M:216:LEU:HD23	1.69	0.73
2:N:153:CYS:O	2:N:156:PRO:HD2	1.89	0.73
1:E:74:VAL:HG12	1:E:75:SER:H	1.53	0.73
1:I:292:ILE:H	1:I:292:ILE:HD12	1.52	0.73
1:Q:38:LYS:HG3	1:Q:39:SER:H	1.54	0.73
1:E:213:ALA:HA	1:E:216:LEU:HD23	1.69	0.73
1:S:80:LEU:HD22	1:S:110:GLN:OE1	1.87	0.73
2:R:198:ALA:HB3	2:R:202:ASN:OD1	1.89	0.73
2:H:153:CYS:O	2:H:156:PRO:HD2	1.88	0.73
2:H:198:ALA:HB3	2:H:202:ASN:OD1	1.89	0.73
1:E:154:LEU:O	1:E:158:VAL:HG23	1.89	0.73
2:F:155:ALA:HB3	2:F:156:PRO:HD3	1.71	0.73
1:O:301:GLY:HA3	1:Q:169:LYS:NZ	2.04	0.72
1:Q:248(A):VAL:HG22	1:Q:249:GLY:N	2.04	0.72
2:R:155:ALA:HB3	2:R:156:PRO:HD3	1.71	0.72
2:N:154:LEU:O	2:N:158:VAL:HG23	1.89	0.72
2:T:198:ALA:HB3	2:T:202:ASN:OD1	1.89	0.72
1:E:248(A):VAL:HG22	1:E:249:GLY:N	2.04	0.72
1:M:301:GLY:HA3	1:S:169:LYS:NZ	2.03	0.72
2:P:154:LEU:O	2:P:158:VAL:HG23	1.89	0.72
1:Q:154:LEU:O	1:Q:158:VAL:HG23	1.89	0.72
1:C:248(A):VAL:HG22	1:C:249:GLY:N	2.04	0.72
1:G:292:ILE:H	1:G:292:ILE:HD12	1.53	0.72
2:F:126:PRO:HB2	2:F:144:ILE:HG22	1.71	0.72
1:M:169:LYS:HZ2	1:S:301:GLY:HA3	1.54	0.72
2:T:155:ALA:HB3	2:T:156:PRO:HD3	1.71	0.72
2:R:126:PRO:HB2	2:R:144:ILE:HG22	1.71	0.72
1:G:245:ASN:HD22	1:E:245:ASN:ND2	1.83	0.72
2:J:198:ALA:HB3	2:J:202:ASN:OD1	1.89	0.72
1:K:82:LEU:HD13	1:K:84:TRP:CZ2	2.25	0.72
1:M:107:LYS:HA	1:M:110:GLN:NE2	2.03	0.72
1:S:154:LEU:O	1:S:158:VAL:HG23	1.89	0.72
1:C:74:VAL:HG12	1:C:75:SER:H	1.53	0.72
2:L:198:ALA:HB3	2:L:202:ASN:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:82:LEU:HD13	1:S:84:TRP:CZ2	2.25	0.72
2:T:91:LEU:HD12	2:T:92:VAL:H	1.55	0.72
1:O:192:ASP:HB3	1:O:195:ARG:HD2	1.72	0.72
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.24	0.72
1:A:245:ASN:HD22	1:C:245:ASN:ND2	1.83	0.72
2:B:198:ALA:HB3	2:B:202:ASN:OD1	1.89	0.72
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.25	0.72
2:L:155:ALA:HB3	2:L:156:PRO:HD3	1.71	0.72
1:S:213:ALA:HA	1:S:216:LEU:HD23	1.69	0.72
2:J:153:CYS:O	2:J:156:PRO:HD2	1.88	0.72
1:K:248(A):VAL:HG22	1:K:249:GLY:N	2.04	0.72
2:D:126:PRO:HB2	2:D:144:ILE:HG22	1.71	0.72
1:G:245:ASN:ND2	1:E:245:ASN:HD22	1.82	0.72
2:L:91:LEU:HD12	2:L:92:VAL:H	1.55	0.72
2:P:198:ALA:HB3	2:P:202:ASN:OD1	1.88	0.72
1:Q:213:ALA:HA	1:Q:216:LEU:HD23	1.69	0.71
2:N:198:ALA:HB3	2:N:202:ASN:OD1	1.89	0.71
1:S:248(A):VAL:HG22	1:S:249:GLY:N	2.04	0.71
1:G:192:ASP:HB3	1:G:195:ARG:HD2	1.72	0.71
2:L:126:PRO:HB2	2:L:144:ILE:HG22	1.71	0.71
1:E:38:LYS:HG3	1:E:39:SER:H	1.54	0.71
2:J:154:LEU:O	2:J:158:VAL:HG23	1.89	0.71
2:B:154:LEU:O	2:B:158:VAL:HG23	1.89	0.71
1:I:192:ASP:HB3	1:I:195:ARG:HD2	1.72	0.71
2:T:126:PRO:HB2	2:T:144:ILE:HG22	1.71	0.71
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.25	0.71
1:I:301:GLY:HA3	1:K:169:LYS:NZ	2.04	0.71
1:S:190:HIS:HB3	1:S:196:ALA:HB2	1.73	0.71
2:R:91:LEU:HD12	2:R:92:VAL:H	1.55	0.71
1:G:245:ASN:HA	1:G:304:MET:HA	1.73	0.71
2:H:9:GLY:O	2:H:13:ARG:HG3	1.91	0.71
1:K:190:HIS:HB3	1:K:196:ALA:HB2	1.73	0.71
1:M:245:ASN:HA	1:M:304:MET:HA	1.73	0.71
1:S:38:LYS:HG3	1:S:39:SER:H	1.54	0.71
1:O:245:ASN:HA	1:O:304:MET:HA	1.73	0.71
2:D:91:LEU:HD12	2:D:92:VAL:H	1.55	0.71
1:I:245:ASN:HA	1:I:304:MET:HA	1.73	0.71
1:M:292:ILE:HD12	1:M:292:ILE:N	2.06	0.71
1:O:292:ILE:HD12	1:O:292:ILE:N	2.06	0.71
1:A:192:ASP:HB3	1:A:195:ARG:HD2	1.72	0.71
2:F:82:LEU:HD13	2:F:84:TRP:CZ2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:122(A):LYS:HD2	1:Q:122(A):LYS:O	1.91	0.70
2:H:154:LEU:O	2:H:158:VAL:HG23	1.89	0.70
1:K:38:LYS:HG3	1:K:39:SER:H	1.54	0.70
1:M:192:ASP:HB3	1:M:195:ARG:HD2	1.72	0.70
1:A:124:ASP:HB2	1:G:124:ASP:OD2	1.83	0.70
1:A:245:ASN:HA	1:A:304:MET:HA	1.73	0.70
2:B:320:ARG:HA	2:B:320:ARG:NE	2.06	0.70
2:J:9:GLY:O	2:J:13:ARG:HG3	1.91	0.70
2:P:9:GLY:O	2:P:13:ARG:HG3	1.91	0.70
2:R:320:ARG:HA	2:R:320:ARG:NE	2.07	0.70
2:D:82:LEU:HD13	2:D:84:TRP:CZ2	2.26	0.70
1:E:123(A):SER:C	1:K:124:ASP:HA	2.16	0.70
1:I:292:ILE:HD12	1:I:292:ILE:N	2.06	0.70
2:T:82:LEU:HD13	2:T:84:TRP:CZ2	2.26	0.70
1:A:292:ILE:HD12	1:A:292:ILE:N	2.06	0.70
2:B:9:GLY:O	2:B:13:ARG:HG3	1.91	0.70
1:C:292:ILE:HD12	1:C:292:ILE:H	1.55	0.70
2:L:82:LEU:HD13	2:L:84:TRP:CZ2	2.26	0.70
2:N:9:GLY:O	2:N:13:ARG:HG3	1.91	0.70
2:T:320:ARG:NE	2:T:320:ARG:HA	2.07	0.70
1:C:292:ILE:HD12	1:C:292:ILE:N	2.07	0.70
1:G:146:ASN:HD22	1:G:321:VAL:HA	1.57	0.70
1:E:190:HIS:HB3	1:E:196:ALA:HB2	1.73	0.70
1:I:124:ASP:HB2	1:M:124:ASP:OD2	1.82	0.70
1:I:169:LYS:NZ	1:K:301:GLY:HA3	2.07	0.70
1:A:146:ASN:HD22	1:A:321:VAL:HA	1.57	0.70
1:A:221:LEU:HD23	1:A:225:LEU:HD11	1.74	0.70
1:A:177:SER:HB3	1:A:234:THR:O	1.92	0.70
1:A:241:ASP:OD1	1:A:306:LYS:HE3	1.91	0.70
1:E:292:ILE:H	1:E:292:ILE:HD12	1.55	0.70
2:J:320:ARG:HA	2:J:320:ARG:NE	2.06	0.70
1:M:169:LYS:NZ	1:S:301:GLY:HA3	2.07	0.70
1:S:292:ILE:H	1:S:292:ILE:HD12	1.56	0.70
1:O:169:LYS:NZ	1:Q:301:GLY:HA3	2.07	0.69
2:P:320:ARG:NE	2:P:320:ARG:HA	2.07	0.69
1:Q:190:HIS:HB3	1:Q:196:ALA:HB2	1.73	0.69
2:B:229:ALA:O	2:B:230:LEU:HD23	1.92	0.69
1:G:221:LEU:HD23	1:G:225:LEU:HD11	1.74	0.69
1:I:241:ASP:OD1	1:I:306:LYS:HE3	1.91	0.69
2:N:320:ARG:NE	2:N:320:ARG:HA	2.06	0.69
1:O:11:ILE:HD11	1:O:317:TYR:HD2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:292:ILE:N	1:Q:292:ILE:HD12	2.07	0.69
1:G:292:ILE:HD12	1:G:292:ILE:N	2.06	0.69
1:I:177:SER:HB3	1:I:234:THR:O	1.92	0.69
1:O:177:SER:HB3	1:O:234:THR:O	1.92	0.69
1:C:190:HIS:HB3	1:C:196:ALA:HB2	1.73	0.69
1:G:241:ASP:OD1	1:G:306:LYS:HE3	1.91	0.69
2:J:229:ALA:O	2:J:230:LEU:HD23	1.92	0.69
1:K:292:ILE:HD12	1:K:292:ILE:N	2.07	0.69
1:M:241:ASP:OD1	1:M:306:LYS:HE3	1.91	0.69
2:N:126:PRO:HB2	2:N:144:ILE:HG22	1.75	0.69
2:R:82:LEU:HD13	2:R:84:TRP:CZ2	2.27	0.69
2:H:320:ARG:NE	2:H:320:ARG:HA	2.06	0.69
2:F:320:ARG:NE	2:F:320:ARG:HA	2.07	0.69
1:O:124:ASP:HB2	1:C:124:ASP:OD2	1.77	0.69
1:Q:292:ILE:HD12	1:Q:292:ILE:H	1.55	0.69
2:H:229:ALA:O	2:H:230:LEU:HD23	1.92	0.69
1:E:292:ILE:HD12	1:E:292:ILE:N	2.07	0.69
1:I:146:ASN:HD22	1:I:321:VAL:HA	1.57	0.69
1:M:11:ILE:HD11	1:M:317:TYR:HD2	1.57	0.69
2:N:133:ASN:C	2:N:133:ASN:HD22	2.00	0.69
1:M:146:ASN:HD22	1:M:321:VAL:HA	1.57	0.69
1:M:154:LEU:O	1:M:158:VAL:HG23	1.93	0.69
1:M:184:LEU:HD13	2:T:184:LEU:HD13	1.74	0.69
1:O:146:ASN:HD22	1:O:321:VAL:HA	1.57	0.69
1:Q:250:VAL:HB	1:Q:254:ASP:OD2	1.93	0.69
2:D:320:ARG:NE	2:D:320:ARG:HA	2.07	0.69
1:G:177:SER:HB3	1:G:234:THR:O	1.92	0.69
2:F:91:LEU:HD12	2:F:92:VAL:H	1.54	0.69
1:I:184:LEU:HD13	2:L:184:LEU:HD13	1.74	0.69
2:J:155:ALA:HB3	2:J:156:PRO:HD3	1.75	0.69
1:K:292:ILE:HD12	1:K:292:ILE:H	1.55	0.69
2:N:155:ALA:HB3	2:N:156:PRO:HD3	1.75	0.69
1:O:184:LEU:HD13	2:R:184:LEU:HD13	1.74	0.69
2:P:229:ALA:O	2:P:230:LEU:HD23	1.92	0.69
1:Q:100:VAL:HG23	1:Q:122(A):LYS:HG2	1.74	0.69
1:A:74:VAL:HG12	1:A:75:SER:N	2.08	0.69
1:G:11:ILE:HD11	1:G:317:TYR:HD2	1.57	0.69
1:G:169:LYS:NZ	1:E:301:GLY:HA3	2.07	0.69
2:H:91:LEU:HD12	2:H:92:VAL:H	1.57	0.69
1:S:250:VAL:HB	1:S:254:ASP:OD2	1.93	0.69
2:P:91:LEU:HD12	2:P:92:VAL:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HD11	1:A:317:TYR:HD2	1.57	0.69
1:G:154:LEU:O	1:G:158:VAL:HG23	1.93	0.69
1:I:154:LEU:O	1:I:158:VAL:HG23	1.93	0.69
1:M:177:SER:HB3	1:M:234:THR:O	1.92	0.69
2:N:229:ALA:O	2:N:230:LEU:HD23	1.92	0.69
1:O:154:LEU:O	1:O:158:VAL:HG23	1.93	0.68
1:A:154:LEU:O	1:A:158:VAL:HG23	1.93	0.68
1:O:74:VAL:HG12	1:O:75:SER:N	2.08	0.68
2:H:155:ALA:HB3	2:H:156:PRO:HD3	1.75	0.68
1:I:169:LYS:HZ2	1:K:301:GLY:HA3	1.58	0.68
1:I:221:LEU:HD23	1:I:225:LEU:HD11	1.74	0.68
1:K:221:LEU:HD23	1:K:225:LEU:HD11	1.75	0.68
2:L:320:ARG:NE	2:L:320:ARG:HA	2.07	0.68
1:G:74:VAL:HG12	1:G:75:SER:N	2.08	0.68
1:I:11:ILE:HD11	1:I:317:TYR:HD2	1.57	0.68
1:O:241:ASP:OD1	1:O:306:LYS:HE3	1.91	0.68
1:A:184:LEU:HD13	2:D:184:LEU:HD13	1.74	0.68
1:C:221:LEU:HD23	1:C:225:LEU:HD11	1.75	0.68
2:J:133:ASN:HD22	2:J:133:ASN:C	2.00	0.68
2:L:181:ASP:CG	2:L:195:ARG:HH11	2.01	0.68
2:T:181:ASP:CG	2:T:195:ARG:HH11	2.01	0.68
1:Q:44:LEU:HD21	1:Q:66:ILE:HD11	1.76	0.68
1:Q:100:VAL:HG23	1:Q:122(A):LYS:HB2	1.76	0.68
2:R:181:ASP:CG	2:R:195:ARG:HH11	2.01	0.68
2:B:155:ALA:HB3	2:B:156:PRO:HD3	1.75	0.68
1:I:226:ASN:OD1	1:K:298:MET:SD	2.52	0.68
2:N:91:LEU:HD12	2:N:92:VAL:H	1.57	0.68
1:A:169:LYS:NZ	1:C:301:GLY:HA3	2.07	0.68
2:B:133:ASN:HD22	2:B:133:ASN:C	2.00	0.68
2:D:181:ASP:CG	2:D:195:ARG:HH11	2.01	0.68
1:G:184:LEU:HD13	2:F:184:LEU:HD13	1.74	0.68
2:J:91:LEU:HD12	2:J:92:VAL:H	1.57	0.68
1:K:250:VAL:HB	1:K:254:ASP:OD2	1.93	0.68
1:S:44:LEU:HD21	1:S:66:ILE:HD11	1.76	0.68
1:S:292:ILE:HD12	1:S:292:ILE:N	2.07	0.68
1:O:221:LEU:HD23	1:O:225:LEU:HD11	1.75	0.68
2:P:155:ALA:HB3	2:P:156:PRO:HD3	1.75	0.68
2:P:210:ALA:O	2:P:214:VAL:HG23	1.94	0.68
1:S:221:LEU:HD23	1:S:225:LEU:HD11	1.76	0.68
1:O:123(A):SER:C	1:C:124:ASP:HA	2.19	0.68
1:O:226:ASN:OD1	1:Q:298:MET:SD	2.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:177:SER:HB3	1:Q:234:THR:O	1.94	0.68
1:K:44:LEU:HD21	1:K:66:ILE:HD11	1.76	0.68
2:F:181:ASP:CG	2:F:195:ARG:HH11	2.01	0.68
1:I:80:LEU:HD21	1:I:110:GLN:OE1	1.93	0.68
2:N:210:ALA:O	2:N:214:VAL:HG23	1.93	0.68
1:Q:221:LEU:HD23	1:Q:225:LEU:HD11	1.76	0.68
2:H:133:ASN:HD22	2:H:133:ASN:C	2.01	0.68
1:E:44:LEU:HD21	1:E:66:ILE:HD11	1.76	0.68
1:M:221:LEU:HD23	1:M:225:LEU:HD11	1.74	0.68
1:G:226:ASN:OD1	1:E:298:MET:SD	2.52	0.67
2:H:210:ALA:O	2:H:214:VAL:HG23	1.93	0.67
1:E:250:VAL:HB	1:E:254:ASP:OD2	1.93	0.67
2:R:229:ALA:O	2:R:230:LEU:HD23	1.95	0.67
1:A:248(A):VAL:HG22	1:A:249:GLY:N	2.08	0.67
2:N:225:LEU:C	2:T:300:MET:HE1	2.19	0.67
2:R:91:LEU:HD12	2:R:92:VAL:N	2.10	0.67
1:G:248(A):VAL:HG22	1:G:249:GLY:N	2.08	0.67
2:J:126:PRO:HB2	2:J:144:ILE:HG22	1.75	0.67
1:K:177:SER:HB3	1:K:234:THR:O	1.94	0.67
1:O:248(A):VAL:HG22	1:O:249:GLY:N	2.08	0.67
1:C:250:VAL:HB	1:C:254:ASP:OD2	1.93	0.67
2:H:225:LEU:C	2:F:300:MET:HE1	2.19	0.67
1:I:33:SER:HA	1:I:75:SER:OG	1.94	0.67
2:J:225:LEU:C	2:L:300:MET:HE1	2.19	0.67
1:M:226:ASN:OD1	1:S:298:MET:SD	2.52	0.67
1:M:248(A):VAL:HG22	1:M:249:GLY:N	2.08	0.67
2:N:178:TYR:HE1	1:S:185:LEU:HD21	1.59	0.67
2:T:229:ALA:O	2:T:230:LEU:HD23	1.94	0.67
1:I:74:VAL:HG12	1:I:75:SER:N	2.08	0.67
2:J:210:ALA:O	2:J:214:VAL:HG23	1.93	0.67
1:M:74:VAL:HG12	1:M:75:SER:N	2.08	0.67
2:H:126:PRO:HB2	2:H:144:ILE:HG22	1.75	0.67
1:E:221:LEU:HD23	1:E:225:LEU:HD11	1.75	0.67
2:P:126:PRO:HB2	2:P:144:ILE:HG22	1.75	0.67
1:C:44:LEU:HD21	1:C:66:ILE:HD11	1.76	0.67
2:L:91:LEU:HD12	2:L:92:VAL:N	2.09	0.67
2:L:229:ALA:O	2:L:230:LEU:HD23	1.94	0.67
1:A:33:SER:HA	1:A:75:SER:OG	1.94	0.67
1:A:228:ILE:HD12	1:C:306:LYS:HE2	1.77	0.67
2:B:91:LEU:HD12	2:B:92:VAL:N	2.10	0.67
2:B:91:LEU:HD12	2:B:92:VAL:H	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LEU:C	2:D:300:MET:HE1	2.19	0.67
2:D:91:LEU:HD12	2:D:92:VAL:N	2.10	0.67
2:D:229:ALA:O	2:D:230:LEU:HD23	1.94	0.67
2:J:91:LEU:HD12	2:J:92:VAL:N	2.10	0.67
1:A:226:ASN:OD1	1:C:298:MET:SD	2.52	0.67
2:B:210:ALA:O	2:B:214:VAL:HG23	1.93	0.67
2:F:91:LEU:HD12	2:F:92:VAL:N	2.10	0.67
1:I:228:ILE:HD12	1:K:306:LYS:HE2	1.77	0.67
2:N:91:LEU:HD12	2:N:92:VAL:N	2.10	0.67
1:S:177:SER:HB3	1:S:234:THR:O	1.94	0.67
2:P:225:LEU:C	2:R:300:MET:HE1	2.20	0.67
1:G:228:ILE:HD12	1:E:306:LYS:HE2	1.77	0.67
1:M:33:SER:HA	1:M:75:SER:OG	1.94	0.67
1:I:248(A):VAL:HG22	1:I:249:GLY:N	2.08	0.66
2:P:133:ASN:HD22	2:P:133:ASN:C	2.00	0.66
2:B:126:PRO:HB2	2:B:144:ILE:HG22	1.75	0.66
1:E:74:VAL:HG12	1:E:75:SER:N	2.10	0.66
1:E:177:SER:HB3	1:E:234:THR:O	1.94	0.66
1:I:129:VAL:HG23	1:I:217:VAL:HG11	1.78	0.66
2:J:242:LEU:HD12	2:J:243:VAL:H	1.60	0.66
2:P:242:LEU:HD12	2:P:243:VAL:H	1.60	0.66
2:P:251:PHE:CE1	2:P:254:GLU:HB2	2.31	0.66
1:I:190:HIS:H	2:L:39:GLN:HE22	1.43	0.66
1:M:129:VAL:HG23	1:M:217:VAL:HG11	1.78	0.66
2:P:91:LEU:HD12	2:P:92:VAL:N	2.10	0.66
2:F:229:ALA:O	2:F:230:LEU:HD23	1.94	0.66
2:J:251:PHE:CE1	2:J:254:GLU:HB2	2.31	0.66
1:K:74:VAL:HG12	1:K:75:SER:N	2.10	0.66
1:M:190:HIS:H	2:T:39:GLN:HE22	1.43	0.66
1:M:228:ILE:HD12	1:S:306:LYS:HE2	1.77	0.66
2:T:91:LEU:HD12	2:T:92:VAL:N	2.10	0.66
1:O:190:HIS:H	2:R:39:GLN:HE22	1.43	0.66
1:O:228:ILE:HD12	1:Q:306:LYS:HE2	1.77	0.66
1:Q:146:ASN:HD22	1:Q:321:VAL:HA	1.60	0.66
1:E:146:ASN:HD22	1:E:321:VAL:HA	1.61	0.66
1:Q:48:SER:HA	2:R:281:ILE:HG21	1.78	0.66
1:C:146:ASN:HD22	1:C:321:VAL:HA	1.60	0.66
1:G:33:SER:HA	1:G:75:SER:OG	1.94	0.66
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.78	0.66
1:E:48:SER:HA	2:F:281:ILE:HG21	1.78	0.66
1:E:123(A):SER:O	1:K:124:ASP:CA	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:241:ASP:OD1	1:S:306:LYS:HE3	1.96	0.66
2:P:178:TYR:HE1	1:Q:185:LEU:HD21	1.59	0.66
1:Q:74:VAL:HG12	1:Q:75:SER:N	2.10	0.66
2:H:91:LEU:HD12	2:H:92:VAL:N	2.10	0.66
2:N:242:LEU:HD12	2:N:243:VAL:H	1.61	0.66
2:P:181:ASP:CG	2:P:195:ARG:HH11	2.04	0.66
1:C:48:SER:HA	2:D:281:ILE:HG21	1.78	0.66
1:C:177:SER:HB3	1:C:234:THR:O	1.94	0.66
1:S:48:SER:HA	2:T:281:ILE:HG21	1.78	0.66
2:B:251:PHE:CE1	2:B:254:GLU:HB2	2.31	0.66
2:H:178:TYR:HE1	1:E:185:LEU:HD21	1.59	0.66
1:K:241:ASP:OD1	1:K:306:LYS:HE3	1.96	0.66
1:S:146:ASN:HD22	1:S:321:VAL:HA	1.61	0.66
1:M:193:LEU:H	1:M:193:LEU:CD1	2.06	0.66
2:T:251:PHE:CE1	2:T:254:GLU:HB2	2.31	0.66
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.78	0.65
2:H:242:LEU:HD12	2:H:243:VAL:H	1.61	0.65
2:H:251:PHE:CE1	2:H:254:GLU:HB2	2.31	0.65
2:N:181:ASP:CG	2:N:195:ARG:HH11	2.04	0.65
1:Q:80:LEU:CD2	1:Q:110:GLN:OE1	2.44	0.65
1:A:190:HIS:H	2:D:39:GLN:HE22	1.43	0.65
2:B:202:ASN:HD22	2:D:281:ILE:H	1.45	0.65
1:C:232:VAL:HG23	1:C:234:THR:HG22	1.79	0.65
2:J:178:TYR:HE1	1:K:185:LEU:HD21	1.59	0.65
1:K:48:SER:HA	2:L:281:ILE:HG21	1.78	0.65
1:Q:232:VAL:HG23	1:Q:234:THR:HG22	1.78	0.65
2:R:154:LEU:HD13	2:R:240:VAL:HG21	1.78	0.65
2:B:178:TYR:HE1	1:C:185:LEU:HD21	1.59	0.65
2:H:181:ASP:CG	2:H:195:ARG:HH11	2.04	0.65
1:E:232:VAL:HG23	1:E:234:THR:HG22	1.79	0.65
1:C:74:VAL:HG12	1:C:75:SER:N	2.10	0.65
2:D:126:PRO:HD2	2:D:143:ILE:O	1.97	0.65
1:E:80:LEU:CD2	1:E:110:GLN:CD	2.58	0.65
1:E:241:ASP:OD1	1:E:306:LYS:HE3	1.96	0.65
2:J:181:ASP:CG	2:J:195:ARG:HH11	2.04	0.65
2:L:15:PHE:CE1	2:L:322:VAL:HG22	2.32	0.65
1:O:100:VAL:HA	1:O:118:ILE:HD13	1.79	0.65
1:Q:101:ASP:CB	1:Q:122(A):LYS:HB3	2.24	0.65
2:B:181:ASP:CG	2:B:195:ARG:HH11	2.04	0.65
2:F:126:PRO:HD2	2:F:143:ILE:O	1.97	0.65
1:K:146:ASN:HD22	1:K:321:VAL:HA	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:SER:HA	1:O:75:SER:OG	1.94	0.65
2:R:126:PRO:HD2	2:R:143:ILE:O	1.97	0.65
2:B:242:LEU:HD12	2:B:243:VAL:H	1.60	0.65
2:D:15:PHE:CE1	2:D:322:VAL:HG22	2.32	0.65
1:G:190:HIS:H	2:F:39:GLN:HE22	1.43	0.65
2:F:251:PHE:CE1	2:F:254:GLU:HB2	2.31	0.65
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.78	0.65
2:R:20:ARG:HH11	2:R:20:ARG:HG3	1.62	0.65
2:H:202:ASN:HD22	2:F:281:ILE:H	1.45	0.65
2:L:251:PHE:CE1	2:L:254:GLU:HB2	2.31	0.65
2:N:251:PHE:CE1	2:N:254:GLU:HB2	2.31	0.65
2:P:42:HIS:CG	1:Q:193:LEU:HD23	2.32	0.65
2:P:82:LEU:HD13	2:P:84:TRP:CZ2	2.32	0.65
2:P:202:ASN:HD22	2:R:281:ILE:H	1.45	0.65
2:R:15:PHE:CE1	2:R:322:VAL:HG22	2.31	0.65
1:Q:110:GLN:HB3	1:S:110:GLN:HB2	1.79	0.65
2:B:42:HIS:CG	1:C:193:LEU:HD23	2.32	0.65
1:G:100:VAL:HA	1:G:118:ILE:HD13	1.79	0.65
1:E:192:ASP:HB3	1:E:195:ARG:HD2	1.79	0.65
1:I:193:LEU:H	1:I:193:LEU:CD1	2.06	0.65
1:M:228:ILE:H	1:M:228:ILE:CD1	2.10	0.65
2:T:15:PHE:CE1	2:T:322:VAL:HG22	2.32	0.65
2:T:126:PRO:HD2	2:T:143:ILE:O	1.97	0.65
1:Q:100:VAL:HG23	1:Q:122(A):LYS:CG	2.27	0.65
1:C:241:ASP:OD1	1:C:306:LYS:HE3	1.96	0.65
2:H:82:LEU:HD13	2:H:84:TRP:CZ2	2.32	0.65
2:F:15:PHE:CE1	2:F:322:VAL:HG22	2.32	0.65
1:S:74:VAL:HG12	1:S:75:SER:N	2.10	0.65
2:D:210:ALA:O	2:D:214:VAL:HG23	1.98	0.64
2:D:251:PHE:CE1	2:D:254:GLU:HB2	2.31	0.64
2:T:154:LEU:HD13	2:T:240:VAL:HG21	1.79	0.64
1:Q:100:VAL:HG23	1:Q:122(A):LYS:CB	2.27	0.64
1:C:170:GLY:HA3	1:C:244:VAL:HG12	1.80	0.64
1:E:170:GLY:HA3	1:E:244:VAL:HG12	1.80	0.64
2:F:154:LEU:HD13	2:F:240:VAL:HG21	1.78	0.64
2:F:210:ALA:O	2:F:214:VAL:HG23	1.98	0.64
2:J:42:HIS:CG	1:K:193:LEU:HD23	2.32	0.64
1:M:100:VAL:HA	1:M:118:ILE:HD13	1.79	0.64
1:Q:124:ASP:HB2	1:S:124:ASP:O	1.97	0.64
1:Q:170:GLY:HA3	1:Q:244:VAL:HG12	1.79	0.64
1:Q:225:LEU:O	1:Q:226:ASN:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HA	1:A:118:ILE:HD13	1.79	0.64
2:D:154:LEU:HD13	2:D:240:VAL:HG21	1.78	0.64
2:F:242:LEU:HD12	2:F:243:VAL:H	1.63	0.64
2:J:82:LEU:HD13	2:J:84:TRP:CZ2	2.32	0.64
2:N:82:LEU:HD13	2:N:84:TRP:CZ2	2.32	0.64
1:Q:192:ASP:HB3	1:Q:195:ARG:HD2	1.79	0.64
1:Q:293:ASP:CB	1:Q:296:LEU:HD12	2.28	0.64
2:B:82:LEU:HD13	2:B:84:TRP:CZ2	2.32	0.64
2:D:242:LEU:HD12	2:D:243:VAL:H	1.63	0.64
2:H:42:HIS:CG	1:E:193:LEU:HD23	2.32	0.64
1:E:320:ARG:NE	1:E:320:ARG:HA	2.12	0.64
1:C:192:ASP:HB3	1:C:195:ARG:HD2	1.79	0.64
1:K:320:ARG:NE	1:K:320:ARG:HA	2.12	0.64
2:N:42:HIS:CG	1:S:193:LEU:HD23	2.32	0.64
1:S:192:ASP:HB3	1:S:195:ARG:HD2	1.78	0.64
2:T:20:ARG:HH11	2:T:20:ARG:HG3	1.62	0.64
2:T:260:ARG:HG2	2:T:273:VAL:HG21	1.80	0.64
1:O:194:ARG:NH1	1:Q:278:LEU:O	2.31	0.64
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.12	0.64
1:E:225:LEU:O	1:E:226:ASN:HB2	1.97	0.64
1:E:293:ASP:CB	1:E:296:LEU:HD12	2.28	0.64
1:K:293:ASP:CB	1:K:296:LEU:HD12	2.28	0.64
2:L:126:PRO:HD2	2:L:143:ILE:O	1.97	0.64
2:L:260:ARG:HG2	2:L:273:VAL:HG21	1.80	0.64
2:T:242:LEU:HD12	2:T:243:VAL:H	1.63	0.64
1:O:279:VAL:CG1	1:Q:204:VAL:HG22	2.28	0.64
1:Q:241:ASP:OD1	1:Q:306:LYS:HE3	1.96	0.64
2:R:251:PHE:CE1	2:R:254:GLU:HB2	2.31	0.64
2:F:182:GLN:HE22	2:F:231:ARG:HB3	1.63	0.64
2:J:202:ASN:HD22	2:L:281:ILE:H	1.45	0.64
1:K:170:GLY:HA3	1:K:244:VAL:HG12	1.79	0.64
1:K:232:VAL:HG23	1:K:234:THR:HG22	1.78	0.64
1:M:133:ASN:HD22	1:M:133:ASN:C	2.05	0.64
1:S:320:ARG:NE	1:S:320:ARG:HA	2.12	0.64
1:Q:182:GLN:HB3	1:Q:199:ALA:HB2	1.80	0.64
2:D:9:GLY:O	2:D:13:ARG:HG3	1.98	0.64
1:K:182:GLN:HB3	1:K:199:ALA:HB2	1.80	0.64
1:S:170:GLY:HA3	1:S:244:VAL:HG12	1.79	0.64
1:S:182:GLN:HB3	1:S:199:ALA:HB2	1.80	0.64
1:S:293:ASP:CB	1:S:296:LEU:HD12	2.28	0.64
2:T:210:ALA:O	2:T:214:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:110:GLN:CB	1:S:110:GLN:HB2	2.28	0.64
1:A:204:VAL:HB	1:A:231:ARG:HB2	1.80	0.64
1:C:320:ARG:NE	1:C:320:ARG:HA	2.12	0.64
1:O:246:ILE:HG13	1:O:247:GLU:H	1.63	0.64
1:O:273:VAL:HG22	1:O:292:ILE:HD13	1.80	0.64
2:R:18:CYS:SG	2:R:319:GLN:HG2	2.38	0.64
2:R:182:GLN:HE22	2:R:231:ARG:HB3	1.63	0.64
2:B:10:ARG:O	2:B:14:ASN:HB2	1.98	0.64
1:G:204:VAL:HB	1:G:231:ARG:HB2	1.80	0.64
1:K:192:ASP:HB3	1:K:195:ARG:HD2	1.79	0.64
2:N:202:ASN:HD22	2:T:281:ILE:H	1.45	0.64
1:O:204:VAL:HB	1:O:231:ARG:HB2	1.80	0.63
2:P:10:ARG:O	2:P:14:ASN:HB2	1.98	0.63
1:A:279:VAL:CG1	1:C:204:VAL:HG22	2.28	0.63
1:G:279:VAL:CG1	1:E:204:VAL:HG22	2.28	0.63
2:F:133:ASN:C	2:F:133:ASN:HD22	2.07	0.63
2:J:10:ARG:O	2:J:14:ASN:HB2	1.98	0.63
2:L:242:LEU:HD12	2:L:243:VAL:H	1.63	0.63
2:T:9:GLY:O	2:T:13:ARG:HG3	1.98	0.63
2:T:18:CYS:SG	2:T:319:GLN:HG2	2.38	0.63
2:P:184:LEU:HD13	1:Q:184:LEU:HD13	1.80	0.63
2:B:177:SER:HB3	2:B:234:THR:O	1.98	0.63
1:C:293:ASP:CB	1:C:296:LEU:HD12	2.28	0.63
1:E:182:GLN:HB3	1:E:199:ALA:HB2	1.80	0.63
1:I:228:ILE:H	1:I:228:ILE:CD1	2.10	0.63
1:I:273:VAL:HG22	1:I:292:ILE:HD13	1.80	0.63
2:L:9:GLY:O	2:L:13:ARG:HG3	1.98	0.63
2:N:177:SER:HB3	2:N:234:THR:O	1.99	0.63
1:O:228:ILE:H	1:O:228:ILE:CD1	2.10	0.63
2:P:177:SER:HB3	2:P:234:THR:O	1.98	0.63
1:A:194:ARG:NH1	1:C:278:LEU:O	2.31	0.63
1:C:225:LEU:O	1:C:226:ASN:HB2	1.97	0.63
2:H:177:SER:HB3	2:H:234:THR:O	1.98	0.63
2:F:20:ARG:HH11	2:F:20:ARG:HG3	1.62	0.63
1:I:100:VAL:HA	1:I:118:ILE:HD13	1.79	0.63
2:N:184:LEU:HD13	1:S:184:LEU:HD13	1.80	0.63
1:S:232:VAL:HG23	1:S:234:THR:HG22	1.79	0.63
1:O:25:LEU:HD22	1:O:25:LEU:N	2.14	0.63
1:O:133:ASN:C	1:O:133:ASN:HD22	2.06	0.63
2:D:133:ASN:C	2:D:133:ASN:HD22	2.07	0.63
1:G:193:LEU:HD12	1:G:193:LEU:N	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:126:PRO:HD2	2:J:143:ILE:O	1.99	0.63
2:L:18:CYS:SG	2:L:319:GLN:HG2	2.38	0.63
1:M:273:VAL:HG22	1:M:292:ILE:HD13	1.80	0.63
2:N:10:ARG:O	2:N:14:ASN:HB2	1.98	0.63
2:L:210:ALA:O	2:L:214:VAL:HG23	1.98	0.63
2:N:260:ARG:HG2	2:N:273:VAL:HG21	1.80	0.63
1:S:225:LEU:O	1:S:226:ASN:HB2	1.97	0.63
2:D:18:CYS:SG	2:D:319:GLN:HG2	2.38	0.63
1:G:273:VAL:HG22	1:G:292:ILE:HD13	1.80	0.63
2:H:10:ARG:O	2:H:14:ASN:HB2	1.98	0.63
2:L:154:LEU:HD13	2:L:240:VAL:HG21	1.78	0.63
1:M:25:LEU:HD22	1:M:25:LEU:N	2.14	0.63
1:M:246:ILE:HG13	1:M:247:GLU:H	1.64	0.63
2:R:9:GLY:O	2:R:13:ARG:HG3	1.98	0.63
2:R:210:ALA:O	2:R:214:VAL:HG23	1.98	0.63
2:D:14:ASN:HB3	2:D:318:SER:OG	1.99	0.63
2:F:14:ASN:HB3	2:F:318:SER:OG	1.99	0.63
2:L:20:ARG:HH11	2:L:20:ARG:HG3	1.61	0.63
1:M:194:ARG:NH1	1:S:278:LEU:O	2.31	0.63
2:F:260:ARG:HG2	2:F:273:VAL:HG21	1.80	0.63
2:J:260:ARG:HG2	2:J:273:VAL:HG21	1.80	0.63
2:L:133:ASN:C	2:L:133:ASN:HD22	2.06	0.63
2:L:293:ASP:CG	2:L:296:LEU:HD12	2.24	0.63
2:P:260:ARG:HG2	2:P:273:VAL:HG21	1.80	0.63
2:R:242:LEU:HD12	2:R:243:VAL:H	1.63	0.63
1:A:25:LEU:HD22	1:A:25:LEU:N	2.14	0.63
1:A:228:ILE:H	1:A:228:ILE:CD1	2.10	0.63
2:D:20:ARG:HH11	2:D:20:ARG:HG3	1.62	0.63
1:G:25:LEU:HD22	1:G:25:LEU:N	2.14	0.63
1:G:194:ARG:NH1	1:E:278:LEU:O	2.31	0.63
1:I:194:ARG:NH1	1:K:278:LEU:O	2.31	0.63
1:K:225:LEU:O	1:K:226:ASN:HB2	1.97	0.63
2:T:133:ASN:C	2:T:133:ASN:HD22	2.06	0.63
1:I:246:ILE:HG13	1:I:247:GLU:H	1.64	0.62
2:T:14:ASN:HB3	2:T:318:SER:OG	1.99	0.62
2:P:182:GLN:HE22	2:P:231:ARG:HB3	1.64	0.62
2:P:293:ASP:CG	2:P:296:LEU:HD12	2.24	0.62
1:A:273:VAL:HG22	1:A:292:ILE:HD13	1.80	0.62
2:D:182:GLN:HE22	2:D:231:ARG:HB3	1.63	0.62
2:F:18:CYS:SG	2:F:319:GLN:HG2	2.38	0.62
2:R:293:ASP:CG	2:R:296:LEU:HD12	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:HB3	1:C:199:ALA:HB2	1.80	0.62
2:F:9:GLY:O	2:F:13:ARG:HG3	1.98	0.62
2:J:184:LEU:HD13	1:K:184:LEU:HD13	1.80	0.62
1:A:133:ASN:C	1:A:133:ASN:HD22	2.06	0.62
2:H:126:PRO:HD2	2:H:143:ILE:O	1.99	0.62
2:H:260:ARG:HG2	2:H:273:VAL:HG21	1.80	0.62
2:L:182:GLN:HE22	2:L:231:ARG:HB3	1.63	0.62
2:N:293:ASP:CG	2:N:296:LEU:HD12	2.25	0.62
2:T:293:ASP:CG	2:T:296:LEU:HD12	2.24	0.62
1:G:29:VAL:HA	1:G:72:LYS:O	2.00	0.62
2:H:293:ASP:CG	2:H:296:LEU:HD12	2.25	0.62
2:F:293:ASP:CG	2:F:296:LEU:HD12	2.24	0.62
1:I:25:LEU:HD22	1:I:25:LEU:N	2.14	0.62
1:I:133:ASN:C	1:I:133:ASN:HD22	2.06	0.62
2:J:177:SER:HB3	2:J:234:THR:O	1.98	0.62
2:J:281:ILE:HB	2:L:202:ASN:ND2	2.15	0.62
2:N:281:ILE:HB	2:T:202:ASN:ND2	2.15	0.62
1:S:29:VAL:HA	1:S:72:LYS:O	2.00	0.62
2:R:260:ARG:HG2	2:R:273:VAL:HG21	1.80	0.62
2:D:260:ARG:HG2	2:D:273:VAL:HG21	1.80	0.62
1:I:279:VAL:CG1	1:K:204:VAL:HG22	2.28	0.62
1:O:306:LYS:HE2	1:Q:228:ILE:HD12	1.82	0.62
1:Q:29:VAL:HA	1:Q:72:LYS:O	2.00	0.62
1:A:29:VAL:HA	1:A:72:LYS:O	2.00	0.62
1:A:110:GLN:HB3	1:G:110:GLN:HB3	1.77	0.62
2:B:126:PRO:HD2	2:B:143:ILE:O	1.99	0.62
1:M:204:VAL:HB	1:M:231:ARG:HB2	1.80	0.62
2:T:182:GLN:HE22	2:T:231:ARG:HB3	1.63	0.62
2:B:281:ILE:HB	2:D:202:ASN:ND2	2.15	0.62
1:G:228:ILE:H	1:G:228:ILE:CD1	2.10	0.62
1:I:204:VAL:HB	1:I:231:ARG:HB2	1.80	0.62
1:K:100:VAL:HA	1:K:118:ILE:HD13	1.82	0.62
1:Q:125:ILE:HG21	1:Q:143:ILE:HG22	1.79	0.62
2:B:260:ARG:HG2	2:B:273:VAL:HG21	1.80	0.62
1:C:246:ILE:HG13	1:C:247:GLU:H	1.65	0.62
2:D:293:ASP:CG	2:D:296:LEU:HD12	2.24	0.62
1:G:133:ASN:C	1:G:133:ASN:HD22	2.05	0.62
2:H:281:ILE:HB	2:F:202:ASN:ND2	2.15	0.62
2:L:153:CYS:O	2:L:156:PRO:HD2	2.00	0.62
2:P:126:PRO:HD2	2:P:143:ILE:O	1.99	0.62
2:R:14:ASN:HB3	2:R:318:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ILE:HG22	2:B:169:LYS:HG2	1.82	0.62
2:D:153:CYS:O	2:D:156:PRO:HD2	2.00	0.62
1:G:250:VAL:HB	1:G:254:ASP:OD2	2.00	0.62
1:M:29:VAL:HA	1:M:72:LYS:O	2.00	0.62
1:Q:246:ILE:HG13	1:Q:247:GLU:H	1.65	0.61
2:R:133:ASN:HD22	2:R:133:ASN:C	2.06	0.61
2:B:293:ASP:CG	2:B:296:LEU:HD12	2.25	0.61
2:F:153:CYS:O	2:F:156:PRO:HD2	2.00	0.61
1:I:31:ASN:OD1	1:I:75:SER:HA	2.00	0.61
2:J:168:ILE:HG22	2:J:169:LYS:HG2	1.82	0.61
2:J:293:ASP:CG	2:J:296:LEU:HD12	2.25	0.61
1:K:107:LYS:HA	1:K:110:GLN:OE1	2.00	0.61
1:M:31:ASN:OD1	1:M:75:SER:HA	2.00	0.61
1:S:100:VAL:HA	1:S:118:ILE:HD13	1.82	0.61
1:A:246:ILE:HG13	1:A:247:GLU:H	1.64	0.61
2:B:182:GLN:HE22	2:B:231:ARG:HB3	1.64	0.61
1:G:246:ILE:HG13	1:G:247:GLU:H	1.64	0.61
1:I:29:VAL:HA	1:I:72:LYS:O	2.00	0.61
1:M:251:THR:HB	1:M:254:ASP:OD1	2.00	0.61
2:P:281:ILE:HB	2:R:202:ASN:ND2	2.15	0.61
2:B:184:LEU:HD13	1:C:184:LEU:HD13	1.80	0.61
1:E:29:VAL:HA	1:E:72:LYS:O	2.00	0.61
1:E:246:ILE:HG13	1:E:247:GLU:H	1.65	0.61
2:L:14:ASN:HB3	2:L:318:SER:OG	1.99	0.61
1:M:250:VAL:HB	1:M:254:ASP:OD2	2.00	0.61
2:N:126:PRO:HD2	2:N:143:ILE:O	1.99	0.61
2:N:168:ILE:HG22	2:N:169:LYS:HG2	1.82	0.61
1:S:246:ILE:HG13	1:S:247:GLU:H	1.65	0.61
2:T:153:CYS:O	2:T:156:PRO:HD2	2.00	0.61
1:O:251:THR:HB	1:O:254:ASP:OD1	2.00	0.61
1:Q:101:ASP:HB3	1:Q:122(A):LYS:CB	2.27	0.61
1:Q:110:GLN:O	1:S:110:GLN:CD	2.43	0.61
1:A:44:LEU:HD21	1:A:66:ILE:HD11	1.82	0.61
1:C:133:ASN:C	1:C:133:ASN:HD22	2.09	0.61
2:H:184:LEU:HD13	1:E:184:LEU:HD13	1.80	0.61
1:I:306:LYS:HE2	1:K:228:ILE:HD12	1.82	0.61
1:M:306:LYS:HE2	1:S:228:ILE:HD12	1.82	0.61
1:C:246:ILE:HG22	1:C:303:ASP:O	2.01	0.61
1:C:273:VAL:HG22	1:C:292:ILE:HD13	1.83	0.61
2:F:120:ALA:O	2:F:145:SER:HB2	2.01	0.61
1:K:246:ILE:HG13	1:K:247:GLU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:LEU:HD21	1:M:66:ILE:HD11	1.82	0.61
2:P:168:ILE:HG22	2:P:169:LYS:HG2	1.82	0.61
2:H:168:ILE:HG22	2:H:169:LYS:HG2	1.82	0.61
1:E:100:VAL:HA	1:E:118:ILE:HD13	1.82	0.61
1:E:273:VAL:HG22	1:E:292:ILE:HD13	1.83	0.61
2:T:120:ALA:O	2:T:145:SER:HB2	2.01	0.61
1:O:191:ARG:NH1	1:O:191:ARG:HB2	2.16	0.61
2:B:183:ARG:HD2	2:B:187:ALA:HB3	1.82	0.61
1:E:246:ILE:HG22	1:E:303:ASP:O	2.00	0.61
2:J:182:GLN:HE22	2:J:231:ARG:HB3	1.64	0.61
1:K:29:VAL:HA	1:K:72:LYS:O	2.00	0.61
2:L:120:ALA:O	2:L:145:SER:HB2	2.01	0.61
1:A:31:ASN:OD1	1:A:75:SER:HA	2.00	0.61
1:A:306:LYS:HE2	1:C:228:ILE:HD12	1.82	0.61
1:G:44:LEU:HD21	1:G:66:ILE:HD11	1.82	0.61
1:G:306:LYS:HE2	1:E:228:ILE:HD12	1.82	0.61
1:E:124:ASP:OD1	1:E:125:ILE:CG1	2.35	0.61
2:J:183:ARG:HD2	2:J:187:ALA:HB3	1.83	0.61
2:N:182:GLN:HE22	2:N:231:ARG:HB3	1.64	0.61
1:S:246:ILE:HG22	1:S:303:ASP:O	2.00	0.61
1:O:44:LEU:HD21	1:O:66:ILE:HD11	1.82	0.61
1:O:201:LEU:HD23	1:O:201:LEU:N	2.16	0.61
1:A:250:VAL:HB	1:A:254:ASP:OD2	2.01	0.61
1:C:31:ASN:OD1	1:C:75:SER:HA	2.01	0.61
2:H:182:GLN:HE22	2:H:231:ARG:HB3	1.64	0.61
1:I:106:GLY:O	1:M:110:GLN:OE1	2.17	0.61
1:K:133:ASN:C	1:K:133:ASN:HD22	2.09	0.61
1:M:279:VAL:CG1	1:S:204:VAL:HG22	2.28	0.61
2:D:120:ALA:O	2:D:145:SER:HB2	2.01	0.60
1:E:165:LEU:C	1:E:246:ILE:HD11	2.26	0.60
1:S:165:LEU:C	1:S:246:ILE:HD11	2.26	0.60
1:C:29:VAL:HA	1:C:72:LYS:O	2.00	0.60
1:G:31:ASN:OD1	1:G:75:SER:HA	2.00	0.60
1:G:251:THR:HB	1:G:254:ASP:OD1	2.00	0.60
1:M:48:SER:HA	2:N:281:ILE:HG21	1.83	0.60
2:N:183:ARG:HD2	2:N:187:ALA:HB3	1.83	0.60
1:O:146:ASN:ND2	1:O:321:VAL:HA	2.16	0.60
2:P:20:ARG:HG3	2:P:20:ARG:HH11	1.66	0.60
1:Q:100:VAL:HA	1:Q:118:ILE:HD13	1.82	0.60
1:Q:246:ILE:HG22	1:Q:303:ASP:O	2.01	0.60
2:R:120:ALA:O	2:R:145:SER:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ARG:NH1	1:G:191:ARG:HB2	2.16	0.60
1:E:31:ASN:OD1	1:E:75:SER:HA	2.01	0.60
1:K:246:ILE:HG22	1:K:303:ASP:O	2.01	0.60
1:M:191:ARG:HB2	1:M:191:ARG:NH1	2.16	0.60
1:O:29:VAL:HA	1:O:72:LYS:O	2.00	0.60
1:Q:31:ASN:OD1	1:Q:75:SER:HA	2.02	0.60
1:Q:133:ASN:C	1:Q:133:ASN:HD22	2.09	0.60
1:Q:273:VAL:HG22	1:Q:292:ILE:HD13	1.83	0.60
1:E:133:ASN:HD22	1:E:133:ASN:C	2.09	0.60
2:F:183:ARG:HD2	2:F:187:ALA:HB3	1.84	0.60
1:I:48:SER:HA	2:J:281:ILE:HG21	1.83	0.60
1:I:110:GLN:HB2	1:M:110:GLN:OE1	2.01	0.60
1:O:31:ASN:OD1	1:O:75:SER:HA	2.00	0.60
2:R:10:ARG:O	2:R:14:ASN:HB2	2.02	0.60
2:R:153:CYS:O	2:R:156:PRO:HD2	2.00	0.60
1:A:123(A):SER:C	1:G:124:ASP:HA	2.26	0.60
1:A:146:ASN:ND2	1:A:321:VAL:HA	2.16	0.60
2:D:183:ARG:HD2	2:D:187:ALA:HB3	1.84	0.60
2:D:281:ILE:O	2:D:284:ARG:HG2	2.02	0.60
1:K:129:VAL:CG2	1:K:217:VAL:HG11	2.31	0.60
1:S:293:ASP:HB3	1:S:296:LEU:HD12	1.83	0.60
1:O:250:VAL:HB	1:O:254:ASP:OD2	2.00	0.60
2:R:281:ILE:O	2:R:284:ARG:HG2	2.01	0.60
2:F:281:ILE:O	2:F:284:ARG:HG2	2.02	0.60
1:I:146:ASN:ND2	1:I:321:VAL:HA	2.16	0.60
1:I:250:VAL:HB	1:I:254:ASP:OD2	2.00	0.60
1:S:133:ASN:C	1:S:133:ASN:HD22	2.09	0.60
1:Q:165:LEU:C	1:Q:246:ILE:HD11	2.26	0.60
1:A:201:LEU:N	1:A:201:LEU:HD23	2.16	0.60
1:C:15:PHE:CE1	1:C:322:VAL:HG22	2.37	0.60
1:I:191:ARG:NH1	1:I:191:ARG:HB2	2.16	0.60
1:K:31:ASN:OD1	1:K:75:SER:HA	2.02	0.60
1:K:154:LEU:HG	1:K:158:VAL:CG2	2.32	0.60
1:K:273:VAL:HG22	1:K:292:ILE:HD13	1.83	0.60
2:L:183:ARG:HD2	2:L:187:ALA:HB3	1.84	0.60
2:T:177:SER:HB3	2:T:234:THR:O	2.02	0.60
2:T:281:ILE:O	2:T:284:ARG:HG2	2.01	0.60
1:Q:85:ALA:HB2	1:Q:112:GLY:HA3	1.84	0.60
1:Q:124:ASP:C	1:Q:125:ILE:HG13	2.26	0.60
1:A:165:LEU:C	1:A:246:ILE:HD11	2.27	0.60
1:A:236:ASN:O	1:A:237:VAL:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:HB	1:A:254:ASP:OD1	2.00	0.60
1:G:201:LEU:HD23	1:G:201:LEU:N	2.16	0.60
2:F:177:SER:HB3	2:F:234:THR:O	2.02	0.60
2:L:10:ARG:O	2:L:14:ASN:HB2	2.02	0.60
1:M:201:LEU:N	1:M:201:LEU:HD23	2.16	0.60
1:O:228:ILE:CD1	1:Q:306:LYS:HE2	2.32	0.60
1:Q:25:LEU:HD22	1:Q:25:LEU:N	2.17	0.60
1:Q:129:VAL:CG2	1:Q:217:VAL:HG11	2.31	0.60
1:C:293:ASP:HB3	1:C:296:LEU:HD12	1.84	0.60
2:D:177:SER:HB3	2:D:234:THR:O	2.02	0.60
1:I:251:THR:HB	1:I:254:ASP:OD1	2.00	0.60
1:K:15:PHE:CE1	1:K:322:VAL:HG22	2.37	0.60
2:L:177:SER:HB3	2:L:234:THR:O	2.02	0.60
2:L:281:ILE:O	2:L:284:ARG:HG2	2.02	0.60
1:M:165:LEU:C	1:M:246:ILE:HD11	2.27	0.60
1:S:154:LEU:HG	1:S:158:VAL:CG2	2.32	0.60
1:Q:30:VAL:HB	1:Q:73:VAL:HG22	1.84	0.60
2:R:183:ARG:HD2	2:R:187:ALA:HB3	1.84	0.60
2:R:221:LEU:HA	2:R:224:LYS:HD2	1.84	0.60
1:A:30:VAL:HB	1:A:73:VAL:HG22	1.84	0.60
1:A:110:GLN:HA	1:G:80:LEU:HD22	1.82	0.60
1:C:100:VAL:HA	1:C:118:ILE:HD13	1.82	0.60
1:C:165:LEU:C	1:C:246:ILE:HD11	2.27	0.60
2:D:10:ARG:O	2:D:14:ASN:HB2	2.02	0.60
1:G:146:ASN:ND2	1:G:321:VAL:HA	2.16	0.60
1:E:251:THR:HG22	1:E:252:ALA:N	2.17	0.60
1:I:44:LEU:HD21	1:I:66:ILE:HD11	1.82	0.60
1:M:30:VAL:HB	1:M:73:VAL:HG22	1.84	0.60
1:M:193:LEU:HD12	1:M:193:LEU:N	2.10	0.60
1:S:25:LEU:N	1:S:25:LEU:HD22	2.17	0.60
1:O:185:LEU:HD21	2:R:178:TYR:HE1	1.67	0.59
1:A:191:ARG:NH1	1:A:191:ARG:HB2	2.16	0.59
2:D:221:LEU:HA	2:D:224:LYS:HD2	1.84	0.59
1:E:293:ASP:HB3	1:E:296:LEU:HD12	1.84	0.59
2:F:10:ARG:O	2:F:14:ASN:HB2	2.02	0.59
2:L:168:ILE:HG22	2:L:169:LYS:HG2	1.85	0.59
1:M:177:SER:HA	1:M:234:THR:HG23	1.84	0.59
1:M:225:LEU:O	1:M:226:ASN:HB2	2.02	0.59
1:M:232:VAL:HG23	1:M:234:THR:HG22	1.84	0.59
2:T:221:LEU:HA	2:T:224:LYS:HD2	1.84	0.59
1:Q:154:LEU:HG	1:Q:158:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ALA:HB2	1:C:112:GLY:HA3	1.84	0.59
1:C:251:THR:HG22	1:C:252:ALA:N	2.17	0.59
1:G:165:LEU:C	1:G:246:ILE:HD11	2.27	0.59
1:I:201:LEU:N	1:I:201:LEU:HD23	2.17	0.59
1:I:232:VAL:HG23	1:I:234:THR:HG22	1.84	0.59
1:I:236:ASN:O	1:I:237:VAL:HB	2.02	0.59
1:K:25:LEU:N	1:K:25:LEU:HD22	2.17	0.59
1:M:146:ASN:ND2	1:M:321:VAL:HA	2.16	0.59
1:Q:25:LEU:HD21	1:Q:326:ASP:HA	1.84	0.59
2:B:78:ASN:OD1	2:B:80:VAL:HG22	2.02	0.59
1:C:30:VAL:HB	1:C:73:VAL:HG22	1.84	0.59
2:D:168:ILE:HG22	2:D:169:LYS:HG2	1.85	0.59
1:E:85:ALA:HB2	1:E:112:GLY:HA3	1.84	0.59
1:E:154:LEU:HG	1:E:158:VAL:CG2	2.32	0.59
2:F:168:ILE:HG22	2:F:169:LYS:HG2	1.85	0.59
1:I:30:VAL:HB	1:I:73:VAL:HG22	1.84	0.59
1:I:193:LEU:HD12	1:I:193:LEU:N	2.10	0.59
1:K:165:LEU:C	1:K:246:ILE:HD11	2.26	0.59
1:M:251:THR:HG22	1:M:252:ALA:N	2.18	0.59
1:O:251:THR:HG22	1:O:252:ALA:N	2.17	0.59
2:P:183:ARG:HD2	2:P:187:ALA:HB3	1.83	0.59
1:A:170:GLY:HA3	1:A:244:VAL:HG12	1.85	0.59
1:C:154:LEU:HG	1:C:158:VAL:CG2	2.32	0.59
1:G:232:VAL:HG23	1:G:234:THR:HG22	1.85	0.59
1:G:236:ASN:O	1:G:237:VAL:HB	2.02	0.59
1:G:251:THR:HG22	1:G:252:ALA:N	2.17	0.59
1:E:30:VAL:HB	1:E:73:VAL:HG22	1.84	0.59
1:I:123(A):SER:C	1:M:124:ASP:HA	2.26	0.59
1:I:225:LEU:O	1:I:226:ASN:HB2	2.02	0.59
1:K:154:LEU:HG	1:K:158:VAL:HG21	1.84	0.59
2:N:20:ARG:HH11	2:N:20:ARG:HG3	1.66	0.59
2:R:177:SER:HB3	2:R:234:THR:O	2.02	0.59
1:A:177:SER:HA	1:A:234:THR:HG23	1.84	0.59
1:G:170:GLY:HA3	1:G:244:VAL:HG12	1.85	0.59
1:G:228:ILE:CD1	1:E:306:LYS:HE2	2.32	0.59
2:H:20:ARG:HG3	2:H:20:ARG:HH11	1.66	0.59
2:H:183:ARG:HD2	2:H:187:ALA:HB3	1.83	0.59
1:E:15:PHE:CE1	1:E:322:VAL:HG22	2.37	0.59
1:E:25:LEU:HD22	1:E:25:LEU:N	2.17	0.59
2:F:221:LEU:HA	2:F:224:LYS:HD2	1.84	0.59
1:I:185:LEU:HD21	2:L:178:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:218:LEU:HB3	2:P:221:LEU:HD23	1.85	0.59
2:R:256:ASN:HD21	2:R:297:THR:CB	2.16	0.59
1:C:25:LEU:HD22	1:C:25:LEU:N	2.17	0.59
2:H:78:ASN:OD1	2:H:80:VAL:HG22	2.02	0.59
1:I:110:GLN:HA	1:M:80:LEU:HD22	1.85	0.59
1:I:228:ILE:CD1	1:K:306:LYS:HE2	2.32	0.59
1:K:293:ASP:HB3	1:K:296:LEU:HD12	1.84	0.59
1:S:15:PHE:CE1	1:S:322:VAL:HG22	2.37	0.59
1:O:236:ASN:O	1:O:237:VAL:HB	2.02	0.59
1:O:246:ILE:HG13	1:O:247:GLU:N	2.18	0.59
1:Q:154:LEU:HG	1:Q:158:VAL:HG21	1.85	0.59
1:Q:293:ASP:HB3	1:Q:296:LEU:HD12	1.84	0.59
1:A:232:VAL:HG23	1:A:234:THR:HG22	1.85	0.59
1:C:25:LEU:HD21	1:C:326:ASP:HA	1.84	0.59
1:C:129:VAL:CG2	1:C:217:VAL:HG11	2.31	0.59
1:E:25:LEU:HD21	1:E:326:ASP:HA	1.85	0.59
1:E:154:LEU:HG	1:E:158:VAL:HG21	1.85	0.59
1:I:177:SER:HA	1:I:234:THR:HG23	1.84	0.59
2:J:218:LEU:HB3	2:J:221:LEU:HD23	1.84	0.59
1:O:193:LEU:HD12	1:O:193:LEU:N	2.10	0.59
1:I:293:ASP:CB	1:I:296:LEU:HD12	2.33	0.59
1:K:251:THR:HG22	1:K:252:ALA:N	2.17	0.59
1:M:185:LEU:HD21	2:T:178:TYR:HE1	1.67	0.59
1:M:228:ILE:CD1	1:S:306:LYS:HE2	2.32	0.59
1:O:48:SER:HA	2:P:281:ILE:HG21	1.83	0.59
1:G:30:VAL:HB	1:G:73:VAL:HG22	1.84	0.59
1:I:170:GLY:HA3	1:I:244:VAL:HG12	1.85	0.59
1:K:246:ILE:HG13	1:K:247:GLU:N	2.18	0.59
1:M:170:GLY:HA3	1:M:244:VAL:HG12	1.85	0.59
1:M:293:ASP:CB	1:M:296:LEU:HD12	2.33	0.59
1:S:154:LEU:HG	1:S:158:VAL:HG21	1.85	0.59
1:S:191:ARG:NH1	1:S:191:ARG:HB2	2.18	0.59
2:T:172:MET:O	2:T:227:GLY:HA3	2.03	0.59
2:T:183:ARG:HD2	2:T:187:ALA:HB3	1.84	0.59
1:O:293:ASP:CB	1:O:296:LEU:HD12	2.33	0.59
2:R:172:MET:O	2:R:227:GLY:HA3	2.03	0.59
1:A:48:SER:HA	2:B:281:ILE:HG21	1.83	0.59
1:A:142:ASN:H	1:G:103:PRO:CG	2.16	0.59
1:A:228:ILE:CD1	1:C:306:LYS:HE2	2.32	0.59
1:C:110:GLN:HE21	1:C:110:GLN:HA	1.67	0.59
2:F:172:MET:O	2:F:227:GLY:HA3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:LEU:C	1:I:246:ILE:HD11	2.27	0.59
1:I:251:THR:HG22	1:I:252:ALA:N	2.18	0.59
2:L:172:MET:O	2:L:227:GLY:HA3	2.03	0.59
1:O:165:LEU:C	1:O:246:ILE:HD11	2.27	0.58
1:O:170:GLY:HA3	1:O:244:VAL:HG12	1.85	0.58
1:Q:191:ARG:NH1	1:Q:191:ARG:HB2	2.18	0.58
2:B:20:ARG:HG3	2:B:20:ARG:HH11	1.66	0.58
1:C:191:ARG:NH1	1:C:191:ARG:HB2	2.18	0.58
1:G:246:ILE:HG13	1:G:247:GLU:N	2.18	0.58
2:L:221:LEU:HA	2:L:224:LYS:HD2	1.84	0.58
1:M:236:ASN:O	1:M:237:VAL:HB	2.02	0.58
1:S:30:VAL:HB	1:S:73:VAL:HG22	1.84	0.58
2:T:10:ARG:O	2:T:14:ASN:HB2	2.02	0.58
1:O:125:ILE:HG23	1:O:143:ILE:O	2.03	0.58
1:O:177:SER:HA	1:O:234:THR:HG23	1.84	0.58
1:Q:15:PHE:CE1	1:Q:322:VAL:HG22	2.37	0.58
1:Q:125:ILE:CG2	1:Q:143:ILE:O	2.44	0.58
1:A:225:LEU:O	1:A:226:ASN:HB2	2.02	0.58
1:C:154:LEU:HG	1:C:158:VAL:HG21	1.85	0.58
1:G:48:SER:HA	2:H:281:ILE:HG21	1.83	0.58
2:F:256:ASN:HD21	2:F:297:THR:CB	2.16	0.58
1:I:110:GLN:NE2	1:M:110:GLN:O	2.37	0.58
1:S:31:ASN:OD1	1:S:75:SER:HA	2.02	0.58
1:S:129:VAL:CG2	1:S:217:VAL:HG11	2.31	0.58
1:S:273:VAL:HG22	1:S:292:ILE:HD13	1.83	0.58
2:T:168:ILE:HG22	2:T:169:LYS:HG2	1.84	0.58
1:O:232:VAL:HG23	1:O:234:THR:HG22	1.85	0.58
1:Q:110:GLN:HB3	1:S:110:GLN:CB	2.32	0.58
1:A:251:THR:HG22	1:A:252:ALA:N	2.17	0.58
2:D:172:MET:O	2:D:227:GLY:HA3	2.03	0.58
2:D:256:ASN:HD21	2:D:297:THR:CB	2.16	0.58
1:G:185:LEU:HD21	2:F:178:TYR:HE1	1.67	0.58
1:E:184:LEU:O	1:E:185:LEU:HD23	2.04	0.58
1:I:246:ILE:HG13	1:I:247:GLU:N	2.18	0.58
1:S:184:LEU:O	1:S:185:LEU:HD23	2.03	0.58
1:Q:251:THR:HG22	1:Q:252:ALA:N	2.18	0.58
2:D:78:ASN:OD1	2:D:80:VAL:HG22	2.04	0.58
1:G:125:ILE:HG23	1:G:143:ILE:O	2.03	0.58
1:G:177:SER:HA	1:G:234:THR:HG23	1.84	0.58
2:F:132:VAL:O	2:F:133:ASN:HB3	2.04	0.58
2:N:132:VAL:O	2:N:133:ASN:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:162:ASP:HB2	1:S:167:ILE:HD12	1.86	0.58
2:T:132:VAL:O	2:T:133:ASN:HB3	2.03	0.58
1:Q:246:ILE:HG13	1:Q:247:GLU:N	2.18	0.58
1:A:246:ILE:HG13	1:A:247:GLU:N	2.18	0.58
1:G:225:LEU:O	1:G:226:ASN:HB2	2.02	0.58
2:H:298:MET:HE1	2:F:226:ASN:OD1	2.04	0.58
1:A:185:LEU:HD21	2:D:178:TYR:HE1	1.67	0.58
1:A:193:LEU:H	1:A:193:LEU:CD1	2.06	0.58
2:B:218:LEU:HB3	2:B:221:LEU:HD23	1.85	0.58
1:C:165:LEU:HD23	1:C:246:ILE:HD13	1.86	0.58
1:K:85:ALA:HB2	1:K:112:GLY:HA3	1.84	0.58
1:K:162:ASP:HB2	1:K:167:ILE:HD12	1.86	0.58
2:N:78:ASN:OD1	2:N:80:VAL:HG22	2.02	0.58
1:S:85:ALA:HB2	1:S:112:GLY:HA3	1.84	0.58
2:P:78:ASN:OD1	2:P:80:VAL:HG22	2.02	0.58
1:A:85:ALA:HB2	1:A:112:GLY:HA3	1.86	0.58
2:H:218:LEU:HB3	2:H:221:LEU:HD23	1.85	0.58
1:K:30:VAL:HB	1:K:73:VAL:HG22	1.84	0.58
2:L:256:ASN:HD21	2:L:297:THR:CB	2.16	0.58
2:T:20:ARG:HG3	2:T:20:ARG:NH1	2.19	0.58
1:O:225:LEU:O	1:O:226:ASN:HB2	2.02	0.58
1:Q:170:GLY:HA3	1:Q:244:VAL:HA	1.86	0.58
1:C:184:LEU:O	1:C:185:LEU:HD23	2.04	0.58
1:G:293:ASP:CB	1:G:296:LEU:HD12	2.33	0.58
2:F:78:ASN:OD1	2:F:80:VAL:HG22	2.04	0.58
1:I:193:LEU:HD23	2:L:42:HIS:CG	2.39	0.58
1:I:211:ALA:O	1:I:214:VAL:HG23	2.04	0.58
2:L:84:TRP:CE3	2:L:84:TRP:HA	2.39	0.58
1:M:246:ILE:HG13	1:M:247:GLU:N	2.18	0.58
2:N:256:ASN:HD21	2:N:297:THR:CB	2.16	0.58
2:T:84:TRP:CE3	2:T:84:TRP:HA	2.39	0.58
2:T:251:PHE:CZ	2:T:254:GLU:HB2	2.39	0.58
1:Q:100:VAL:O	1:Q:122(A):LYS:HB2	2.04	0.58
1:G:85:ALA:HB2	1:G:112:GLY:HA3	1.86	0.58
1:E:129:VAL:CG2	1:E:217:VAL:HG11	2.31	0.58
2:F:84:TRP:HA	2:F:84:TRP:CE3	2.39	0.58
2:F:251:PHE:CZ	2:F:254:GLU:HB2	2.39	0.58
2:J:78:ASN:OD1	2:J:80:VAL:HG22	2.02	0.58
1:M:211:ALA:O	1:M:214:VAL:HG23	2.04	0.58
1:M:306:LYS:HE2	1:S:228:ILE:CD1	2.34	0.58
2:N:298:MET:HE1	2:T:226:ASN:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:25:LEU:HD21	1:S:326:ASP:HA	1.84	0.58
1:S:248:LYS:HG2	1:S:248(A):VAL:N	2.19	0.58
2:T:78:ASN:OD1	2:T:80:VAL:HG22	2.04	0.58
1:O:30:VAL:HB	1:O:73:VAL:HG22	1.84	0.58
1:O:182:GLN:HB3	1:O:199:ALA:HB2	1.86	0.58
2:P:96:THR:OG1	2:P:98:VAL:HG22	2.04	0.58
2:P:132:VAL:O	2:P:133:ASN:HB3	2.03	0.58
1:C:162:ASP:HB2	1:C:167:ILE:HD12	1.86	0.58
2:D:132:VAL:O	2:D:133:ASN:HB3	2.04	0.58
2:H:132:VAL:O	2:H:133:ASN:HB3	2.03	0.58
1:E:66:ILE:O	1:E:67:ASP:HB2	2.04	0.58
1:E:191:ARG:HB2	1:E:191:ARG:NH1	2.18	0.58
2:J:20:ARG:HH11	2:J:20:ARG:HG3	1.66	0.58
1:K:25:LEU:HD21	1:K:326:ASP:HA	1.84	0.58
1:M:85:ALA:HB2	1:M:112:GLY:HA3	1.86	0.58
1:Q:248:LYS:HG2	1:Q:248(A):VAL:N	2.19	0.57
1:A:293:ASP:CB	1:A:296:LEU:HD12	2.33	0.57
2:B:256:ASN:HD21	2:B:297:THR:CB	2.16	0.57
1:C:110:GLN:HA	1:C:110:GLN:NE2	2.19	0.57
1:E:162:ASP:HB2	1:E:167:ILE:HD12	1.86	0.57
1:E:248:LYS:HG2	1:E:248(A):VAL:N	2.19	0.57
1:I:125:ILE:HG23	1:I:143:ILE:O	2.03	0.57
1:I:142:ASN:H	1:M:103:PRO:CG	2.17	0.57
2:J:256:ASN:HD21	2:J:297:THR:CB	2.16	0.57
2:L:78:ASN:OD1	2:L:80:VAL:HG22	2.04	0.57
2:L:251:PHE:CZ	2:L:254:GLU:HB2	2.39	0.57
1:O:85:ALA:HB2	1:O:112:GLY:HA3	1.85	0.57
2:P:221:LEU:HA	2:P:224:LYS:HD2	1.86	0.57
1:Q:184:LEU:O	1:Q:185:LEU:HD23	2.03	0.57
2:R:78:ASN:OD1	2:R:80:VAL:HG22	2.04	0.57
2:R:84:TRP:HA	2:R:84:TRP:CE3	2.39	0.57
2:R:168:ILE:HG22	2:R:169:LYS:HG2	1.85	0.57
1:A:125:ILE:HG23	1:A:143:ILE:O	2.03	0.57
1:A:246:ILE:HG22	1:A:303:ASP:O	2.04	0.57
2:B:298:MET:HE1	2:D:226:ASN:OD1	2.04	0.57
2:D:84:TRP:CE3	2:D:84:TRP:HA	2.39	0.57
2:H:256:ASN:HD21	2:H:297:THR:CB	2.16	0.57
1:E:165:LEU:HD23	1:E:246:ILE:HD13	1.86	0.57
2:J:132:VAL:O	2:J:133:ASN:HB3	2.04	0.57
1:K:248:LYS:HG2	1:K:248(A):VAL:N	2.19	0.57
1:M:125:ILE:HG23	1:M:143:ILE:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:96:THR:OG1	2:N:98:VAL:HG22	2.04	0.57
2:N:218:LEU:HB3	2:N:221:LEU:HD23	1.85	0.57
1:O:193:LEU:HD23	2:R:42:HIS:CG	2.39	0.57
1:Q:165:LEU:HD23	1:Q:246:ILE:HD13	1.86	0.57
2:R:84:TRP:HA	2:R:84:TRP:HE3	1.70	0.57
1:G:211:ALA:O	1:G:214:VAL:HG23	2.04	0.57
1:I:85:ALA:HB2	1:I:112:GLY:HA3	1.85	0.57
2:J:298:MET:HE1	2:L:226:ASN:OD1	2.04	0.57
1:M:182:GLN:HB3	1:M:199:ALA:HB2	1.86	0.57
1:M:193:LEU:HD23	2:T:42:HIS:CG	2.39	0.57
1:M:246:ILE:HG22	1:M:303:ASP:O	2.04	0.57
2:T:256:ASN:HD21	2:T:297:THR:CB	2.16	0.57
1:O:211:ALA:O	1:O:214:VAL:HG23	2.04	0.57
1:Q:162:ASP:HB2	1:Q:167:ILE:HD12	1.86	0.57
1:C:248:LYS:HG2	1:C:248(A):VAL:N	2.19	0.57
2:H:96:THR:OG1	2:H:98:VAL:HG22	2.04	0.57
1:I:182:GLN:HB3	1:I:199:ALA:HB2	1.86	0.57
1:S:66:ILE:O	1:S:67:ASP:HB2	2.04	0.57
1:A:193:LEU:HD23	2:D:42:HIS:CG	2.39	0.57
1:G:246:ILE:HG22	1:G:303:ASP:O	2.04	0.57
2:J:96:THR:OG1	2:J:98:VAL:HG22	2.04	0.57
1:K:191:ARG:NH1	1:K:191:ARG:HB2	2.18	0.57
2:L:84:TRP:HA	2:L:84:TRP:HE3	1.69	0.57
2:L:132:VAL:O	2:L:133:ASN:HB3	2.04	0.57
2:N:271:LEU:HG	2:N:272:SER:N	2.19	0.57
1:S:139:HIS:O	1:S:139(A):ASP:HB2	2.05	0.57
1:S:246:ILE:HG13	1:S:247:GLU:N	2.18	0.57
2:P:171:THR:HB	2:R:306:LYS:HE2	1.86	0.57
2:P:271:LEU:HG	2:P:272:SER:N	2.19	0.57
2:P:300:MET:HE1	2:R:225:LEU:C	2.30	0.57
2:B:96:THR:OG1	2:B:98:VAL:HG22	2.04	0.57
2:B:271:LEU:HG	2:B:272:SER:N	2.19	0.57
1:C:154:LEU:C	1:C:158:VAL:HG23	2.30	0.57
2:D:1:LEU:HD22	2:D:329:ALA:HA	1.87	0.57
1:G:228:ILE:HG21	1:E:296:LEU:CD2	2.35	0.57
2:H:271:LEU:HG	2:H:272:SER:N	2.19	0.57
1:E:139:HIS:O	1:E:139(A):ASP:HB2	2.05	0.57
2:F:1:LEU:HD22	2:F:329:ALA:HA	1.87	0.57
1:I:246:ILE:HG22	1:I:303:ASP:O	2.05	0.57
1:K:66:ILE:O	1:K:67:ASP:HB2	2.04	0.57
1:K:184:LEU:O	1:K:185:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:ARG:HG3	2:L:20:ARG:NH1	2.19	0.57
1:O:228:ILE:HG21	1:Q:296:LEU:CD2	2.35	0.57
2:P:256:ASN:HD21	2:P:297:THR:CB	2.16	0.57
1:Q:154:LEU:C	1:Q:158:VAL:HG23	2.30	0.57
2:R:20:ARG:HG3	2:R:20:ARG:NH1	2.19	0.57
2:R:251:PHE:CZ	2:R:254:GLU:HB2	2.39	0.57
1:G:193:LEU:HD23	2:F:42:HIS:CG	2.39	0.57
2:N:221:LEU:HA	2:N:224:LYS:HD2	1.86	0.57
1:S:165:LEU:HD23	1:S:246:ILE:HD13	1.86	0.57
1:O:306:LYS:HE2	1:Q:228:ILE:CD1	2.34	0.57
1:C:204:VAL:HB	1:C:231:ARG:HB2	1.86	0.57
2:H:171:THR:HB	2:F:306:LYS:HE2	1.86	0.57
2:J:300:MET:HE1	2:L:225:LEU:C	2.30	0.57
1:K:165:LEU:HD23	1:K:246:ILE:HD13	1.86	0.57
1:O:177:SER:CB	1:O:234:THR:O	2.53	0.57
1:C:66:ILE:O	1:C:67:ASP:HB2	2.04	0.57
1:C:246:ILE:HG13	1:C:247:GLU:N	2.18	0.57
2:D:84:TRP:HA	2:D:84:TRP:HE3	1.70	0.57
2:D:251:PHE:CZ	2:D:254:GLU:HB2	2.39	0.57
1:I:170:GLY:HA3	1:I:244:VAL:HA	1.87	0.57
2:N:133:ASN:C	2:N:133:ASN:ND2	2.62	0.57
1:Q:66:ILE:O	1:Q:67:ASP:HB2	2.04	0.57
2:R:132:VAL:O	2:R:133:ASN:HB3	2.04	0.57
1:A:228:ILE:HG21	1:C:296:LEU:CD2	2.35	0.57
2:B:132:VAL:O	2:B:133:ASN:HB3	2.03	0.57
1:G:66:ILE:O	1:G:67:ASP:HB2	2.05	0.57
1:G:170:GLY:HA3	1:G:244:VAL:HA	1.87	0.57
2:F:20:ARG:HG3	2:F:20:ARG:NH1	2.19	0.57
1:I:306:LYS:HE2	1:K:228:ILE:CD1	2.34	0.57
2:J:171:THR:HB	2:L:306:LYS:HE2	1.86	0.57
2:J:271:LEU:HG	2:J:272:SER:N	2.19	0.57
1:K:204:VAL:HB	1:K:231:ARG:HB2	1.86	0.57
1:M:66:ILE:O	1:M:67:ASP:HB2	2.05	0.57
2:N:120:ALA:O	2:N:145:SER:HB2	2.05	0.57
1:O:168:VAL:HG12	1:O:169:LYS:CG	2.33	0.56
1:A:306:LYS:HE2	1:C:228:ILE:CD1	2.34	0.56
2:B:134:GLU:OE1	2:B:134:GLU:N	2.33	0.56
2:B:221:LEU:HA	2:B:224:LYS:HD2	1.86	0.56
1:E:154:LEU:C	1:E:158:VAL:HG23	2.30	0.56
1:M:228:ILE:HG21	1:S:296:LEU:CD2	2.35	0.56
2:N:171:THR:HB	2:T:306:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:300:MET:HE1	2:T:225:LEU:C	2.30	0.56
2:T:84:TRP:HA	2:T:84:TRP:HE3	1.70	0.56
2:P:298:MET:HE1	2:R:226:ASN:OD1	2.04	0.56
1:A:182:GLN:HB3	1:A:199:ALA:HB2	1.86	0.56
2:B:84:TRP:HA	2:B:84:TRP:CE3	2.40	0.56
1:C:139:HIS:O	1:C:139(A):ASP:HB2	2.05	0.56
1:G:248:LYS:HG2	1:G:248(A):VAL:N	2.21	0.56
1:E:170:GLY:HA3	1:E:244:VAL:HA	1.86	0.56
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.86	0.56
1:S:170:GLY:HA3	1:S:244:VAL:HA	1.86	0.56
2:R:1:LEU:HD22	2:R:329:ALA:HA	1.87	0.56
2:R:209:GLY:O	2:R:211:ALA:N	2.39	0.56
1:A:248:LYS:HG2	1:A:248(A):VAL:N	2.21	0.56
2:D:209:GLY:O	2:D:211:ALA:N	2.39	0.56
1:G:182:GLN:HB3	1:G:199:ALA:HB2	1.86	0.56
1:E:110:GLN:HB2	1:K:110:GLN:HB3	1.87	0.56
1:E:124:ASP:CB	1:K:124:ASP:OD2	2.44	0.56
1:E:246:ILE:HG13	1:E:247:GLU:N	2.18	0.56
1:K:170:GLY:HA3	1:K:244:VAL:HA	1.86	0.56
1:M:248:LYS:HG2	1:M:248(A):VAL:N	2.21	0.56
1:O:110:GLN:C	1:O:110:GLN:CD	2.73	0.56
1:O:246:ILE:HG22	1:O:303:ASP:O	2.04	0.56
2:P:84:TRP:HA	2:P:84:TRP:CE3	2.41	0.56
1:A:170:GLY:HA3	1:A:244:VAL:HA	1.88	0.56
1:A:211:ALA:O	1:A:214:VAL:HG23	2.04	0.56
2:B:120:ALA:O	2:B:145:SER:HB2	2.05	0.56
2:B:133:ASN:C	2:B:133:ASN:ND2	2.62	0.56
2:B:156:PRO:O	2:B:160:VAL:HG23	2.06	0.56
2:D:20:ARG:HG3	2:D:20:ARG:NH1	2.19	0.56
1:G:154:LEU:HG	1:G:158:VAL:HG21	1.88	0.56
1:G:232:VAL:O	1:G:234:THR:HG22	2.06	0.56
2:F:84:TRP:HA	2:F:84:TRP:HE3	1.69	0.56
1:K:139:HIS:O	1:K:139(A):ASP:HB2	2.05	0.56
1:K:246:ILE:N	1:K:303:ASP:O	2.39	0.56
1:S:154:LEU:C	1:S:158:VAL:HG23	2.30	0.56
1:S:204:VAL:HB	1:S:231:ARG:HB2	1.86	0.56
1:O:193:LEU:H	1:O:193:LEU:CD1	2.06	0.56
1:O:248:LYS:HG2	1:O:248(A):VAL:N	2.20	0.56
1:Q:125:ILE:HG23	1:Q:143:ILE:HG22	1.87	0.56
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.86	0.56
2:B:171:THR:HB	2:D:306:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:GLN:OE1	2:B:231:ARG:HD2	2.06	0.56
2:H:84:TRP:HA	2:H:84:TRP:CE3	2.41	0.56
2:H:120:ALA:O	2:H:145:SER:HB2	2.05	0.56
1:E:246:ILE:N	1:E:303:ASP:O	2.39	0.56
2:F:156:PRO:O	2:F:160:VAL:HG23	2.06	0.56
1:I:80:LEU:HD22	1:I:110:GLN:CD	2.31	0.56
1:I:154:LEU:HG	1:I:158:VAL:HG21	1.88	0.56
1:I:174:THR:O	1:I:174:THR:HG23	2.06	0.56
1:Q:110:GLN:HE22	1:S:109:ILE:HB	1.71	0.56
1:A:154:LEU:HG	1:A:158:VAL:HG21	1.88	0.56
1:C:110:GLN:NE2	1:C:110:GLN:CA	2.68	0.56
2:D:156:PRO:O	2:D:160:VAL:HG23	2.06	0.56
1:G:174:THR:HG23	1:G:174:THR:O	2.06	0.56
1:G:177:SER:CB	1:G:234:THR:O	2.53	0.56
2:H:156:PRO:O	2:H:160:VAL:HG23	2.06	0.56
2:H:300:MET:HE1	2:F:225:LEU:C	2.30	0.56
1:I:177:SER:CB	1:I:234:THR:O	2.53	0.56
2:J:182:GLN:OE1	2:J:231:ARG:HD2	2.06	0.56
2:J:221:LEU:HA	2:J:224:LYS:HD2	1.86	0.56
1:O:162:ASP:HB2	1:O:167:ILE:HD12	1.88	0.56
1:O:174:THR:HG23	1:O:174:THR:O	2.06	0.56
1:O:293:ASP:HB3	1:O:296:LEU:HD12	1.88	0.56
1:A:177:SER:CB	1:A:234:THR:O	2.53	0.56
2:B:281:ILE:HB	2:D:202:ASN:HD21	1.71	0.56
1:C:170:GLY:HA3	1:C:244:VAL:HA	1.86	0.56
2:H:221:LEU:HA	2:H:224:LYS:HD2	1.86	0.56
2:F:209:GLY:O	2:F:211:ALA:N	2.38	0.56
2:L:1:LEU:HD22	2:L:329:ALA:HA	1.87	0.56
2:N:182:GLN:OE1	2:N:231:ARG:HD2	2.06	0.56
2:T:209:GLY:O	2:T:211:ALA:N	2.39	0.56
2:P:182:GLN:OE1	2:P:231:ARG:HD2	2.06	0.56
2:P:251:PHE:CZ	2:P:254:GLU:HB2	2.41	0.56
1:Q:139:HIS:O	1:Q:139(A):ASP:HB2	2.05	0.56
1:A:60:ILE:HB	1:A:63:THR:O	2.06	0.56
1:A:66:ILE:O	1:A:67:ASP:HB2	2.05	0.56
2:B:300:MET:HE1	2:D:225:LEU:C	2.30	0.56
1:I:228:ILE:HG21	1:K:296:LEU:CD2	2.35	0.56
1:I:232:VAL:O	1:I:234:THR:HG22	2.06	0.56
2:J:84:TRP:HA	2:J:84:TRP:CE3	2.40	0.56
1:M:154:LEU:HG	1:M:158:VAL:HG21	1.88	0.56
1:A:162:ASP:HB2	1:A:167:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:O	1:A:234:THR:HG22	2.05	0.56
1:I:248:LYS:HG2	1:I:248(A):VAL:N	2.21	0.56
1:O:154:LEU:HG	1:O:158:VAL:HG21	1.88	0.56
1:A:174:THR:HG23	1:A:174:THR:O	2.06	0.56
1:G:60:ILE:HB	1:G:63:THR:O	2.06	0.56
1:G:306:LYS:HE2	1:E:228:ILE:CD1	2.34	0.56
2:H:182:GLN:OE1	2:H:231:ARG:HD2	2.06	0.56
2:H:281:ILE:HB	2:F:202:ASN:HD21	1.71	0.56
2:J:251:PHE:CZ	2:J:254:GLU:HB2	2.41	0.56
2:J:281:ILE:HB	2:L:202:ASN:HD21	1.71	0.56
1:O:66:ILE:O	1:O:67:ASP:HB2	2.05	0.55
1:O:170:GLY:HA3	1:O:244:VAL:HA	1.87	0.55
2:B:251:PHE:CZ	2:B:254:GLU:HB2	2.41	0.55
1:G:162:ASP:HB2	1:G:167:ILE:HD12	1.88	0.55
1:E:110:GLN:CB	1:K:110:GLN:HB3	2.36	0.55
1:I:162:ASP:HB2	1:I:167:ILE:HD12	1.88	0.55
1:M:60:ILE:HB	1:M:63:THR:O	2.06	0.55
1:O:232:VAL:O	1:O:234:THR:HG22	2.05	0.55
2:P:134:GLU:OE1	2:P:134:GLU:N	2.33	0.55
2:J:156:PRO:O	2:J:160:VAL:HG23	2.06	0.55
1:M:177:SER:CB	1:M:234:THR:O	2.53	0.55
2:N:251:PHE:CZ	2:N:254:GLU:HB2	2.41	0.55
1:S:251:THR:HG22	1:S:252:ALA:N	2.17	0.55
2:P:120:ALA:O	2:P:145:SER:HB2	2.05	0.55
1:I:66:ILE:O	1:I:67:ASP:HB2	2.05	0.55
1:K:228:ILE:HD13	1:K:228:ILE:N	2.17	0.55
2:N:84:TRP:HE3	2:N:84:TRP:HA	1.72	0.55
2:N:156:PRO:O	2:N:160:VAL:HG23	2.06	0.55
2:N:228:ILE:CD1	2:T:296:LEU:HD22	2.37	0.55
1:O:60:ILE:HB	1:O:63:THR:O	2.06	0.55
2:R:156:PRO:O	2:R:160:VAL:HG23	2.06	0.55
1:A:228:ILE:HD13	1:A:228:ILE:N	2.14	0.55
2:B:84:TRP:HA	2:B:84:TRP:HE3	1.71	0.55
1:G:193:LEU:H	1:G:193:LEU:CD1	2.06	0.55
2:J:84:TRP:HA	2:J:84:TRP:HE3	1.71	0.55
1:K:154:LEU:C	1:K:158:VAL:HG23	2.30	0.55
1:S:246:ILE:N	1:S:303:ASP:O	2.39	0.55
2:T:1:LEU:HD22	2:T:329:ALA:HA	1.87	0.55
2:B:202:ASN:HD21	2:D:281:ILE:CB	2.19	0.55
2:J:120:ALA:O	2:J:145:SER:HB2	2.05	0.55
2:N:84:TRP:HA	2:N:84:TRP:CE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:281:ILE:HB	2:T:202:ASN:HD21	1.71	0.55
1:Q:246:ILE:N	1:Q:303:ASP:O	2.39	0.55
1:A:293:ASP:HB3	1:A:296:LEU:HD12	1.88	0.55
2:J:228:ILE:CD1	2:L:296:LEU:HD22	2.37	0.55
2:L:193:LEU:H	2:L:193:LEU:CD1	2.06	0.55
2:L:209:GLY:O	2:L:211:ALA:N	2.39	0.55
1:M:162:ASP:HB2	1:M:167:ILE:HD12	1.88	0.55
1:M:170:GLY:HA3	1:M:244:VAL:HA	1.87	0.55
2:P:156:PRO:O	2:P:160:VAL:HG23	2.06	0.55
1:Q:174:THR:O	1:Q:174:THR:HG23	2.07	0.55
1:C:251:THR:HB	1:C:254:ASP:OD1	2.07	0.55
2:L:156:PRO:O	2:L:160:VAL:HG23	2.06	0.55
1:M:168:VAL:HG12	1:M:169:LYS:CG	2.33	0.55
2:N:139:HIS:HE1	2:N:332:TRP:CE3	2.25	0.55
2:P:281:ILE:HB	2:R:202:ASN:HD21	1.71	0.55
1:Q:251:THR:HB	1:Q:254:ASP:OD1	2.07	0.55
2:R:193:LEU:H	2:R:193:LEU:CD1	2.07	0.55
2:H:202:ASN:HD21	2:F:281:ILE:CB	2.19	0.55
1:E:174:THR:HG23	1:E:174:THR:O	2.07	0.55
1:K:174:THR:HG23	1:K:174:THR:O	2.07	0.55
2:L:49:ILE:HD11	2:L:235:PRO:HB2	1.89	0.55
1:C:177:SER:HA	1:C:234:THR:HG23	1.88	0.55
1:C:246:ILE:N	1:C:303:ASP:O	2.39	0.55
2:H:251:PHE:CZ	2:H:254:GLU:HB2	2.41	0.55
1:E:251:THR:HB	1:E:254:ASP:OD1	2.07	0.55
1:M:232:VAL:O	1:M:234:THR:HG22	2.06	0.55
1:S:177:SER:HA	1:S:234:THR:HG23	1.88	0.55
2:T:49:ILE:HD11	2:T:235:PRO:HB2	1.89	0.55
2:P:139:HIS:HE1	2:P:332:TRP:CE3	2.25	0.55
2:H:228:ILE:CD1	2:F:296:LEU:HD22	2.37	0.55
2:F:256:ASN:HD21	2:F:297:THR:HG21	1.72	0.55
2:P:202:ASN:HD21	2:R:281:ILE:CB	2.19	0.54
2:R:18:CYS:HG	2:R:319:GLN:HG2	1.72	0.54
2:B:185:LEU:O	2:B:186:ASP:C	2.50	0.54
1:I:293:ASP:HB3	1:I:296:LEU:HD12	1.88	0.54
1:K:236:ASN:O	1:K:237:VAL:HB	2.07	0.54
2:L:256:ASN:HD21	2:L:297:THR:HG21	1.72	0.54
2:P:84:TRP:HA	2:P:84:TRP:HE3	1.72	0.54
2:P:171:THR:CB	2:R:306:LYS:HE2	2.37	0.54
1:Q:168:VAL:HG12	1:Q:169:LYS:CG	2.36	0.54
1:A:193:LEU:HD12	1:A:193:LEU:N	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:TRP:HA	2:H:84:TRP:HE3	1.72	0.54
2:H:133:ASN:C	2:H:133:ASN:ND2	2.62	0.54
1:I:233:PRO:HB2	1:K:233:PRO:HB2	1.90	0.54
2:J:171:THR:CB	2:L:306:LYS:HE2	2.37	0.54
1:K:177:SER:HA	1:K:234:THR:HG23	1.89	0.54
1:Q:177:SER:HA	1:Q:234:THR:HG23	1.88	0.54
2:B:20:ARG:HG3	2:B:20:ARG:NH1	2.23	0.54
2:D:256:ASN:HD21	2:D:297:THR:HG21	1.73	0.54
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.88	0.54
2:H:20:ARG:HG3	2:H:20:ARG:NH1	2.23	0.54
2:J:133:ASN:C	2:J:133:ASN:ND2	2.62	0.54
1:S:236:ASN:O	1:S:237:VAL:HB	2.08	0.54
1:S:251:THR:HB	1:S:254:ASP:OD1	2.07	0.54
2:P:185:LEU:O	2:P:186:ASP:C	2.50	0.54
2:B:139:HIS:HE1	2:B:332:TRP:CE3	2.25	0.54
1:I:60:ILE:HB	1:I:63:THR:O	2.06	0.54
2:J:139:HIS:HE1	2:J:332:TRP:CE3	2.25	0.54
1:M:174:THR:HG23	1:M:174:THR:O	2.06	0.54
1:S:174:THR:HG23	1:S:174:THR:O	2.07	0.54
2:P:226:ASN:HB3	2:R:298:MET:HE1	1.89	0.54
2:P:228:ILE:CD1	2:R:296:LEU:HD22	2.36	0.54
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.07	0.54
1:A:200:ALA:C	1:A:201:LEU:HD23	2.33	0.54
2:B:172:MET:O	2:B:227:GLY:HA3	2.08	0.54
2:B:226:ASN:HB3	2:D:298:MET:HE1	1.90	0.54
2:H:134:GLU:OE1	2:H:134:GLU:N	2.33	0.54
2:H:139:HIS:HE1	2:H:332:TRP:CE3	2.26	0.54
2:H:185:LEU:O	2:H:186:ASP:C	2.50	0.54
2:H:226:ASN:HB3	2:F:298:MET:HE1	1.90	0.54
1:I:123(A):SER:O	1:M:124:ASP:CA	2.47	0.54
1:K:251:THR:HB	1:K:254:ASP:OD1	2.07	0.54
2:T:156:PRO:O	2:T:160:VAL:HG23	2.06	0.54
1:Q:259:PHE:O	1:Q:263:ALA:N	2.41	0.54
1:Q:272:ASP:HB2	1:Q:288:PHE:CE2	2.43	0.54
2:B:228:ILE:CD1	2:D:296:LEU:HD22	2.36	0.54
1:G:200:ALA:C	1:G:201:LEU:HD23	2.33	0.54
1:G:233:PRO:HB2	1:E:233:PRO:HB2	1.90	0.54
2:F:157:PHE:HB2	2:F:259:PHE:CE1	2.43	0.54
2:L:25:LEU:HD11	2:L:325:ALA:HB1	1.89	0.54
2:L:157:PHE:HB2	2:L:259:PHE:CE1	2.43	0.54
1:M:233:PRO:HB2	1:S:233:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:256:ASN:HD21	2:T:297:THR:HG21	1.72	0.54
2:R:256:ASN:ND2	2:R:297:THR:HG21	2.22	0.54
2:B:171:THR:CB	2:D:306:LYS:HE2	2.37	0.54
1:C:259:PHE:O	1:C:263:ALA:N	2.41	0.54
1:G:259:PHE:O	1:G:263:ALA:N	2.41	0.54
1:K:232:VAL:O	1:K:234:THR:N	2.41	0.54
2:N:20:ARG:HG3	2:N:20:ARG:NH1	2.23	0.54
2:N:171:THR:CB	2:T:306:LYS:HE2	2.37	0.54
2:P:18:CYS:SG	2:P:319:GLN:HG2	2.48	0.54
2:R:256:ASN:HD21	2:R:297:THR:HG21	1.73	0.54
2:B:18:CYS:SG	2:B:319:GLN:HG2	2.48	0.54
1:C:174:THR:HG23	1:C:174:THR:O	2.07	0.54
1:G:60:ILE:HG22	1:G:60(A):ASP:N	2.23	0.54
2:H:18:CYS:SG	2:H:319:GLN:HG2	2.48	0.54
2:F:49:ILE:HD11	2:F:235:PRO:HB2	1.89	0.54
1:I:200:ALA:C	1:I:201:LEU:HD23	2.33	0.54
1:K:168:VAL:HG12	1:K:169:LYS:CG	2.36	0.54
2:L:256:ASN:ND2	2:L:297:THR:HG21	2.22	0.54
1:M:200:ALA:C	1:M:201:LEU:HD23	2.33	0.54
1:S:146:ASN:ND2	1:S:321:VAL:HA	2.23	0.54
1:O:200:ALA:C	1:O:201:LEU:HD23	2.33	0.54
2:P:28:VAL:HG23	2:P:29:VAL:HG12	1.90	0.54
1:A:60:ILE:HG22	1:A:60(A):ASP:N	2.23	0.54
1:A:233:PRO:HB2	1:C:233:PRO:HB2	1.90	0.54
1:C:232:VAL:O	1:C:234:THR:N	2.41	0.54
1:C:272:ASP:HB2	1:C:288:PHE:CE2	2.43	0.54
2:D:185:LEU:O	2:D:186:ASP:C	2.51	0.54
2:H:172:MET:O	2:H:227:GLY:HA3	2.08	0.54
1:E:177:SER:HA	1:E:234:THR:HG23	1.88	0.54
1:E:272:ASP:HB2	1:E:288:PHE:CE2	2.43	0.54
2:F:256:ASN:ND2	2:F:297:THR:HG21	2.22	0.54
1:S:232:VAL:O	1:S:234:THR:N	2.41	0.54
2:P:20:ARG:HG3	2:P:20:ARG:NH1	2.23	0.54
1:Q:232:VAL:O	1:Q:234:THR:N	2.41	0.54
1:Q:232:VAL:O	1:Q:234:THR:HG22	2.08	0.54
1:G:228:ILE:HG21	1:E:296:LEU:HD22	1.90	0.54
1:G:320:ARG:HA	1:G:320:ARG:NE	2.23	0.54
2:H:171:THR:CB	2:F:306:LYS:HE2	2.37	0.54
1:I:320:ARG:NE	1:I:320:ARG:HA	2.23	0.54
2:J:18:CYS:SG	2:J:319:GLN:HG2	2.48	0.54
2:R:25:LEU:HD11	2:R:325:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:49:ILE:HD11	2:R:235:PRO:HB2	1.89	0.53
1:A:25:LEU:N	1:A:25:LEU:CD2	2.72	0.53
1:A:320:ARG:NE	1:A:320:ARG:HA	2.23	0.53
1:C:225:LEU:O	1:C:226:ASN:CB	2.57	0.53
2:D:49:ILE:HD11	2:D:235:PRO:HB2	1.89	0.53
2:D:157:PHE:HB2	2:D:259:PHE:CE1	2.43	0.53
1:E:18:CYS:O	1:E:20:ARG:HG2	2.08	0.53
1:I:228:ILE:HG21	1:K:296:LEU:HD22	1.90	0.53
1:S:225:LEU:O	1:S:226:ASN:CB	2.57	0.53
1:O:54:LYS:O	1:O:55:ALA:HB2	2.08	0.53
1:O:60:ILE:HG22	1:O:60(A):ASP:N	2.23	0.53
1:O:77:ARG:O	1:O:79:PRO:HD3	2.09	0.53
1:O:228:ILE:HG21	1:Q:296:LEU:HD22	1.90	0.53
2:P:31:ASN:OD1	2:P:74:VAL:HG23	2.08	0.53
2:P:172:MET:O	2:P:227:GLY:HA3	2.08	0.53
2:P:245:GLN:OE1	2:R:245:GLN:OE1	2.27	0.53
1:Q:129:VAL:O	1:Q:130:VAL:C	2.52	0.53
1:A:77:ARG:O	1:A:79:PRO:HD3	2.09	0.53
1:A:209:GLY:O	1:A:211:ALA:N	2.41	0.53
2:D:256:ASN:ND2	2:D:297:THR:HG21	2.22	0.53
1:G:54:LYS:O	1:G:55:ALA:HB2	2.09	0.53
1:I:77:ARG:O	1:I:79:PRO:HD3	2.08	0.53
2:J:20:ARG:HG3	2:J:20:ARG:NH1	2.23	0.53
2:J:80:VAL:HG23	2:J:81:ASN:OD1	2.08	0.53
1:K:18:CYS:O	1:K:20:ARG:HG2	2.09	0.53
1:M:25:LEU:N	1:M:25:LEU:CD2	2.71	0.53
1:M:209:GLY:O	1:M:211:ALA:N	2.41	0.53
1:M:293:ASP:HB3	1:M:296:LEU:HD12	1.88	0.53
2:N:94:GLU:OE1	2:N:99:PHE:HB2	2.08	0.53
1:S:232:VAL:O	1:S:234:THR:HG22	2.08	0.53
1:O:165:LEU:HD23	1:O:246:ILE:HD13	1.91	0.53
1:O:228:ILE:HD13	1:O:228:ILE:N	2.13	0.53
1:O:233:PRO:HB2	1:Q:233:PRO:HB2	1.90	0.53
2:P:80:VAL:HG23	2:P:81:ASN:OD1	2.08	0.53
2:R:286:THR:HG22	2:R:288:VAL:HG22	1.90	0.53
1:A:165:LEU:HD23	1:A:246:ILE:HD13	1.91	0.53
2:B:28:VAL:HG23	2:B:29:VAL:HG12	1.90	0.53
1:G:25:LEU:N	1:G:25:LEU:CD2	2.71	0.53
1:E:225:LEU:O	1:E:226:ASN:CB	2.57	0.53
1:E:232:VAL:O	1:E:234:THR:N	2.41	0.53
1:I:209:GLY:O	1:I:211:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:PHE:O	1:I:263:ALA:N	2.41	0.53
1:K:232:VAL:O	1:K:234:THR:HG22	2.08	0.53
1:K:272:ASP:HB2	1:K:288:PHE:CE2	2.43	0.53
1:M:54:LYS:O	1:M:55:ALA:HB2	2.08	0.53
1:M:259:PHE:O	1:M:263:ALA:N	2.41	0.53
1:O:25:LEU:N	1:O:25:LEU:CD2	2.71	0.53
1:O:209:GLY:O	1:O:211:ALA:N	2.41	0.53
2:P:133:ASN:C	2:P:133:ASN:ND2	2.62	0.53
2:R:157:PHE:HB2	2:R:259:PHE:CE1	2.43	0.53
1:A:228:ILE:HG21	1:C:296:LEU:HD22	1.90	0.53
1:E:236:ASN:O	1:E:237:VAL:HB	2.08	0.53
1:E:259:PHE:O	1:E:263:ALA:N	2.41	0.53
2:J:281:ILE:O	2:J:284:ARG:HG2	2.09	0.53
1:S:218:LEU:HB3	1:S:221:LEU:HD13	1.91	0.53
2:T:256:ASN:ND2	2:T:297:THR:HG21	2.22	0.53
1:Q:146:ASN:ND2	1:Q:321:VAL:HA	2.23	0.53
2:F:185:LEU:O	2:F:186:ASP:C	2.51	0.53
1:I:54:LYS:O	1:I:55:ALA:HB2	2.09	0.53
2:J:185:LEU:O	2:J:186:ASP:C	2.50	0.53
2:J:226:ASN:HB3	2:L:298:MET:HE1	1.89	0.53
1:K:129:VAL:O	1:K:130:VAL:C	2.52	0.53
2:N:18:CYS:SG	2:N:319:GLN:HG2	2.48	0.53
2:T:25:LEU:HD11	2:T:325:ALA:HB1	1.89	0.53
1:O:320:ARG:HA	1:O:320:ARG:NE	2.23	0.53
1:A:54:LYS:O	1:A:55:ALA:HB2	2.08	0.53
1:A:272:ASP:HB2	1:A:288:PHE:CE2	2.44	0.53
1:G:165:LEU:HD23	1:G:246:ILE:HD13	1.91	0.53
2:H:28:VAL:HG23	2:H:29:VAL:HG12	1.90	0.53
1:M:60:ILE:HG22	1:M:60(A):ASP:N	2.23	0.53
1:S:177:SER:CB	1:S:234:THR:O	2.56	0.53
1:S:259:PHE:O	1:S:263:ALA:N	2.41	0.53
1:S:272:ASP:HB2	1:S:288:PHE:CE2	2.43	0.53
1:Q:18:CYS:O	1:Q:20:ARG:HG2	2.09	0.53
1:Q:177:SER:CB	1:Q:234:THR:O	2.56	0.53
1:C:177:SER:CB	1:C:234:THR:O	2.56	0.53
2:D:25:LEU:HD11	2:D:325:ALA:HB1	1.89	0.53
1:E:146:ASN:ND2	1:E:321:VAL:HA	2.23	0.53
2:F:80:VAL:HG23	2:F:81:ASN:OD1	2.08	0.53
1:I:25:LEU:N	1:I:25:LEU:CD2	2.71	0.53
2:J:94:GLU:OE1	2:J:99:PHE:HB2	2.08	0.53
2:J:172:MET:O	2:J:227:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:228:ILE:HG21	1:S:296:LEU:HD22	1.90	0.53
1:O:79:PRO:HA	1:O:82:LEU:HG	1.91	0.53
2:B:281:ILE:O	2:B:284:ARG:HG2	2.09	0.53
1:C:146:ASN:ND2	1:C:321:VAL:HA	2.23	0.53
1:C:232:VAL:O	1:C:234:THR:HG22	2.08	0.53
1:C:236:ASN:O	1:C:237:VAL:HB	2.08	0.53
2:H:80:VAL:HG23	2:H:81:ASN:OD1	2.08	0.53
2:L:128:TYR:HA	2:L:133:ASN:HD21	1.74	0.53
2:L:271:LEU:HG	2:L:272:SER:N	2.24	0.53
2:N:172:MET:O	2:N:227:GLY:HA3	2.08	0.53
1:S:18:CYS:O	1:S:20:ARG:HG2	2.08	0.53
2:T:133:ASN:C	2:T:133:ASN:ND2	2.67	0.53
2:T:157:PHE:HB2	2:T:259:PHE:CE1	2.43	0.53
2:P:281:ILE:O	2:P:284:ARG:HG2	2.09	0.53
2:R:14:ASN:ND2	2:R:314:GLU:HB3	2.24	0.53
1:C:18:CYS:O	1:C:20:ARG:HG2	2.08	0.53
1:G:209:GLY:O	1:G:211:ALA:N	2.42	0.53
2:H:14:ASN:HB3	2:H:318:SER:OG	2.09	0.53
1:E:110:GLN:HB2	1:K:110:GLN:CB	2.39	0.53
2:N:286:THR:HG22	2:N:288:VAL:HG22	1.91	0.53
1:O:18:CYS:O	1:O:20:ARG:HG2	2.10	0.53
1:O:259:PHE:O	1:O:263:ALA:N	2.41	0.53
2:R:128:TYR:HA	2:R:133:ASN:HD21	1.74	0.53
1:A:259:PHE:O	1:A:263:ALA:N	2.41	0.53
2:B:80:VAL:HG23	2:B:81:ASN:OD1	2.08	0.53
2:D:28:VAL:HG23	2:D:29:VAL:HG12	1.91	0.53
2:D:128:TYR:HA	2:D:133:ASN:HD21	1.74	0.53
2:H:281:ILE:O	2:H:284:ARG:HG2	2.09	0.53
1:E:123(A):SER:C	1:K:124:ASP:CA	2.82	0.53
2:F:286:THR:HG22	2:F:288:VAL:HG22	1.90	0.53
1:I:129:VAL:O	1:I:130:VAL:C	2.52	0.53
2:J:14:ASN:HB3	2:J:318:SER:OG	2.09	0.53
2:J:31:ASN:OD1	2:J:74:VAL:HG23	2.08	0.53
1:K:209:GLY:O	1:K:211:ALA:N	2.42	0.53
1:K:259:PHE:O	1:K:263:ALA:N	2.41	0.53
2:L:185:LEU:O	2:L:186:ASP:C	2.51	0.53
2:N:167:ILE:HG23	2:N:244:VAL:HB	1.91	0.53
2:N:245:GLN:OE1	2:T:245:GLN:OE1	2.27	0.53
1:S:248:LYS:HG2	1:S:248(A):VAL:H	1.75	0.53
1:Q:172:MET:HE3	1:Q:172:MET:C	2.35	0.52
1:Q:248:LYS:HG2	1:Q:248(A):VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:28:VAL:HG23	2:R:29:VAL:HG12	1.91	0.52
2:R:271:LEU:HG	2:R:272:SER:N	2.24	0.52
2:B:14:ASN:HB3	2:B:318:SER:OG	2.09	0.52
1:C:172:MET:HE3	1:C:172:MET:C	2.35	0.52
2:D:80:VAL:HG23	2:D:81:ASN:OD1	2.08	0.52
2:D:286:THR:HG22	2:D:288:VAL:HG22	1.90	0.52
1:G:77:ARG:O	1:G:79:PRO:HD3	2.09	0.52
1:G:248:LYS:HG2	1:G:248(A):VAL:H	1.75	0.52
2:H:245:GLN:OE1	2:F:245:GLN:OE1	2.27	0.52
1:E:218:LEU:HB3	1:E:221:LEU:HD13	1.91	0.52
1:E:232:VAL:O	1:E:234:THR:HG22	2.08	0.52
2:F:28:VAL:HG23	2:F:29:VAL:HG12	1.91	0.52
1:I:18:CYS:O	1:I:20:ARG:HG2	2.10	0.52
2:J:28:VAL:HG23	2:J:29:VAL:HG12	1.90	0.52
1:K:177:SER:CB	1:K:234:THR:O	2.56	0.52
2:L:80:VAL:HG23	2:L:81:ASN:OD1	2.08	0.52
1:M:25:LEU:HD21	1:M:326:ASP:HA	1.91	0.52
2:N:31:ASN:OD1	2:N:74:VAL:HG23	2.08	0.52
2:N:80:VAL:HG23	2:N:81:ASN:OD1	2.08	0.52
2:T:80:VAL:HG23	2:T:81:ASN:OD1	2.09	0.52
2:T:185:LEU:O	2:T:186:ASP:C	2.51	0.52
2:P:94:GLU:OE1	2:P:99:PHE:HB2	2.08	0.52
2:R:80:VAL:HG23	2:R:81:ASN:OD1	2.08	0.52
2:R:133:ASN:C	2:R:133:ASN:ND2	2.67	0.52
1:A:25:LEU:HD21	1:A:326:ASP:HA	1.91	0.52
1:E:209:GLY:O	1:E:211:ALA:N	2.42	0.52
2:J:286:THR:HG22	2:J:288:VAL:HG22	1.91	0.52
1:K:218:LEU:HB3	1:K:221:LEU:HD13	1.91	0.52
1:S:209:GLY:O	1:S:211:ALA:N	2.42	0.52
2:T:18:CYS:HG	2:T:319:GLN:HG2	1.74	0.52
2:T:128:TYR:HA	2:T:133:ASN:HD21	1.74	0.52
2:T:286:THR:HG22	2:T:288:VAL:HG22	1.90	0.52
1:O:246:ILE:N	1:O:303:ASP:O	2.42	0.52
2:B:245:GLN:OE1	2:D:245:GLN:OE1	2.27	0.52
1:C:209:GLY:O	1:C:211:ALA:N	2.42	0.52
2:H:31:ASN:OD1	2:H:74:VAL:HG23	2.08	0.52
2:H:94:GLU:OE1	2:H:99:PHE:HB2	2.09	0.52
1:I:25:LEU:HD21	1:I:326:ASP:HA	1.91	0.52
1:I:60:ILE:HG22	1:I:60(A):ASP:N	2.23	0.52
2:J:170:GLY:HA2	2:L:304:MET:SD	2.50	0.52
2:L:133:ASN:C	2:L:133:ASN:ND2	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:PRO:HA	1:M:82:LEU:HG	1.90	0.52
1:M:139:HIS:O	1:M:139(A):ASP:HB2	2.10	0.52
1:M:246:ILE:N	1:M:303:ASP:O	2.43	0.52
1:M:272:ASP:HB2	1:M:288:PHE:CE2	2.44	0.52
2:N:281:ILE:O	2:N:284:ARG:HG2	2.09	0.52
2:T:25:LEU:HD21	2:T:326:ASP:CA	2.38	0.52
1:Q:225:LEU:O	1:Q:226:ASN:CB	2.57	0.52
1:A:18:CYS:O	1:A:20:ARG:HG2	2.10	0.52
1:A:191:ARG:HB2	1:A:191:ARG:HH11	1.75	0.52
2:B:94:GLU:OE1	2:B:99:PHE:HB2	2.09	0.52
1:C:129:VAL:O	1:C:130:VAL:C	2.52	0.52
1:G:18:CYS:O	1:G:20:ARG:HG2	2.09	0.52
1:G:139:HIS:O	1:G:139(A):ASP:HB2	2.10	0.52
1:E:177:SER:CB	1:E:234:THR:O	2.56	0.52
2:F:14:ASN:ND2	2:F:314:GLU:HB3	2.24	0.52
1:I:110:GLN:HB2	1:M:110:GLN:CD	2.34	0.52
2:J:167:ILE:HG23	2:J:244:VAL:HB	1.92	0.52
1:K:172:MET:HE3	1:K:172:MET:C	2.34	0.52
1:M:18:CYS:O	1:M:20:ARG:HG2	2.10	0.52
1:M:20:ARG:HH21	1:M:319:GLN:HE22	1.58	0.52
2:N:151:THR:OG1	2:N:210:ALA:HA	2.10	0.52
1:S:172:MET:HE3	1:S:172:MET:C	2.35	0.52
2:T:271:LEU:HG	2:T:272:SER:N	2.24	0.52
2:R:185:LEU:O	2:R:186:ASP:C	2.51	0.52
1:A:248:LYS:HG2	1:A:248(A):VAL:H	1.75	0.52
2:B:31:ASN:OD1	2:B:74:VAL:HG23	2.08	0.52
2:B:151:THR:OG1	2:B:210:ALA:HA	2.10	0.52
1:G:246:ILE:N	1:G:303:ASP:O	2.42	0.52
2:F:25:LEU:HD11	2:F:325:ALA:HB1	1.89	0.52
1:I:165:LEU:HD23	1:I:246:ILE:HD13	1.91	0.52
1:K:146:ASN:ND2	1:K:321:VAL:HA	2.23	0.52
1:K:225:LEU:O	1:K:226:ASN:CB	2.57	0.52
2:L:270:ILE:O	2:L:288:VAL:HB	2.10	0.52
1:M:129:VAL:O	1:M:130:VAL:C	2.52	0.52
1:M:320:ARG:HA	1:M:320:ARG:NE	2.23	0.52
2:N:185:LEU:O	2:N:186:ASP:C	2.50	0.52
2:T:218:LEU:HB3	2:T:221:LEU:HD23	1.92	0.52
1:O:272:ASP:HB2	1:O:288:PHE:CE2	2.44	0.52
1:A:79:PRO:HA	1:A:82:LEU:HG	1.90	0.52
1:A:140:VAL:O	1:A:141:ALA:O	2.28	0.52
1:C:218:LEU:HB3	1:C:221:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:LEU:HG	2:D:272:SER:N	2.24	0.52
1:G:140:VAL:O	1:G:141:ALA:O	2.28	0.52
1:G:191:ARG:HB2	1:G:191:ARG:HH11	1.75	0.52
1:E:130:VAL:HB	1:E:320:ARG:HD3	1.92	0.52
1:M:77:ARG:O	1:M:79:PRO:HD3	2.09	0.52
1:M:248:LYS:HG2	1:M:248(A):VAL:H	1.74	0.52
2:N:193:LEU:H	2:N:193:LEU:CD1	2.06	0.52
2:T:193:LEU:H	2:T:193:LEU:CD1	2.06	0.52
1:O:15:PHE:CE1	1:O:322:VAL:HG22	2.45	0.52
1:O:248:LYS:HG2	1:O:248(A):VAL:H	1.74	0.52
1:A:246:ILE:N	1:A:303:ASP:O	2.42	0.52
2:B:170:GLY:HA2	2:D:304:MET:SD	2.50	0.52
2:D:18:CYS:HG	2:D:319:GLN:HG2	1.74	0.52
1:G:25:LEU:HD21	1:G:326:ASP:HA	1.91	0.52
1:I:79:PRO:HA	1:I:82:LEU:HG	1.90	0.52
1:I:272:ASP:HB2	1:I:288:PHE:CE2	2.44	0.52
2:N:28:VAL:HG23	2:N:29:VAL:HG12	1.90	0.52
2:N:226:ASN:HB3	2:T:298:MET:HE1	1.90	0.52
2:T:14:ASN:ND2	2:T:314:GLU:HB3	2.24	0.52
1:O:140:VAL:O	1:O:141:ALA:O	2.28	0.52
2:P:170:GLY:HA2	2:R:304:MET:SD	2.49	0.52
1:C:248:LYS:HG2	1:C:248(A):VAL:H	1.75	0.52
1:C:248(A):VAL:HG13	1:C:249:GLY:N	2.19	0.52
2:D:14:ASN:ND2	2:D:314:GLU:HB3	2.24	0.52
1:E:172:MET:C	1:E:172:MET:HE3	2.34	0.52
2:F:193:LEU:H	2:F:193:LEU:CD1	2.06	0.52
1:I:15:PHE:CE1	1:I:322:VAL:HG22	2.45	0.52
1:I:246:ILE:N	1:I:303:ASP:O	2.43	0.52
2:L:286:THR:HG22	2:L:288:VAL:HG22	1.90	0.52
1:S:129:VAL:O	1:S:130:VAL:C	2.52	0.52
2:T:209:GLY:C	2:T:211:ALA:N	2.68	0.52
1:O:25:LEU:CD2	1:O:25:LEU:H	2.23	0.52
1:O:80:LEU:HD23	1:O:110:GLN:OE1	2.09	0.52
1:O:129:VAL:O	1:O:130:VAL:C	2.52	0.52
1:Q:209:GLY:O	1:Q:211:ALA:N	2.42	0.52
1:A:129:VAL:O	1:A:130:VAL:C	2.53	0.52
2:H:170:GLY:HA2	2:F:304:MET:SD	2.50	0.52
2:H:286:THR:HG22	2:H:288:VAL:HG22	1.91	0.52
1:E:168:VAL:HG12	1:E:169:LYS:CG	2.36	0.52
2:F:128:TYR:HA	2:F:133:ASN:HD21	1.74	0.52
1:I:140:VAL:O	1:I:141:ALA:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:151:THR:OG1	2:J:210:ALA:HA	2.10	0.52
2:L:14:ASN:ND2	2:L:314:GLU:HB3	2.24	0.52
1:M:232:VAL:O	1:M:234:THR:N	2.43	0.52
1:A:15:PHE:CE1	1:A:322:VAL:HG22	2.45	0.52
1:A:232:VAL:O	1:A:234:THR:N	2.43	0.52
2:B:25:LEU:HD11	2:B:325:ALA:HB1	1.92	0.52
2:B:226:ASN:CB	2:D:298:MET:HE1	2.40	0.52
1:C:130:VAL:HB	1:C:320:ARG:HD3	1.92	0.52
1:G:232:VAL:O	1:G:234:THR:N	2.43	0.52
2:F:270:ILE:O	2:F:288:VAL:HB	2.10	0.52
2:F:271:LEU:HG	2:F:272:SER:N	2.24	0.52
2:J:192:ASP:O	2:J:194:ARG:N	2.43	0.52
1:M:154:LEU:C	1:M:158:VAL:HG23	2.35	0.52
1:M:165:LEU:HD23	1:M:246:ILE:HD13	1.91	0.52
1:S:130:VAL:HB	1:S:320:ARG:HD3	1.92	0.52
2:P:306:LYS:HE2	2:R:171:THR:HB	1.92	0.51
1:A:139:HIS:O	1:A:139(A):ASP:HB2	2.10	0.51
1:G:25:LEU:CD2	1:G:25:LEU:H	2.23	0.51
1:G:79:PRO:HA	1:G:82:LEU:HG	1.90	0.51
2:J:25:LEU:HD11	2:J:325:ALA:HB1	1.92	0.51
2:L:213:ALA:O	2:L:216:LEU:HB2	2.11	0.51
2:N:14:ASN:HB3	2:N:318:SER:OG	2.10	0.51
2:T:28:VAL:HG23	2:T:29:VAL:HG12	1.91	0.51
1:O:194:ARG:NH2	1:Q:277:PRO:HA	2.26	0.51
2:P:25:LEU:HD11	2:P:325:ALA:HB1	1.92	0.51
1:A:154:LEU:C	1:A:158:VAL:HG23	2.35	0.51
1:G:272:ASP:HB2	1:G:288:PHE:CE2	2.44	0.51
2:H:151:THR:OG1	2:H:210:ALA:HA	2.10	0.51
1:E:248(A):VAL:HG13	1:E:249:GLY:N	2.19	0.51
2:F:133:ASN:C	2:F:133:ASN:ND2	2.68	0.51
2:J:245:GLN:OE1	2:L:245:GLN:OE1	2.27	0.51
1:K:130:VAL:HB	1:K:320:ARG:HD3	1.92	0.51
2:L:84:TRP:CE3	2:L:89:ILE:HG13	2.46	0.51
1:M:140:VAL:O	1:M:141:ALA:O	2.28	0.51
2:N:25:LEU:HD11	2:N:325:ALA:HB1	1.92	0.51
2:T:270:ILE:O	2:T:288:VAL:HB	2.10	0.51
2:P:192:ASP:O	2:P:194:ARG:N	2.43	0.51
2:R:213:ALA:O	2:R:216:LEU:HB2	2.10	0.51
2:B:286:THR:HG22	2:B:288:VAL:HG22	1.91	0.51
2:H:226:ASN:CB	2:F:298:MET:HE1	2.41	0.51
2:J:134:GLU:OE1	2:J:134:GLU:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:MET:HE3	1:K:172:MET:O	2.10	0.51
2:L:28:VAL:HG23	2:L:29:VAL:HG12	1.91	0.51
2:L:209:GLY:C	2:L:211:ALA:N	2.68	0.51
2:N:170:GLY:HA2	2:T:304:MET:SD	2.50	0.51
1:S:149:CYS:HB3	3:S:401:NAD:H5N	1.92	0.51
1:O:154:LEU:HG	1:O:158:VAL:CG2	2.41	0.51
2:P:226:ASN:CB	2:R:298:MET:HE1	2.40	0.51
1:A:110:GLN:HB2	1:G:110:GLN:HB2	1.88	0.51
1:G:95:GLY:HA2	1:G:119:THR:OG1	2.11	0.51
2:H:192:ASP:O	2:H:194:ARG:N	2.43	0.51
1:E:129:VAL:O	1:E:130:VAL:C	2.52	0.51
1:I:248:LYS:HG2	1:I:248(A):VAL:H	1.75	0.51
1:K:149:CYS:HB3	3:K:401:NAD:H5N	1.93	0.51
1:K:248(A):VAL:HG13	1:K:249:GLY:N	2.19	0.51
2:L:218:LEU:HB3	2:L:221:LEU:HD23	1.92	0.51
1:M:95:GLY:HA2	1:M:119:THR:OG1	2.11	0.51
1:M:191:ARG:HB2	1:M:191:ARG:HH11	1.75	0.51
1:Q:130:VAL:HB	1:Q:320:ARG:HD3	1.92	0.51
2:R:179:THR:OG1	2:R:231:ARG:NH1	2.44	0.51
2:R:218:LEU:HB3	2:R:221:LEU:HD23	1.92	0.51
1:A:142:ASN:H	1:G:103:PRO:HG2	1.76	0.51
1:A:283:PHE:CE2	1:A:310:TRP:CD1	2.99	0.51
2:D:270:ILE:O	2:D:288:VAL:HB	2.10	0.51
1:G:168:VAL:HB	1:G:245:ASN:O	2.11	0.51
2:H:25:LEU:HD11	2:H:325:ALA:HB1	1.92	0.51
1:K:248:LYS:HG2	1:K:248(A):VAL:H	1.75	0.51
1:M:15:PHE:CE1	1:M:322:VAL:HG22	2.45	0.51
2:N:134:GLU:OE1	2:N:134:GLU:N	2.33	0.51
1:S:172:MET:HE3	1:S:172:MET:O	2.10	0.51
1:O:25:LEU:HD21	1:O:326:ASP:HA	1.91	0.51
1:O:218:LEU:HB3	1:O:221:LEU:HD13	1.92	0.51
1:O:232:VAL:O	1:O:234:THR:N	2.43	0.51
1:O:298:MET:O	1:O:298:MET:HG3	2.11	0.51
2:P:209:GLY:O	2:P:211:ALA:N	2.44	0.51
1:Q:218:LEU:HB3	1:Q:221:LEU:HD13	1.91	0.51
1:C:192:ASP:O	1:C:194:ARG:N	2.44	0.51
2:D:25:LEU:HD21	2:D:326:ASP:CA	2.38	0.51
2:H:306:LYS:HE2	2:F:171:THR:HB	1.92	0.51
1:I:25:LEU:CD2	1:I:25:LEU:H	2.23	0.51
2:J:202:ASN:HD21	2:L:281:ILE:CB	2.19	0.51
2:J:226:ASN:CB	2:L:298:MET:HE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:192:ASP:C	1:K:194:ARG:H	2.19	0.51
2:P:167:ILE:HG23	2:P:244:VAL:HB	1.92	0.51
1:Q:79:PRO:HA	1:Q:82:LEU:HG	1.92	0.51
1:A:168:VAL:HB	1:A:245:ASN:O	2.11	0.51
1:C:172:MET:HE3	1:C:172:MET:O	2.11	0.51
1:I:95:GLY:HA2	1:I:119:THR:OG1	2.11	0.51
1:I:283:PHE:CE2	1:I:310:TRP:CD1	2.99	0.51
1:M:25:LEU:CD2	1:M:25:LEU:H	2.23	0.51
2:N:209:GLY:O	2:N:211:ALA:N	2.44	0.51
2:T:213:ALA:O	2:T:216:LEU:HB2	2.10	0.51
1:O:283:PHE:CE2	1:O:310:TRP:CD1	2.99	0.51
2:P:14:ASN:HB3	2:P:318:SER:OG	2.10	0.51
1:A:32:ASP:O	1:A:34:GLY:N	2.44	0.51
2:B:192:ASP:O	2:B:194:ARG:N	2.43	0.51
1:C:192:ASP:C	1:C:194:ARG:H	2.19	0.51
1:C:293:ASP:HB3	1:C:296:LEU:HB2	1.93	0.51
2:D:213:ALA:O	2:D:216:LEU:HB2	2.11	0.51
2:D:218:LEU:HB3	2:D:221:LEU:HD23	1.92	0.51
2:H:209:GLY:O	2:H:211:ALA:N	2.44	0.51
1:E:192:ASP:O	1:E:194:ARG:N	2.44	0.51
2:F:213:ALA:O	2:F:216:LEU:HB2	2.11	0.51
2:J:306:LYS:HE2	2:L:171:THR:HB	1.92	0.51
1:K:79:PRO:HA	1:K:82:LEU:HG	1.92	0.51
1:K:293:ASP:HB3	1:K:296:LEU:HB2	1.93	0.51
1:O:191:ARG:HB2	1:O:191:ARG:HH11	1.75	0.51
1:O:283:PHE:CE2	1:O:310:TRP:CG	2.99	0.51
2:P:84:TRP:CE3	2:P:89:ILE:HG13	2.46	0.51
2:P:151:THR:OG1	2:P:210:ALA:HA	2.10	0.51
1:Q:101:ASP:N	1:Q:122(A):LYS:HB2	2.25	0.51
2:R:84:TRP:CE3	2:R:89:ILE:HG13	2.46	0.51
2:R:270:ILE:O	2:R:288:VAL:HB	2.10	0.51
1:C:60:ILE:HB	1:C:63:THR:O	2.11	0.51
2:D:25:LEU:CD2	2:D:326:ASP:HA	2.39	0.51
2:D:179:THR:OG1	2:D:231:ARG:NH1	2.44	0.51
2:H:84:TRP:CE3	2:H:89:ILE:HG13	2.46	0.51
2:H:167:ILE:HG23	2:H:244:VAL:HB	1.92	0.51
1:E:60:ILE:HB	1:E:63:THR:O	2.11	0.51
1:E:77:ARG:O	1:E:79:PRO:HD3	2.11	0.51
1:E:172:MET:HE3	1:E:172:MET:O	2.11	0.51
1:E:293:ASP:HB3	1:E:296:LEU:HB2	1.93	0.51
1:I:298:MET:HG3	1:I:298:MET:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:60:ILE:HB	1:K:63:THR:O	2.11	0.51
2:L:25:LEU:HD21	2:L:326:ASP:CA	2.38	0.51
2:L:139:HIS:HE1	2:L:332:TRP:CE3	2.29	0.51
2:N:192:ASP:O	2:N:194:ARG:N	2.43	0.51
1:O:139:HIS:O	1:O:139(A):ASP:HB2	2.10	0.51
1:O:142:ASN:H	1:C:103:PRO:CG	2.24	0.51
1:O:154:LEU:C	1:O:158:VAL:HG23	2.35	0.51
2:R:209:GLY:C	2:R:211:ALA:N	2.68	0.51
1:A:25:LEU:CD2	1:A:25:LEU:H	2.23	0.51
1:A:298:MET:HG3	1:A:298:MET:O	2.11	0.51
2:B:226:ASN:OD1	2:D:298:MET:HE1	2.11	0.51
2:D:209:GLY:C	2:D:211:ALA:N	2.68	0.51
1:G:154:LEU:C	1:G:158:VAL:HG23	2.35	0.51
1:G:194:ARG:NH2	1:E:277:PRO:HA	2.25	0.51
1:G:283:PHE:CE2	1:G:310:TRP:CD1	2.99	0.51
1:G:298:MET:HG3	1:G:298:MET:O	2.11	0.51
2:F:84:TRP:CE3	2:F:89:ILE:HG13	2.46	0.51
1:I:139:HIS:O	1:I:139(A):ASP:HB2	2.10	0.51
2:J:84:TRP:CE3	2:J:89:ILE:HG13	2.46	0.51
2:J:209:GLY:O	2:J:211:ALA:N	2.44	0.51
1:K:140:VAL:O	1:K:141:ALA:O	2.29	0.51
2:L:18:CYS:HG	2:L:319:GLN:HG2	1.76	0.51
1:M:32:ASP:O	1:M:34:GLY:N	2.44	0.51
1:M:154:LEU:HG	1:M:158:VAL:CG2	2.41	0.51
1:M:218:LEU:HB3	1:M:221:LEU:HD13	1.92	0.51
1:S:25:LEU:N	1:S:25:LEU:CD2	2.74	0.51
1:O:95:GLY:HA2	1:O:119:THR:OG1	2.11	0.50
2:P:98:VAL:HG23	2:P:99:PHE:N	2.26	0.50
2:P:286:THR:HG22	2:P:288:VAL:HG22	1.91	0.50
1:Q:60:ILE:HB	1:Q:63:THR:O	2.11	0.50
1:Q:293:ASP:HB3	1:Q:296:LEU:HB2	1.93	0.50
2:R:139:HIS:HE1	2:R:332:TRP:CE3	2.30	0.50
2:B:84:TRP:CE3	2:B:89:ILE:HG13	2.46	0.50
2:D:84:TRP:CE3	2:D:89:ILE:HG13	2.46	0.50
1:G:15:PHE:CE1	1:G:322:VAL:HG22	2.45	0.50
1:G:129:VAL:O	1:G:130:VAL:C	2.52	0.50
1:E:248:LYS:HG2	1:E:248(A):VAL:H	1.75	0.50
1:K:84:TRP:HA	1:K:84:TRP:CE3	2.46	0.50
2:L:179:THR:OG1	2:L:231:ARG:NH1	2.44	0.50
1:M:168:VAL:HB	1:M:245:ASN:O	2.11	0.50
2:N:226:ASN:CB	2:T:298:MET:HE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:60:ILE:HB	1:S:63:THR:O	2.11	0.50
1:O:168:VAL:HB	1:O:245:ASN:O	2.11	0.50
1:Q:110:GLN:HB3	1:S:110:GLN:OE1	2.12	0.50
2:R:82:LEU:O	2:R:111:ALA:HB1	2.12	0.50
1:A:20:ARG:HH21	1:A:319:GLN:HE22	1.58	0.50
1:A:194:ARG:NH2	1:C:277:PRO:HA	2.26	0.50
2:B:209:GLY:O	2:B:211:ALA:N	2.44	0.50
2:B:306:LYS:HE2	2:D:171:THR:HB	1.92	0.50
1:C:79:PRO:HA	1:C:82:LEU:HG	1.92	0.50
1:C:140:VAL:O	1:C:141:ALA:O	2.29	0.50
1:E:54:LYS:O	1:E:55:ALA:HB2	2.12	0.50
1:E:79:PRO:HA	1:E:82:LEU:HG	1.92	0.50
2:F:82:LEU:O	2:F:111:ALA:HB1	2.12	0.50
2:F:218:LEU:HB3	2:F:221:LEU:HD23	1.92	0.50
1:I:168:VAL:HG12	1:I:169:LYS:CG	2.33	0.50
1:I:298:MET:SD	1:K:226:ASN:OD1	2.70	0.50
2:J:3:VAL:HG12	2:J:4:ALA:N	2.27	0.50
1:M:194:ARG:NH2	1:S:277:PRO:HA	2.26	0.50
1:M:283:PHE:CE2	1:M:310:TRP:CG	2.99	0.50
2:N:202:ASN:HD21	2:T:281:ILE:CB	2.19	0.50
2:N:283:PHE:CE2	2:N:310:TRP:CD1	3.00	0.50
1:S:168:VAL:HG12	1:S:169:LYS:CG	2.36	0.50
1:S:192:ASP:C	1:S:194:ARG:H	2.19	0.50
1:S:293:ASP:HB3	1:S:296:LEU:HB2	1.93	0.50
1:O:20:ARG:HH21	1:O:319:GLN:HE22	1.58	0.50
2:P:3:VAL:HG12	2:P:4:ALA:N	2.27	0.50
1:Q:84:TRP:HA	1:Q:84:TRP:CE3	2.47	0.50
1:Q:172:MET:HE3	1:Q:172:MET:O	2.11	0.50
1:Q:192:ASP:C	1:Q:194:ARG:H	2.20	0.50
1:Q:192:ASP:O	1:Q:194:ARG:N	2.44	0.50
2:D:82:LEU:O	2:D:111:ALA:HB1	2.12	0.50
1:G:32:ASP:O	1:G:34:GLY:N	2.44	0.50
1:G:168:VAL:HG12	1:G:169:LYS:CG	2.33	0.50
1:G:283:PHE:CE2	1:G:310:TRP:CG	2.99	0.50
1:E:25:LEU:N	1:E:25:LEU:CD2	2.75	0.50
1:E:140:VAL:O	1:E:141:ALA:O	2.29	0.50
1:E:251:THR:O	1:E:255:VAL:HG23	2.12	0.50
1:K:173:THR:HG22	1:K:174:THR:N	2.26	0.50
1:S:77:ARG:O	1:S:79:PRO:HD3	2.11	0.50
1:S:140:VAL:O	1:S:141:ALA:O	2.29	0.50
1:O:124:ASP:OD1	1:O:125:ILE:CG1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:219:PRO:HD2	1:O:220:GLN:NE2	2.26	0.50
1:O:298:MET:SD	1:Q:226:ASN:OD1	2.70	0.50
2:P:226:ASN:OD1	2:R:298:MET:HE1	2.11	0.50
2:R:283:PHE:CE2	2:R:310:TRP:CD1	3.00	0.50
1:A:154:LEU:HG	1:A:158:VAL:CG2	2.41	0.50
2:B:167:ILE:HG23	2:B:244:VAL:HB	1.92	0.50
1:C:173:THR:HG22	1:C:174:THR:N	2.26	0.50
2:D:139:HIS:HE1	2:D:332:TRP:CE3	2.30	0.50
2:H:98:VAL:HG23	2:H:99:PHE:N	2.26	0.50
1:E:132:VAL:HG12	1:E:133:ASN:N	2.27	0.50
2:F:179:THR:OG1	2:F:231:ARG:NH1	2.44	0.50
1:I:20:ARG:HH21	1:I:319:GLN:HE22	1.58	0.50
1:K:25:LEU:N	1:K:25:LEU:CD2	2.75	0.50
1:K:228:ILE:H	1:K:228:ILE:CD1	2.18	0.50
1:S:84:TRP:HA	1:S:84:TRP:CE3	2.46	0.50
2:T:84:TRP:CE3	2:T:89:ILE:HG13	2.46	0.50
1:O:173:THR:HG22	1:O:174:THR:N	2.27	0.50
1:Q:251:THR:O	1:Q:255:VAL:HG23	2.12	0.50
1:A:95:GLY:HA2	1:A:119:THR:OG1	2.11	0.50
1:A:251:THR:O	1:A:255:VAL:HG23	2.12	0.50
1:C:168:VAL:HG12	1:C:169:LYS:CG	2.36	0.50
1:G:12:GLY:O	1:G:15:PHE:HB3	2.12	0.50
1:G:132:VAL:HG12	1:G:133:ASN:N	2.27	0.50
1:G:218:LEU:HB3	1:G:221:LEU:HD13	1.92	0.50
1:E:149:CYS:HB3	3:E:401:NAD:H5N	1.93	0.50
1:I:154:LEU:C	1:I:158:VAL:HG23	2.35	0.50
1:I:272:ASP:HB2	1:I:288:PHE:CD2	2.47	0.50
1:I:318:SER:O	1:I:322:VAL:HG23	2.12	0.50
1:K:77:ARG:O	1:K:79:PRO:HD3	2.11	0.50
1:M:219:PRO:HD2	1:M:220:GLN:NE2	2.27	0.50
2:N:82:LEU:O	2:N:111:ALA:HB1	2.12	0.50
2:N:226:ASN:OD1	2:T:298:MET:HE1	2.11	0.50
1:S:79:PRO:HA	1:S:82:LEU:HG	1.92	0.50
1:S:165:LEU:HB3	1:S:246:ILE:HD11	1.94	0.50
1:O:12:GLY:O	1:O:15:PHE:HB3	2.12	0.50
1:O:133:ASN:C	1:O:133:ASN:ND2	2.70	0.50
1:O:154:LEU:O	1:O:155:ALA:C	2.55	0.50
1:Q:54:LYS:O	1:Q:55:ALA:HB2	2.12	0.50
1:A:133:ASN:C	1:A:133:ASN:ND2	2.70	0.50
1:A:218:LEU:HB3	1:A:221:LEU:HD13	1.93	0.50
1:C:272:ASP:HB2	1:C:288:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:ASN:C	1:G:133:ASN:ND2	2.70	0.50
1:G:165:LEU:HB3	1:G:246:ILE:HD11	1.94	0.50
2:H:226:ASN:OD1	2:F:298:MET:HE1	2.11	0.50
1:E:192:ASP:C	1:E:194:ARG:H	2.20	0.50
2:F:25:LEU:CD2	2:F:326:ASP:HA	2.39	0.50
1:I:32:ASP:O	1:I:34:GLY:N	2.44	0.50
1:I:283:PHE:CE2	1:I:310:TRP:CG	2.99	0.50
2:J:213:ALA:O	2:J:216:LEU:HB2	2.12	0.50
1:S:192:ASP:O	1:S:194:ARG:N	2.44	0.50
1:S:272:ASP:HB2	1:S:288:PHE:CD2	2.47	0.50
2:T:179:THR:OG1	2:T:231:ARG:NH1	2.44	0.50
1:O:165:LEU:HB3	1:O:246:ILE:HD11	1.94	0.50
2:P:283:PHE:CE2	2:P:310:TRP:CD1	3.00	0.50
1:A:12:GLY:O	1:A:15:PHE:HB3	2.12	0.50
1:A:283:PHE:CE2	1:A:310:TRP:CG	3.00	0.50
1:C:84:TRP:HA	1:C:84:TRP:CE3	2.46	0.50
1:C:132:VAL:HG12	1:C:133:ASN:N	2.27	0.50
1:C:251:THR:O	1:C:255:VAL:HG23	2.12	0.50
1:G:154:LEU:HG	1:G:158:VAL:CG2	2.41	0.50
1:G:219:PRO:HD2	1:G:220:GLN:NE2	2.27	0.50
1:G:272:ASP:HB2	1:G:288:PHE:CD2	2.47	0.50
2:H:15:PHE:CE1	2:H:322:VAL:HG22	2.47	0.50
2:F:283:PHE:CE2	2:F:310:TRP:CD1	3.00	0.50
1:I:194:ARG:NH2	1:K:277:PRO:HA	2.26	0.50
1:I:219:PRO:HD2	1:I:220:GLN:NE2	2.27	0.50
2:J:15:PHE:CE1	2:J:322:VAL:HG22	2.47	0.50
2:J:226:ASN:OD1	2:L:298:MET:HE1	2.11	0.50
1:M:12:GLY:O	1:M:15:PHE:HB3	2.12	0.50
1:M:130:VAL:HB	1:M:320:ARG:HD3	1.94	0.50
1:M:132:VAL:HG12	1:M:133:ASN:N	2.27	0.50
2:N:84:TRP:CE3	2:N:89:ILE:HG13	2.46	0.50
2:D:283:PHE:CE2	2:D:310:TRP:CD1	3.00	0.50
2:F:209:GLY:C	2:F:211:ALA:N	2.68	0.50
1:I:12:GLY:O	1:I:15:PHE:HB3	2.12	0.50
1:I:187:ALA:O	1:I:196:ALA:HB1	2.12	0.50
1:I:232:VAL:O	1:I:234:THR:N	2.43	0.50
2:L:283:PHE:CE2	2:L:310:TRP:CD1	3.00	0.50
2:N:213:ALA:O	2:N:216:LEU:HB2	2.12	0.50
1:S:95:GLY:HA2	1:S:119:THR:OG1	2.12	0.50
1:O:318:SER:O	1:O:322:VAL:HG23	2.12	0.50
2:P:213:ALA:O	2:P:216:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:25:LEU:N	1:Q:25:LEU:CD2	2.75	0.50
1:C:54:LYS:O	1:C:55:ALA:HB2	2.12	0.50
2:D:192:ASP:O	2:D:194:ARG:N	2.45	0.50
1:G:298:MET:SD	1:E:226:ASN:OD1	2.70	0.50
1:E:84:TRP:HA	1:E:84:TRP:CE3	2.46	0.50
1:I:168:VAL:HB	1:I:245:ASN:O	2.11	0.50
1:I:220:GLN:H	1:I:220:GLN:CD	2.20	0.50
1:I:228:ILE:HD13	1:I:228:ILE:N	2.13	0.50
1:K:192:ASP:O	1:K:194:ARG:N	2.44	0.50
2:L:82:LEU:O	2:L:111:ALA:HB1	2.12	0.50
2:L:182:GLN:OE1	2:L:231:ARG:HD2	2.12	0.50
1:M:283:PHE:CE2	1:M:310:TRP:CD1	2.99	0.50
1:O:220:GLN:H	1:O:220:GLN:CD	2.20	0.49
1:O:234:THR:O	1:O:234:THR:HG23	2.12	0.49
1:Q:77:ARG:O	1:Q:79:PRO:HD3	2.11	0.49
1:Q:140:VAL:O	1:Q:141:ALA:O	2.29	0.49
2:R:192:ASP:O	2:R:194:ARG:N	2.45	0.49
1:C:149:CYS:HB3	3:C:401:NAD:H5N	1.93	0.49
1:G:173:THR:HG22	1:G:174:THR:N	2.27	0.49
1:G:251:THR:O	1:G:255:VAL:HG23	2.12	0.49
2:F:139:HIS:HE1	2:F:332:TRP:CE3	2.30	0.49
1:I:165:LEU:HB3	1:I:246:ILE:HD11	1.94	0.49
1:K:54:LYS:O	1:K:55:ALA:HB2	2.12	0.49
1:K:272:ASP:HB2	1:K:288:PHE:CD2	2.47	0.49
2:L:25:LEU:CD2	2:L:326:ASP:HA	2.39	0.49
2:L:192:ASP:O	2:L:194:ARG:N	2.45	0.49
1:M:165:LEU:HB3	1:M:246:ILE:HD11	1.94	0.49
1:M:173:THR:HG22	1:M:174:THR:N	2.27	0.49
1:M:184:LEU:O	1:M:185:LEU:HD23	2.12	0.49
1:M:251:THR:O	1:M:255:VAL:HG23	2.12	0.49
1:M:298:MET:HG3	1:M:298:MET:O	2.11	0.49
1:S:12:GLY:O	1:S:15:PHE:HB3	2.12	0.49
2:T:328:VAL:O	2:T:332:TRP:HB2	2.12	0.49
2:R:85:GLY:CA	2:R:112:GLY:HA3	2.42	0.49
1:A:132:VAL:HG12	1:A:133:ASN:N	2.28	0.49
1:A:219:PRO:HD2	1:A:220:GLN:NE2	2.27	0.49
2:B:98:VAL:HG23	2:B:99:PHE:N	2.26	0.49
2:F:182:GLN:OE1	2:F:231:ARG:HD2	2.12	0.49
2:F:328:VAL:O	2:F:332:TRP:HB2	2.12	0.49
1:I:234:THR:O	1:I:234:THR:HG23	2.12	0.49
1:K:95:GLY:HA2	1:K:119:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:85:GLY:CA	2:L:112:GLY:HA3	2.42	0.49
2:L:328:VAL:O	2:L:332:TRP:HB2	2.12	0.49
1:M:187:ALA:O	1:M:196:ALA:HB1	2.12	0.49
2:N:306:LYS:HE2	2:T:171:THR:HB	1.92	0.49
2:T:139:HIS:HE1	2:T:332:TRP:CE3	2.30	0.49
1:O:272:ASP:HB2	1:O:288:PHE:CD2	2.47	0.49
2:P:82:LEU:O	2:P:111:ALA:HB1	2.12	0.49
1:Q:12:GLY:O	1:Q:15:PHE:HB3	2.12	0.49
1:Q:248(A):VAL:HG13	1:Q:249:GLY:N	2.19	0.49
2:R:182:GLN:OE1	2:R:231:ARG:HD2	2.12	0.49
1:C:77:ARG:O	1:C:79:PRO:HD3	2.11	0.49
1:G:234:THR:O	1:G:234:THR:HG23	2.12	0.49
1:E:272:ASP:HB2	1:E:288:PHE:CD2	2.47	0.49
2:F:25:LEU:HD21	2:F:326:ASP:CA	2.38	0.49
1:I:135:LYS:C	1:I:137:TYR:H	2.21	0.49
1:I:154:LEU:HG	1:I:158:VAL:CG2	2.41	0.49
1:I:173:THR:HG22	1:I:174:THR:N	2.27	0.49
2:J:283:PHE:CE2	2:J:310:TRP:CD1	3.00	0.49
1:K:251:THR:O	1:K:255:VAL:HG23	2.12	0.49
2:L:96:THR:OG1	2:L:98:VAL:HG22	2.12	0.49
1:M:154:LEU:O	1:M:155:ALA:C	2.55	0.49
1:S:251:THR:O	1:S:255:VAL:HG23	2.12	0.49
2:T:25:LEU:CD2	2:T:326:ASP:HA	2.39	0.49
2:T:82:LEU:O	2:T:111:ALA:HB1	2.12	0.49
1:O:187:ALA:O	1:O:196:ALA:HB1	2.12	0.49
1:O:251:THR:O	1:O:255:VAL:HG23	2.12	0.49
2:R:217:VAL:C	2:R:219:PRO:HD3	2.38	0.49
1:A:165:LEU:HB3	1:A:246:ILE:HD11	1.94	0.49
1:A:168:VAL:HG12	1:A:169:LYS:CG	2.33	0.49
1:A:298:MET:SD	1:C:226:ASN:OD1	2.70	0.49
2:B:3:VAL:HG12	2:B:4:ALA:N	2.27	0.49
1:G:187:ALA:O	1:G:196:ALA:HB1	2.12	0.49
1:I:218:LEU:HB3	1:I:221:LEU:HD13	1.92	0.49
2:J:82:LEU:O	2:J:111:ALA:HB1	2.12	0.49
1:K:165:LEU:HB3	1:K:246:ILE:HD11	1.94	0.49
1:M:298:MET:SD	1:S:226:ASN:OD1	2.70	0.49
1:S:132:VAL:HG12	1:S:133:ASN:N	2.27	0.49
2:T:96:THR:OG1	2:T:98:VAL:HG22	2.12	0.49
2:T:192:ASP:O	2:T:194:ARG:N	2.45	0.49
2:T:283:PHE:CE2	2:T:310:TRP:CD1	3.00	0.49
1:O:132:VAL:HG12	1:O:133:ASN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:15:PHE:CE1	2:P:322:VAL:HG22	2.47	0.49
1:Q:95:GLY:HA2	1:Q:119:THR:OG1	2.12	0.49
1:C:12:GLY:O	1:C:15:PHE:HB3	2.13	0.49
2:D:181:ASP:CG	2:D:195:ARG:NH1	2.70	0.49
2:H:283:PHE:CE2	2:H:310:TRP:CD1	3.00	0.49
2:F:96:THR:OG1	2:F:98:VAL:HG22	2.12	0.49
2:F:217:VAL:C	2:F:219:PRO:HD3	2.38	0.49
2:J:228:ILE:HD13	2:L:296:LEU:HD22	1.95	0.49
1:M:220:GLN:CD	1:M:220:GLN:H	2.20	0.49
1:M:272:ASP:HB2	1:M:288:PHE:CD2	2.47	0.49
2:N:202:ASN:HD22	2:T:281:ILE:N	2.11	0.49
1:S:54:LYS:O	1:S:55:ALA:HB2	2.12	0.49
2:T:182:GLN:OE1	2:T:231:ARG:HD2	2.12	0.49
2:B:283:PHE:CE2	2:B:310:TRP:CD1	3.00	0.49
2:D:182:GLN:OE1	2:D:231:ARG:HD2	2.12	0.49
1:G:184:LEU:O	1:G:185:LEU:HD23	2.12	0.49
1:G:318:SER:O	1:G:322:VAL:HG23	2.12	0.49
1:E:110:GLN:CD	1:K:110:GLN:O	2.55	0.49
1:E:173:THR:HG22	1:E:174:THR:N	2.26	0.49
2:F:181:ASP:CG	2:F:195:ARG:NH1	2.70	0.49
1:I:9:GLY:O	1:I:10:ARG:C	2.55	0.49
1:I:41:THR:O	1:I:42:HIS:C	2.56	0.49
1:I:130:VAL:HB	1:I:320:ARG:HD3	1.94	0.49
1:I:251:THR:O	1:I:255:VAL:HG23	2.12	0.49
1:M:135:LYS:C	1:M:137:TYR:H	2.21	0.49
2:N:98:VAL:HG23	2:N:99:PHE:N	2.27	0.49
1:O:41:THR:O	1:O:42:HIS:C	2.56	0.49
1:O:135:LYS:C	1:O:137:TYR:H	2.21	0.49
2:P:228:ILE:HD13	2:R:296:LEU:HD22	1.95	0.49
2:P:270:ILE:O	2:P:288:VAL:HB	2.13	0.49
1:A:252:ALA:O	1:A:254:ASP:N	2.46	0.49
2:B:270:ILE:O	2:B:288:VAL:HB	2.13	0.49
1:C:25:LEU:N	1:C:25:LEU:CD2	2.75	0.49
2:D:85:GLY:CA	2:D:112:GLY:HA3	2.42	0.49
2:D:133:ASN:C	2:D:133:ASN:ND2	2.67	0.49
1:G:20:ARG:HH21	1:G:319:GLN:HE22	1.58	0.49
2:H:228:ILE:HD13	2:F:296:LEU:HD22	1.95	0.49
1:E:242:LEU:HD11	1:E:244:VAL:HG13	1.95	0.49
1:I:252:ALA:O	1:I:254:ASP:N	2.46	0.49
2:N:3:VAL:HG12	2:N:4:ALA:N	2.27	0.49
2:N:15:PHE:CE1	2:N:322:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:220:GLN:CD	1:S:220:GLN:H	2.21	0.49
1:S:228:ILE:H	1:S:228:ILE:CD1	2.17	0.49
2:P:25:LEU:HD21	2:P:326:ASP:CA	2.39	0.49
1:Q:25:LEU:CD2	1:Q:25:LEU:H	2.26	0.49
1:Q:272:ASP:HB2	1:Q:288:PHE:CD2	2.47	0.49
2:R:181:ASP:CG	2:R:195:ARG:NH1	2.70	0.49
1:A:125:ILE:HG23	1:A:143:ILE:HG22	1.95	0.49
1:A:154:LEU:O	1:A:155:ALA:C	2.55	0.49
1:A:187:ALA:O	1:A:196:ALA:HB1	2.12	0.49
1:A:272:ASP:HB2	1:A:288:PHE:CD2	2.47	0.49
1:A:318:SER:O	1:A:322:VAL:HG23	2.12	0.49
2:B:82:LEU:O	2:B:111:ALA:HB1	2.12	0.49
1:C:95:GLY:HA2	1:C:119:THR:OG1	2.12	0.49
2:D:217:VAL:C	2:D:219:PRO:HD3	2.38	0.49
2:D:328:VAL:O	2:D:332:TRP:HB2	2.12	0.49
2:H:3:VAL:HG12	2:H:4:ALA:N	2.27	0.49
1:E:220:GLN:CD	1:E:220:GLN:H	2.21	0.49
1:I:191:ARG:HB2	1:I:191:ARG:HH11	1.75	0.49
1:K:132:VAL:HG12	1:K:133:ASN:N	2.27	0.49
1:K:242:LEU:HD11	1:K:244:VAL:HG13	1.95	0.49
1:M:125:ILE:HG23	1:M:143:ILE:HG22	1.95	0.49
2:N:228:ILE:HD13	2:T:296:LEU:HD22	1.95	0.49
1:O:9:GLY:O	1:O:10:ARG:C	2.55	0.49
1:Q:132:VAL:HG12	1:Q:133:ASN:N	2.27	0.49
2:R:96:THR:OG1	2:R:98:VAL:HG22	2.12	0.49
1:A:123(A):SER:O	1:G:124:ASP:CA	2.48	0.49
1:C:110:GLN:CD	1:C:110:GLN:N	2.71	0.49
1:C:242:LEU:HD11	1:C:244:VAL:HG13	1.95	0.49
2:H:162:ASP:C	2:H:164:LYS:H	2.21	0.49
2:H:273:VAL:HG12	2:H:274:CYS:N	2.28	0.49
1:E:95:GLY:HA2	1:E:119:THR:OG1	2.12	0.49
2:J:202:ASN:HD22	2:L:281:ILE:N	2.11	0.49
1:S:173:THR:HG22	1:S:174:THR:N	2.26	0.49
1:Q:173:THR:HG22	1:Q:174:THR:N	2.26	0.49
1:Q:239:VAL:CG2	1:Q:308:VAL:HG13	2.43	0.49
2:R:328:VAL:O	2:R:332:TRP:HB2	2.12	0.49
1:A:135:LYS:C	1:A:137:TYR:H	2.21	0.49
2:B:273:VAL:HG12	2:B:274:CYS:N	2.28	0.49
1:C:154:LEU:O	1:C:155:ALA:C	2.56	0.49
1:C:239:VAL:CG2	1:C:308:VAL:HG13	2.43	0.49
1:G:135:LYS:C	1:G:137:TYR:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:LEU:O	1:G:155:ALA:C	2.55	0.49
2:H:82:LEU:O	2:H:111:ALA:HB1	2.12	0.49
2:H:213:ALA:O	2:H:216:LEU:HB2	2.12	0.49
1:E:12:GLY:O	1:E:15:PHE:HB3	2.13	0.49
1:E:32:ASP:O	1:E:34:GLY:N	2.45	0.49
1:E:239:VAL:CG2	1:E:308:VAL:HG13	2.43	0.49
2:J:162:ASP:C	2:J:164:LYS:H	2.21	0.49
2:L:217:VAL:C	2:L:219:PRO:HD3	2.38	0.49
2:N:162:ASP:C	2:N:164:LYS:H	2.21	0.49
2:T:85:GLY:CA	2:T:112:GLY:HA3	2.42	0.49
1:O:166:GLY:O	1:O:246:ILE:HD12	2.13	0.48
1:Q:32:ASP:O	1:Q:34:GLY:N	2.45	0.48
1:Q:242:LEU:HD11	1:Q:244:VAL:HG13	1.95	0.48
2:R:94:GLU:OE1	2:R:99:PHE:HB2	2.13	0.48
1:A:184:LEU:O	1:A:185:LEU:HD23	2.12	0.48
2:B:15:PHE:CE1	2:B:322:VAL:HG22	2.47	0.48
2:D:96:THR:OG1	2:D:98:VAL:HG22	2.12	0.48
2:H:270:ILE:O	2:H:288:VAL:HB	2.13	0.48
2:F:85:GLY:CA	2:F:112:GLY:HA3	2.42	0.48
1:I:125:ILE:HG23	1:I:143:ILE:HG22	1.95	0.48
1:I:166:GLY:O	1:I:246:ILE:HD12	2.13	0.48
1:K:12:GLY:O	1:K:15:PHE:HB3	2.13	0.48
2:N:217:VAL:C	2:N:219:PRO:HD3	2.39	0.48
1:S:242:LEU:HD11	1:S:244:VAL:HG13	1.95	0.48
1:O:225:LEU:O	1:O:226:ASN:CB	2.61	0.48
2:P:162:ASP:C	2:P:164:LYS:H	2.21	0.48
2:P:202:ASN:HD22	2:R:281:ILE:N	2.11	0.48
2:R:158:VAL:HG13	2:R:167:ILE:CD1	2.43	0.48
1:A:41:THR:O	1:A:42:HIS:C	2.56	0.48
2:B:213:ALA:O	2:B:216:LEU:HB2	2.12	0.48
1:G:125:ILE:HG23	1:G:143:ILE:HG22	1.95	0.48
1:G:252:ALA:O	1:G:254:ASP:N	2.46	0.48
2:F:94:GLU:OE1	2:F:99:PHE:HB2	2.13	0.48
2:F:192:ASP:O	2:F:194:ARG:N	2.45	0.48
1:I:154:LEU:O	1:I:155:ALA:C	2.55	0.48
2:L:94:GLU:OE1	2:L:99:PHE:HB2	2.13	0.48
1:M:166:GLY:O	1:M:246:ILE:HD12	2.13	0.48
1:M:318:SER:O	1:M:322:VAL:HG23	2.12	0.48
2:N:49:ILE:HD11	2:N:235:PRO:HB2	1.95	0.48
2:T:158:VAL:HG13	2:T:167:ILE:CD1	2.43	0.48
2:T:217:VAL:C	2:T:219:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:49:ILE:HD11	2:P:235:PRO:HB2	1.96	0.48
1:Q:165:LEU:HB3	1:Q:246:ILE:HD11	1.94	0.48
1:G:130:VAL:HB	1:G:320:ARG:HD3	1.94	0.48
1:E:270:VAL:HG13	1:E:289:SER:HB2	1.95	0.48
1:I:184:LEU:O	1:I:185:LEU:HD23	2.12	0.48
2:J:209:GLY:C	2:J:211:ALA:N	2.71	0.48
2:J:229:ALA:C	2:J:230:LEU:HD23	2.39	0.48
2:N:273:VAL:HG12	2:N:274:CYS:N	2.28	0.48
2:T:134:GLU:OE1	2:T:134:GLU:N	2.38	0.48
1:O:110:GLN:HA	1:C:80:LEU:HD22	1.94	0.48
1:O:125:ILE:HG23	1:O:143:ILE:HG22	1.95	0.48
2:P:209:GLY:C	2:P:211:ALA:N	2.71	0.48
1:A:9:GLY:O	1:A:10:ARG:C	2.55	0.48
1:A:173:THR:HG22	1:A:174:THR:N	2.27	0.48
1:A:220:GLN:H	1:A:220:GLN:CD	2.20	0.48
1:C:25:LEU:CD2	1:C:25:LEU:H	2.26	0.48
1:C:252:ALA:O	1:C:254:ASP:N	2.47	0.48
1:G:41:THR:O	1:G:42:HIS:C	2.56	0.48
1:E:165:LEU:HB3	1:E:246:ILE:HD11	1.94	0.48
1:E:239:VAL:HB	1:E:310:TRP:CZ3	2.49	0.48
1:I:132:VAL:HG12	1:I:133:ASN:N	2.27	0.48
1:I:142:ASN:H	1:M:103:PRO:HG2	1.78	0.48
2:J:98:VAL:HG23	2:J:99:PHE:N	2.27	0.48
1:Q:239:VAL:HB	1:Q:310:TRP:CZ3	2.49	0.48
2:D:158:VAL:HG13	2:D:167:ILE:CD1	2.43	0.48
1:G:225:LEU:O	1:G:226:ASN:CB	2.61	0.48
1:M:270:VAL:HG13	1:M:289:SER:HB2	1.95	0.48
1:S:239:VAL:CG2	1:S:308:VAL:HG13	2.43	0.48
1:O:11:ILE:HG23	1:O:12:GLY:N	2.29	0.48
1:O:130:VAL:HB	1:O:320:ARG:HD3	1.94	0.48
1:O:221:LEU:O	1:O:222:LYS:C	2.56	0.48
1:Q:240:VAL:CG2	1:Q:309:ALA:HB3	2.44	0.48
1:Q:252:ALA:O	1:Q:254:ASP:N	2.47	0.48
1:A:244:VAL:O	1:A:244:VAL:HG23	2.14	0.48
1:A:307:VAL:HG12	1:A:308:VAL:N	2.29	0.48
2:B:166:GLY:O	2:B:246:VAL:HA	2.14	0.48
2:B:228:ILE:HD13	2:D:296:LEU:HD22	1.95	0.48
1:C:165:LEU:HB3	1:C:246:ILE:HD11	1.94	0.48
1:C:220:GLN:H	1:C:220:GLN:CD	2.21	0.48
2:D:151:THR:OG1	2:D:210:ALA:HA	2.13	0.48
1:E:228:ILE:H	1:E:228:ILE:CD1	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:ASP:OD1	1:I:125:ILE:CG1	2.40	0.48
2:J:217:VAL:C	2:J:219:PRO:HD3	2.38	0.48
1:K:154:LEU:O	1:K:155:ALA:C	2.56	0.48
1:K:220:GLN:H	1:K:220:GLN:CD	2.21	0.48
1:K:239:VAL:CG2	1:K:308:VAL:HG13	2.43	0.48
1:K:240:VAL:CG2	1:K:309:ALA:HB3	2.44	0.48
1:K:252:ALA:O	1:K:254:ASP:N	2.47	0.48
1:M:234:THR:O	1:M:234:THR:HG23	2.12	0.48
1:M:252:ALA:O	1:M:254:ASP:N	2.46	0.48
1:A:124:ASP:OD1	1:A:125:ILE:CG1	2.40	0.48
1:A:270:VAL:HG13	1:A:289:SER:HB2	1.95	0.48
1:C:32:ASP:O	1:C:34:GLY:N	2.45	0.48
1:C:240:VAL:CG2	1:C:309:ALA:HB3	2.44	0.48
1:G:9:GLY:O	1:G:10:ARG:C	2.55	0.48
2:H:209:GLY:C	2:H:211:ALA:N	2.71	0.48
2:J:179:THR:OG1	2:J:231:ARG:NH1	2.47	0.48
2:J:273:VAL:HG12	2:J:274:CYS:N	2.28	0.48
1:K:10:ARG:O	1:K:14:ASN:HB2	2.14	0.48
1:K:20:ARG:HH21	1:K:319:GLN:HE22	1.62	0.48
1:K:32:ASP:O	1:K:34:GLY:N	2.45	0.48
1:M:9:GLY:O	1:M:10:ARG:C	2.55	0.48
1:M:225:LEU:O	1:M:226:ASN:CB	2.61	0.48
2:N:270:ILE:O	2:N:288:VAL:HB	2.13	0.48
1:O:184:LEU:O	1:O:185:LEU:HD23	2.12	0.48
1:O:270:VAL:HG13	1:O:289:SER:HB2	1.95	0.48
1:A:166:GLY:O	1:A:246:ILE:HD12	2.13	0.48
2:B:179:THR:OG1	2:B:231:ARG:NH1	2.47	0.48
1:C:9:GLY:O	1:C:10:ARG:C	2.57	0.48
1:C:270:VAL:HG13	1:C:289:SER:HB2	1.94	0.48
1:G:221:LEU:O	1:G:222:LYS:C	2.56	0.48
2:F:10:ARG:NH1	2:F:47:ASP:OD1	2.43	0.48
1:K:11:ILE:CG2	1:K:12:GLY:N	2.77	0.48
1:S:25:LEU:CD2	1:S:25:LEU:H	2.26	0.48
2:T:94:GLU:OE1	2:T:99:PHE:HB2	2.14	0.48
1:O:110:GLN:CG	1:C:110:GLN:HB3	2.43	0.48
1:O:307:VAL:HG12	1:O:308:VAL:N	2.29	0.48
2:P:229:ALA:C	2:P:230:LEU:HD23	2.38	0.48
1:Q:220:GLN:H	1:Q:220:GLN:CD	2.21	0.48
1:Q:298:MET:HG3	1:Q:298:MET:O	2.14	0.48
2:R:25:LEU:HD21	2:R:326:ASP:CA	2.37	0.48
1:A:130:VAL:HB	1:A:320:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:ARG:NH1	2:D:47:ASP:OD1	2.43	0.48
1:G:270:VAL:HG13	1:G:289:SER:HB2	1.95	0.48
1:G:307:VAL:HG12	1:G:308:VAL:N	2.29	0.48
2:H:179:THR:OG1	2:H:231:ARG:NH1	2.47	0.48
1:I:248(A):VAL:HG13	1:I:249:GLY:N	2.18	0.48
2:J:193:LEU:H	2:J:193:LEU:CD1	2.06	0.48
1:M:41:THR:O	1:M:42:HIS:C	2.56	0.48
2:N:25:LEU:CD2	2:N:326:ASP:HA	2.40	0.48
2:N:229:ALA:C	2:N:230:LEU:HD23	2.39	0.48
1:O:244:VAL:HG23	1:O:244:VAL:O	2.14	0.48
1:Q:20:ARG:HH21	1:Q:319:GLN:HE22	1.62	0.48
1:Q:270:VAL:HG13	1:Q:289:SER:HB2	1.94	0.48
1:A:11:ILE:HG23	1:A:12:GLY:N	2.29	0.48
1:A:225:LEU:O	1:A:226:ASN:CB	2.61	0.48
2:B:162:ASP:C	2:B:164:LYS:H	2.21	0.48
2:B:217:VAL:C	2:B:219:PRO:HD3	2.38	0.48
1:G:82:LEU:HA	1:G:83:PRO:HD3	1.68	0.48
1:G:293:ASP:HB3	1:G:296:LEU:HB2	1.96	0.48
2:H:217:VAL:C	2:H:219:PRO:HD3	2.39	0.48
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.44	0.48
1:I:293:ASP:HB3	1:I:296:LEU:HB2	1.96	0.48
2:J:166:GLY:O	2:J:246:VAL:HA	2.14	0.48
1:K:240:VAL:O	1:K:308:VAL:HA	2.14	0.48
2:L:151:THR:OG1	2:L:210:ALA:HA	2.13	0.48
2:N:25:LEU:HD21	2:N:326:ASP:CA	2.39	0.48
2:N:157:PHE:HB2	2:N:259:PHE:CE1	2.49	0.48
1:S:270:VAL:HG13	1:S:289:SER:HB2	1.94	0.48
2:T:129:VAL:HB	2:T:132:VAL:HB	1.96	0.48
2:T:151:THR:OG1	2:T:210:ALA:HA	2.13	0.48
2:T:162:ASP:C	2:T:164:LYS:H	2.22	0.48
1:O:123(A):SER:O	1:C:124:ASP:CA	2.47	0.47
1:O:252:ALA:O	1:O:254:ASP:N	2.46	0.47
2:R:100:VAL:HA	2:R:118:ILE:HD13	1.96	0.47
2:R:162:ASP:C	2:R:164:LYS:H	2.22	0.47
1:A:235:PRO:O	1:A:236:ASN:HB2	2.14	0.47
2:B:49:ILE:HD11	2:B:235:PRO:HB2	1.96	0.47
1:C:133:ASN:C	1:C:133:ASN:ND2	2.72	0.47
2:D:162:ASP:C	2:D:164:LYS:H	2.22	0.47
1:G:220:GLN:H	1:G:220:GLN:CD	2.20	0.47
1:E:20:ARG:HH21	1:E:319:GLN:HE22	1.62	0.47
1:E:240:VAL:O	1:E:308:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:LEU:O	1:I:226:ASN:CB	2.61	0.47
2:J:49:ILE:HD11	2:J:235:PRO:HB2	1.96	0.47
2:J:270:ILE:O	2:J:288:VAL:HB	2.13	0.47
1:K:239:VAL:HB	1:K:310:TRP:CZ3	2.49	0.47
2:L:10:ARG:NH1	2:L:47:ASP:OD1	2.43	0.47
1:M:293:ASP:HB3	1:M:296:LEU:HB2	1.96	0.47
2:N:25:LEU:HD22	2:N:25:LEU:N	2.29	0.47
1:O:235:PRO:O	1:O:236:ASN:HB2	2.14	0.47
2:P:217:VAL:C	2:P:219:PRO:HD3	2.38	0.47
1:C:11:ILE:CG2	1:C:12:GLY:N	2.77	0.47
1:C:240:VAL:O	1:C:308:VAL:HA	2.14	0.47
2:D:100:VAL:HA	2:D:118:ILE:HD13	1.96	0.47
1:E:11:ILE:CG2	1:E:12:GLY:N	2.77	0.47
1:K:298:MET:HG3	1:K:298:MET:O	2.14	0.47
2:L:134:GLU:OE1	2:L:134:GLU:N	2.38	0.47
2:L:158:VAL:HG13	2:L:167:ILE:CD1	2.44	0.47
2:N:14:ASN:OD1	2:N:50:LEU:HD11	2.14	0.47
1:S:9:GLY:O	1:S:10:ARG:C	2.57	0.47
1:S:32:ASP:O	1:S:34:GLY:N	2.45	0.47
1:S:135:LYS:C	1:S:137:TYR:H	2.22	0.47
1:S:239:VAL:HB	1:S:310:TRP:CZ3	2.49	0.47
1:O:293:ASP:HB3	1:O:296:LEU:HB2	1.96	0.47
2:P:14:ASN:OD1	2:P:50:LEU:HD11	2.14	0.47
1:Q:10:ARG:O	1:Q:14:ASN:HB2	2.14	0.47
1:Q:125:ILE:HG23	1:Q:143:ILE:C	2.36	0.47
1:Q:135:LYS:C	1:Q:137:TYR:H	2.22	0.47
1:A:186:ASP:HA	1:A:196:ALA:O	2.14	0.47
1:A:221:LEU:O	1:A:222:LYS:C	2.56	0.47
1:A:293:ASP:HB3	1:A:296:LEU:HB2	1.97	0.47
2:B:14:ASN:OD1	2:B:50:LEU:HD11	2.14	0.47
2:B:218:LEU:HB3	2:B:221:LEU:CD2	2.44	0.47
1:G:11:ILE:CG2	1:G:12:GLY:N	2.78	0.47
1:G:186:ASP:HA	1:G:196:ALA:O	2.14	0.47
1:E:9:GLY:O	1:E:10:ARG:C	2.57	0.47
1:E:110:GLN:CB	1:K:110:GLN:NE2	2.78	0.47
1:I:235:PRO:O	1:I:236:ASN:HB2	2.14	0.47
1:I:270:VAL:HG13	1:I:289:SER:HB2	1.95	0.47
2:J:14:ASN:OD1	2:J:50:LEU:HD11	2.14	0.47
1:K:270:VAL:HG13	1:K:289:SER:HB2	1.94	0.47
2:L:162:ASP:C	2:L:164:LYS:H	2.23	0.47
1:M:244:VAL:HG23	1:M:244:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:179:THR:OG1	2:N:231:ARG:NH1	2.47	0.47
2:N:218:LEU:HB3	2:N:221:LEU:CD2	2.44	0.47
1:S:10:ARG:O	1:S:14:ASN:HB2	2.14	0.47
1:O:186:ASP:HA	1:O:196:ALA:O	2.14	0.47
1:Q:149:CYS:HB3	3:Q:401:NAD:H5N	1.95	0.47
1:Q:228:ILE:H	1:Q:228:ILE:CD1	2.18	0.47
1:Q:240:VAL:O	1:Q:308:VAL:HA	2.14	0.47
2:R:218:LEU:HA	2:R:218:LEU:HD23	1.77	0.47
1:A:11:ILE:CG2	1:A:12:GLY:N	2.78	0.47
2:B:157:PHE:HB2	2:B:259:PHE:CE1	2.49	0.47
1:C:125:ILE:HA	1:C:126:PRO:HD3	1.63	0.47
1:C:135:LYS:C	1:C:137:TYR:H	2.22	0.47
2:D:94:GLU:OE1	2:D:99:PHE:HB2	2.14	0.47
1:G:235:PRO:O	1:G:236:ASN:HB2	2.14	0.47
2:H:166:GLY:O	2:H:246:VAL:HA	2.14	0.47
1:E:125:ILE:HG23	1:E:143:ILE:O	2.14	0.47
1:E:135:LYS:C	1:E:137:TYR:H	2.22	0.47
1:E:154:LEU:O	1:E:155:ALA:C	2.56	0.47
2:F:100:VAL:HA	2:F:118:ILE:HD13	1.96	0.47
1:I:226:ASN:OD1	1:I:227:GLY:N	2.48	0.47
1:K:25:LEU:CD2	1:K:25:LEU:H	2.26	0.47
1:K:226:ASN:OD1	1:K:227:GLY:N	2.47	0.47
1:S:154:LEU:O	1:S:155:ALA:C	2.56	0.47
2:T:31:ASN:OD1	2:T:74:VAL:HG23	2.14	0.47
1:O:32:ASP:O	1:O:34:GLY:N	2.44	0.47
1:O:192:ASP:O	1:O:194:ARG:N	2.48	0.47
2:P:218:LEU:HB3	2:P:221:LEU:CD2	2.44	0.47
2:P:273:VAL:HG12	2:P:274:CYS:N	2.28	0.47
1:Q:271:LEU:HG	1:Q:272:ASP:N	2.29	0.47
2:R:31:ASN:OD1	2:R:74:VAL:HG23	2.15	0.47
2:R:151:THR:OG1	2:R:210:ALA:HA	2.13	0.47
1:A:205:PRO:HA	1:A:230:LEU:HD23	1.97	0.47
1:A:234:THR:O	1:A:234:THR:HG23	2.12	0.47
2:B:229:ALA:C	2:B:230:LEU:HD23	2.39	0.47
1:C:228:ILE:HD13	1:C:228:ILE:N	2.18	0.47
1:G:192:ASP:O	1:G:194:ARG:N	2.48	0.47
2:H:14:ASN:OD1	2:H:50:LEU:HD11	2.14	0.47
1:E:10:ARG:O	1:E:14:ASN:HB2	2.14	0.47
1:E:252:ALA:O	1:E:254:ASP:N	2.47	0.47
2:J:279:VAL:O	2:J:280:SER:C	2.57	0.47
1:K:293:ASP:CG	1:K:296:LEU:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:11:ILE:CG2	1:S:12:GLY:N	2.77	0.47
1:S:191:ARG:HB2	1:S:191:ARG:HH11	1.79	0.47
1:S:240:VAL:CG2	1:S:309:ALA:HB3	2.44	0.47
1:S:298:MET:HG3	1:S:298:MET:O	2.14	0.47
1:Q:154:LEU:O	1:Q:155:ALA:C	2.56	0.47
1:Q:293:ASP:CG	1:Q:296:LEU:HD12	2.40	0.47
1:Q:327:LEU:O	1:Q:330:ASN:N	2.48	0.47
2:R:129:VAL:HB	2:R:132:VAL:HB	1.96	0.47
1:A:226:ASN:OD1	1:A:227:GLY:N	2.48	0.47
1:C:221:LEU:O	1:C:222:LYS:C	2.58	0.47
1:C:298:MET:HG3	1:C:298:MET:O	2.14	0.47
1:G:9:GLY:O	1:G:11:ILE:N	2.48	0.47
1:G:166:GLY:O	1:G:246:ILE:HD12	2.13	0.47
2:H:279:VAL:O	2:H:280:SER:C	2.57	0.47
1:K:318:SER:O	1:K:322:VAL:HG23	2.15	0.47
2:L:167:ILE:HG23	2:L:244:VAL:HB	1.96	0.47
1:M:9:GLY:O	1:M:11:ILE:N	2.48	0.47
2:N:129:VAL:H	2:N:133:ASN:HD21	1.63	0.47
2:N:166:GLY:O	2:N:246:VAL:HA	2.14	0.47
1:O:123(A):SER:C	1:C:124:ASP:CA	2.88	0.47
2:P:279:VAL:O	2:P:280:SER:C	2.57	0.47
1:Q:226:ASN:OD1	1:Q:227:GLY:N	2.48	0.47
2:R:167:ILE:HG23	2:R:244:VAL:HB	1.97	0.47
2:B:20:ARG:HE	2:B:319:GLN:HE22	1.63	0.47
1:C:125:ILE:HG23	1:C:143:ILE:O	2.15	0.47
1:C:204:VAL:HA	1:C:205:PRO:HD3	1.77	0.47
1:C:239:VAL:HB	1:C:310:TRP:CZ3	2.49	0.47
1:C:327:LEU:O	1:C:330:ASN:N	2.48	0.47
2:D:129:VAL:HB	2:D:132:VAL:HB	1.96	0.47
1:G:11:ILE:HG23	1:G:12:GLY:N	2.29	0.47
1:G:74:VAL:CG1	1:G:75:SER:N	2.78	0.47
1:G:205:PRO:HA	1:G:230:LEU:HD23	1.97	0.47
2:H:49:ILE:HD11	2:H:235:PRO:HB2	1.96	0.47
1:E:25:LEU:CD2	1:E:25:LEU:H	2.26	0.47
1:E:109:ILE:HB	1:K:110:GLN:HE22	1.79	0.47
1:E:226:ASN:OD1	1:E:227:GLY:N	2.47	0.47
1:E:271:LEU:HG	1:E:272:ASP:N	2.29	0.47
1:E:327:LEU:O	1:E:330:ASN:N	2.48	0.47
2:F:31:ASN:OD1	2:F:74:VAL:HG23	2.14	0.47
2:F:151:THR:OG1	2:F:210:ALA:HA	2.13	0.47
2:F:158:VAL:HG13	2:F:167:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ASP:C	2:F:164:LYS:H	2.22	0.47
1:I:9:GLY:O	1:I:11:ILE:N	2.48	0.47
1:I:11:ILE:CG2	1:I:12:GLY:N	2.77	0.47
1:I:192:ASP:O	1:I:194:ARG:N	2.48	0.47
1:I:205:PRO:HA	1:I:230:LEU:HD23	1.97	0.47
2:J:25:LEU:HD22	2:J:25:LEU:N	2.29	0.47
2:J:161:LEU:HD13	2:J:244:VAL:HG21	1.97	0.47
2:J:218:LEU:HB3	2:J:221:LEU:CD2	2.44	0.47
1:K:271:LEU:HG	1:K:272:ASP:N	2.30	0.47
1:M:11:ILE:CG2	1:M:12:GLY:N	2.78	0.47
1:M:84:TRP:HA	1:M:84:TRP:CE3	2.50	0.47
1:M:186:ASP:HA	1:M:196:ALA:O	2.14	0.47
1:M:192:ASP:O	1:M:194:ARG:N	2.48	0.47
2:N:209:GLY:C	2:N:211:ALA:N	2.71	0.47
2:N:271:LEU:HG	2:N:272:SER:H	1.80	0.47
2:N:279:VAL:O	2:N:280:SER:C	2.57	0.47
1:S:14:ASN:HB3	1:S:318:SER:OG	2.15	0.47
1:S:125:ILE:HG23	1:S:143:ILE:O	2.14	0.47
1:S:240:VAL:O	1:S:308:VAL:HA	2.14	0.47
1:S:271:LEU:HG	1:S:272:ASP:N	2.30	0.47
2:T:16:LEU:HD23	2:T:16:LEU:O	2.15	0.47
1:O:204:VAL:HA	1:Q:279:VAL:HG12	1.97	0.47
1:Q:124:ASP:O	1:Q:125:ILE:CB	2.63	0.47
1:A:9:GLY:O	1:A:11:ILE:N	2.48	0.47
1:C:193:LEU:H	1:C:193:LEU:CD1	2.26	0.47
1:C:271:LEU:HG	1:C:272:ASP:N	2.30	0.47
1:C:293:ASP:CG	1:C:296:LEU:HD12	2.40	0.47
2:H:138:THR:C	2:H:140:ALA:H	2.23	0.47
2:H:157:PHE:HB2	2:H:259:PHE:CE1	2.50	0.47
2:H:229:ALA:C	2:H:230:LEU:HD23	2.39	0.47
1:E:125:ILE:HG23	1:E:143:ILE:HG22	1.97	0.47
1:E:293:ASP:CG	1:E:296:LEU:HD12	2.40	0.47
1:I:186:ASP:HA	1:I:196:ALA:O	2.14	0.47
1:I:221:LEU:O	1:I:222:LYS:C	2.56	0.47
2:J:157:PHE:HB2	2:J:259:PHE:CE1	2.50	0.47
1:M:129:VAL:CG2	1:M:217:VAL:HG11	2.45	0.47
1:M:226:ASN:OD1	1:M:227:GLY:N	2.48	0.47
2:T:100:VAL:HA	2:T:118:ILE:HD13	1.96	0.47
2:T:272:SER:O	2:T:291:THR:HA	2.15	0.47
1:O:9:GLY:O	1:O:11:ILE:N	2.48	0.47
1:O:129:VAL:CG2	1:O:217:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:183:ARG:HG2	1:O:187:ALA:HB3	1.97	0.47
1:A:124:ASP:O	1:G:124:ASP:OD2	2.27	0.47
1:A:135:LYS:O	1:A:137:TYR:N	2.48	0.47
1:C:20:ARG:HH21	1:C:319:GLN:HE22	1.62	0.47
1:C:76:ASN:ND2	1:C:81:LYS:HD2	2.30	0.47
2:D:20:ARG:HE	2:D:319:GLN:HE22	1.62	0.47
1:G:135:LYS:O	1:G:137:TYR:N	2.48	0.47
1:G:244:VAL:HG23	1:G:244:VAL:O	2.14	0.47
2:H:202:ASN:HD22	2:F:281:ILE:N	2.11	0.47
2:H:218:LEU:HB3	2:H:221:LEU:CD2	2.44	0.47
1:E:168:VAL:HB	1:E:245:ASN:O	2.15	0.47
1:I:192:ASP:C	1:I:194:ARG:H	2.23	0.47
1:K:11:ILE:HG23	1:K:12:GLY:N	2.30	0.47
2:L:16:LEU:HD23	2:L:16:LEU:O	2.15	0.47
2:L:240:VAL:CG1	2:L:309:ALA:HB3	2.45	0.47
1:M:11:ILE:HG23	1:M:12:GLY:N	2.29	0.47
1:M:90:ASP:HA	1:M:114:LYS:CG	2.45	0.47
1:M:235:PRO:O	1:M:236:ASN:HB2	2.14	0.47
2:N:138:THR:C	2:N:140:ALA:H	2.23	0.47
1:S:221:LEU:O	1:S:222:LYS:C	2.57	0.47
1:S:252:ALA:O	1:S:254:ASP:N	2.47	0.47
1:S:318:SER:O	1:S:322:VAL:HG23	2.15	0.47
1:S:327:LEU:O	1:S:330:ASN:N	2.48	0.47
2:T:167:ILE:HG23	2:T:244:VAL:HB	1.97	0.47
1:O:226:ASN:OD1	1:O:227:GLY:N	2.48	0.47
2:P:25:LEU:CD2	2:P:326:ASP:HA	2.40	0.47
2:P:157:PHE:HB2	2:P:259:PHE:CE1	2.50	0.47
2:P:166:GLY:O	2:P:246:VAL:HA	2.14	0.47
2:P:179:THR:OG1	2:P:231:ARG:NH1	2.47	0.47
1:Q:193:LEU:H	1:Q:193:LEU:CD1	2.26	0.47
1:Q:318:SER:O	1:Q:322:VAL:HG23	2.15	0.47
1:A:192:ASP:O	1:A:194:ARG:N	2.48	0.47
1:A:204:VAL:HA	1:C:279:VAL:HG12	1.97	0.47
1:C:318:SER:O	1:C:322:VAL:HG23	2.15	0.47
1:G:226:ASN:OD1	1:G:227:GLY:N	2.48	0.47
1:G:327:LEU:O	1:G:330:ASN:N	2.47	0.47
2:H:20:ARG:HE	2:H:319:GLN:HE22	1.63	0.47
1:K:9:GLY:O	1:K:10:ARG:C	2.57	0.47
2:L:129:VAL:HB	2:L:132:VAL:HB	1.96	0.47
1:M:135:LYS:O	1:M:137:TYR:N	2.48	0.47
1:M:228:ILE:HD13	1:M:228:ILE:N	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:84:TRP:HA	1:S:84:TRP:HE3	1.80	0.47
2:P:154:LEU:HD21	2:P:172:MET:HG2	1.97	0.46
1:Q:9:GLY:O	1:Q:10:ARG:C	2.57	0.46
2:R:138:THR:C	2:R:140:ALA:H	2.23	0.46
2:B:322:VAL:O	2:B:326:ASP:HB2	2.15	0.46
1:C:84:TRP:HA	1:C:84:TRP:HE3	1.80	0.46
1:C:291:THR:O	1:C:310:TRP:N	2.39	0.46
2:D:193:LEU:H	2:D:193:LEU:CD1	2.07	0.46
1:G:239:VAL:CG2	1:G:308:VAL:HG13	2.46	0.46
2:F:129:VAL:HB	2:F:132:VAL:HB	1.96	0.46
1:I:11:ILE:HG23	1:I:12:GLY:N	2.29	0.46
1:I:162:ASP:CA	1:I:167:ILE:HG13	2.45	0.46
1:I:244:VAL:O	1:I:244:VAL:HG23	2.14	0.46
2:J:322:VAL:O	2:J:326:ASP:HB2	2.15	0.46
1:K:133:ASN:C	1:K:133:ASN:ND2	2.72	0.46
1:K:135:LYS:C	1:K:137:TYR:H	2.22	0.46
2:L:272:SER:O	2:L:291:THR:HA	2.15	0.46
1:M:162:ASP:CA	1:M:167:ILE:HG13	2.45	0.46
1:M:192:ASP:C	1:M:194:ARG:H	2.23	0.46
1:M:221:LEU:O	1:M:222:LYS:C	2.56	0.46
2:N:193:LEU:HD12	2:N:193:LEU:N	2.12	0.46
2:T:138:THR:C	2:T:140:ALA:H	2.23	0.46
1:O:11:ILE:CG2	1:O:12:GLY:N	2.78	0.46
1:O:90:ASP:HA	1:O:114:LYS:CG	2.46	0.46
2:P:322:VAL:O	2:P:326:ASP:HB2	2.15	0.46
1:Q:283:PHE:CE2	1:Q:310:TRP:CG	3.04	0.46
1:A:74:VAL:CG1	1:A:75:SER:N	2.78	0.46
1:A:90:ASP:HA	1:A:114:LYS:CG	2.45	0.46
2:B:25:LEU:HD22	2:B:25:LEU:N	2.29	0.46
2:B:279:VAL:O	2:B:280:SER:C	2.57	0.46
1:C:14:ASN:HB3	1:C:318:SER:OG	2.15	0.46
1:C:125:ILE:HG23	1:C:143:ILE:HG22	1.97	0.46
1:C:226:ASN:OD1	1:C:227:GLY:N	2.48	0.46
2:D:16:LEU:HD23	2:D:16:LEU:O	2.15	0.46
2:D:31:ASN:OD1	2:D:74:VAL:HG23	2.15	0.46
2:D:276:GLU:O	2:D:278:LEU:HG	2.16	0.46
1:G:204:VAL:HA	1:E:279:VAL:HG12	1.97	0.46
2:H:16:LEU:O	2:H:16:LEU:HD23	2.15	0.46
2:H:154:LEU:HD21	2:H:172:MET:HG2	1.97	0.46
1:E:298:MET:HG3	1:E:298:MET:O	2.14	0.46
2:F:18:CYS:HG	2:F:319:GLN:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:LYS:O	1:I:137:TYR:N	2.48	0.46
2:J:79:PRO:O	2:J:81:ASN:N	2.49	0.46
2:J:154:LEU:HD21	2:J:172:MET:HG2	1.97	0.46
1:M:307:VAL:HG12	1:M:308:VAL:N	2.29	0.46
1:M:327:LEU:O	1:M:330:ASN:N	2.47	0.46
2:N:158:VAL:HG13	2:N:167:ILE:CD1	2.46	0.46
2:N:161:LEU:HD13	2:N:244:VAL:HG21	1.97	0.46
1:S:293:ASP:CG	1:S:296:LEU:HD12	2.40	0.46
2:T:98:VAL:HG23	2:T:99:PHE:N	2.31	0.46
1:O:192:ASP:C	1:O:194:ARG:H	2.23	0.46
1:O:205:PRO:HA	1:O:230:LEU:HD23	1.97	0.46
2:P:129:VAL:H	2:P:133:ASN:HD21	1.63	0.46
1:Q:41:THR:O	1:Q:42:HIS:C	2.59	0.46
2:R:10:ARG:NH1	2:R:47:ASP:OD1	2.43	0.46
1:A:84:TRP:CE3	1:A:84:TRP:HA	2.50	0.46
1:A:192:ASP:C	1:A:194:ARG:H	2.23	0.46
1:A:204:VAL:HA	1:A:205:PRO:HD3	1.78	0.46
1:C:10:ARG:O	1:C:14:ASN:HB2	2.14	0.46
1:G:90:ASP:HA	1:G:114:LYS:CG	2.45	0.46
1:G:192:ASP:C	1:G:194:ARG:H	2.23	0.46
2:H:25:LEU:N	2:H:25:LEU:HD22	2.30	0.46
2:H:120:ALA:HB1	2:H:121:PRO:CD	2.46	0.46
1:E:14:ASN:HB3	1:E:318:SER:OG	2.15	0.46
2:F:276:GLU:O	2:F:278:LEU:HG	2.16	0.46
2:J:138:THR:C	2:J:140:ALA:H	2.23	0.46
1:M:239:VAL:CG2	1:M:308:VAL:HG13	2.46	0.46
2:N:79:PRO:O	2:N:81:ASN:N	2.49	0.46
2:N:120:ALA:HB1	2:N:121:PRO:CD	2.46	0.46
1:S:20:ARG:HH21	1:S:319:GLN:HE22	1.62	0.46
1:O:198:ALA:CB	1:O:201:LEU:HG	2.46	0.46
1:O:248(A):VAL:HG13	1:O:249:GLY:N	2.18	0.46
2:P:120:ALA:HB1	2:P:121:PRO:CD	2.45	0.46
2:R:272:SER:O	2:R:291:THR:HA	2.15	0.46
1:C:168:VAL:HB	1:C:245:ASN:O	2.15	0.46
1:G:183:ARG:HG2	1:G:187:ALA:HB3	1.97	0.46
1:G:198:ALA:CB	1:G:201:LEU:HG	2.45	0.46
2:H:79:PRO:O	2:H:81:ASN:N	2.48	0.46
2:F:20:ARG:HE	2:F:319:GLN:HE22	1.62	0.46
2:F:167:ILE:HG23	2:F:244:VAL:HB	1.97	0.46
1:K:41:THR:O	1:K:42:HIS:C	2.58	0.46
1:K:215:SER:HB3	1:K:222:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:LEU:O	1:K:222:LYS:C	2.58	0.46
2:L:31:ASN:OD1	2:L:74:VAL:HG23	2.14	0.46
2:L:106:GLY:O	2:L:109:LEU:N	2.49	0.46
2:N:16:LEU:O	2:N:16:LEU:HD23	2.15	0.46
2:N:256:ASN:ND2	2:N:297:THR:HG21	2.31	0.46
1:S:76:ASN:ND2	1:S:81:LYS:HD2	2.30	0.46
2:T:181:ASP:CG	2:T:195:ARG:NH1	2.70	0.46
1:O:327:LEU:O	1:O:330:ASN:N	2.48	0.46
2:P:79:PRO:O	2:P:81:ASN:N	2.49	0.46
2:P:256:ASN:ND2	2:P:297:THR:HG21	2.31	0.46
1:Q:76:ASN:ND2	1:Q:81:LYS:HD2	2.30	0.46
1:Q:221:LEU:O	1:Q:222:LYS:C	2.57	0.46
2:R:16:LEU:O	2:R:16:LEU:HD23	2.15	0.46
2:R:240:VAL:CG1	2:R:309:ALA:HB3	2.45	0.46
1:A:135:LYS:C	1:A:137:TYR:N	2.74	0.46
2:B:193:LEU:H	2:B:193:LEU:CD1	2.06	0.46
2:H:158:VAL:HG13	2:H:167:ILE:CD1	2.46	0.46
2:H:322:VAL:O	2:H:326:ASP:HB2	2.15	0.46
1:E:84:TRP:HA	1:E:84:TRP:HE3	1.80	0.46
1:E:193:LEU:H	1:E:193:LEU:CD1	2.26	0.46
2:F:138:THR:C	2:F:140:ALA:H	2.23	0.46
1:I:142:ASN:H	1:M:103:PRO:HG3	1.81	0.46
1:K:307:VAL:HG12	1:K:308:VAL:N	2.30	0.46
2:L:276:GLU:O	2:L:278:LEU:HG	2.16	0.46
1:M:198:ALA:CB	1:M:201:LEU:HG	2.46	0.46
1:M:248(A):VAL:CG2	1:M:249:GLY:N	2.75	0.46
1:S:125:ILE:HG23	1:S:143:ILE:HG22	1.97	0.46
1:S:226:ASN:OD1	1:S:227:GLY:N	2.48	0.46
2:T:240:VAL:CG1	2:T:309:ALA:HB3	2.45	0.46
1:O:74:VAL:CG1	1:O:75:SER:N	2.78	0.46
2:P:25:LEU:HD22	2:P:25:LEU:N	2.29	0.46
2:P:138:THR:C	2:P:140:ALA:H	2.23	0.46
1:Q:107:LYS:HA	1:Q:110:GLN:CD	2.41	0.46
1:Q:307:VAL:HG12	1:Q:308:VAL:N	2.30	0.46
2:R:25:LEU:CD2	2:R:326:ASP:HA	2.39	0.46
2:R:161:LEU:HD13	2:R:244:VAL:HG21	1.98	0.46
1:A:142:ASN:H	1:G:103:PRO:HG3	1.79	0.46
1:A:239:VAL:CG2	1:A:308:VAL:HG13	2.45	0.46
2:B:120:ALA:HB1	2:B:121:PRO:CD	2.46	0.46
1:G:84:TRP:HA	1:G:84:TRP:CE3	2.50	0.46
1:G:162:ASP:CA	1:G:167:ILE:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:PHE:CZ	1:I:310:TRP:CD1	3.04	0.46
2:J:106:GLY:O	2:J:109:LEU:N	2.49	0.46
2:J:158:VAL:HG13	2:J:167:ILE:CD1	2.46	0.46
1:K:125:ILE:HG23	1:K:143:ILE:O	2.15	0.46
1:K:168:VAL:HB	1:K:245:ASN:O	2.15	0.46
2:L:100:VAL:HA	2:L:118:ILE:HD13	1.96	0.46
2:L:138:THR:C	2:L:140:ALA:H	2.23	0.46
2:N:169:LYS:HE3	2:T:303:ASP:OD1	2.16	0.46
1:S:215:SER:HB3	1:S:222:LYS:HA	1.98	0.46
1:O:135:LYS:O	1:O:137:TYR:N	2.48	0.46
2:P:161:LEU:HD13	2:P:244:VAL:HG21	1.97	0.46
1:Q:11:ILE:CG2	1:Q:12:GLY:N	2.77	0.46
2:R:276:GLU:O	2:R:278:LEU:HG	2.16	0.46
1:A:327:LEU:O	1:A:330:ASN:N	2.48	0.46
2:B:79:PRO:O	2:B:81:ASN:N	2.48	0.46
2:B:256:ASN:ND2	2:B:297:THR:HG21	2.31	0.46
1:E:221:LEU:O	1:E:222:LYS:C	2.58	0.46
2:F:272:SER:O	2:F:291:THR:HA	2.15	0.46
1:K:14:ASN:HB3	1:K:318:SER:OG	2.15	0.46
1:K:76:ASN:ND2	1:K:81:LYS:HD2	2.30	0.46
2:N:280:SER:O	2:N:282:ASP:N	2.49	0.46
1:S:133:ASN:C	1:S:133:ASN:ND2	2.72	0.46
1:S:168:VAL:HB	1:S:245:ASN:O	2.15	0.46
2:T:106:GLY:O	2:T:109:LEU:N	2.49	0.46
2:T:276:GLU:O	2:T:278:LEU:HG	2.16	0.46
2:P:20:ARG:HE	2:P:319:GLN:HE22	1.63	0.46
1:A:283:PHE:CZ	1:A:310:TRP:CD1	3.04	0.46
2:B:16:LEU:O	2:B:16:LEU:HD23	2.15	0.46
2:B:154:LEU:HD21	2:B:172:MET:HG2	1.97	0.46
1:G:283:PHE:CZ	1:G:310:TRP:CD1	3.04	0.46
1:E:283:PHE:CE2	1:E:310:TRP:CG	3.03	0.46
1:E:318:SER:O	1:E:322:VAL:HG23	2.15	0.46
1:I:236:ASN:O	1:I:237:VAL:CB	2.64	0.46
1:I:307:VAL:HG12	1:I:308:VAL:N	2.29	0.46
2:L:161:LEU:HD13	2:L:244:VAL:HG21	1.98	0.46
1:M:283:PHE:CZ	1:M:310:TRP:CD1	3.04	0.46
1:O:135:LYS:C	1:O:137:TYR:N	2.74	0.46
2:P:16:LEU:O	2:P:16:LEU:HD23	2.15	0.46
1:Q:121:PRO:O	1:Q:122:ALA:O	2.33	0.46
2:R:106:GLY:O	2:R:109:LEU:N	2.49	0.46
1:A:198:ALA:CB	1:A:201:LEU:HG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:HE3	2:D:303:ASP:OD1	2.16	0.46
1:C:191:ARG:HB2	1:C:191:ARG:HH11	1.79	0.46
1:C:228:ILE:H	1:C:228:ILE:CD1	2.18	0.46
2:D:256:ASN:HD21	2:D:297:THR:CG2	2.29	0.46
1:G:204:VAL:HA	1:G:205:PRO:HD3	1.78	0.46
2:H:256:ASN:ND2	2:H:297:THR:HG21	2.31	0.46
1:E:191:ARG:HB2	1:E:191:ARG:HH11	1.79	0.46
2:F:256:ASN:HD21	2:F:297:THR:CG2	2.29	0.46
1:I:84:TRP:CE3	1:I:84:TRP:HA	2.50	0.46
2:L:98:VAL:HG23	2:L:99:PHE:N	2.31	0.46
2:L:181:ASP:CG	2:L:195:ARG:NH1	2.70	0.46
1:M:135:LYS:C	1:M:137:TYR:N	2.74	0.46
1:M:209:GLY:C	1:M:211:ALA:N	2.74	0.46
1:M:248(A):VAL:HG13	1:M:249:GLY:N	2.18	0.46
2:N:154:LEU:HD21	2:N:172:MET:HG2	1.97	0.46
1:S:9:GLY:O	1:S:11:ILE:N	2.49	0.46
1:S:198:ALA:CB	1:S:201:LEU:HG	2.46	0.46
1:S:283:PHE:CE2	1:S:310:TRP:CG	3.04	0.46
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.50	0.46
2:P:85:GLY:CA	2:P:112:GLY:HA3	2.46	0.46
2:P:169:LYS:HE3	2:R:303:ASP:OD1	2.16	0.46
1:Q:271:LEU:HG	1:Q:272:ASP:H	1.81	0.46
1:A:82:LEU:HA	1:A:83:PRO:HD3	1.68	0.46
1:A:162:ASP:CA	1:A:167:ILE:HG13	2.45	0.46
1:A:183:ARG:HG2	1:A:187:ALA:HB3	1.97	0.46
2:B:138:THR:C	2:B:140:ALA:H	2.23	0.46
2:B:202:ASN:HD22	2:D:281:ILE:N	2.11	0.46
1:C:240:VAL:HG22	1:C:309:ALA:HB3	1.98	0.46
2:D:167:ILE:HG23	2:D:244:VAL:HB	1.97	0.46
2:D:240:VAL:CG1	2:D:309:ALA:HB3	2.45	0.46
2:D:272:SER:O	2:D:291:THR:HA	2.15	0.46
1:G:209:GLY:C	1:G:211:ALA:N	2.74	0.46
1:E:133:ASN:C	1:E:133:ASN:ND2	2.72	0.46
1:E:198:ALA:CB	1:E:201:LEU:HG	2.47	0.46
1:E:228:ILE:HD13	1:E:228:ILE:N	2.17	0.46
2:F:16:LEU:HD23	2:F:16:LEU:O	2.15	0.46
2:F:106:GLY:O	2:F:109:LEU:N	2.49	0.46
1:I:90:ASP:HA	1:I:114:LYS:CG	2.45	0.46
1:I:198:ALA:CB	1:I:201:LEU:HG	2.46	0.46
2:J:272:SER:O	2:J:291:THR:HA	2.16	0.46
1:K:209:GLY:C	1:K:211:ALA:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:CYS:SG	2:L:319:GLN:OE1	2.74	0.46
1:M:205:PRO:HA	1:M:230:LEU:HD23	1.97	0.46
2:N:79:PRO:O	2:N:80:VAL:C	2.59	0.46
2:N:322:VAL:O	2:N:326:ASP:HB2	2.15	0.46
1:S:11:ILE:HG23	1:S:12:GLY:N	2.30	0.46
2:T:256:ASN:HD21	2:T:297:THR:CG2	2.29	0.46
1:O:239:VAL:CG2	1:O:308:VAL:HG13	2.46	0.45
2:P:280:SER:O	2:P:282:ASP:N	2.49	0.45
2:P:303:ASP:OD1	2:R:169:LYS:HE3	2.17	0.45
1:Q:133:ASN:C	1:Q:133:ASN:ND2	2.72	0.45
2:R:98:VAL:HG23	2:R:99:PHE:N	2.31	0.45
1:A:293:ASP:CG	1:A:296:LEU:HD12	2.41	0.45
2:B:317:TYR:O	2:B:320:ARG:HB2	2.16	0.45
1:C:82:LEU:HA	1:C:83:PRO:HD3	1.72	0.45
1:C:327:LEU:O	1:C:328:VAL:C	2.59	0.45
2:H:129:VAL:H	2:H:133:ASN:HD21	1.63	0.45
2:H:272:SER:O	2:H:291:THR:HA	2.16	0.45
1:E:76:ASN:ND2	1:E:81:LYS:HD2	2.30	0.45
2:F:240:VAL:CG1	2:F:309:ALA:HB3	2.45	0.45
1:I:183:ARG:HG2	1:I:187:ALA:HB3	1.97	0.45
2:J:169:LYS:HE3	2:L:303:ASP:OD1	2.16	0.45
1:K:191:ARG:HB2	1:K:191:ARG:HH11	1.80	0.45
2:L:28:VAL:C	2:L:71:ILE:HG23	2.42	0.45
2:L:138:THR:C	2:L:140:ALA:N	2.74	0.45
2:N:106:GLY:O	2:N:109:LEU:N	2.49	0.45
2:T:108:HIS:HB2	2:T:116:VAL:HG21	1.99	0.45
1:O:142:ASN:H	1:C:103:PRO:HG2	1.80	0.45
2:P:106:GLY:O	2:P:109:LEU:N	2.49	0.45
2:P:139:HIS:CE1	2:P:332:TRP:CE3	3.04	0.45
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.17	0.45
1:Q:191:ARG:HB2	1:Q:191:ARG:HH11	1.80	0.45
2:R:256:ASN:HD21	2:R:297:THR:CG2	2.29	0.45
1:A:129:VAL:CG2	1:A:217:VAL:HG11	2.45	0.45
2:B:85:GLY:CA	2:B:112:GLY:HA3	2.47	0.45
2:B:161:LEU:HD13	2:B:244:VAL:HG21	1.97	0.45
2:D:106:GLY:O	2:D:109:LEU:N	2.49	0.45
1:G:293:ASP:CG	1:G:296:LEU:HD12	2.41	0.45
2:H:85:GLY:CA	2:H:112:GLY:HA3	2.46	0.45
1:E:41:THR:O	1:E:42:HIS:C	2.58	0.45
1:E:307:VAL:HG12	1:E:308:VAL:N	2.31	0.45
2:J:85:GLY:CA	2:J:112:GLY:HA3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:120:ALA:HB1	2:J:121:PRO:CD	2.46	0.45
2:J:256:ASN:ND2	2:J:297:THR:HG21	2.31	0.45
2:J:276:GLU:O	2:J:278:LEU:HG	2.17	0.45
2:J:280:SER:O	2:J:282:ASP:N	2.49	0.45
2:J:303:ASP:OD1	2:L:169:LYS:HE3	2.17	0.45
1:K:60:ILE:HG22	1:K:60(A):ASP:N	2.31	0.45
1:K:125:ILE:HG23	1:K:143:ILE:HG22	1.97	0.45
1:K:283:PHE:CE2	1:K:310:TRP:CG	3.04	0.45
2:N:210:ALA:HA	2:N:213:ALA:HB3	1.98	0.45
2:T:129:VAL:O	2:T:130:VAL:C	2.59	0.45
1:O:162:ASP:CA	1:O:167:ILE:HG13	2.45	0.45
1:O:209:GLY:O	1:O:210:ALA:C	2.60	0.45
2:P:210:ALA:HA	2:P:213:ALA:HB3	1.98	0.45
2:P:271:LEU:HG	2:P:272:SER:H	1.80	0.45
1:Q:11:ILE:HG23	1:Q:12:GLY:N	2.30	0.45
1:Q:84:TRP:HA	1:Q:84:TRP:HE3	1.81	0.45
2:R:28:VAL:C	2:R:71:ILE:HG23	2.42	0.45
2:R:138:THR:C	2:R:140:ALA:N	2.75	0.45
1:A:211:ALA:HB1	1:A:226:ASN:HA	1.98	0.45
2:B:79:PRO:O	2:B:80:VAL:C	2.59	0.45
2:B:129:VAL:H	2:B:133:ASN:HD21	1.63	0.45
2:B:271:LEU:HG	2:B:272:SER:H	1.80	0.45
2:B:272:SER:O	2:B:291:THR:HA	2.17	0.45
1:C:11:ILE:HG23	1:C:12:GLY:N	2.30	0.45
1:C:41:THR:O	1:C:42:HIS:C	2.58	0.45
1:C:104:GLY:O	1:C:107:LYS:HG3	2.17	0.45
1:C:283:PHE:CE2	1:C:310:TRP:CG	3.04	0.45
2:H:276:GLU:O	2:H:278:LEU:HG	2.17	0.45
2:F:209:GLY:O	2:F:210:ALA:C	2.60	0.45
1:I:202:ASN:OD1	1:K:281:VAL:HB	2.17	0.45
2:J:317:TYR:O	2:J:320:ARG:HB2	2.16	0.45
1:K:84:TRP:HA	1:K:84:TRP:HE3	1.81	0.45
2:L:20:ARG:HE	2:L:319:GLN:HE22	1.63	0.45
2:L:108:HIS:HB2	2:L:116:VAL:HG21	1.99	0.45
2:L:256:ASN:HD21	2:L:297:THR:CG2	2.29	0.45
1:M:211:ALA:HB1	1:M:226:ASN:HA	1.98	0.45
2:N:272:SER:O	2:N:291:THR:HA	2.17	0.45
2:N:284:ARG:O	2:N:285:CYS:C	2.60	0.45
1:S:104:GLY:O	1:S:107:LYS:HG3	2.17	0.45
1:S:327:LEU:O	1:S:328:VAL:C	2.59	0.45
2:T:18:CYS:SG	2:T:319:GLN:OE1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:218:LEU:HD23	2:T:218:LEU:HA	1.77	0.45
2:P:117:LEU:HD23	2:P:117:LEU:C	2.42	0.45
1:Q:55:ALA:O	1:Q:57:VAL:HG23	2.17	0.45
1:Q:168:VAL:HB	1:Q:245:ASN:O	2.15	0.45
2:B:158:VAL:HG13	2:B:167:ILE:CD1	2.46	0.45
2:B:209:GLY:C	2:B:211:ALA:N	2.71	0.45
2:B:276:GLU:O	2:B:278:LEU:HG	2.17	0.45
1:C:307:VAL:HG12	1:C:308:VAL:N	2.31	0.45
2:H:25:LEU:HD21	2:H:326:ASP:CA	2.39	0.45
2:H:202:ASN:ND2	2:F:281:ILE:H	2.14	0.45
2:H:271:LEU:HG	2:H:272:SER:H	1.80	0.45
2:H:280:SER:O	2:H:282:ASP:N	2.49	0.45
2:H:317:TYR:O	2:H:320:ARG:HB2	2.17	0.45
1:E:11:ILE:HG23	1:E:12:GLY:N	2.30	0.45
1:E:104:GLY:O	1:E:107:LYS:HG3	2.17	0.45
1:E:327:LEU:O	1:E:328:VAL:C	2.59	0.45
1:I:204:VAL:HA	1:K:279:VAL:HG12	1.97	0.45
1:I:239:VAL:CG2	1:I:308:VAL:HG13	2.46	0.45
2:J:16:LEU:O	2:J:16:LEU:HD23	2.15	0.45
2:J:117:LEU:HD23	2:J:117:LEU:C	2.42	0.45
1:K:62:GLU:C	1:K:63:THR:OG1	2.60	0.45
2:N:317:TYR:O	2:N:320:ARG:HB2	2.16	0.45
1:O:283:PHE:CZ	1:O:310:TRP:CD1	3.04	0.45
2:P:272:SER:O	2:P:291:THR:HA	2.17	0.45
1:A:209:GLY:C	1:A:211:ALA:N	2.74	0.45
1:C:187:ALA:O	1:C:196:ALA:HB1	2.17	0.45
1:C:198:ALA:CB	1:C:201:LEU:HG	2.46	0.45
1:C:289:SER:OG	1:C:320:ARG:HD2	2.17	0.45
2:D:138:THR:C	2:D:140:ALA:N	2.74	0.45
1:G:10:ARG:O	1:G:14:ASN:HB2	2.17	0.45
1:G:228:ILE:CD1	1:G:228:ILE:N	2.77	0.45
1:E:62:GLU:C	1:E:63:THR:OG1	2.60	0.45
1:E:271:LEU:HG	1:E:272:ASP:H	1.81	0.45
1:E:289:SER:OG	1:E:320:ARG:HD2	2.17	0.45
1:I:10:ARG:O	1:I:14:ASN:HB2	2.17	0.45
1:I:211:ALA:HB1	1:I:226:ASN:HA	1.98	0.45
2:J:16:LEU:O	2:J:18(A):TRP:HB3	2.17	0.45
2:J:284:ARG:O	2:J:285:CYS:C	2.60	0.45
2:L:322:VAL:O	2:L:326:ASP:HB2	2.17	0.45
1:M:133:ASN:C	1:M:133:ASN:ND2	2.70	0.45
1:M:291:THR:O	1:M:310:TRP:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:60:ILE:HG22	1:S:60(A):ASP:N	2.31	0.45
2:T:10:ARG:NH1	2:T:47:ASP:OD1	2.43	0.45
2:T:28:VAL:C	2:T:71:ILE:HG23	2.42	0.45
1:O:202:ASN:OD1	1:Q:281:VAL:HB	2.17	0.45
2:P:138:THR:C	2:P:140:ALA:N	2.75	0.45
2:P:233:PRO:HB2	2:R:233:PRO:HB2	1.99	0.45
1:Q:14:ASN:HB3	1:Q:318:SER:OG	2.15	0.45
1:Q:62:GLU:C	1:Q:63:THR:OG1	2.60	0.45
1:Q:198:ALA:CB	1:Q:201:LEU:HG	2.46	0.45
2:R:129:VAL:O	2:R:130:VAL:C	2.59	0.45
1:A:10:ARG:O	1:A:14:ASN:HB2	2.17	0.45
1:A:209:GLY:O	1:A:210:ALA:C	2.60	0.45
2:B:210:ALA:HA	2:B:213:ALA:HB3	1.98	0.45
2:B:233:PRO:HB2	2:D:233:PRO:HB2	1.99	0.45
1:C:209:GLY:O	1:C:210:ALA:C	2.60	0.45
1:C:211:ALA:HB1	1:C:226:ASN:HA	1.98	0.45
1:C:271:LEU:HG	1:C:272:ASP:H	1.82	0.45
2:H:210:ALA:HA	2:H:213:ALA:HB3	1.98	0.45
2:H:233:PRO:HB2	2:F:233:PRO:HB2	1.99	0.45
1:E:55:ALA:O	1:E:57:VAL:HG23	2.17	0.45
1:I:228:ILE:CD1	1:I:228:ILE:N	2.76	0.45
1:K:198:ALA:CB	1:K:201:LEU:HG	2.47	0.45
2:L:129:VAL:O	2:L:130:VAL:C	2.59	0.45
1:M:125:ILE:HA	1:M:126:PRO:HD3	1.65	0.45
1:M:183:ARG:HG2	1:M:187:ALA:HB3	1.97	0.45
1:O:289:SER:OG	1:O:320:ARG:HD2	2.17	0.45
2:P:16:LEU:O	2:P:18(A):TRP:HB3	2.17	0.45
1:Q:205:PRO:HA	1:Q:230:LEU:HD23	1.99	0.45
2:R:134:GLU:OE1	2:R:134:GLU:N	2.38	0.45
1:A:23:SER:HA	1:A:24:PRO:HD3	1.82	0.45
2:B:280:SER:O	2:B:282:ASP:N	2.49	0.45
1:C:9:GLY:O	1:C:11:ILE:N	2.49	0.45
1:C:215:SER:HB3	1:C:222:LYS:HA	1.98	0.45
1:C:239:VAL:HG23	1:C:309:ALA:O	2.17	0.45
2:D:209:GLY:O	2:D:210:ALA:C	2.60	0.45
1:G:248(A):VAL:HG13	1:G:249:GLY:N	2.18	0.45
2:H:161:LEU:HD13	2:H:244:VAL:HG21	1.97	0.45
2:H:169:LYS:HE3	2:F:303:ASP:OD1	2.16	0.45
1:E:135:LYS:C	1:E:137:TYR:N	2.75	0.45
1:E:135:LYS:O	1:E:137:TYR:N	2.50	0.45
1:E:211:ALA:HB1	1:E:226:ASN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:VAL:HG22	1:E:309:ALA:HB3	1.98	0.45
2:F:98:VAL:HG23	2:F:99:PHE:N	2.31	0.45
1:I:129:VAL:CG2	1:I:217:VAL:HG11	2.45	0.45
1:I:239:VAL:HB	1:I:310:TRP:CZ3	2.52	0.45
1:I:248(A):VAL:CG1	1:I:249:GLY:H	2.13	0.45
2:J:139:HIS:CE1	2:J:332:TRP:CE3	3.04	0.45
2:J:165:PHE:O	2:J:246:VAL:HB	2.17	0.45
2:J:210:ALA:HA	2:J:213:ALA:HB3	1.98	0.45
1:K:9:GLY:O	1:K:11:ILE:N	2.49	0.45
1:K:265:GLY:HA3	1:K:266:PRO:HD3	1.84	0.45
1:M:82:LEU:HA	1:M:83:PRO:HD3	1.69	0.45
1:M:202:ASN:OD1	1:S:281:VAL:HB	2.17	0.45
1:M:239:VAL:HB	1:M:310:TRP:CZ3	2.52	0.45
1:S:190:HIS:CE1	1:S:195:ARG:HD2	2.52	0.45
1:O:76:ASN:ND2	1:O:81:LYS:HD2	2.32	0.45
2:P:158:VAL:HG13	2:P:167:ILE:CD1	2.46	0.45
1:Q:110:GLN:O	1:S:110:GLN:OE1	2.34	0.45
1:Q:124:ASP:O	1:Q:125:ILE:HB	2.17	0.45
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	1.99	0.45
1:C:55:ALA:O	1:C:57:VAL:HG23	2.17	0.45
2:D:129:VAL:O	2:D:130:VAL:C	2.59	0.45
1:G:209:GLY:O	1:G:210:ALA:C	2.60	0.45
2:H:25:LEU:CD2	2:H:326:ASP:HA	2.40	0.45
2:H:117:LEU:HD23	2:H:117:LEU:C	2.42	0.45
2:H:174:THR:HG23	2:H:229:ALA:CB	2.47	0.45
2:H:193:LEU:H	2:H:193:LEU:CD1	2.06	0.45
1:E:9:GLY:O	1:E:11:ILE:N	2.49	0.45
1:E:60:ILE:HG22	1:E:60(A):ASP:N	2.31	0.45
2:F:322:VAL:O	2:F:326:ASP:HB2	2.17	0.45
1:I:110:GLN:CG	1:M:110:GLN:HB3	2.47	0.45
1:K:190:HIS:CE1	1:K:195:ARG:HD2	2.52	0.45
1:S:41:THR:O	1:S:42:HIS:C	2.58	0.45
2:T:161:LEU:HD13	2:T:244:VAL:HG21	1.98	0.45
2:P:1:LEU:HD22	2:P:329:ALA:HA	1.98	0.45
2:P:317:TYR:O	2:P:320:ARG:HB2	2.16	0.45
1:Q:9:GLY:O	1:Q:11:ILE:N	2.49	0.45
1:Q:154:LEU:HA	1:Q:154:LEU:HD12	1.79	0.45
1:Q:165:LEU:CG	1:Q:246:ILE:HG12	2.43	0.45
1:Q:239:VAL:HG23	1:Q:309:ALA:O	2.17	0.45
1:A:202:ASN:OD1	1:C:281:VAL:HB	2.17	0.45
2:B:117:LEU:HD23	2:B:117:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:ASN:ND2	2:H:314:GLU:HB3	2.32	0.45
1:E:205:PRO:HA	1:E:230:LEU:HD23	1.99	0.45
2:F:28:VAL:C	2:F:71:ILE:HG23	2.41	0.45
2:J:20:ARG:HE	2:J:319:GLN:HE22	1.63	0.45
1:K:51:GLY:O	1:K:52:THR:C	2.60	0.45
1:K:104:GLY:O	1:K:107:LYS:HG3	2.17	0.45
1:K:239:VAL:HG23	1:K:309:ALA:O	2.17	0.45
1:M:204:VAL:HA	1:S:279:VAL:HG12	1.97	0.45
2:N:1:LEU:HD22	2:N:329:ALA:HA	1.98	0.45
2:N:85:GLY:CA	2:N:112:GLY:HA3	2.47	0.45
2:N:276:GLU:O	2:N:278:LEU:HG	2.17	0.45
1:S:186:ASP:HA	1:S:196:ALA:O	2.17	0.45
1:S:307:VAL:HG12	1:S:308:VAL:N	2.30	0.45
2:T:322:VAL:O	2:T:326:ASP:HB2	2.17	0.45
1:O:211:ALA:HB1	1:O:226:ASN:HA	1.98	0.45
1:O:293:ASP:CG	1:O:296:LEU:HD12	2.41	0.45
2:P:276:GLU:O	2:P:278:LEU:HG	2.17	0.45
1:Q:135:LYS:O	1:Q:137:TYR:N	2.50	0.45
2:B:1:LEU:HD22	2:B:329:ALA:HA	1.98	0.45
2:B:165:PHE:O	2:B:246:VAL:HB	2.17	0.45
2:B:202:ASN:ND2	2:D:281:ILE:H	2.13	0.45
1:C:62:GLU:C	1:C:63:THR:OG1	2.60	0.45
2:D:138:THR:C	2:D:140:ALA:H	2.23	0.45
2:D:322:VAL:O	2:D:326:ASP:HB2	2.17	0.45
2:H:79:PRO:O	2:H:80:VAL:C	2.59	0.45
2:H:139:HIS:CE1	2:H:332:TRP:CE3	3.04	0.45
1:E:215:SER:HB3	1:E:222:LYS:HA	1.98	0.45
1:E:283:PHE:CE2	1:E:310:TRP:CD1	3.05	0.45
2:F:129:VAL:O	2:F:130:VAL:C	2.59	0.45
1:K:135:LYS:C	1:K:137:TYR:N	2.75	0.45
1:K:271:LEU:HG	1:K:272:ASP:H	1.81	0.45
2:L:209:GLY:O	2:L:210:ALA:C	2.60	0.45
1:M:10:ARG:O	1:M:14:ASN:HB2	2.17	0.45
1:S:55:ALA:O	1:S:57:VAL:HG23	2.17	0.45
1:S:283:PHE:CE2	1:S:310:TRP:CD1	3.05	0.45
1:O:276:ILE:O	1:O:278:LEU:HG	2.18	0.44
2:P:236:ASN:O	2:P:237:VAL:HB	2.17	0.44
1:Q:51:GLY:O	1:Q:52:THR:C	2.60	0.44
1:Q:60:ILE:HG22	1:Q:60(A):ASP:N	2.31	0.44
1:Q:209:GLY:C	1:Q:211:ALA:N	2.74	0.44
2:R:20:ARG:HE	2:R:319:GLN:HE22	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:129:VAL:H	2:R:133:ASN:HD21	1.65	0.44
2:B:25:LEU:HD21	2:B:326:ASP:CA	2.39	0.44
2:B:106:GLY:O	2:B:109:LEU:N	2.49	0.44
1:G:76:ASN:ND2	1:G:81:LYS:HD2	2.32	0.44
2:H:284:ARG:O	2:H:285:CYS:C	2.60	0.44
2:H:328:VAL:O	2:H:332:TRP:HB2	2.17	0.44
1:E:82:LEU:HA	1:E:83:PRO:HD3	1.72	0.44
1:E:265:GLY:HA3	1:E:266:PRO:HD3	1.84	0.44
2:F:108:HIS:HB2	2:F:116:VAL:HG21	1.99	0.44
2:F:161:LEU:HD13	2:F:244:VAL:HG21	1.98	0.44
1:I:20:ARG:HH21	1:I:319:GLN:NE2	2.15	0.44
1:I:293:ASP:CG	1:I:296:LEU:HD12	2.42	0.44
1:I:327:LEU:O	1:I:330:ASN:N	2.48	0.44
2:J:129:VAL:H	2:J:133:ASN:HD21	1.63	0.44
1:K:55:ALA:O	1:K:57:VAL:HG23	2.16	0.44
1:K:205:PRO:HA	1:K:230:LEU:HD23	1.99	0.44
1:K:240:VAL:HG22	1:K:309:ALA:HB3	1.98	0.44
1:K:254:ASP:O	1:K:255:VAL:C	2.60	0.44
1:K:327:LEU:O	1:K:328:VAL:C	2.59	0.44
1:M:209:GLY:O	1:M:210:ALA:C	2.60	0.44
1:M:289:SER:OG	1:M:320:ARG:HD2	2.17	0.44
1:S:90:ASP:HA	1:S:114:LYS:HG2	1.99	0.44
1:S:271:LEU:HG	1:S:272:ASP:H	1.82	0.44
2:T:20:ARG:HE	2:T:319:GLN:HE22	1.62	0.44
1:O:215:SER:HB3	1:O:222:LYS:HA	1.99	0.44
1:Q:186:ASP:HA	1:Q:196:ALA:O	2.17	0.44
1:Q:228:ILE:HD13	1:Q:228:ILE:N	2.18	0.44
1:Q:240:VAL:HG22	1:Q:309:ALA:HB3	1.98	0.44
1:Q:327:LEU:O	1:Q:328:VAL:C	2.59	0.44
2:R:209:GLY:O	2:R:210:ALA:C	2.60	0.44
1:A:228:ILE:CD1	1:A:228:ILE:N	2.77	0.44
2:B:16:LEU:O	2:B:18(A):TRP:HB3	2.17	0.44
2:B:25:LEU:CD2	2:B:326:ASP:HA	2.40	0.44
2:B:303:ASP:OD1	2:D:169:LYS:HE3	2.16	0.44
1:C:135:LYS:C	1:C:137:TYR:N	2.75	0.44
2:H:106:GLY:O	2:H:109:LEU:N	2.49	0.44
2:H:218:LEU:HD23	2:H:218:LEU:HA	1.75	0.44
2:H:303:ASP:OD1	2:F:169:LYS:HE3	2.17	0.44
1:E:187:ALA:O	1:E:196:ALA:HB1	2.17	0.44
1:I:232:VAL:HA	1:I:233:PRO:HD3	1.87	0.44
2:J:271:LEU:HG	2:J:272:SER:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:ASP:HA	1:K:114:LYS:HG2	1.99	0.44
1:K:135:LYS:O	1:K:137:TYR:N	2.50	0.44
1:M:76:ASN:ND2	1:M:81:LYS:HD2	2.32	0.44
2:N:117:LEU:HD23	2:N:117:LEU:C	2.42	0.44
2:N:233:PRO:HB2	2:T:233:PRO:HB2	1.99	0.44
2:N:236:ASN:O	2:N:237:VAL:HB	2.18	0.44
1:O:236:ASN:O	1:O:237:VAL:CB	2.64	0.44
2:P:14:ASN:ND2	2:P:314:GLU:HB3	2.32	0.44
1:Q:82:LEU:HA	1:Q:83:PRO:HD3	1.72	0.44
1:A:76:ASN:ND2	1:A:81:LYS:HD2	2.32	0.44
1:A:239:VAL:HB	1:A:310:TRP:CZ3	2.52	0.44
1:A:289:SER:OG	1:A:320:ARG:HD2	2.17	0.44
2:B:174:THR:HG23	2:B:229:ALA:CB	2.47	0.44
1:C:165:LEU:CG	1:C:246:ILE:HG12	2.43	0.44
1:C:186:ASP:HA	1:C:196:ALA:O	2.17	0.44
1:C:205:PRO:HA	1:C:230:LEU:HD23	1.99	0.44
2:D:28:VAL:C	2:D:71:ILE:HG23	2.42	0.44
1:E:190:HIS:CE1	1:E:195:ARG:HD2	2.52	0.44
2:F:18:CYS:SG	2:F:319:GLN:OE1	2.74	0.44
1:I:125:ILE:HA	1:I:126:PRO:HD3	1.65	0.44
1:I:154:LEU:HD12	1:I:154:LEU:HA	1.84	0.44
1:I:209:GLY:O	1:I:210:ALA:C	2.60	0.44
2:J:138:THR:C	2:J:140:ALA:N	2.75	0.44
2:J:279:VAL:HG23	2:L:202:ASN:ND2	2.33	0.44
1:K:187:ALA:O	1:K:196:ALA:HB1	2.17	0.44
1:K:289:SER:OG	1:K:320:ARG:HD2	2.17	0.44
1:M:23:SER:HA	1:M:24:PRO:HD3	1.82	0.44
1:M:236:ASN:O	1:M:237:VAL:CB	2.64	0.44
1:S:187:ALA:O	1:S:196:ALA:HB1	2.17	0.44
2:T:229:ALA:C	2:T:230:LEU:HD23	2.42	0.44
1:O:15:PHE:O	1:O:16:LEU:C	2.61	0.44
1:Q:235:PRO:O	1:Q:236:ASN:HB2	2.17	0.44
2:B:139:HIS:CE1	2:B:332:TRP:CE3	3.04	0.44
2:B:306:LYS:HE2	2:D:171:THR:CB	2.48	0.44
1:C:60:ILE:HG22	1:C:60(A):ASP:N	2.31	0.44
1:G:62:GLU:O	1:G:63:THR:OG1	2.35	0.44
2:H:165:PHE:O	2:H:246:VAL:HB	2.17	0.44
2:H:236:ASN:O	2:H:237:VAL:HB	2.17	0.44
2:H:306:LYS:HE2	2:F:171:THR:CB	2.48	0.44
1:E:186:ASP:HA	1:E:196:ALA:O	2.17	0.44
1:E:239:VAL:HG23	1:E:309:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:LEU:HD12	1:E:243:VAL:H	1.83	0.44
1:I:141:ALA:HA	1:M:103:PRO:HG2	1.99	0.44
2:J:233:PRO:HB2	2:L:233:PRO:HB2	1.99	0.44
1:K:192:ASP:C	1:K:194:ARG:N	2.76	0.44
2:L:197:ARG:O	2:L:199:ALA:N	2.51	0.44
1:M:293:ASP:CG	1:M:296:LEU:HD12	2.41	0.44
2:N:303:ASP:OD1	2:T:169:LYS:HE3	2.17	0.44
2:N:328:VAL:O	2:N:332:TRP:HB2	2.17	0.44
1:S:239:VAL:HG23	1:S:309:ALA:O	2.17	0.44
2:T:176:HIS:HA	2:T:238:SER:HB3	2.00	0.44
2:P:165:PHE:O	2:P:246:VAL:HB	2.17	0.44
2:P:279:VAL:HG23	2:R:202:ASN:ND2	2.33	0.44
2:P:306:LYS:HE2	2:R:171:THR:CB	2.48	0.44
2:B:14:ASN:ND2	2:B:314:GLU:HB3	2.32	0.44
1:C:192:ASP:C	1:C:194:ARG:N	2.76	0.44
1:C:242:LEU:HD12	1:C:243:VAL:H	1.82	0.44
2:D:98:VAL:HG23	2:D:99:PHE:N	2.31	0.44
1:G:202:ASN:OD1	1:E:281:VAL:HB	2.17	0.44
1:G:215:SER:HB3	1:G:222:LYS:HA	1.99	0.44
1:E:165:LEU:CG	1:E:246:ILE:HG12	2.43	0.44
1:I:82:LEU:HA	1:I:83:PRO:HD3	1.68	0.44
2:J:174:THR:HG23	2:J:229:ALA:CB	2.47	0.44
2:J:228:ILE:HD12	2:L:296:LEU:HD22	1.99	0.44
2:N:228:ILE:HD12	2:T:296:LEU:HD22	1.99	0.44
2:N:306:LYS:HE2	2:T:171:THR:CB	2.48	0.44
1:S:3:VAL:HG21	1:S:25:LEU:HD12	2.00	0.44
1:S:51:GLY:O	1:S:52:THR:C	2.60	0.44
1:S:240:VAL:HG22	1:S:309:ALA:HB3	1.98	0.44
2:T:197:ARG:O	2:T:199:ALA:N	2.51	0.44
2:T:209:GLY:O	2:T:210:ALA:C	2.60	0.44
1:O:10:ARG:O	1:O:14:ASN:HB2	2.17	0.44
2:P:256:ASN:HD21	2:P:297:THR:HG21	1.83	0.44
1:Q:166:GLY:O	1:Q:246:ILE:HD12	2.18	0.44
1:Q:215:SER:HB3	1:Q:222:LYS:HA	1.98	0.44
1:A:215:SER:HB3	1:A:222:LYS:HA	1.99	0.44
2:B:279:VAL:HG23	2:D:202:ASN:ND2	2.33	0.44
2:B:284:ARG:O	2:B:285:CYS:C	2.60	0.44
1:C:74:VAL:CG1	1:C:75:SER:N	2.80	0.44
1:C:283:PHE:CE2	1:C:310:TRP:CD1	3.05	0.44
2:D:108:HIS:HB2	2:D:116:VAL:HG21	1.99	0.44
1:G:20:ARG:HH21	1:G:319:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.98	0.44
1:G:289:SER:OG	1:G:320:ARG:HD2	2.17	0.44
2:H:1:LEU:HD22	2:H:329:ALA:HA	1.98	0.44
2:J:1:LEU:HD22	2:J:329:ALA:HA	1.98	0.44
2:J:14:ASN:ND2	2:J:314:GLU:HB3	2.32	0.44
2:J:328:VAL:O	2:J:332:TRP:HB2	2.17	0.44
1:K:283:PHE:CE2	1:K:310:TRP:CD1	3.05	0.44
1:K:327:LEU:O	1:K:330:ASN:N	2.48	0.44
2:N:16:LEU:O	2:N:18(A):TRP:HB3	2.17	0.44
1:S:135:LYS:O	1:S:137:TYR:N	2.50	0.44
1:S:242:LEU:HD12	1:S:243:VAL:H	1.83	0.44
1:O:37:VAL:HG11	1:O:59:ILE:HG23	2.00	0.44
1:O:161:LEU:HB2	1:O:167:ILE:HD11	2.00	0.44
2:P:15:PHE:CE1	2:P:321:VAL:HG12	2.53	0.44
1:Q:168:VAL:O	1:Q:169:LYS:HB3	2.18	0.44
1:Q:211:ALA:O	1:Q:214:VAL:HG23	2.18	0.44
1:Q:289:SER:OG	1:Q:320:ARG:HD2	2.17	0.44
2:R:322:VAL:O	2:R:326:ASP:HB2	2.17	0.44
1:A:161:LEU:HB2	1:A:167:ILE:HD11	2.00	0.44
2:B:328:VAL:O	2:B:332:TRP:HB2	2.17	0.44
1:C:135:LYS:O	1:C:137:TYR:N	2.50	0.44
1:C:209:GLY:C	1:C:211:ALA:N	2.74	0.44
1:C:254:ASP:O	1:C:255:VAL:C	2.60	0.44
1:G:161:LEU:HB2	1:G:167:ILE:HD11	2.00	0.44
1:E:51:GLY:O	1:E:52:THR:C	2.60	0.44
2:F:236:ASN:O	2:F:237:VAL:HB	2.18	0.44
2:J:306:LYS:HE2	2:L:171:THR:CB	2.48	0.44
1:K:186:ASP:HA	1:K:196:ALA:O	2.17	0.44
1:K:235:PRO:O	1:K:236:ASN:HB2	2.17	0.44
2:L:273:VAL:HG12	2:L:274:CYS:N	2.33	0.44
2:N:298:MET:HE1	2:T:226:ASN:CG	2.43	0.44
1:S:211:ALA:O	1:S:214:VAL:HG23	2.18	0.44
1:O:125:ILE:CG2	1:O:143:ILE:HG22	2.48	0.44
1:O:239:VAL:HB	1:O:310:TRP:CZ3	2.52	0.44
2:P:79:PRO:O	2:P:80:VAL:C	2.59	0.44
2:P:174:THR:HG23	2:P:229:ALA:CB	2.48	0.44
2:P:197:ARG:NH1	2:R:282:ASP:OD2	2.51	0.44
1:Q:90:ASP:HA	1:Q:114:LYS:HG2	1.99	0.44
1:Q:104:GLY:O	1:Q:107:LYS:HG3	2.17	0.44
2:R:108:HIS:HB2	2:R:116:VAL:HG21	1.99	0.44
2:R:197:ARG:O	2:R:199:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLY:HA3	1:C:266:PRO:HD3	1.84	0.44
2:D:154:LEU:HD21	2:D:172:MET:HG2	2.00	0.44
2:H:15:PHE:CE1	2:H:321:VAL:HG12	2.53	0.44
1:E:162:ASP:CA	1:E:167:ILE:HG13	2.48	0.44
1:E:209:GLY:O	1:E:210:ALA:C	2.60	0.44
1:E:254:ASP:O	1:E:255:VAL:C	2.61	0.44
1:I:76:ASN:ND2	1:I:81:LYS:HD2	2.32	0.44
2:J:242:LEU:HD12	2:J:243:VAL:N	2.30	0.44
2:J:298:MET:HE1	2:L:226:ASN:CG	2.43	0.44
1:K:168:VAL:O	1:K:169:LYS:HB3	2.18	0.44
1:K:242:LEU:HD12	1:K:243:VAL:H	1.83	0.44
2:N:14:ASN:ND2	2:N:314:GLU:HB3	2.32	0.44
2:N:20:ARG:HE	2:N:319:GLN:HE22	1.63	0.44
2:N:139:HIS:CE1	2:N:332:TRP:CE3	3.04	0.44
1:S:90:ASP:HA	1:S:114:LYS:CG	2.48	0.44
1:S:289:SER:OG	1:S:320:ARG:HD2	2.17	0.44
2:T:273:VAL:HG12	2:T:274:CYS:N	2.33	0.44
1:O:149:CYS:HB3	3:O:401:NAD:H5N	2.00	0.44
2:P:172:MET:HE2	2:P:173:THR:N	2.33	0.44
2:P:284:ARG:O	2:P:285:CYS:C	2.60	0.44
2:P:298:MET:HE1	2:R:226:ASN:CG	2.43	0.44
1:Q:209:GLY:O	1:Q:210:ALA:C	2.60	0.44
1:C:235:PRO:O	1:C:236:ASN:HB2	2.17	0.44
2:D:236:ASN:O	2:D:237:VAL:HB	2.18	0.44
1:G:37:VAL:HG11	1:G:59:ILE:HG23	2.00	0.44
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.83	0.44
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.44	0.44
1:G:168:VAL:O	1:G:169:LYS:HB3	2.18	0.44
2:H:138:THR:C	2:H:140:ALA:N	2.75	0.44
1:E:90:ASP:HA	1:E:114:LYS:CG	2.48	0.44
1:E:168:VAL:O	1:E:169:LYS:HB3	2.18	0.44
1:I:84:TRP:HA	1:I:84:TRP:HE3	1.83	0.44
1:I:135:LYS:C	1:I:137:TYR:N	2.74	0.44
2:J:79:PRO:O	2:J:80:VAL:C	2.59	0.44
1:K:155:ALA:HB3	1:K:156:PRO:CD	2.42	0.44
2:L:154:LEU:HD21	2:L:172:MET:HG2	2.00	0.44
2:L:229:ALA:C	2:L:230:LEU:HD23	2.42	0.44
1:M:155:ALA:HB3	1:M:156:PRO:CD	2.43	0.44
2:N:165:PHE:O	2:N:246:VAL:HB	2.17	0.44
2:N:197:ARG:NH1	2:T:282:ASP:OD2	2.51	0.44
2:N:279:VAL:HG23	2:T:202:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:162:ASP:CA	1:S:167:ILE:HG13	2.48	0.44
1:S:192:ASP:C	1:S:194:ARG:N	2.76	0.44
1:S:209:GLY:O	1:S:210:ALA:C	2.60	0.44
1:S:235:PRO:O	1:S:236:ASN:HB2	2.17	0.44
1:O:62:GLU:C	1:O:63:THR:OG1	2.61	0.43
1:O:265:GLY:HA3	1:O:266:PRO:HD3	1.84	0.43
2:P:108:HIS:HB2	2:P:116:VAL:HG21	2.00	0.43
2:P:110:GLN:C	2:P:112:GLY:H	2.26	0.43
2:P:328:VAL:O	2:P:332:TRP:HB2	2.17	0.43
1:Q:162:ASP:CA	1:Q:167:ILE:HG13	2.48	0.43
2:R:236:ASN:O	2:R:237:VAL:HB	2.18	0.43
1:A:14:ASN:HB3	1:A:318:SER:OG	2.18	0.43
1:A:84:TRP:HA	1:A:84:TRP:HE3	1.83	0.43
1:C:168:VAL:O	1:C:169:LYS:HB3	2.18	0.43
2:D:18:CYS:SG	2:D:319:GLN:OE1	2.74	0.43
2:D:161:LEU:HD13	2:D:244:VAL:HG21	1.98	0.43
2:D:229:ALA:C	2:D:230:LEU:HD23	2.42	0.43
1:G:14:ASN:HB3	1:G:318:SER:OG	2.18	0.43
1:G:149:CYS:HB3	3:G:401:NAD:H5N	2.00	0.43
1:G:236:ASN:O	1:G:237:VAL:CB	2.64	0.43
2:H:279:VAL:HG23	2:F:202:ASN:ND2	2.33	0.43
1:E:90:ASP:HA	1:E:114:LYS:HG2	1.99	0.43
1:E:291:THR:O	1:E:310:TRP:N	2.39	0.43
2:F:197:ARG:O	2:F:199:ALA:N	2.51	0.43
2:F:273:VAL:HG12	2:F:274:CYS:N	2.33	0.43
1:I:15:PHE:O	1:I:16:LEU:C	2.61	0.43
2:J:15:PHE:CE1	2:J:321:VAL:HG12	2.53	0.43
2:J:202:ASN:ND2	2:L:281:ILE:H	2.14	0.43
2:J:256:ASN:HD21	2:J:297:THR:HG21	1.83	0.43
1:K:3:VAL:HG21	1:K:25:LEU:HD12	2.00	0.43
2:L:236:ASN:O	2:L:237:VAL:HB	2.18	0.43
1:M:149:CYS:HB3	3:M:401:NAD:H5N	2.00	0.43
2:N:15:PHE:CE1	2:N:321:VAL:HG12	2.53	0.43
2:T:154:LEU:HD21	2:T:172:MET:HG2	2.00	0.43
1:O:185:LEU:HD23	1:O:185:LEU:HA	1.85	0.43
2:P:228:ILE:HD12	2:R:296:LEU:HD22	1.99	0.43
1:Q:283:PHE:CE2	1:Q:310:TRP:CD1	3.05	0.43
2:R:18:CYS:SG	2:R:319:GLN:OE1	2.74	0.43
1:A:168:VAL:O	1:A:169:LYS:HB3	2.18	0.43
1:A:276:ILE:O	1:A:278:LEU:HG	2.18	0.43
1:C:3:VAL:HG21	1:C:25:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:HIS:CE1	1:C:195:ARG:HD2	2.52	0.43
1:C:257:ASN:HA	1:C:260:ARG:HD2	2.00	0.43
1:C:279:VAL:O	1:C:280:SER:C	2.61	0.43
1:G:62:GLU:C	1:G:63:THR:OG1	2.61	0.43
2:H:256:ASN:HD21	2:H:297:THR:HG21	1.83	0.43
1:E:3:VAL:HG21	1:E:25:LEU:HD12	2.00	0.43
2:F:138:THR:C	2:F:140:ALA:N	2.75	0.43
2:F:229:ALA:C	2:F:230:LEU:HD23	2.43	0.43
1:I:149:CYS:HB3	3:I:401:NAD:H5N	2.00	0.43
1:I:161:LEU:HB2	1:I:167:ILE:HD11	2.00	0.43
1:I:289:SER:OG	1:I:320:ARG:HD2	2.17	0.43
2:J:236:ASN:O	2:J:237:VAL:HB	2.18	0.43
1:K:209:GLY:O	1:K:210:ALA:C	2.60	0.43
2:L:176:HIS:HA	2:L:238:SER:HB3	2.00	0.43
1:M:232:VAL:HA	1:M:233:PRO:HD3	1.87	0.43
1:S:135:LYS:C	1:S:137:TYR:N	2.75	0.43
1:S:154:LEU:HD12	1:S:154:LEU:HA	1.79	0.43
1:S:168:VAL:O	1:S:169:LYS:HB3	2.18	0.43
1:S:205:PRO:HA	1:S:230:LEU:HD23	1.99	0.43
1:S:257:ASN:HA	1:S:260:ARG:HD2	2.00	0.43
2:T:236:ASN:O	2:T:237:VAL:HB	2.18	0.43
1:Q:190:HIS:CE1	1:Q:195:ARG:HD2	2.52	0.43
2:R:192:ASP:C	2:R:194:ARG:H	2.26	0.43
1:A:15:PHE:O	1:A:16:LEU:C	2.61	0.43
1:A:20:ARG:HH21	1:A:319:GLN:NE2	2.15	0.43
2:B:138:THR:C	2:B:140:ALA:N	2.75	0.43
2:B:236:ASN:O	2:B:237:VAL:HB	2.17	0.43
1:C:155:ALA:HB3	1:C:156:PRO:CD	2.42	0.43
1:G:239:VAL:HB	1:G:310:TRP:CZ3	2.52	0.43
2:H:197:ARG:NH1	2:F:282:ASP:OD2	2.51	0.43
2:H:298:MET:HE1	2:F:226:ASN:CG	2.43	0.43
1:E:235:PRO:O	1:E:236:ASN:HB2	2.17	0.43
1:E:279:VAL:O	1:E:280:SER:C	2.61	0.43
1:I:62:GLU:C	1:I:63:THR:OG1	2.61	0.43
2:J:172:MET:HE2	2:J:173:THR:N	2.33	0.43
1:K:162:ASP:CA	1:K:167:ILE:HG13	2.48	0.43
2:L:256:ASN:HD22	2:L:256:ASN:N	2.16	0.43
1:M:20:ARG:HH21	1:M:319:GLN:NE2	2.15	0.43
2:N:110:GLN:C	2:N:112:GLY:H	2.26	0.43
1:S:62:GLU:C	1:S:63:THR:OG1	2.60	0.43
1:S:165:LEU:CG	1:S:246:ILE:HG12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:254:ASP:O	1:S:255:VAL:C	2.60	0.43
1:S:291:THR:O	1:S:310:TRP:N	2.39	0.43
2:T:129:VAL:H	2:T:133:ASN:HD21	1.65	0.43
1:O:251:THR:CG2	1:O:252:ALA:H	2.28	0.43
1:O:327:LEU:O	1:O:328:VAL:C	2.61	0.43
2:P:242:LEU:HD12	2:P:243:VAL:N	2.30	0.43
1:Q:234:THR:O	1:Q:234:THR:HG23	2.19	0.43
2:B:172:MET:HE2	2:B:173:THR:N	2.33	0.43
2:B:192:ASP:C	2:B:194:ARG:H	2.27	0.43
2:B:298:MET:HE1	2:D:226:ASN:CG	2.43	0.43
1:C:90:ASP:HA	1:C:114:LYS:CG	2.48	0.43
1:C:162:ASP:CA	1:C:167:ILE:HG13	2.48	0.43
2:D:153:CYS:SG	2:D:311:TYR:CD1	3.12	0.43
1:G:15:PHE:O	1:G:16:LEU:C	2.61	0.43
1:G:276:ILE:O	1:G:278:LEU:HG	2.17	0.43
1:E:209:GLY:C	1:E:211:ALA:N	2.74	0.43
1:E:211:ALA:O	1:E:214:VAL:HG23	2.18	0.43
1:I:215:SER:HB3	1:I:222:LYS:HA	2.00	0.43
2:N:174:THR:HG23	2:N:229:ALA:CB	2.47	0.43
1:S:166:GLY:O	1:S:246:ILE:HD12	2.18	0.43
1:O:20:ARG:HH21	1:O:319:GLN:NE2	2.15	0.43
1:O:82:LEU:HA	1:O:83:PRO:HD3	1.68	0.43
2:P:221:LEU:HD22	2:P:221:LEU:N	2.34	0.43
1:Q:279:VAL:O	1:Q:280:SER:C	2.61	0.43
2:R:279:VAL:O	2:R:280:SER:C	2.62	0.43
1:A:236:ASN:O	1:A:237:VAL:CB	2.64	0.43
2:B:221:LEU:HD22	2:B:221:LEU:N	2.34	0.43
2:B:256:ASN:HD21	2:B:297:THR:HG21	1.83	0.43
1:C:51:GLY:O	1:C:52:THR:C	2.60	0.43
1:C:159:LYS:O	1:C:160:VAL:C	2.62	0.43
1:C:211:ALA:O	1:C:214:VAL:HG23	2.18	0.43
1:C:234:THR:O	1:C:234:THR:HG23	2.19	0.43
2:D:129:VAL:H	2:D:133:ASN:HD21	1.65	0.43
2:D:221:LEU:HD22	2:D:221:LEU:N	2.33	0.43
2:H:16:LEU:O	2:H:18(A):TRP:HB3	2.17	0.43
1:E:166:GLY:O	1:E:246:ILE:HD12	2.18	0.43
2:F:153:CYS:SG	2:F:311:TYR:CD1	3.12	0.43
2:J:110:GLN:C	2:J:112:GLY:H	2.26	0.43
1:K:211:ALA:HB1	1:K:226:ASN:HA	1.99	0.43
2:L:20:ARG:HH12	2:L:322:VAL:HG12	1.84	0.43
2:L:192:ASP:C	2:L:194:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:221:LEU:HD22	2:L:221:LEU:N	2.33	0.43
1:M:37:VAL:HG11	1:M:59:ILE:HG23	2.00	0.43
1:M:161:LEU:HB2	1:M:167:ILE:HD11	2.00	0.43
2:N:172:MET:HE2	2:N:173:THR:N	2.33	0.43
1:S:161:LEU:HB2	1:S:167:ILE:HD11	2.01	0.43
2:T:81:ASN:O	2:T:82:LEU:C	2.62	0.43
1:O:159:LYS:O	1:O:160:VAL:C	2.62	0.43
1:O:204:VAL:HA	1:O:205:PRO:HD3	1.78	0.43
1:Q:271:LEU:CD1	1:Q:292:ILE:HD11	2.35	0.43
2:R:25:LEU:HD22	2:R:25:LEU:N	2.34	0.43
2:R:182:GLN:HE22	2:R:231:ARG:CB	2.31	0.43
2:R:221:LEU:HD22	2:R:221:LEU:N	2.34	0.43
2:R:239:VAL:HB	2:R:310:TRP:CE3	2.54	0.43
2:R:271:LEU:HG	2:R:272:SER:H	1.84	0.43
1:A:279:VAL:O	1:A:280:SER:C	2.62	0.43
2:B:132:VAL:O	2:B:132:VAL:HG12	2.18	0.43
2:D:197:ARG:O	2:D:199:ALA:N	2.51	0.43
1:G:271:LEU:HG	1:G:272:ASP:N	2.34	0.43
1:E:161:LEU:HB2	1:E:167:ILE:HD11	2.01	0.43
1:I:62:GLU:O	1:I:63:THR:OG1	2.35	0.43
1:I:110:GLN:CB	1:M:110:GLN:OE1	2.67	0.43
1:I:124:ASP:O	1:M:124:ASP:OD2	2.26	0.43
1:I:240:VAL:O	1:I:308:VAL:HA	2.19	0.43
2:J:221:LEU:HD22	2:J:221:LEU:N	2.34	0.43
2:J:289:SER:OG	2:J:320:ARG:HD2	2.19	0.43
1:M:276:ILE:O	1:M:278:LEU:HG	2.18	0.43
1:M:327:LEU:O	1:M:328:VAL:C	2.61	0.43
2:N:132:VAL:O	2:N:132:VAL:HG12	2.19	0.43
2:N:240:VAL:CG1	2:N:309:ALA:HB3	2.49	0.43
2:T:320:ARG:HA	2:T:320:ARG:HE	1.83	0.43
1:O:254:ASP:O	1:O:255:VAL:C	2.62	0.43
2:P:138:THR:O	2:P:140:ALA:N	2.52	0.43
1:Q:135:LYS:C	1:Q:137:TYR:N	2.75	0.43
1:Q:242:LEU:HD12	1:Q:243:VAL:H	1.83	0.43
2:R:153:CYS:SG	2:R:311:TYR:CD1	3.12	0.43
2:R:229:ALA:C	2:R:230:LEU:HD23	2.43	0.43
1:A:37:VAL:HG11	1:A:59:ILE:HG23	2.00	0.43
1:A:62:GLU:C	1:A:63:THR:OG1	2.61	0.43
1:A:149:CYS:HB3	3:A:401:NAD:H5N	2.00	0.43
2:B:228:ILE:HG13	2:B:229:ALA:N	2.34	0.43
2:B:317:TYR:O	2:B:320:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:182:GLN:HE22	2:D:231:ARG:CB	2.31	0.43
3:D:401:NAD:H2N	3:D:401:NAD:H2D	1.71	0.43
1:G:135:LYS:C	1:G:137:TYR:N	2.74	0.43
1:G:248(A):VAL:CG1	1:G:249:GLY:H	2.14	0.43
1:G:254:ASP:O	1:G:255:VAL:C	2.62	0.43
1:G:279:VAL:O	1:G:280:SER:C	2.62	0.43
2:H:110:GLN:C	2:H:112:GLY:H	2.26	0.43
2:H:172:MET:HE2	2:H:173:THR:N	2.33	0.43
2:H:228:ILE:HD12	2:F:296:LEU:HD22	2.00	0.43
2:H:240:VAL:CG1	2:H:309:ALA:HB3	2.49	0.43
1:E:204:VAL:HA	1:E:205:PRO:HD3	1.77	0.43
2:F:239:VAL:HB	2:F:310:TRP:CE3	2.54	0.43
1:I:125:ILE:CG2	1:I:143:ILE:HG22	2.48	0.43
1:I:209:GLY:C	1:I:211:ALA:N	2.74	0.43
1:I:254:ASP:O	1:I:255:VAL:C	2.62	0.43
1:I:276:ILE:O	1:I:278:LEU:HG	2.17	0.43
1:K:166:GLY:O	1:K:246:ILE:HD12	2.18	0.43
1:K:211:ALA:O	1:K:214:VAL:HG23	2.18	0.43
2:L:317:TYR:O	2:L:318:SER:C	2.62	0.43
1:M:168:VAL:O	1:M:169:LYS:HB3	2.18	0.43
1:M:215:SER:HB3	1:M:222:LYS:HA	1.99	0.43
1:M:271:LEU:HG	1:M:272:ASP:N	2.34	0.43
2:N:218:LEU:HD23	2:N:218:LEU:HA	1.75	0.43
2:N:228:ILE:HG13	2:N:229:ALA:N	2.34	0.43
2:N:289:SER:OG	2:N:320:ARG:HD2	2.19	0.43
2:T:221:LEU:HD22	2:T:221:LEU:N	2.33	0.43
1:O:84:TRP:HA	1:O:84:TRP:HE3	1.83	0.43
1:O:155:ALA:HB3	1:O:156:PRO:CD	2.43	0.43
1:O:248:LYS:CG	1:O:248(A):VAL:H	2.32	0.43
2:P:218:LEU:HA	2:P:218:LEU:HD23	1.75	0.43
2:P:240:VAL:CG1	2:P:309:ALA:HB3	2.49	0.43
2:P:289:SER:OG	2:P:320:ARG:HD2	2.19	0.43
1:Q:125:ILE:HG12	1:Q:143:ILE:CG2	2.48	0.43
2:R:139:HIS:CE1	2:R:332:TRP:CE3	3.07	0.43
2:R:273:VAL:HG12	2:R:274:CYS:N	2.33	0.43
2:R:317:TYR:O	2:R:318:SER:C	2.62	0.43
1:A:327:LEU:O	1:A:328:VAL:C	2.61	0.43
2:D:89:ILE:HG21	2:D:92:VAL:HG23	2.01	0.43
2:D:218:LEU:HB3	2:D:221:LEU:CD2	2.49	0.43
2:D:279:VAL:O	2:D:280:SER:C	2.62	0.43
1:G:125:ILE:CG2	1:G:143:ILE:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:VAL:O	1:G:308:VAL:HA	2.19	0.43
2:H:108:HIS:HB2	2:H:116:VAL:HG21	2.00	0.43
2:H:289:SER:OG	2:H:320:ARG:HD2	2.19	0.43
2:F:218:LEU:HB3	2:F:221:LEU:CD2	2.49	0.43
1:I:168:VAL:O	1:I:169:LYS:HB3	2.18	0.43
1:K:161:LEU:HB2	1:K:167:ILE:HD11	2.01	0.43
1:K:248:LYS:CG	1:K:248(A):VAL:N	2.82	0.43
1:K:279:VAL:O	1:K:280:SER:C	2.61	0.43
2:L:25:LEU:HD22	2:L:25:LEU:N	2.34	0.43
2:L:239:VAL:HB	2:L:310:TRP:CE3	2.54	0.43
1:M:62:GLU:C	1:M:63:THR:OG1	2.61	0.43
2:N:81:ASN:O	2:N:82:LEU:C	2.62	0.43
2:N:138:THR:C	2:N:140:ALA:N	2.75	0.43
2:N:221:LEU:N	2:N:221:LEU:HD22	2.34	0.43
1:S:211:ALA:HB1	1:S:226:ASN:HA	1.99	0.43
1:S:234:THR:O	1:S:234:THR:HG23	2.19	0.43
1:S:248:LYS:CG	1:S:248(A):VAL:N	2.82	0.43
2:T:20:ARG:HH12	2:T:322:VAL:HG12	1.84	0.43
1:O:14:ASN:HB3	1:O:318:SER:OG	2.18	0.43
1:O:209:GLY:C	1:O:211:ALA:N	2.74	0.43
2:P:192:ASP:C	2:P:194:ARG:H	2.26	0.43
1:Q:3:VAL:HG21	1:Q:25:LEU:HD12	2.00	0.43
2:R:18:CYS:HG	2:R:319:GLN:CD	2.27	0.43
2:R:89:ILE:HG21	2:R:92:VAL:HG23	2.01	0.43
2:R:154:LEU:HD21	2:R:172:MET:HG2	2.00	0.43
1:A:159:LYS:O	1:A:160:VAL:C	2.62	0.43
1:A:254:ASP:O	1:A:255:VAL:C	2.62	0.43
1:C:161:LEU:HB2	1:C:167:ILE:HD11	2.01	0.43
1:C:166:GLY:O	1:C:246:ILE:HD12	2.18	0.43
2:D:218:LEU:HA	2:D:218:LEU:HD23	1.77	0.43
2:D:239:VAL:HB	2:D:310:TRP:CE3	2.54	0.43
2:H:159:LYS:O	2:H:163:GLN:HB3	2.19	0.43
2:H:221:LEU:HD22	2:H:221:LEU:N	2.34	0.43
1:E:155:ALA:HB3	1:E:156:PRO:CD	2.42	0.43
1:E:257:ASN:HA	1:E:260:ARG:HD2	2.00	0.43
2:F:25:LEU:HD22	2:F:25:LEU:N	2.34	0.43
2:F:129:VAL:H	2:F:133:ASN:HD21	1.65	0.43
1:I:327:LEU:O	1:I:328:VAL:C	2.61	0.43
2:J:108:HIS:HB2	2:J:116:VAL:HG21	2.00	0.43
2:N:45:LYS:NZ	2:N:55:ALA:O	2.50	0.43
2:N:66:VAL:O	2:N:66:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:209:GLY:C	1:S:211:ALA:N	2.74	0.43
2:T:79:PRO:O	2:T:80:VAL:C	2.62	0.43
2:T:239:VAL:HB	2:T:310:TRP:CE3	2.54	0.43
1:Q:198:ALA:HB3	1:Q:201:LEU:HG	2.01	0.43
1:Q:254:ASP:O	1:Q:255:VAL:C	2.60	0.43
1:Q:257:ASN:HA	1:Q:260:ARG:HD2	2.00	0.43
1:A:240:VAL:O	1:A:308:VAL:HA	2.19	0.43
2:B:15:PHE:CE1	2:B:321:VAL:HG12	2.53	0.43
2:B:138:THR:O	2:B:140:ALA:N	2.52	0.43
2:B:289:SER:OG	2:B:320:ARG:HD2	2.19	0.43
1:C:90:ASP:HA	1:C:114:LYS:HG2	1.99	0.43
2:D:317:TYR:O	2:D:318:SER:C	2.62	0.43
2:H:192:ASP:C	2:H:194:ARG:H	2.27	0.43
2:F:139:HIS:CE1	2:F:332:TRP:CE3	3.07	0.43
2:F:192:ASP:C	2:F:194:ARG:H	2.27	0.43
2:F:317:TYR:O	2:F:318:SER:C	2.62	0.43
1:I:279:VAL:O	1:I:280:SER:C	2.62	0.43
2:J:197:ARG:NH1	2:L:282:ASP:OD2	2.51	0.43
1:K:248:LYS:CG	1:K:248(A):VAL:H	2.32	0.43
1:M:254:ASP:O	1:M:255:VAL:C	2.62	0.43
2:N:192:ASP:C	2:N:194:ARG:H	2.27	0.43
1:S:198:ALA:HB3	1:S:201:LEU:HG	2.01	0.43
2:T:23:SER:C	2:T:25:LEU:N	2.76	0.43
2:T:138:THR:C	2:T:140:ALA:N	2.75	0.43
2:T:154:LEU:HD12	2:T:157:PHE:CZ	2.54	0.43
2:T:260:ARG:O	2:T:261:GLU:C	2.62	0.43
1:O:51:GLY:O	1:O:52:THR:C	2.62	0.42
1:Q:90:ASP:HA	1:Q:114:LYS:CG	2.48	0.42
1:Q:124:ASP:C	1:Q:125:ILE:CG1	2.90	0.42
1:Q:161:LEU:HB2	1:Q:167:ILE:HD11	2.01	0.42
2:R:101:ASP:O	2:R:102:ARG:C	2.62	0.42
2:B:101:ASP:O	2:B:102:ARG:C	2.62	0.42
2:D:25:LEU:HD22	2:D:25:LEU:N	2.34	0.42
2:H:204:VAL:HB	2:H:231:ARG:HB2	2.01	0.42
1:E:192:ASP:C	1:E:194:ARG:N	2.76	0.42
1:E:198:ALA:HB3	1:E:201:LEU:HG	2.01	0.42
1:E:248:LYS:CG	1:E:248(A):VAL:H	2.32	0.42
2:F:23:SER:C	2:F:25:LEU:N	2.76	0.42
2:F:154:LEU:HD21	2:F:172:MET:HG2	2.00	0.42
2:F:218:LEU:HD23	2:F:218:LEU:HA	1.77	0.42
2:F:221:LEU:HD22	2:F:221:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ASN:HB3	1:I:318:SER:OG	2.18	0.42
1:I:37:VAL:HG11	1:I:59:ILE:HG23	2.00	0.42
1:K:90:ASP:HA	1:K:114:LYS:CG	2.48	0.42
2:L:3:VAL:HG12	2:L:4:ALA:N	2.34	0.42
2:L:45:LYS:NZ	2:L:55:ALA:O	2.51	0.42
1:M:14:ASN:HB3	1:M:318:SER:OG	2.18	0.42
2:N:242:LEU:HD12	2:N:243:VAL:N	2.30	0.42
2:T:317:TYR:O	2:T:318:SER:C	2.62	0.42
1:O:279:VAL:O	1:O:280:SER:C	2.62	0.42
2:P:81:ASN:O	2:P:82:LEU:C	2.62	0.42
2:P:101:ASP:O	2:P:102:ARG:C	2.62	0.42
2:P:132:VAL:O	2:P:132:VAL:HG12	2.18	0.42
2:R:81:ASN:O	2:R:82:LEU:C	2.62	0.42
2:R:284:ARG:O	2:R:285:CYS:C	2.62	0.42
1:A:108:HIS:HB2	1:A:116:VAL:HG21	2.01	0.42
2:B:45:LYS:NZ	2:B:55:ALA:O	2.51	0.42
2:B:66:VAL:O	2:B:66:VAL:HG12	2.19	0.42
2:B:110:GLN:C	2:B:112:GLY:N	2.77	0.42
2:B:197:ARG:NH1	2:D:282:ASP:OD2	2.51	0.42
2:B:204:VAL:HB	2:B:231:ARG:HB2	2.01	0.42
2:D:192:ASP:C	2:D:194:ARG:H	2.26	0.42
2:D:256:ASN:N	2:D:256:ASN:HD22	2.16	0.42
2:D:273:VAL:HG12	2:D:274:CYS:N	2.33	0.42
2:D:312:ASP:OD1	2:D:315:TRP:N	2.48	0.42
1:G:125:ILE:HA	1:G:126:PRO:HD3	1.65	0.42
1:G:159:LYS:O	1:G:160:VAL:C	2.62	0.42
1:G:248:LYS:CG	1:G:248(A):VAL:H	2.32	0.42
2:F:176:HIS:HA	2:F:238:SER:HB3	2.00	0.42
1:I:74:VAL:CG1	1:I:75:SER:H	2.27	0.42
1:I:133:ASN:C	1:I:133:ASN:ND2	2.70	0.42
1:K:198:ALA:HB3	1:K:201:LEU:HG	2.01	0.42
2:L:101:ASP:O	2:L:102:ARG:C	2.62	0.42
2:L:129:VAL:H	2:L:133:ASN:HD21	1.65	0.42
1:M:84:TRP:HA	1:M:84:TRP:HE3	1.83	0.42
1:M:108:HIS:HB2	1:M:116:VAL:HG21	2.02	0.42
2:N:106:GLY:C	2:N:108:HIS:N	2.77	0.42
2:N:256:ASN:HD21	2:N:297:THR:HG21	1.83	0.42
2:T:284:ARG:O	2:T:285:CYS:C	2.62	0.42
1:O:125:ILE:HA	1:O:126:PRO:HD3	1.65	0.42
1:O:170:GLY:HA2	1:Q:304:MET:SD	2.60	0.42
1:O:215:SER:O	1:O:217:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:202:ASN:ND2	2:R:281:ILE:H	2.14	0.42
2:R:3:VAL:HG12	2:R:4:ALA:N	2.34	0.42
2:R:37:VAL:HG13	2:R:64:ILE:CG2	2.50	0.42
2:R:84:TRP:CE3	2:R:84:TRP:CA	3.03	0.42
2:R:176:HIS:HA	2:R:238:SER:HB3	2.00	0.42
1:A:125:ILE:CG2	1:A:143:ILE:HG22	2.48	0.42
1:C:248(A):VAL:CG1	1:C:249:GLY:H	2.15	0.42
2:D:23:SER:C	2:D:25:LEU:N	2.76	0.42
2:D:37:VAL:HG13	2:D:64:ILE:CG2	2.50	0.42
2:D:271:LEU:HG	2:D:272:SER:H	1.84	0.42
2:D:327:ILE:O	2:D:330:ASN:O	2.37	0.42
2:H:81:ASN:O	2:H:82:LEU:C	2.61	0.42
1:E:248:LYS:CG	1:E:248(A):VAL:N	2.82	0.42
1:E:283:PHE:CZ	1:E:310:TRP:CD1	3.07	0.42
2:F:84:TRP:CE3	2:F:84:TRP:CA	3.02	0.42
2:F:101:ASP:O	2:F:102:ARG:C	2.62	0.42
2:F:279:VAL:O	2:F:280:SER:C	2.62	0.42
2:F:327:ILE:O	2:F:330:ASN:O	2.37	0.42
1:I:108:HIS:HB2	1:I:116:VAL:HG21	2.02	0.42
2:J:25:LEU:HD21	2:J:326:ASP:CA	2.39	0.42
2:J:138:THR:O	2:J:140:ALA:N	2.52	0.42
2:J:193:LEU:HD12	2:J:193:LEU:N	2.12	0.42
2:J:228:ILE:HG13	2:J:229:ALA:N	2.34	0.42
2:J:240:VAL:CG1	2:J:309:ALA:HB3	2.49	0.42
2:L:182:GLN:HE22	2:L:231:ARG:CB	2.31	0.42
2:L:271:LEU:HG	2:L:272:SER:H	1.84	0.42
2:L:320:ARG:HA	2:L:320:ARG:HE	1.83	0.42
2:N:138:THR:O	2:N:140:ALA:N	2.52	0.42
2:T:84:TRP:CE3	2:T:84:TRP:CA	3.03	0.42
2:T:153:CYS:SG	2:T:311:TYR:CD1	3.12	0.42
2:P:3:VAL:HG21	2:P:25:LEU:HD12	2.01	0.42
2:P:228:ILE:HG13	2:P:229:ALA:N	2.34	0.42
1:A:248(A):VAL:HG13	1:A:249:GLY:N	2.19	0.42
1:A:296:LEU:CD2	1:C:228:ILE:HG21	2.50	0.42
2:B:110:GLN:C	2:B:112:GLY:H	2.26	0.42
2:B:159:LYS:O	2:B:163:GLN:HB3	2.19	0.42
2:B:228:ILE:HD12	2:D:296:LEU:HD22	1.99	0.42
2:B:240:VAL:CG1	2:B:309:ALA:HB3	2.49	0.42
1:C:198:ALA:HB3	1:C:201:LEU:HG	2.01	0.42
2:D:3:VAL:HG12	2:D:4:ALA:N	2.34	0.42
2:D:176:HIS:HA	2:D:238:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ARG:O	2:D:261:GLU:C	2.62	0.42
1:G:108:HIS:HB2	1:G:116:VAL:HG21	2.01	0.42
1:G:327:LEU:O	1:G:328:VAL:C	2.61	0.42
2:H:132:VAL:O	2:H:132:VAL:HG12	2.18	0.42
2:H:138:THR:O	2:H:140:ALA:N	2.52	0.42
1:E:219:PRO:HD2	1:E:220:GLN:NE2	2.35	0.42
1:E:234:THR:O	1:E:234:THR:HG23	2.19	0.42
2:F:16:LEU:O	2:F:18(A):TRP:HB3	2.20	0.42
2:F:45:LYS:NZ	2:F:55:ALA:O	2.51	0.42
1:I:159:LYS:O	1:I:160:VAL:C	2.62	0.42
1:K:283:PHE:CZ	1:K:310:TRP:CD1	3.08	0.42
2:L:84:TRP:CE3	2:L:84:TRP:CA	3.02	0.42
2:L:105:ALA:HB2	2:L:118:ILE:HD11	2.02	0.42
2:L:299:VAL:CG1	2:L:300:MET:N	2.83	0.42
1:M:15:PHE:O	1:M:16:LEU:C	2.61	0.42
1:M:125:ILE:CG2	1:M:143:ILE:HG22	2.48	0.42
2:N:108:HIS:HB2	2:N:116:VAL:HG21	2.00	0.42
2:N:159:LYS:O	2:N:163:GLN:HB3	2.19	0.42
1:S:8:PHE:CB	1:S:32:ASP:HB2	2.50	0.42
1:S:18(A):TRP:O	1:S:20:ARG:HB2	2.20	0.42
1:S:170:GLY:CA	1:S:244:VAL:HG12	2.48	0.42
1:S:201:LEU:N	1:S:201:LEU:HD23	2.35	0.42
1:S:219:PRO:HD2	1:S:220:GLN:NE2	2.35	0.42
2:T:192:ASP:CG	2:T:195:ARG:HG3	2.45	0.42
2:T:256:ASN:HD22	2:T:256:ASN:N	2.17	0.42
2:P:320:ARG:HA	2:P:320:ARG:HE	1.84	0.42
1:Q:18(A):TRP:O	1:Q:20:ARG:HB2	2.20	0.42
1:Q:159:LYS:O	1:Q:160:VAL:C	2.62	0.42
2:R:174:THR:HG23	2:R:229:ALA:CB	2.50	0.42
2:R:218:LEU:HB3	2:R:221:LEU:CD2	2.49	0.42
2:R:293:ASP:OD1	2:R:296:LEU:HD12	2.20	0.42
1:A:215:SER:O	1:A:217:VAL:N	2.52	0.42
1:A:248:LYS:CG	1:A:248(A):VAL:H	2.32	0.42
2:B:39:GLN:H	2:B:39:GLN:HG2	1.68	0.42
2:D:174:THR:HG23	2:D:229:ALA:CB	2.50	0.42
1:G:170:GLY:HA2	1:E:304:MET:SD	2.60	0.42
2:H:101:ASP:O	2:H:102:ARG:C	2.62	0.42
2:H:106:GLY:C	2:H:108:HIS:N	2.77	0.42
1:E:232:VAL:HA	1:E:233:PRO:HD3	1.89	0.42
3:F:401:NAD:H2N	3:F:401:NAD:H2D	1.71	0.42
1:I:170:GLY:HA2	1:K:304:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:SER:C	2:L:25:LEU:N	2.76	0.42
2:L:81:ASN:O	2:L:82:LEU:C	2.62	0.42
1:M:90:ASP:HA	1:M:114:LYS:HG2	2.01	0.42
1:M:215:SER:O	1:M:217:VAL:N	2.53	0.42
1:M:279:VAL:O	1:M:280:SER:C	2.62	0.42
2:T:89:ILE:HG21	2:T:92:VAL:HG23	2.01	0.42
2:T:139:HIS:CE1	2:T:332:TRP:CE3	3.07	0.42
2:T:192:ASP:C	2:T:194:ARG:H	2.26	0.42
2:T:218:LEU:HB3	2:T:221:LEU:CD2	2.49	0.42
2:T:242:LEU:HD12	2:T:243:VAL:N	2.32	0.42
2:T:279:VAL:O	2:T:280:SER:C	2.62	0.42
2:T:327:ILE:O	2:T:330:ASN:O	2.37	0.42
1:O:240:VAL:O	1:O:308:VAL:HA	2.19	0.42
1:O:271:LEU:HG	1:O:272:ASP:N	2.34	0.42
2:P:181:ASP:CG	2:P:195:ARG:NH1	2.75	0.42
2:P:204:VAL:HB	2:P:231:ARG:HB2	2.01	0.42
1:A:90:ASP:HA	1:A:114:LYS:HG2	2.01	0.42
1:A:141:ALA:HA	1:G:103:PRO:HG2	2.00	0.42
2:B:108:HIS:HB2	2:B:116:VAL:HG21	2.00	0.42
1:C:283:PHE:CZ	1:C:310:TRP:CD1	3.08	0.42
1:G:296:LEU:CD2	1:E:228:ILE:HG21	2.50	0.42
2:H:29:VAL:HG21	2:H:84:TRP:HZ3	1.85	0.42
2:H:110:GLN:C	2:H:112:GLY:N	2.77	0.42
2:H:228:ILE:HG13	2:H:229:ALA:N	2.34	0.42
2:F:79:PRO:O	2:F:80:VAL:C	2.62	0.42
1:I:172:MET:HE3	1:I:172:MET:C	2.45	0.42
1:I:248:LYS:CG	1:I:248(A):VAL:H	2.32	0.42
1:I:271:LEU:HG	1:I:272:ASP:N	2.34	0.42
2:J:81:ASN:O	2:J:82:LEU:C	2.62	0.42
2:J:84:TRP:CE3	2:J:84:TRP:CA	3.02	0.42
2:L:37:VAL:HG13	2:L:64:ILE:CG2	2.50	0.42
2:L:79:PRO:O	2:L:80:VAL:C	2.62	0.42
2:L:192:ASP:CG	2:L:195:ARG:HG3	2.45	0.42
1:M:251:THR:CG2	1:M:252:ALA:H	2.28	0.42
2:N:84:TRP:CE3	2:N:84:TRP:CA	3.02	0.42
2:T:182:GLN:HE22	2:T:231:ARG:CB	2.31	0.42
1:O:108:HIS:HB2	1:O:116:VAL:HG21	2.01	0.42
1:Q:312:ASP:OD1	1:Q:312:ASP:C	2.63	0.42
2:R:154:LEU:HD12	2:R:157:PHE:CZ	2.54	0.42
2:R:192:ASP:CG	2:R:195:ARG:HG3	2.45	0.42
1:A:3:VAL:HG12	1:A:4:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PRO:HD2	1:C:220:GLN:NE2	2.35	0.42
2:D:15:PHE:CE1	2:D:322:VAL:CG2	3.02	0.42
2:D:39:GLN:H	2:D:39:GLN:HG2	1.68	0.42
2:D:81:ASN:O	2:D:82:LEU:C	2.62	0.42
2:D:154:LEU:HD12	2:D:157:PHE:CZ	2.54	0.42
2:F:37:VAL:HG13	2:F:64:ILE:CG2	2.50	0.42
2:F:110:GLN:C	2:F:112:GLY:H	2.28	0.42
2:F:174:THR:HG23	2:F:229:ALA:CB	2.50	0.42
2:F:322:VAL:O	2:F:326:ASP:N	2.48	0.42
1:I:296:LEU:CD2	1:K:228:ILE:HG21	2.50	0.42
1:K:8:PHE:CB	1:K:32:ASP:HB2	2.50	0.42
1:K:257:ASN:HA	1:K:260:ARG:HD2	2.00	0.42
2:L:154:LEU:HD12	2:L:157:PHE:CZ	2.54	0.42
2:N:129:VAL:O	2:N:130:VAL:C	2.63	0.42
2:N:204:VAL:HB	2:N:231:ARG:HB2	2.01	0.42
2:N:320:ARG:HA	2:N:320:ARG:HE	1.84	0.42
1:S:159:LYS:O	1:S:160:VAL:C	2.62	0.42
1:S:283:PHE:CZ	1:S:310:TRP:CD1	3.08	0.42
2:T:117:LEU:C	2:T:117:LEU:HD23	2.45	0.42
2:T:202:ASN:O	2:T:233:PRO:HD3	2.20	0.42
1:O:228:ILE:CD1	1:O:228:ILE:N	2.76	0.42
1:O:296:LEU:CD2	1:Q:228:ILE:HG21	2.50	0.42
1:Q:102:GLY:CA	1:Q:124:ASP:OD1	2.68	0.42
2:R:16:LEU:O	2:R:18(A):TRP:HB3	2.20	0.42
1:A:62:GLU:O	1:A:63:THR:OG1	2.35	0.42
1:A:170:GLY:HA2	1:C:304:MET:SD	2.60	0.42
1:A:312:ASP:OD1	1:A:312:ASP:C	2.63	0.42
1:C:232:VAL:HA	1:C:233:PRO:HD3	1.89	0.42
2:D:84:TRP:CE3	2:D:84:TRP:CA	3.03	0.42
2:D:202:ASN:O	2:D:233:PRO:HD3	2.20	0.42
2:D:293:ASP:OD1	2:D:296:LEU:HD12	2.20	0.42
1:G:11:ILE:HD12	1:G:11:ILE:HA	1.92	0.42
2:H:209:GLY:O	2:H:210:ALA:C	2.63	0.42
2:F:20:ARG:HH12	2:F:322:VAL:HG12	1.84	0.42
1:I:51:GLY:O	1:I:52:THR:C	2.62	0.42
1:I:90:ASP:HA	1:I:114:LYS:HG2	2.01	0.42
1:I:123(A):SER:C	1:M:124:ASP:CA	2.92	0.42
2:J:23:SER:C	2:J:25:LEU:N	2.77	0.42
2:J:25:LEU:CD2	2:J:326:ASP:HA	2.40	0.42
2:J:132:VAL:O	2:J:132:VAL:HG12	2.19	0.42
2:J:159:LYS:O	2:J:163:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:ASP:OD1	1:K:312:ASP:C	2.63	0.42
2:L:117:LEU:C	2:L:117:LEU:HD23	2.45	0.42
2:L:139:HIS:CE1	2:L:332:TRP:CE3	3.07	0.42
2:N:190:HIS:ND1	2:N:191:ARG:N	2.68	0.42
1:S:8:PHE:HB2	1:S:32:ASP:HB2	2.02	0.42
1:S:234:THR:HA	1:S:235:PRO:HD2	1.90	0.42
2:P:163:GLN:HG2	2:P:163:GLN:O	2.20	0.42
2:P:226:ASN:CG	2:R:298:MET:HE1	2.45	0.42
1:Q:11:ILE:HD11	1:Q:317:TYR:CD2	2.41	0.42
1:Q:84:TRP:CE3	1:Q:84:TRP:CA	3.03	0.42
2:R:256:ASN:N	2:R:256:ASN:HD22	2.17	0.42
1:A:125:ILE:HA	1:A:126:PRO:HD3	1.65	0.42
1:G:215:SER:O	1:G:217:VAL:N	2.53	0.42
1:G:312:ASP:OD1	1:G:312:ASP:C	2.63	0.42
2:H:3:VAL:HG21	2:H:25:LEU:HD12	2.01	0.42
2:H:66:VAL:O	2:H:66:VAL:HG12	2.19	0.42
1:E:18(A):TRP:O	1:E:20:ARG:HB2	2.19	0.42
1:E:157:PHE:CD1	1:E:157:PHE:C	2.98	0.42
2:F:154:LEU:HD12	2:F:157:PHE:CZ	2.54	0.42
2:F:192:ASP:CG	2:F:195:ARG:HG3	2.45	0.42
2:F:256:ASN:N	2:F:256:ASN:HD22	2.17	0.42
2:F:271:LEU:HG	2:F:272:SER:H	1.84	0.42
2:F:284:ARG:O	2:F:285:CYS:C	2.62	0.42
1:I:110:GLN:CD	1:M:110:GLN:C	2.85	0.42
1:I:215:SER:O	1:I:217:VAL:N	2.53	0.42
1:I:312:ASP:OD1	1:I:312:ASP:C	2.63	0.42
2:J:110:GLN:C	2:J:112:GLY:N	2.77	0.42
2:L:110:GLN:C	2:L:112:GLY:H	2.28	0.42
2:L:284:ARG:O	2:L:285:CYS:C	2.62	0.42
1:M:162:ASP:HA	1:M:167:ILE:HG13	2.02	0.42
2:N:101:ASP:O	2:N:102:ARG:C	2.62	0.42
2:T:16:LEU:O	2:T:18(A):TRP:HB3	2.20	0.42
1:O:139:HIS:C	1:O:140:VAL:H	2.28	0.42
1:O:168:VAL:O	1:O:169:LYS:HB3	2.18	0.42
2:P:66:VAL:O	2:P:66:VAL:HG12	2.19	0.42
2:P:256:ASN:N	2:P:256:ASN:HD22	2.18	0.42
1:C:201:LEU:N	1:C:201:LEU:HD23	2.35	0.42
2:D:139:HIS:CE1	2:D:332:TRP:CE3	3.07	0.42
2:D:284:ARG:O	2:D:285:CYS:C	2.62	0.42
1:G:90:ASP:HA	1:G:114:LYS:HG2	2.02	0.42
1:G:172:MET:HE3	1:G:172:MET:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:PHE:O	1:K:16:LEU:C	2.63	0.42
1:M:296:LEU:CD2	1:S:228:ILE:HG21	2.50	0.42
2:N:163:GLN:O	2:N:163:GLN:HG2	2.20	0.42
2:N:182:GLN:HE22	2:N:231:ARG:CB	2.32	0.42
2:N:232:VAL:HG11	2:T:232:VAL:HG21	2.02	0.42
1:S:251:THR:CG2	1:S:252:ALA:H	2.26	0.42
1:O:172:MET:HE3	1:O:172:MET:C	2.45	0.41
2:P:45:LYS:NZ	2:P:55:ALA:O	2.50	0.41
2:P:129:VAL:O	2:P:130:VAL:C	2.63	0.41
1:Q:8:PHE:HB2	1:Q:32:ASP:HB2	2.02	0.41
1:Q:192:ASP:C	1:Q:194:ARG:N	2.76	0.41
2:R:202:ASN:O	2:R:233:PRO:HD3	2.20	0.41
3:R:401:NAD:H2N	3:R:401:NAD:H2D	1.72	0.41
2:H:232:VAL:HA	2:H:233:PRO:HD3	1.90	0.41
1:E:8:PHE:CB	1:E:32:ASP:HB2	2.50	0.41
1:E:74:VAL:CG1	1:E:75:SER:N	2.80	0.41
1:E:84:TRP:CE3	1:E:84:TRP:CA	3.03	0.41
2:F:89:ILE:HG21	2:F:92:VAL:HG23	2.01	0.41
2:F:202:ASN:O	2:F:233:PRO:HD3	2.20	0.41
1:I:198:ALA:HB3	1:I:201:LEU:HG	2.02	0.41
1:I:204:VAL:HA	1:I:205:PRO:HD3	1.78	0.41
1:I:265:GLY:HA3	1:I:266:PRO:HD3	1.84	0.41
1:I:277:PRO:HA	1:K:194:ARG:NH2	2.35	0.41
1:K:84:TRP:CE3	1:K:84:TRP:CA	3.03	0.41
1:K:201:LEU:N	1:K:201:LEU:HD23	2.35	0.41
1:K:219:PRO:HD2	1:K:220:GLN:NE2	2.35	0.41
2:L:327:ILE:O	2:L:330:ASN:O	2.37	0.41
1:M:240:VAL:O	1:M:308:VAL:HA	2.19	0.41
1:M:248:LYS:CG	1:M:248(A):VAL:H	2.32	0.41
2:N:23:SER:C	2:N:25:LEU:N	2.77	0.41
2:N:232:VAL:HA	2:N:233:PRO:HD3	1.90	0.41
1:S:84:TRP:CE3	1:S:84:TRP:CA	3.03	0.41
2:P:29:VAL:HG21	2:P:84:TRP:HZ3	1.85	0.41
2:P:106:GLY:C	2:P:108:HIS:N	2.77	0.41
2:P:190:HIS:ND1	2:P:191:ARG:N	2.68	0.41
1:Q:10:ARG:NH1	1:Q:47:ASP:OD2	2.48	0.41
1:Q:248:LYS:CG	1:Q:248(A):VAL:H	2.32	0.41
1:Q:283:PHE:CZ	1:Q:310:TRP:CD1	3.08	0.41
1:Q:291:THR:O	1:Q:310:TRP:N	2.39	0.41
1:A:232:VAL:HA	1:A:233:PRO:HD3	1.87	0.41
1:A:271:LEU:HG	1:A:272:ASP:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:VAL:HA	2:B:118:ILE:HD13	2.02	0.41
2:B:129:VAL:O	2:B:130:VAL:C	2.63	0.41
2:B:198:ALA:O	2:B:199:ALA:HB3	2.21	0.41
2:B:232:VAL:HA	2:B:233:PRO:HD3	1.90	0.41
1:C:96:THR:OG1	1:C:98:VAL:HG23	2.21	0.41
1:C:248:LYS:CG	1:C:248(A):VAL:H	2.32	0.41
2:D:20:ARG:HH12	2:D:322:VAL:HG12	1.84	0.41
2:D:94:GLU:HA	2:D:94:GLU:OE2	2.21	0.41
1:G:184:LEU:CD1	2:F:184:LEU:HD13	2.49	0.41
1:G:248:LYS:CG	1:G:248(A):VAL:N	2.83	0.41
2:H:84:TRP:CE3	2:H:84:TRP:CA	3.02	0.41
2:H:190:HIS:CB	2:H:196:ALA:HB2	2.43	0.41
1:E:96:THR:OG1	1:E:98:VAL:HG23	2.20	0.41
2:F:81:ASN:O	2:F:82:LEU:C	2.62	0.41
2:F:106:GLY:C	2:F:108:HIS:N	2.78	0.41
2:F:117:LEU:HD23	2:F:117:LEU:C	2.45	0.41
2:F:242:LEU:HD12	2:F:243:VAL:N	2.32	0.41
2:F:260:ARG:O	2:F:261:GLU:C	2.62	0.41
1:I:139:HIS:C	1:I:140:VAL:H	2.28	0.41
2:J:3:VAL:HG21	2:J:25:LEU:HD12	2.01	0.41
1:K:170:GLY:CA	1:K:244:VAL:HG12	2.48	0.41
2:L:279:VAL:O	2:L:280:SER:C	2.62	0.41
1:M:38:LYS:HG3	1:M:39:SER:N	2.27	0.41
1:M:170:GLY:HA2	1:S:304:MET:SD	2.60	0.41
1:M:172:MET:C	1:M:172:MET:HE3	2.45	0.41
1:M:198:ALA:HB3	1:M:201:LEU:HG	2.03	0.41
1:M:248:LYS:CG	1:M:248(A):VAL:N	2.83	0.41
2:N:3:VAL:HG21	2:N:25:LEU:HD12	2.01	0.41
2:N:226:ASN:CG	2:T:298:MET:HE1	2.45	0.41
1:S:157:PHE:CD1	1:S:157:PHE:C	2.98	0.41
1:S:204:VAL:HA	1:S:205:PRO:HD3	1.77	0.41
1:S:228:ILE:HD13	1:S:228:ILE:N	2.17	0.41
2:T:25:LEU:N	2:T:25:LEU:HD22	2.34	0.41
2:T:105:ALA:HB2	2:T:118:ILE:HD11	2.02	0.41
2:T:106:GLY:C	2:T:108:HIS:N	2.78	0.41
2:P:159:LYS:O	2:P:163:GLN:HB3	2.19	0.41
1:Q:124:ASP:HA	1:S:124:ASP:CA	2.40	0.41
1:Q:161:LEU:HD23	1:Q:161:LEU:HA	1.93	0.41
2:R:106:GLY:C	2:R:108:HIS:N	2.78	0.41
2:R:118:ILE:C	2:R:120:ALA:H	2.28	0.41
1:A:291:THR:O	1:A:310:TRP:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:GLN:HG2	2:B:163:GLN:O	2.20	0.41
2:B:209:GLY:O	2:B:210:ALA:C	2.63	0.41
2:B:304:MET:SD	2:D:170:GLY:HA2	2.60	0.41
1:C:248:LYS:CG	1:C:248(A):VAL:N	2.82	0.41
1:C:281:VAL:O	1:C:281:VAL:CG1	2.69	0.41
1:C:312:ASP:C	1:C:312:ASP:OD1	2.63	0.41
2:D:192:ASP:C	2:D:194:ARG:N	2.79	0.41
2:H:163:GLN:HG2	2:H:163:GLN:O	2.20	0.41
2:H:181:ASP:CG	2:H:195:ARG:NH1	2.75	0.41
2:H:232:VAL:HG11	2:F:232:VAL:HG21	2.02	0.41
2:F:105:ALA:HB2	2:F:118:ILE:HD11	2.02	0.41
2:F:333:GLN:H	2:F:333:GLN:HG2	1.71	0.41
1:I:239:VAL:HG23	1:I:309:ALA:O	2.20	0.41
2:J:129:VAL:O	2:J:130:VAL:C	2.63	0.41
2:J:163:GLN:HG2	2:J:163:GLN:O	2.20	0.41
2:J:232:VAL:HG11	2:L:232:VAL:HG21	2.02	0.41
1:K:74:VAL:CG1	1:K:75:SER:H	2.29	0.41
1:K:234:THR:O	1:K:234:THR:HG23	2.19	0.41
2:L:242:LEU:HD12	2:L:243:VAL:N	2.32	0.41
1:S:74:VAL:CG1	1:S:75:SER:H	2.29	0.41
1:S:279:VAL:O	1:S:280:SER:C	2.61	0.41
3:T:401:NAD:H2N	3:T:401:NAD:H2D	1.71	0.41
2:P:39:GLN:HE22	1:Q:190:HIS:N	2.08	0.41
2:P:84:TRP:CE3	2:P:84:TRP:CA	3.03	0.41
2:R:23:SER:C	2:R:25:LEU:N	2.76	0.41
2:R:29:VAL:HG21	2:R:84:TRP:HZ3	1.86	0.41
2:R:94:GLU:HA	2:R:94:GLU:OE2	2.21	0.41
2:R:181:ASP:OD1	2:R:195:ARG:HD3	2.21	0.41
1:A:172:MET:HE3	1:A:172:MET:C	2.45	0.41
2:B:106:GLY:C	2:B:108:HIS:N	2.77	0.41
2:D:16:LEU:O	2:D:18(A):TRP:HB3	2.20	0.41
1:G:17:ARG:NE	1:G:53:PHE:CD1	2.89	0.41
1:G:139:HIS:C	1:G:140:VAL:H	2.28	0.41
1:G:239:VAL:HG23	1:G:309:ALA:O	2.20	0.41
2:H:242:LEU:HD12	2:H:243:VAL:N	2.30	0.41
2:F:3:VAL:HG12	2:F:4:ALA:N	2.35	0.41
2:F:293:ASP:OD1	2:F:296:LEU:HD12	2.20	0.41
1:I:17:ARG:NE	1:I:53:PHE:CD1	2.89	0.41
2:J:29:VAL:HG21	2:J:84:TRP:HZ3	1.85	0.41
2:J:101:ASP:O	2:J:102:ARG:C	2.62	0.41
2:J:192:ASP:C	2:J:194:ARG:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:204:VAL:HB	2:J:231:ARG:HB2	2.01	0.41
2:J:209:GLY:O	2:J:210:ALA:C	2.63	0.41
2:J:256:ASN:N	2:J:256:ASN:HD22	2.18	0.41
2:J:317:TYR:O	2:J:320:ARG:N	2.51	0.41
2:J:320:ARG:HA	2:J:320:ARG:HE	1.83	0.41
1:K:18(A):TRP:O	1:K:20:ARG:HB2	2.19	0.41
1:K:139:HIS:C	1:K:140:VAL:H	2.29	0.41
1:K:157:PHE:CD1	1:K:157:PHE:C	2.99	0.41
2:L:29:VAL:HG21	2:L:84:TRP:HZ3	1.86	0.41
2:L:106:GLY:C	2:L:108:HIS:N	2.78	0.41
2:L:192:ASP:C	2:L:194:ARG:N	2.79	0.41
2:L:221:LEU:HD22	2:L:221:LEU:H	1.85	0.41
2:N:202:ASN:ND2	2:T:281:ILE:H	2.13	0.41
2:N:317:TYR:O	2:N:320:ARG:N	2.51	0.41
1:S:139:HIS:C	1:S:140:VAL:H	2.29	0.41
2:T:29:VAL:HG21	2:T:84:TRP:HZ3	1.86	0.41
2:T:37:VAL:HG13	2:T:64:ILE:CG2	2.50	0.41
2:T:192:ASP:C	2:T:194:ARG:N	2.79	0.41
1:O:23:SER:HA	1:O:24:PRO:HD3	1.82	0.41
1:Q:8:PHE:CB	1:Q:32:ASP:HB2	2.50	0.41
1:Q:101:ASP:CA	1:Q:122(A):LYS:HB3	2.50	0.41
1:Q:248:LYS:CG	1:Q:248(A):VAL:N	2.82	0.41
1:Q:251:THR:CG2	1:Q:252:ALA:H	2.27	0.41
1:Q:281:VAL:O	1:Q:281:VAL:HG12	2.20	0.41
2:R:20:ARG:HH12	2:R:322:VAL:HG12	1.84	0.41
2:R:110:GLN:C	2:R:112:GLY:H	2.28	0.41
2:R:117:LEU:HD23	2:R:117:LEU:C	2.45	0.41
1:A:17:ARG:NE	1:A:53:PHE:CD1	2.89	0.41
1:A:38:LYS:HG3	1:A:39:SER:N	2.27	0.41
1:A:162:ASP:HB2	1:A:167:ILE:CD1	2.51	0.41
1:A:277:PRO:HA	1:C:194:ARG:NH2	2.35	0.41
1:A:281:VAL:O	1:A:281:VAL:HG12	2.21	0.41
2:B:3:VAL:HG21	2:B:25:LEU:HD12	2.01	0.41
2:B:81:ASN:O	2:B:82:LEU:C	2.62	0.41
1:C:8:PHE:CB	1:C:32:ASP:HB2	2.50	0.41
1:C:154:LEU:HA	1:C:154:LEU:HD12	1.79	0.41
1:C:157:PHE:CD1	1:C:157:PHE:C	2.98	0.41
2:D:79:PRO:O	2:D:80:VAL:C	2.62	0.41
2:D:317:TYR:O	2:D:320:ARG:HB2	2.21	0.41
1:G:155:ALA:HB3	1:G:156:PRO:CD	2.43	0.41
2:H:304:MET:SD	2:F:170:GLY:HA2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:ASP:C	1:E:312:ASP:OD1	2.63	0.41
2:F:94:GLU:OE2	2:F:94:GLU:HA	2.21	0.41
2:F:118:ILE:C	2:F:120:ALA:H	2.29	0.41
2:F:138:THR:O	2:F:140:ALA:N	2.54	0.41
2:J:190:HIS:ND1	2:J:191:ARG:N	2.68	0.41
1:K:281:VAL:O	1:K:281:VAL:CG1	2.69	0.41
2:L:198:ALA:HB1	2:L:201:LEU:HG	2.03	0.41
2:L:260:ARG:O	2:L:261:GLU:C	2.62	0.41
1:M:192:ASP:CB	1:M:195:ARG:HD2	2.46	0.41
2:N:29:VAL:HG21	2:N:84:TRP:HZ3	1.85	0.41
1:S:248:LYS:CG	1:S:248(A):VAL:H	2.32	0.41
1:S:312:ASP:C	1:S:312:ASP:OD1	2.63	0.41
2:T:110:GLN:C	2:T:112:GLY:H	2.28	0.41
2:T:293:ASP:OD1	2:T:296:LEU:HD12	2.20	0.41
1:O:17:ARG:NE	1:O:53:PHE:CD1	2.89	0.41
1:O:161:LEU:HD23	1:O:161:LEU:HA	1.90	0.41
1:Q:96:THR:OG1	1:Q:98:VAL:HG23	2.21	0.41
1:Q:236:ASN:O	1:Q:237:VAL:CB	2.69	0.41
1:A:51:GLY:O	1:A:52:THR:C	2.62	0.41
1:A:165:LEU:CG	1:A:246:ILE:HG12	2.45	0.41
2:B:181:ASP:CG	2:B:195:ARG:NH1	2.75	0.41
2:B:226:ASN:CG	2:D:298:MET:HE1	2.45	0.41
1:C:8:PHE:HB2	1:C:32:ASP:HB2	2.02	0.41
1:C:281:VAL:O	1:C:281:VAL:HG12	2.20	0.41
2:D:29:VAL:HG21	2:D:84:TRP:HZ3	1.86	0.41
2:D:110:GLN:C	2:D:112:GLY:H	2.28	0.41
2:D:299:VAL:CG1	2:D:300:MET:N	2.83	0.41
1:G:51:GLY:O	1:G:52:THR:C	2.62	0.41
2:H:190:HIS:ND1	2:H:191:ARG:N	2.68	0.41
2:H:256:ASN:N	2:H:256:ASN:HD22	2.18	0.41
2:H:320:ARG:HA	2:H:320:ARG:HE	1.84	0.41
1:E:201:LEU:N	1:E:201:LEU:HD23	2.35	0.41
1:E:281:VAL:O	1:E:281:VAL:CG1	2.69	0.41
1:I:11:ILE:HD12	1:I:11:ILE:HA	1.92	0.41
1:I:162:ASP:HA	1:I:167:ILE:HG13	2.02	0.41
1:I:278:LEU:HB3	1:I:282:ASP:OD2	2.21	0.41
1:K:185:LEU:HD23	1:K:185:LEU:HA	1.88	0.41
2:L:89:ILE:HG21	2:L:92:VAL:HG23	2.01	0.41
2:L:194:ARG:C	2:L:196:ALA:N	2.78	0.41
2:L:317:TYR:O	2:L:320:ARG:HB2	2.21	0.41
1:M:51:GLY:O	1:M:52:THR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:GLU:O	1:M:63:THR:OG1	2.35	0.41
1:S:15:PHE:O	1:S:16:LEU:C	2.63	0.41
2:T:101:ASP:O	2:T:102:ARG:C	2.62	0.41
2:T:174:THR:HG23	2:T:229:ALA:CB	2.50	0.41
1:O:239:VAL:HG23	1:O:309:ALA:O	2.20	0.41
1:O:312:ASP:OD1	1:O:312:ASP:C	2.63	0.41
2:P:90:ASP:HA	2:P:114:LYS:HD2	2.03	0.41
2:P:110:GLN:C	2:P:112:GLY:N	2.77	0.41
2:P:192:ASP:C	2:P:194:ARG:N	2.78	0.41
2:P:232:VAL:HG11	2:R:232:VAL:HG21	2.02	0.41
2:P:304:MET:SD	2:R:170:GLY:HA2	2.60	0.41
1:Q:139:HIS:C	1:Q:140:VAL:H	2.29	0.41
1:Q:157:PHE:CD1	1:Q:157:PHE:C	2.98	0.41
1:Q:201:LEU:N	1:Q:201:LEU:HD23	2.35	0.41
1:Q:219:PRO:HD2	1:Q:220:GLN:NE2	2.35	0.41
2:B:84:TRP:CE3	2:B:84:TRP:CA	3.02	0.41
2:D:105:ALA:HB2	2:D:118:ILE:HD11	2.02	0.41
2:D:242:LEU:HD12	2:D:243:VAL:N	2.32	0.41
1:G:198:ALA:HB3	1:G:201:LEU:HG	2.02	0.41
2:H:226:ASN:CG	2:F:298:MET:HE1	2.45	0.41
1:E:139:HIS:C	1:E:140:VAL:H	2.29	0.41
2:F:15:PHE:CE1	2:F:322:VAL:CG2	3.02	0.41
2:F:317:TYR:O	2:F:320:ARG:HB2	2.21	0.41
2:F:320:ARG:HA	2:F:320:ARG:HE	1.83	0.41
1:I:154:LEU:HD12	1:I:157:PHE:CE2	2.56	0.41
2:J:20:ARG:HH12	2:J:322:VAL:HG12	1.86	0.41
2:J:89:ILE:HG21	2:J:92:VAL:HG23	2.02	0.41
2:J:181:ASP:CG	2:J:195:ARG:NH1	2.75	0.41
2:J:304:MET:SD	2:L:170:GLY:HA2	2.61	0.41
2:L:181:ASP:OD1	2:L:195:ARG:HD3	2.21	0.41
2:L:293:ASP:OD1	2:L:296:LEU:HD12	2.20	0.41
1:M:17:ARG:NE	1:M:53:PHE:CD1	2.89	0.41
1:M:74:VAL:CG1	1:M:75:SER:H	2.27	0.41
1:M:265:GLY:HA3	1:M:266:PRO:HD3	1.85	0.41
2:N:256:ASN:HD22	2:N:256:ASN:N	2.18	0.41
1:S:228:ILE:CD1	1:S:228:ILE:N	2.82	0.41
1:O:90:ASP:HA	1:O:114:LYS:HG2	2.02	0.41
1:O:110:GLN:HG3	1:C:110:GLN:HB3	2.03	0.41
1:Q:256:ASN:O	1:Q:259:PHE:N	2.54	0.41
1:Q:307:VAL:CG1	1:Q:308:VAL:N	2.84	0.41
2:R:105:ALA:HB2	2:R:118:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:198:ALA:HB1	2:R:201:LEU:HG	2.03	0.41
2:R:260:ARG:O	2:R:261:GLU:C	2.62	0.41
2:R:312:ASP:OD1	2:R:315:TRP:N	2.48	0.41
1:A:110:GLN:CD	1:G:110:GLN:O	2.58	0.41
2:B:29:VAL:HG21	2:B:84:TRP:HZ3	1.85	0.41
2:B:90:ASP:HA	2:B:114:LYS:HD2	2.03	0.41
2:B:190:HIS:ND1	2:B:191:ARG:N	2.68	0.41
2:D:106:GLY:C	2:D:108:HIS:N	2.78	0.41
2:D:192:ASP:CG	2:D:195:ARG:HG3	2.45	0.41
1:G:3:VAL:HG12	1:G:4:ALA:N	2.35	0.41
1:G:281:VAL:O	1:G:281:VAL:HG12	2.21	0.41
2:H:129:VAL:O	2:H:130:VAL:C	2.63	0.41
2:H:182:GLN:HE22	2:H:231:ARG:CB	2.32	0.41
1:E:170:GLY:CA	1:E:244:VAL:HG12	2.48	0.41
1:I:138:GLY:O	1:I:139:HIS:C	2.64	0.41
1:I:281:VAL:O	1:I:281:VAL:HG12	2.20	0.41
2:J:106:GLY:C	2:J:108:HIS:N	2.77	0.41
2:J:192:ASP:C	2:J:194:ARG:N	2.79	0.41
1:K:8:PHE:HB2	1:K:32:ASP:HB2	2.02	0.41
1:K:159:LYS:O	1:K:160:VAL:C	2.62	0.41
1:K:228:ILE:CD1	1:K:228:ILE:N	2.82	0.41
2:L:16:LEU:O	2:L:18(A):TRP:HB3	2.20	0.41
2:L:94:GLU:HA	2:L:94:GLU:OE2	2.21	0.41
2:L:138:THR:O	2:L:140:ALA:N	2.54	0.41
2:L:153:CYS:SG	2:L:311:TYR:CD1	3.12	0.41
2:L:166:GLY:O	2:L:246:VAL:HA	2.21	0.41
2:L:174:THR:HG23	2:L:229:ALA:CB	2.50	0.41
2:L:202:ASN:O	2:L:233:PRO:HD3	2.20	0.41
2:L:218:LEU:HB3	2:L:221:LEU:CD2	2.49	0.41
1:M:139:HIS:C	1:M:140:VAL:H	2.28	0.41
1:M:234:THR:HA	1:M:235:PRO:HD2	1.88	0.41
1:M:277:PRO:HA	1:S:194:ARG:NH2	2.35	0.41
1:M:312:ASP:OD1	1:M:312:ASP:C	2.63	0.41
2:N:11:ILE:HD13	2:N:11:ILE:HA	1.92	0.41
2:N:192:ASP:C	2:N:194:ARG:N	2.79	0.41
1:S:256:ASN:O	1:S:259:PHE:N	2.54	0.41
2:T:198:ALA:HB1	2:T:201:LEU:HG	2.03	0.41
2:T:317:TYR:O	2:T:320:ARG:HB2	2.21	0.41
1:O:3:VAL:HG12	1:O:4:ALA:N	2.35	0.41
1:O:110:GLN:HB2	1:C:110:GLN:CG	2.49	0.41
1:O:248:LYS:CG	1:O:248(A):VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:277:PRO:HA	1:Q:194:ARG:NH2	2.35	0.41
2:P:20:ARG:HH12	2:P:322:VAL:HG12	1.86	0.41
2:P:89:ILE:HG21	2:P:92:VAL:HG23	2.02	0.41
2:P:132:VAL:HG21	2:P:155:ALA:HB1	2.03	0.41
2:P:182:GLN:HE22	2:P:231:ARG:CB	2.32	0.41
2:P:209:GLY:O	2:P:210:ALA:C	2.63	0.41
1:Q:121:PRO:C	1:Q:122:ALA:O	2.62	0.41
1:Q:155:ALA:HB3	1:Q:156:PRO:CD	2.42	0.41
2:R:185:LEU:O	2:R:187:ALA:N	2.54	0.41
2:R:192:ASP:C	2:R:194:ARG:N	2.79	0.41
2:R:221:LEU:HD22	2:R:221:LEU:H	1.86	0.41
2:R:228:ILE:HG13	2:R:229:ALA:N	2.36	0.41
2:R:327:ILE:O	2:R:330:ASN:O	2.37	0.41
1:A:109:ILE:HB	1:G:110:GLN:OE1	2.21	0.41
1:A:139:HIS:C	1:A:140:VAL:H	2.28	0.41
1:A:192:ASP:CB	1:A:195:ARG:HD2	2.46	0.41
1:A:239:VAL:HG23	1:A:309:ALA:O	2.20	0.41
2:B:89:ILE:HG21	2:B:92:VAL:HG23	2.02	0.41
2:B:132:VAL:HG21	2:B:155:ALA:HB1	2.03	0.41
2:B:232:VAL:HG11	2:D:232:VAL:HG21	2.02	0.41
2:B:256:ASN:N	2:B:256:ASN:HD22	2.18	0.41
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.20	0.41
1:C:108:HIS:HB2	1:C:116:VAL:HG21	2.03	0.41
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.93	0.41
1:C:170:GLY:CA	1:C:244:VAL:HG12	2.48	0.41
1:C:236:ASN:O	1:C:237:VAL:CB	2.69	0.41
2:D:45:LYS:NZ	2:D:55:ALA:O	2.51	0.41
2:D:132:VAL:HG21	2:D:155:ALA:HB1	2.03	0.41
2:D:138:THR:O	2:D:140:ALA:N	2.54	0.41
2:D:198:ALA:HB1	2:D:201:LEU:HG	2.03	0.41
2:D:213:ALA:O	2:D:214:VAL:C	2.64	0.41
2:D:221:LEU:HD22	2:D:221:LEU:H	1.86	0.41
2:D:333:GLN:H	2:D:333:GLN:HG2	1.71	0.41
1:G:162:ASP:HB2	1:G:167:ILE:CD1	2.51	0.41
2:H:20:ARG:HH12	2:H:322:VAL:HG12	1.86	0.41
2:H:90:ASP:HA	2:H:114:LYS:HD2	2.03	0.41
2:H:100:VAL:HA	2:H:118:ILE:HD13	2.02	0.41
2:H:132:VAL:HG21	2:H:155:ALA:HB1	2.03	0.41
1:E:8:PHE:HB2	1:E:32:ASP:HB2	2.02	0.41
1:E:256:ASN:O	1:E:259:PHE:N	2.54	0.41
2:F:192:ASP:C	2:F:194:ARG:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:198:ALA:HB1	2:F:201:LEU:HG	2.03	0.41
2:F:221:LEU:HD22	2:F:221:LEU:H	1.86	0.41
2:F:299:VAL:CG1	2:F:300:MET:N	2.83	0.41
1:I:3:VAL:HG12	1:I:4:ALA:N	2.35	0.41
1:I:192:ASP:CB	1:I:195:ARG:HD2	2.46	0.41
2:J:66:VAL:O	2:J:66:VAL:HG12	2.19	0.41
2:J:226:ASN:CG	2:L:298:MET:HE1	2.45	0.41
2:J:298:MET:HE1	2:L:226:ASN:HB3	2.03	0.41
1:K:165:LEU:CG	1:K:246:ILE:HG12	2.43	0.41
1:K:200:ALA:C	1:K:201:LEU:HD23	2.46	0.41
2:L:118:ILE:C	2:L:120:ALA:H	2.28	0.41
2:L:185:LEU:O	2:L:187:ALA:N	2.54	0.41
2:L:218:LEU:HD23	2:L:218:LEU:HA	1.77	0.41
1:M:159:LYS:O	1:M:160:VAL:C	2.62	0.41
1:M:239:VAL:HG23	1:M:309:ALA:O	2.20	0.41
2:N:20:ARG:HH12	2:N:322:VAL:HG12	1.86	0.41
2:N:100:VAL:HA	2:N:118:ILE:HD13	2.02	0.41
1:S:96:THR:OG1	1:S:98:VAL:HG23	2.21	0.41
1:S:115:LYS:HE3	1:S:137:TYR:OH	2.21	0.41
1:S:307:VAL:CG1	1:S:308:VAL:N	2.84	0.41
2:T:3:VAL:HG12	2:T:4:ALA:N	2.35	0.41
2:T:15:PHE:CE1	2:T:322:VAL:CG2	3.02	0.41
2:T:181:ASP:OD1	2:T:195:ARG:HD3	2.21	0.41
1:O:226:ASN:HB3	1:Q:300:MET:SD	2.61	0.41
1:O:281:VAL:O	1:O:281:VAL:HG12	2.20	0.41
2:P:41:SER:O	2:P:42:HIS:C	2.64	0.41
2:P:193:LEU:H	2:P:193:LEU:CD1	2.06	0.41
1:Q:74:VAL:CG1	1:Q:75:SER:H	2.29	0.41
1:Q:200:ALA:C	1:Q:201:LEU:HD23	2.46	0.41
2:R:299:VAL:CG1	2:R:300:MET:N	2.83	0.41
1:A:194:ARG:CZ	1:C:277:PRO:HA	2.51	0.41
1:A:265:GLY:HA3	1:A:266:PRO:HD3	1.84	0.41
1:C:84:TRP:CE3	1:C:84:TRP:CA	3.03	0.41
2:D:118:ILE:C	2:D:120:ALA:H	2.29	0.41
2:D:320:ARG:HA	2:D:320:ARG:HE	1.83	0.41
2:H:198:ALA:O	2:H:199:ALA:HB3	2.21	0.41
1:E:108:HIS:HB2	1:E:116:VAL:HG21	2.03	0.41
1:E:281:VAL:O	1:E:281:VAL:HG12	2.20	0.41
2:F:39:GLN:H	2:F:39:GLN:HG2	1.68	0.41
2:F:166:GLY:O	2:F:246:VAL:HA	2.21	0.41
2:F:181:ASP:OD1	2:F:195:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:ALA:O	2:F:214:VAL:C	2.64	0.41
2:J:198:ALA:O	2:J:199:ALA:HB3	2.21	0.41
1:M:60:ILE:CG2	1:M:60(A):ASP:N	2.84	0.41
1:M:165:LEU:CG	1:M:246:ILE:HG12	2.45	0.41
1:M:307:VAL:CG1	1:M:308:VAL:N	2.84	0.41
2:N:132:VAL:HG21	2:N:155:ALA:HB1	2.03	0.41
2:N:192:ASP:CG	2:N:195:ARG:HG3	2.46	0.41
2:N:203:ILE:HG12	2:N:232:VAL:HG12	2.03	0.41
2:N:209:GLY:O	2:N:210:ALA:C	2.63	0.41
1:S:200:ALA:C	1:S:201:LEU:HD23	2.46	0.41
1:S:213:ALA:O	1:S:214:VAL:C	2.64	0.41
2:T:94:GLU:HA	2:T:94:GLU:OE2	2.21	0.41
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.51	0.40
1:O:198:ALA:HB3	1:O:201:LEU:HG	2.02	0.40
1:O:215:SER:O	1:O:216:LEU:C	2.64	0.40
1:O:248(A):VAL:CG1	1:O:249:GLY:N	2.83	0.40
2:R:79:PRO:O	2:R:80:VAL:C	2.62	0.40
2:R:138:THR:O	2:R:140:ALA:N	2.54	0.40
1:A:198:ALA:HB3	1:A:201:LEU:HG	2.02	0.40
2:B:192:ASP:C	2:B:194:ARG:N	2.79	0.40
2:B:298:MET:HE1	2:D:226:ASN:HB3	2.03	0.40
1:C:15:PHE:O	1:C:16:LEU:C	2.63	0.40
1:C:139:HIS:C	1:C:140:VAL:H	2.29	0.40
1:C:251:THR:CG2	1:C:252:ALA:H	2.27	0.40
1:C:256:ASN:O	1:C:259:PHE:N	2.54	0.40
1:G:194:ARG:CZ	1:E:277:PRO:HA	2.51	0.40
2:H:89:ILE:HG21	2:H:92:VAL:HG23	2.02	0.40
2:H:192:ASP:C	2:H:194:ARG:N	2.79	0.40
1:E:15:PHE:O	1:E:16:LEU:C	2.63	0.40
1:I:190:HIS:CE1	1:I:195:ARG:HD2	2.56	0.40
2:J:132:VAL:HG21	2:J:155:ALA:HB1	2.03	0.40
1:M:154:LEU:HD12	1:M:157:PHE:CE2	2.56	0.40
1:M:194:ARG:CZ	1:S:277:PRO:HA	2.51	0.40
2:N:298:MET:HE1	2:T:226:ASN:HB3	2.03	0.40
1:S:31:ASN:HA	1:S:74:VAL:O	2.21	0.40
2:T:138:THR:O	2:T:140:ALA:N	2.54	0.40
1:O:38:LYS:HG3	1:O:39:SER:N	2.27	0.40
1:O:215:SER:C	1:O:217:VAL:N	2.79	0.40
2:P:100:VAL:HA	2:P:118:ILE:HD13	2.02	0.40
2:P:182:GLN:HE21	2:P:204:VAL:HG21	1.86	0.40
2:P:198:ALA:O	2:P:199:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:GLY:CA	1:Q:244:VAL:HG12	2.48	0.40
2:R:209:GLY:C	2:R:211:ALA:H	2.30	0.40
2:R:210:ALA:HA	2:R:213:ALA:HB3	2.02	0.40
1:A:226:ASN:HB3	1:C:300:MET:SD	2.61	0.40
2:B:41:SER:O	2:B:42:HIS:C	2.64	0.40
2:B:299:VAL:CG1	2:B:300:MET:N	2.85	0.40
2:D:101:ASP:O	2:D:102:ARG:C	2.62	0.40
2:D:117:LEU:C	2:D:117:LEU:HD23	2.45	0.40
1:G:138:GLY:O	1:G:139:HIS:C	2.64	0.40
1:G:154:LEU:HD12	1:G:157:PHE:CE2	2.56	0.40
1:G:157:PHE:CD1	1:G:157:PHE:C	2.99	0.40
1:G:162:ASP:HA	1:G:167:ILE:HG13	2.02	0.40
1:E:259:PHE:O	1:E:260:ARG:C	2.65	0.40
1:E:307:VAL:CG1	1:E:308:VAL:N	2.84	0.40
2:F:204:VAL:HB	2:F:231:ARG:HB2	2.04	0.40
1:I:162:ASP:HB2	1:I:167:ILE:CD1	2.51	0.40
2:J:203:ILE:HG12	2:J:232:VAL:HG12	2.03	0.40
1:K:96:THR:OG1	1:K:98:VAL:HG23	2.21	0.40
1:K:256:ASN:O	1:K:259:PHE:N	2.54	0.40
1:K:281:VAL:O	1:K:281:VAL:HG12	2.20	0.40
1:M:240:VAL:HG22	1:M:309:ALA:HB3	2.04	0.40
2:N:41:SER:O	2:N:42:HIS:C	2.64	0.40
2:N:89:ILE:HG21	2:N:92:VAL:HG23	2.02	0.40
2:N:299:VAL:CG1	2:N:300:MET:N	2.85	0.40
2:T:194:ARG:C	2:T:196:ALA:N	2.78	0.40
1:O:190:HIS:CE1	1:O:195:ARG:HD2	2.57	0.40
2:P:202:ASN:ND2	2:R:281:ILE:CB	2.75	0.40
2:P:317:TYR:O	2:P:318:SER:C	2.64	0.40
1:Q:108:HIS:HB2	1:Q:116:VAL:HG21	2.04	0.40
2:R:317:TYR:O	2:R:320:ARG:HB2	2.21	0.40
2:B:242:LEU:HD12	2:B:243:VAL:N	2.30	0.40
2:D:37:VAL:CG1	2:D:64:ILE:HG22	2.52	0.40
2:D:228:ILE:HG13	2:D:229:ALA:N	2.36	0.40
1:G:226:ASN:HB3	1:E:300:MET:SD	2.62	0.40
1:G:277:PRO:HA	1:E:194:ARG:NH2	2.36	0.40
2:H:23:SER:C	2:H:25:LEU:N	2.77	0.40
1:E:74:VAL:CG1	1:E:75:SER:H	2.29	0.40
1:E:159:LYS:O	1:E:160:VAL:C	2.62	0.40
2:F:185:LEU:O	2:F:187:ALA:N	2.54	0.40
1:I:60:ILE:CG2	1:I:60(A):ASP:N	2.84	0.40
1:I:89:ILE:O	1:I:114:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:LEU:CD1	2:L:184:LEU:HD13	2.49	0.40
1:I:194:ARG:CZ	1:K:277:PRO:HA	2.51	0.40
2:J:299:VAL:CG1	2:J:300:MET:N	2.85	0.40
2:J:317:TYR:O	2:J:318:SER:C	2.64	0.40
1:K:115:LYS:HE3	1:K:137:TYR:OH	2.21	0.40
1:K:236:ASN:O	1:K:237:VAL:CB	2.69	0.40
2:L:322:VAL:O	2:L:326:ASP:N	2.48	0.40
1:M:161:LEU:HD23	1:M:161:LEU:HA	1.90	0.40
1:M:240:VAL:CG2	1:M:309:ALA:HB3	2.52	0.40
2:N:90:ASP:HA	2:N:114:LYS:HD2	2.03	0.40
1:S:126:PRO:HD2	1:S:143:ILE:O	2.21	0.40
1:S:162:ASP:HB2	1:S:167:ILE:CD1	2.51	0.40
1:S:281:VAL:O	1:S:281:VAL:CG1	2.69	0.40
1:O:74:VAL:CG1	1:O:75:SER:H	2.27	0.40
1:O:154:LEU:HD12	1:O:157:PHE:CE2	2.56	0.40
1:Q:217:VAL:O	1:Q:218:LEU:HD12	2.22	0.40
1:Q:281:VAL:O	1:Q:281:VAL:CG1	2.69	0.40
1:A:157:PHE:CD1	1:A:157:PHE:C	2.99	0.40
1:A:292:ILE:H	1:A:292:ILE:CD1	2.30	0.40
2:B:118:ILE:C	2:B:120:ALA:H	2.29	0.40
1:C:115:LYS:HE3	1:C:137:TYR:OH	2.21	0.40
1:C:217:VAL:O	1:C:218:LEU:HD12	2.22	0.40
2:D:204:VAL:HB	2:D:231:ARG:HB2	2.04	0.40
1:G:15:PHE:O	1:G:18:CYS:N	2.55	0.40
1:G:259:PHE:O	1:G:260:ARG:C	2.65	0.40
2:H:182:GLN:HE21	2:H:204:VAL:HG21	1.86	0.40
1:E:145:SER:C	1:E:147:ALA:H	2.30	0.40
1:E:200:ALA:C	1:E:201:LEU:HD23	2.46	0.40
2:F:29:VAL:HG21	2:F:84:TRP:HZ3	1.86	0.40
2:F:132:VAL:HG21	2:F:155:ALA:HB1	2.03	0.40
1:I:157:PHE:CD1	1:I:157:PHE:C	3.00	0.40
2:J:100:VAL:HA	2:J:118:ILE:HD13	2.02	0.40
1:K:45:LYS:O	1:K:52:THR:HA	2.22	0.40
1:K:244:VAL:HG23	1:K:244:VAL:O	2.22	0.40
2:L:132:VAL:HG21	2:L:155:ALA:HB1	2.03	0.40
2:L:323:ASP:HA	2:L:326:ASP:HB2	2.04	0.40
3:L:401:NAD:H2D	3:L:401:NAD:H2N	1.69	0.40
1:M:259:PHE:O	1:M:260:ARG:C	2.65	0.40
1:S:45:LYS:O	1:S:52:THR:HA	2.21	0.40
1:S:271:LEU:CD1	1:S:292:ILE:HD11	2.35	0.40
2:T:16:LEU:HD23	2:T:16:LEU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:299:VAL:CG1	2:T:300:MET:N	2.83	0.40
1:O:157:PHE:CD1	1:O:157:PHE:C	2.99	0.40
1:O:278:LEU:HB3	1:O:282:ASP:OD2	2.21	0.40
2:P:118:ILE:C	2:P:120:ALA:H	2.29	0.40
1:Q:278:LEU:HB3	1:Q:282:ASP:OD2	2.22	0.40
2:R:15:PHE:CE1	2:R:322:VAL:CG2	3.02	0.40
2:R:23:SER:C	2:R:25:LEU:H	2.30	0.40
2:R:37:VAL:CG1	2:R:64:ILE:HG22	2.52	0.40
2:R:166:GLY:O	2:R:246:VAL:HA	2.22	0.40
2:R:333:GLN:H	2:R:333:GLN:HG2	1.71	0.40
1:A:162:ASP:HA	1:A:167:ILE:HG13	2.02	0.40
1:A:240:VAL:HG22	1:A:309:ALA:HB3	2.03	0.40
2:B:317:TYR:O	2:B:318:SER:C	2.64	0.40
1:E:20:ARG:HH21	1:E:319:GLN:NE2	2.20	0.40
1:E:43:LEU:HD23	1:E:43:LEU:HA	1.78	0.40
1:I:15:PHE:O	1:I:18:CYS:N	2.55	0.40
1:K:108:HIS:HB2	1:K:116:VAL:HG21	2.04	0.40
1:K:307:VAL:CG1	1:K:308:VAL:N	2.84	0.40
2:L:210:ALA:HA	2:L:213:ALA:HB3	2.02	0.40
1:M:138:GLY:O	1:M:139:HIS:C	2.64	0.40
1:M:226:ASN:HB3	1:S:300:MET:SD	2.61	0.40
2:N:235:PRO:O	2:N:236:ASN:HB2	2.21	0.40
1:S:281:VAL:O	1:S:281:VAL:HG12	2.20	0.40
2:T:23:SER:C	2:T:25:LEU:H	2.30	0.40
2:T:221:LEU:HD22	2:T:221:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	337/451 (75%)	237 (70%)	67 (20%)	33 (10%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	340/451 (75%)	236 (69%)	73 (22%)	31 (9%)	0	8
1	E	340/451 (75%)	236 (69%)	75 (22%)	29 (8%)	0	9
1	G	337/451 (75%)	237 (70%)	67 (20%)	33 (10%)	0	7
1	I	337/451 (75%)	237 (70%)	67 (20%)	33 (10%)	0	7
1	K	340/451 (75%)	236 (69%)	75 (22%)	29 (8%)	0	9
1	M	337/451 (75%)	237 (70%)	66 (20%)	34 (10%)	0	7
1	O	337/451 (75%)	237 (70%)	66 (20%)	34 (10%)	0	7
1	Q	337/451 (75%)	236 (70%)	69 (20%)	32 (10%)	0	8
1	S	339/451 (75%)	236 (70%)	73 (22%)	30 (9%)	0	8
2	B	335/337 (99%)	265 (79%)	51 (15%)	19 (6%)	1	14
2	D	335/337 (99%)	265 (79%)	55 (16%)	15 (4%)	2	17
2	F	335/337 (99%)	264 (79%)	55 (16%)	16 (5%)	2	16
2	H	335/337 (99%)	265 (79%)	52 (16%)	18 (5%)	1	15
2	J	335/337 (99%)	265 (79%)	52 (16%)	18 (5%)	1	15
2	L	335/337 (99%)	264 (79%)	56 (17%)	15 (4%)	2	17
2	N	335/337 (99%)	265 (79%)	52 (16%)	18 (5%)	1	15
2	P	335/337 (99%)	264 (79%)	53 (16%)	18 (5%)	1	15
2	R	335/337 (99%)	264 (79%)	55 (16%)	16 (5%)	2	16
2	T	335/337 (99%)	264 (79%)	55 (16%)	16 (5%)	2	16
All	All	6731/7880 (85%)	5010 (74%)	1234 (18%)	487 (7%)	2	11

All (487) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	10	ARG
1	O	141	ALA
1	O	193	LEU
1	O	248(A)	VAL
2	P	133	ASN
2	P	198	ALA
2	P	280	SER
1	Q	10	ARG
1	Q	122	ALA
1	Q	141	ALA
1	Q	248(A)	VAL

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Mol	Chain	Res	Type
1	Q	252	ALA
2	R	133	ASN
2	R	198	ALA
2	R	280	SER
1	A	10	ARG
1	A	141	ALA
1	A	193	LEU
1	A	248(A)	VAL
2	B	133	ASN
2	B	198	ALA
2	B	280	SER
1	C	10	ARG
1	C	141	ALA
1	C	248(A)	VAL
1	C	252	ALA
2	D	133	ASN
2	D	198	ALA
2	D	280	SER
1	G	10	ARG
1	G	141	ALA
1	G	193	LEU
1	G	248(A)	VAL
2	H	133	ASN
2	H	198	ALA
2	H	280	SER
1	E	10	ARG
1	E	141	ALA
1	E	248(A)	VAL
1	E	252	ALA
2	F	133	ASN
2	F	198	ALA
2	F	280	SER
1	I	10	ARG
1	I	141	ALA
1	I	193	LEU
1	I	248(A)	VAL
2	J	133	ASN
2	J	198	ALA
2	J	280	SER
1	K	10	ARG
1	K	141	ALA
1	K	248(A)	VAL

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Mol	Chain	Res	Type
1	K	252	ALA
2	L	133	ASN
2	L	198	ALA
2	L	280	SER
1	M	10	ARG
1	M	141	ALA
1	M	193	LEU
1	M	248(A)	VAL
2	N	133	ASN
2	N	198	ALA
2	N	280	SER
1	S	10	ARG
1	S	141	ALA
1	S	248(A)	VAL
1	S	252	ALA
2	T	133	ASN
2	T	198	ALA
2	T	280	SER
1	O	18(B)	HIS
1	O	165	LEU
1	O	198	ALA
1	O	210	ALA
1	O	226	ASN
1	O	233	PRO
1	O	252	ALA
1	O	253	GLU
2	P	80	VAL
2	P	186	ASP
2	P	193	LEU
2	P	210	ALA
2	P	281	ILE
1	Q	18(B)	HIS
1	Q	165	LEU
1	Q	193	LEU
1	Q	198	ALA
1	Q	210	ALA
1	Q	226	ASN
1	Q	233	PRO
1	Q	253	GLU
2	R	186	ASP
2	R	193	LEU
2	R	210	ALA

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Mol	Chain	Res	Type
1	A	18(B)	HIS
1	A	165	LEU
1	A	198	ALA
1	A	210	ALA
1	A	226	ASN
1	A	233	PRO
1	A	252	ALA
1	A	253	GLU
2	B	80	VAL
2	B	186	ASP
2	B	193	LEU
2	B	210	ALA
2	B	281	ILE
1	C	18(B)	HIS
1	C	165	LEU
1	C	193	LEU
1	C	198	ALA
1	C	210	ALA
1	C	226	ASN
1	C	233	PRO
1	C	253	GLU
2	D	186	ASP
2	D	193	LEU
2	D	210	ALA
1	G	18(B)	HIS
1	G	165	LEU
1	G	198	ALA
1	G	210	ALA
1	G	226	ASN
1	G	233	PRO
1	G	252	ALA
1	G	253	GLU
2	H	80	VAL
2	H	186	ASP
2	H	193	LEU
2	H	210	ALA
2	H	281	ILE
1	E	18(B)	HIS
1	E	165	LEU
1	E	193	LEU
1	E	198	ALA
1	E	210	ALA

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Mol	Chain	Res	Type
1	E	226	ASN
1	E	233	PRO
1	E	253	GLU
2	F	186	ASP
2	F	193	LEU
2	F	210	ALA
1	I	18(B)	HIS
1	I	165	LEU
1	I	198	ALA
1	I	210	ALA
1	I	226	ASN
1	I	233	PRO
1	I	252	ALA
1	I	253	GLU
2	J	80	VAL
2	J	186	ASP
2	J	193	LEU
2	J	210	ALA
2	J	281	ILE
1	K	18(B)	HIS
1	K	165	LEU
1	K	193	LEU
1	K	198	ALA
1	K	210	ALA
1	K	226	ASN
1	K	233	PRO
1	K	253	GLU
2	L	186	ASP
2	L	193	LEU
2	L	210	ALA
1	M	18(B)	HIS
1	M	165	LEU
1	M	198	ALA
1	M	210	ALA
1	M	226	ASN
1	M	233	PRO
1	M	252	ALA
1	M	253	GLU
2	N	80	VAL
2	N	186	ASP
2	N	193	LEU
2	N	210	ALA

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Mol	Chain	Res	Type
2	N	281	ILE
1	S	18(B)	HIS
1	S	165	LEU
1	S	193	LEU
1	S	198	ALA
1	S	210	ALA
1	S	226	ASN
1	S	233	PRO
1	S	253	GLU
2	T	186	ASP
2	T	193	LEU
2	T	210	ALA
1	O	22	ASP
1	O	33	SER
1	O	136	ASP
1	O	213	ALA
1	O	216	LEU
2	P	130	VAL
2	P	233	PRO
2	P	237	VAL
2	P	252	ALA
1	Q	22	ASP
1	Q	136	ASP
1	Q	186	ASP
1	Q	237	VAL
2	R	130	VAL
2	R	233	PRO
2	R	237	VAL
2	R	252	ALA
1	A	22	ASP
1	A	33	SER
1	A	136	ASP
1	A	213	ALA
1	A	216	LEU
2	B	130	VAL
2	B	233	PRO
2	B	237	VAL
2	B	252	ALA
1	C	22	ASP
1	C	136	ASP
1	C	186	ASP
1	C	237	VAL

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Mol	Chain	Res	Type
2	D	130	VAL
2	D	233	PRO
2	D	237	VAL
2	D	252	ALA
1	G	22	ASP
1	G	33	SER
1	G	136	ASP
1	G	213	ALA
1	G	216	LEU
2	H	130	VAL
2	H	233	PRO
2	H	237	VAL
2	H	252	ALA
1	E	22	ASP
1	E	136	ASP
1	E	186	ASP
1	E	237	VAL
2	F	130	VAL
2	F	233	PRO
2	F	237	VAL
2	F	252	ALA
1	I	22	ASP
1	I	33	SER
1	I	136	ASP
1	I	213	ALA
1	I	216	LEU
2	J	130	VAL
2	J	233	PRO
2	J	237	VAL
2	J	252	ALA
1	K	22	ASP
1	K	136	ASP
1	K	186	ASP
1	K	237	VAL
2	L	130	VAL
2	L	233	PRO
2	L	237	VAL
2	L	252	ALA
1	M	22	ASP
1	M	33	SER
1	M	136	ASP
1	M	213	ALA

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Mol	Chain	Res	Type
1	M	216	LEU
2	N	130	VAL
2	N	233	PRO
2	N	237	VAL
2	N	252	ALA
1	S	22	ASP
1	S	136	ASP
1	S	186	ASP
1	S	213	ALA
1	S	237	VAL
2	T	130	VAL
2	T	233	PRO
2	T	237	VAL
2	T	252	ALA
1	O	34	GLY
1	O	139	HIS
1	O	237	VAL
1	O	249	GLY
2	P	163	GLN
2	P	287	ASP
1	Q	33	SER
1	Q	38	LYS
1	Q	139	HIS
1	Q	213	ALA
1	Q	249	GLY
2	R	80	VAL
2	R	281	ILE
2	R	313	ASN
1	A	34	GLY
1	A	139	HIS
1	A	237	VAL
1	A	249	GLY
2	B	163	GLN
2	B	287	ASP
1	C	33	SER
1	C	38	LYS
1	C	139	HIS
1	C	213	ALA
1	C	249	GLY
2	D	80	VAL
2	D	281	ILE
2	D	313	ASN

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Mol	Chain	Res	Type
1	G	34	GLY
1	G	139	HIS
1	G	237	VAL
1	G	249	GLY
2	H	163	GLN
2	H	287	ASP
1	E	33	SER
1	E	38	LYS
1	E	139	HIS
1	E	213	ALA
1	E	249	GLY
2	F	80	VAL
2	F	281	ILE
2	F	313	ASN
1	I	34	GLY
1	I	139	HIS
1	I	186	ASP
1	I	237	VAL
1	I	249	GLY
2	J	163	GLN
2	J	287	ASP
1	K	33	SER
1	K	38	LYS
1	K	139	HIS
1	K	213	ALA
1	K	249	GLY
2	L	80	VAL
2	L	281	ILE
2	L	313	ASN
1	M	34	GLY
1	M	139	HIS
1	M	186	ASP
1	M	237	VAL
1	M	249	GLY
2	N	163	GLN
2	N	287	ASP
1	S	33	SER
1	S	38	LYS
1	S	139	HIS
1	S	249	GLY
2	T	80	VAL
2	T	281	ILE

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Mol	Chain	Res	Type
2	T	313	ASN
1	O	21	LYS
1	O	38	LYS
1	O	60(A)	ASP
1	O	123(A)	SER
1	O	186	ASP
1	O	191	ARG
2	P	219	PRO
1	Q	21	LYS
1	Q	34	GLY
1	A	21	LYS
1	A	38	LYS
1	A	60(A)	ASP
1	A	186	ASP
1	A	191	ARG
2	B	219	PRO
1	C	21	LYS
1	C	34	GLY
1	G	21	LYS
1	G	38	LYS
1	G	60(A)	ASP
1	G	186	ASP
1	G	191	ARG
2	H	219	PRO
1	E	21	LYS
1	E	34	GLY
1	I	21	LYS
1	I	38	LYS
1	I	60(A)	ASP
1	I	191	ARG
1	K	21	LYS
1	K	34	GLY
1	M	21	LYS
1	M	38	LYS
1	M	60(A)	ASP
1	M	191	ARG
1	S	21	LYS
1	S	34	GLY
1	O	207	SER
1	O	281	VAL
2	P	139	HIS
2	P	147	ALA

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Mol	Chain	Res	Type
1	Q	55	ALA
1	Q	125	ILE
1	Q	166	GLY
1	Q	216	LEU
2	R	119	THR
2	R	219	PRO
1	A	123(A)	SER
1	A	281	VAL
2	B	119	THR
2	B	139	HIS
2	B	147	ALA
1	C	55	ALA
1	C	166	GLY
1	C	216	LEU
2	D	119	THR
2	D	219	PRO
1	G	123(A)	SER
1	G	281	VAL
2	H	139	HIS
2	H	147	ALA
1	E	166	GLY
1	E	216	LEU
2	F	119	THR
2	F	219	PRO
1	I	123(A)	SER
1	I	281	VAL
2	J	139	HIS
2	J	147	ALA
2	J	219	PRO
1	K	166	GLY
1	K	216	LEU
2	L	119	THR
2	L	219	PRO
1	M	123(A)	SER
1	M	207	SER
1	M	281	VAL
2	N	139	HIS
2	N	147	ALA
2	N	219	PRO
1	S	55	ALA
1	S	166	GLY
1	S	216	LEU

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Mol	Chain	Res	Type
2	T	119	THR
2	T	219	PRO
1	O	166	GLY
1	Q	328	VAL
1	A	166	GLY
1	C	328	VAL
1	G	166	GLY
1	E	328	VAL
1	I	166	GLY
1	K	328	VAL
1	M	166	GLY
1	S	328	VAL
1	O	104	GLY
1	O	130	VAL
1	Q	130	VAL
1	A	104	GLY
1	A	130	VAL
1	C	130	VAL
1	G	104	GLY
1	G	130	VAL
1	E	130	VAL
1	E	155	ALA
1	I	104	GLY
1	I	130	VAL
1	I	328	VAL
1	K	130	VAL
1	M	104	GLY
1	M	130	VAL
1	S	130	VAL
1	O	155	ALA
1	O	328	VAL
2	P	166	GLY
1	Q	155	ALA
1	Q	281	VAL
1	A	155	ALA
1	A	328	VAL
2	B	166	GLY
1	C	155	ALA
1	C	281	VAL
1	G	155	ALA
1	G	328	VAL
1	E	281	VAL

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Mol	Chain	Res	Type
1	I	155	ALA
2	J	166	GLY
1	K	155	ALA
1	K	281	VAL
1	M	155	ALA
1	M	328	VAL
2	N	166	GLY
1	S	155	ALA
1	S	281	VAL
2	H	166	GLY
2	R	277	PRO
1	C	180	GLY
2	F	277	PRO
2	T	277	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/370 (76%)	254 (91%)	26 (9%)	8	26
1	C	282/370 (76%)	255 (90%)	27 (10%)	8	25
1	E	282/370 (76%)	256 (91%)	26 (9%)	8	27
1	G	280/370 (76%)	256 (91%)	24 (9%)	10	29
1	I	280/370 (76%)	256 (91%)	24 (9%)	10	29
1	K	282/370 (76%)	257 (91%)	25 (9%)	9	28
1	M	280/370 (76%)	256 (91%)	24 (9%)	10	29
1	O	280/370 (76%)	256 (91%)	24 (9%)	10	29
1	Q	280/370 (76%)	252 (90%)	28 (10%)	7	24
1	S	281/370 (76%)	256 (91%)	25 (9%)	9	28
2	B	279/279 (100%)	262 (94%)	17 (6%)	17	38
2	D	279/279 (100%)	263 (94%)	16 (6%)	18	40
2	F	279/279 (100%)	263 (94%)	16 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	279/279 (100%)	262 (94%)	17 (6%)	17	38
2	J	279/279 (100%)	262 (94%)	17 (6%)	17	38
2	L	279/279 (100%)	263 (94%)	16 (6%)	18	40
2	N	279/279 (100%)	262 (94%)	17 (6%)	17	38
2	P	279/279 (100%)	263 (94%)	16 (6%)	18	40
2	R	279/279 (100%)	263 (94%)	16 (6%)	18	40
2	T	279/279 (100%)	263 (94%)	16 (6%)	18	40
All	All	5597/6490 (86%)	5180 (92%)	417 (8%)	14	33

All (417) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	16	LEU
1	O	23	SER
1	O	25	LEU
1	O	37	VAL
1	O	84	TRP
1	O	94	GLU
1	O	98	VAL
1	O	127	THR
1	O	133	ASN
1	O	152	ASN
1	O	169	LYS
1	O	172	MET
1	O	183	ARG
1	O	191	ARG
1	O	201	LEU
1	O	218	LEU
1	O	220	GLN
1	O	228	ILE
1	O	254	ASP
1	O	279	VAL
1	O	292	ILE
1	O	313	ASN
1	O	319	GLN
1	O	326	ASP
2	P	14	ASN
2	P	18	CYS
2	P	18(A)	TRP
2	P	18(B)	HIS

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Mol	Chain	Res	Type
2	P	25	LEU
2	P	39	GLN
2	P	84	TRP
2	P	92	VAL
2	P	133	ASN
2	P	152	ASN
2	P	172	MET
2	P	204	VAL
2	P	216	LEU
2	P	281	ILE
2	P	291	THR
2	P	326	ASP
1	Q	14	ASN
1	Q	16	LEU
1	Q	23	SER
1	Q	25	LEU
1	Q	37	VAL
1	Q	63	THR
1	Q	84	TRP
1	Q	94	GLU
1	Q	98	VAL
1	Q	122(A)	LYS
1	Q	124	ASP
1	Q	127	THR
1	Q	133	ASN
1	Q	152	ASN
1	Q	169	LYS
1	Q	172	MET
1	Q	183	ARG
1	Q	191	ARG
1	Q	201	LEU
1	Q	220	GLN
1	Q	228	ILE
1	Q	254	ASP
1	Q	279	VAL
1	Q	292	ILE
1	Q	313	ASN
1	Q	319	GLN
1	Q	326	ASP
1	Q	333	PRO
2	R	14	ASN
2	R	18	CYS

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Mol	Chain	Res	Type
2	R	18(A)	TRP
2	R	18(B)	HIS
2	R	39	GLN
2	R	84	TRP
2	R	92	VAL
2	R	133	ASN
2	R	152	ASN
2	R	172	MET
2	R	204	VAL
2	R	216	LEU
2	R	281	ILE
2	R	291	THR
2	R	326	ASP
2	R	333	GLN
1	A	16	LEU
1	A	23	SER
1	A	25	LEU
1	A	37	VAL
1	A	84	TRP
1	A	94	GLU
1	A	98	VAL
1	A	110	GLN
1	A	127	THR
1	A	133	ASN
1	A	152	ASN
1	A	169	LYS
1	A	172	MET
1	A	183	ARG
1	A	191	ARG
1	A	193	LEU
1	A	201	LEU
1	A	218	LEU
1	A	220	GLN
1	A	228	ILE
1	A	254	ASP
1	A	279	VAL
1	A	292	ILE
1	A	313	ASN
1	A	319	GLN
1	A	326	ASP
2	B	14	ASN
2	B	18	CYS

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Mol	Chain	Res	Type
2	B	18(A)	TRP
2	B	18(B)	HIS
2	B	25	LEU
2	B	39	GLN
2	B	84	TRP
2	B	92	VAL
2	B	133	ASN
2	B	152	ASN
2	B	172	MET
2	B	204	VAL
2	B	216	LEU
2	B	281	ILE
2	B	291	THR
2	B	302	ASP
2	B	326	ASP
1	C	14	ASN
1	C	16	LEU
1	C	23	SER
1	C	25	LEU
1	C	37	VAL
1	C	63	THR
1	C	84	TRP
1	C	94	GLU
1	C	98	VAL
1	C	110	GLN
1	C	127	THR
1	C	133	ASN
1	C	152	ASN
1	C	169	LYS
1	C	172	MET
1	C	183	ARG
1	C	191	ARG
1	C	201	LEU
1	C	220	GLN
1	C	228	ILE
1	C	254	ASP
1	C	279	VAL
1	C	292	ILE
1	C	313	ASN
1	C	319	GLN
1	C	326	ASP
1	C	333	PRO

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Mol	Chain	Res	Type
2	D	14	ASN
2	D	18	CYS
2	D	18(A)	TRP
2	D	18(B)	HIS
2	D	39	GLN
2	D	84	TRP
2	D	92	VAL
2	D	133	ASN
2	D	152	ASN
2	D	172	MET
2	D	204	VAL
2	D	216	LEU
2	D	281	ILE
2	D	291	THR
2	D	326	ASP
2	D	333	GLN
1	G	16	LEU
1	G	23	SER
1	G	25	LEU
1	G	37	VAL
1	G	84	TRP
1	G	94	GLU
1	G	98	VAL
1	G	127	THR
1	G	133	ASN
1	G	152	ASN
1	G	169	LYS
1	G	172	MET
1	G	183	ARG
1	G	191	ARG
1	G	201	LEU
1	G	218	LEU
1	G	220	GLN
1	G	228	ILE
1	G	254	ASP
1	G	279	VAL
1	G	292	ILE
1	G	313	ASN
1	G	319	GLN
1	G	326	ASP
2	H	14	ASN
2	H	18	CYS

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Mol	Chain	Res	Type
2	H	18(A)	TRP
2	H	18(B)	HIS
2	H	25	LEU
2	H	39	GLN
2	H	84	TRP
2	H	92	VAL
2	H	133	ASN
2	H	152	ASN
2	H	172	MET
2	H	204	VAL
2	H	216	LEU
2	H	281	ILE
2	H	291	THR
2	H	302	ASP
2	H	326	ASP
1	E	14	ASN
1	E	16	LEU
1	E	23	SER
1	E	25	LEU
1	E	37	VAL
1	E	63	THR
1	E	84	TRP
1	E	94	GLU
1	E	98	VAL
1	E	127	THR
1	E	133	ASN
1	E	152	ASN
1	E	169	LYS
1	E	172	MET
1	E	183	ARG
1	E	191	ARG
1	E	201	LEU
1	E	220	GLN
1	E	228	ILE
1	E	254	ASP
1	E	279	VAL
1	E	292	ILE
1	E	313	ASN
1	E	319	GLN
1	E	326	ASP
1	E	333	PRO
2	F	14	ASN

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Mol	Chain	Res	Type
2	F	18	CYS
2	F	18(A)	TRP
2	F	18(B)	HIS
2	F	39	GLN
2	F	84	TRP
2	F	92	VAL
2	F	133	ASN
2	F	152	ASN
2	F	172	MET
2	F	204	VAL
2	F	216	LEU
2	F	281	ILE
2	F	291	THR
2	F	326	ASP
2	F	333	GLN
1	I	16	LEU
1	I	23	SER
1	I	25	LEU
1	I	37	VAL
1	I	84	TRP
1	I	94	GLU
1	I	98	VAL
1	I	127	THR
1	I	133	ASN
1	I	152	ASN
1	I	169	LYS
1	I	172	MET
1	I	183	ARG
1	I	191	ARG
1	I	201	LEU
1	I	218	LEU
1	I	220	GLN
1	I	228	ILE
1	I	254	ASP
1	I	279	VAL
1	I	292	ILE
1	I	313	ASN
1	I	319	GLN
1	I	326	ASP
2	J	14	ASN
2	J	18	CYS
2	J	18(A)	TRP

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Mol	Chain	Res	Type
2	J	18(B)	HIS
2	J	25	LEU
2	J	39	GLN
2	J	84	TRP
2	J	92	VAL
2	J	133	ASN
2	J	152	ASN
2	J	172	MET
2	J	204	VAL
2	J	216	LEU
2	J	281	ILE
2	J	291	THR
2	J	302	ASP
2	J	326	ASP
1	K	14	ASN
1	K	16	LEU
1	K	23	SER
1	K	25	LEU
1	K	37	VAL
1	K	63	THR
1	K	84	TRP
1	K	94	GLU
1	K	98	VAL
1	K	127	THR
1	K	133	ASN
1	K	152	ASN
1	K	169	LYS
1	K	172	MET
1	K	183	ARG
1	K	191	ARG
1	K	201	LEU
1	K	220	GLN
1	K	228	ILE
1	K	254	ASP
1	K	279	VAL
1	K	292	ILE
1	K	313	ASN
1	K	319	GLN
1	K	326	ASP
2	L	14	ASN
2	L	18	CYS
2	L	18(A)	TRP

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Mol	Chain	Res	Type
2	L	18(B)	HIS
2	L	39	GLN
2	L	84	TRP
2	L	92	VAL
2	L	133	ASN
2	L	152	ASN
2	L	172	MET
2	L	204	VAL
2	L	216	LEU
2	L	281	ILE
2	L	291	THR
2	L	326	ASP
2	L	333	GLN
1	M	16	LEU
1	M	23	SER
1	M	25	LEU
1	M	37	VAL
1	M	84	TRP
1	M	94	GLU
1	M	98	VAL
1	M	127	THR
1	M	133	ASN
1	M	152	ASN
1	M	169	LYS
1	M	172	MET
1	M	183	ARG
1	M	191	ARG
1	M	201	LEU
1	M	218	LEU
1	M	220	GLN
1	M	228	ILE
1	M	254	ASP
1	M	279	VAL
1	M	292	ILE
1	M	313	ASN
1	M	319	GLN
1	M	326	ASP
2	N	14	ASN
2	N	18	CYS
2	N	18(A)	TRP
2	N	18(B)	HIS
2	N	25	LEU

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Mol	Chain	Res	Type
2	N	39	GLN
2	N	84	TRP
2	N	92	VAL
2	N	133	ASN
2	N	152	ASN
2	N	172	MET
2	N	204	VAL
2	N	216	LEU
2	N	281	ILE
2	N	291	THR
2	N	302	ASP
2	N	326	ASP
1	S	14	ASN
1	S	16	LEU
1	S	23	SER
1	S	25	LEU
1	S	37	VAL
1	S	63	THR
1	S	84	TRP
1	S	94	GLU
1	S	98	VAL
1	S	127	THR
1	S	133	ASN
1	S	152	ASN
1	S	169	LYS
1	S	172	MET
1	S	183	ARG
1	S	191	ARG
1	S	201	LEU
1	S	220	GLN
1	S	228	ILE
1	S	254	ASP
1	S	279	VAL
1	S	292	ILE
1	S	313	ASN
1	S	319	GLN
1	S	326	ASP
2	T	14	ASN
2	T	18	CYS
2	T	18(A)	TRP
2	T	18(B)	HIS
2	T	39	GLN

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Mol	Chain	Res	Type
2	T	84	TRP
2	T	92	VAL
2	T	133	ASN
2	T	152	ASN
2	T	172	MET
2	T	204	VAL
2	T	216	LEU
2	T	281	ILE
2	T	291	THR
2	T	326	ASP
2	T	333	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	14	ASN
1	O	220	GLN
1	O	245	ASN
1	O	319	GLN
1	O	330	ASN
2	P	14	ASN
2	P	39	GLN
2	P	42	HIS
2	P	133	ASN
2	P	139	HIS
2	P	152	ASN
2	P	176	HIS
2	P	182	GLN
2	P	202	ASN
2	P	256	ASN
2	P	319	GLN
2	P	333	GLN
1	Q	18(B)	HIS
1	Q	220	GLN
1	Q	319	GLN
1	Q	330	ASN
2	R	14	ASN
2	R	39	GLN
2	R	42	HIS
2	R	133	ASN
2	R	139	HIS
2	R	152	ASN

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Mol	Chain	Res	Type
2	R	182	GLN
2	R	202	ASN
2	R	256	ASN
2	R	319	GLN
2	R	333	GLN
1	A	14	ASN
1	A	146	ASN
1	A	220	GLN
1	A	245	ASN
1	A	319	GLN
1	A	330	ASN
2	B	14	ASN
2	B	39	GLN
2	B	42	HIS
2	B	133	ASN
2	B	139	HIS
2	B	152	ASN
2	B	176	HIS
2	B	182	GLN
2	B	202	ASN
2	B	256	ASN
2	B	319	GLN
2	B	333	GLN
1	C	110	GLN
1	C	182	GLN
1	C	220	GLN
1	C	319	GLN
1	C	330	ASN
2	D	14	ASN
2	D	39	GLN
2	D	133	ASN
2	D	139	HIS
2	D	152	ASN
2	D	182	GLN
2	D	202	ASN
2	D	256	ASN
2	D	319	GLN
2	D	333	GLN
1	G	220	GLN
1	G	245	ASN
1	G	319	GLN
1	G	330	ASN

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Mol	Chain	Res	Type
2	H	14	ASN
2	H	39	GLN
2	H	42	HIS
2	H	133	ASN
2	H	139	HIS
2	H	152	ASN
2	H	176	HIS
2	H	182	GLN
2	H	202	ASN
2	H	256	ASN
2	H	319	GLN
2	H	333	GLN
1	E	18(B)	HIS
1	E	182	GLN
1	E	220	GLN
1	E	319	GLN
1	E	330	ASN
2	F	14	ASN
2	F	39	GLN
2	F	133	ASN
2	F	139	HIS
2	F	152	ASN
2	F	163	GLN
2	F	182	GLN
2	F	202	ASN
2	F	256	ASN
2	F	319	GLN
2	F	333	GLN
1	I	14	ASN
1	I	146	ASN
1	I	220	GLN
1	I	245	ASN
1	I	319	GLN
1	I	330	ASN
2	J	14	ASN
2	J	39	GLN
2	J	42	HIS
2	J	133	ASN
2	J	139	HIS
2	J	152	ASN
2	J	176	HIS
2	J	182	GLN

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Mol	Chain	Res	Type
2	J	202	ASN
2	J	256	ASN
2	J	319	GLN
2	J	333	GLN
1	K	110	GLN
1	K	220	GLN
1	K	319	GLN
1	K	330	ASN
2	L	14	ASN
2	L	39	GLN
2	L	133	ASN
2	L	139	HIS
2	L	182	GLN
2	L	202	ASN
2	L	256	ASN
2	L	319	GLN
2	L	333	GLN
1	M	220	GLN
1	M	245	ASN
1	M	319	GLN
1	M	330	ASN
2	N	14	ASN
2	N	39	GLN
2	N	42	HIS
2	N	133	ASN
2	N	139	HIS
2	N	152	ASN
2	N	176	HIS
2	N	182	GLN
2	N	202	ASN
2	N	256	ASN
2	N	319	GLN
2	N	333	GLN
1	S	18(B)	HIS
1	S	182	GLN
1	S	220	GLN
1	S	319	GLN
1	S	330	ASN
2	T	14	ASN
2	T	39	GLN
2	T	133	ASN
2	T	139	HIS

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Mol	Chain	Res	Type
2	T	152	ASN
2	T	182	GLN
2	T	202	ASN
2	T	256	ASN
2	T	319	GLN
2	T	333	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAD	G	401	-	46,48,48	0.58	1 (2%)	64,73,73	0.54	1 (1%)
3	NAD	M	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.54	1 (1%)
3	NAD	R	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.52	1 (1%)
3	NAD	A	401	-	46,48,48	0.60	1 (2%)	64,73,73	0.54	1 (1%)
3	NAD	S	401	-	46,48,48	0.60	1 (2%)	64,73,73	0.53	1 (1%)
3	NAD	T	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.52	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	E	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.54	1 (1%)
3	NAD	F	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.52	1 (1%)
3	NAD	P	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.68	2 (3%)
3	NAD	O	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.53	1 (1%)
3	NAD	N	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.67	2 (3%)
3	NAD	D	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.52	1 (1%)
3	NAD	H	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.67	2 (3%)
3	NAD	Q	401	-	46,48,48	0.63	1 (2%)	64,73,73	0.55	1 (1%)
3	NAD	L	401	-	46,48,48	0.58	1 (2%)	64,73,73	0.52	1 (1%)
3	NAD	K	401	-	46,48,48	0.60	1 (2%)	64,73,73	0.53	1 (1%)
3	NAD	C	401	-	46,48,48	0.61	1 (2%)	64,73,73	0.54	1 (1%)
3	NAD	J	400	-	46,48,48	0.62	1 (2%)	64,73,73	0.70	2 (3%)
3	NAD	B	401	-	46,48,48	0.62	1 (2%)	64,73,73	0.66	2 (3%)
3	NAD	I	401	-	46,48,48	0.59	1 (2%)	64,73,73	0.54	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	G	401	-	-	19/30/62/62	0/5/5/5
3	NAD	M	401	-	-	19/30/62/62	0/5/5/5
3	NAD	R	401	-	-	20/30/62/62	0/5/5/5
3	NAD	A	401	-	-	19/30/62/62	0/5/5/5
3	NAD	S	401	-	-	19/30/62/62	0/5/5/5
3	NAD	T	401	-	-	20/30/62/62	0/5/5/5
3	NAD	E	401	-	-	19/30/62/62	0/5/5/5
3	NAD	F	401	-	-	20/30/62/62	0/5/5/5
3	NAD	P	401	-	-	15/30/62/62	0/5/5/5
3	NAD	O	401	-	-	19/30/62/62	0/5/5/5
3	NAD	N	401	-	-	15/30/62/62	0/5/5/5
3	NAD	D	401	-	-	20/30/62/62	0/5/5/5
3	NAD	H	401	-	-	14/30/62/62	0/5/5/5
3	NAD	Q	401	-	-	10/30/62/62	0/5/5/5
3	NAD	L	401	-	-	20/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	K	401	-	-	19/30/62/62	0/5/5/5
3	NAD	C	401	-	-	20/30/62/62	0/5/5/5
3	NAD	J	400	-	-	14/30/62/62	0/5/5/5
3	NAD	B	401	-	-	16/30/62/62	0/5/5/5
3	NAD	I	401	-	-	19/30/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	401	NAD	C2N-N1N	2.85	1.38	1.35
3	H	401	NAD	C2N-N1N	2.66	1.37	1.35
3	E	401	NAD	C2N-N1N	2.65	1.37	1.35
3	B	401	NAD	C2N-N1N	2.64	1.37	1.35
3	J	400	NAD	C2N-N1N	2.63	1.37	1.35
3	N	401	NAD	C2N-N1N	2.62	1.37	1.35
3	K	401	NAD	C2N-N1N	2.57	1.37	1.35
3	C	401	NAD	C2N-N1N	2.57	1.37	1.35
3	P	401	NAD	C2N-N1N	2.55	1.37	1.35
3	S	401	NAD	C2N-N1N	2.55	1.37	1.35
3	A	401	NAD	C2N-N1N	2.47	1.37	1.35
3	R	401	NAD	C2N-N1N	2.46	1.37	1.35
3	D	401	NAD	C2N-N1N	2.46	1.37	1.35
3	T	401	NAD	C2N-N1N	2.45	1.37	1.35
3	I	401	NAD	C2N-N1N	2.45	1.37	1.35
3	M	401	NAD	C2N-N1N	2.42	1.37	1.35
3	F	401	NAD	C2N-N1N	2.41	1.37	1.35
3	G	401	NAD	C2N-N1N	2.40	1.37	1.35
3	L	401	NAD	C2N-N1N	2.40	1.37	1.35
3	O	401	NAD	C2N-N1N	2.38	1.37	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	400	NAD	C6N-N1N-C2N	-3.26	119.10	121.88
3	P	401	NAD	C6N-N1N-C2N	-3.23	119.13	121.88
3	N	401	NAD	C6N-N1N-C2N	-3.05	119.28	121.88
3	H	401	NAD	C6N-N1N-C2N	-3.02	119.31	121.88
3	B	401	NAD	C6N-N1N-C2N	-2.91	119.40	121.88
3	E	401	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
3	S	401	NAD	C6N-N1N-C2N	-2.48	119.77	121.88
3	A	401	NAD	C6N-N1N-C2N	-2.48	119.77	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	401	NAD	C6N-N1N-C2N	-2.47	119.77	121.88
3	C	401	NAD	C6N-N1N-C2N	-2.47	119.78	121.88
3	G	401	NAD	C6N-N1N-C2N	-2.47	119.78	121.88
3	B	401	NAD	C4D-O4D-C1D	-2.46	107.67	109.92
3	Q	401	NAD	C6N-N1N-C2N	-2.46	119.78	121.88
3	K	401	NAD	C6N-N1N-C2N	-2.46	119.79	121.88
3	J	400	NAD	C4D-O4D-C1D	-2.45	107.68	109.92
3	I	401	NAD	C6N-N1N-C2N	-2.45	119.79	121.88
3	O	401	NAD	C6N-N1N-C2N	-2.43	119.81	121.88
3	N	401	NAD	C4D-O4D-C1D	-2.38	107.75	109.92
3	H	401	NAD	C4D-O4D-C1D	-2.37	107.76	109.92
3	L	401	NAD	C6N-N1N-C2N	-2.26	119.96	121.88
3	T	401	NAD	C6N-N1N-C2N	-2.19	120.01	121.88
3	R	401	NAD	C6N-N1N-C2N	-2.16	120.04	121.88
3	F	401	NAD	C6N-N1N-C2N	-2.16	120.04	121.88
3	D	401	NAD	C6N-N1N-C2N	-2.15	120.05	121.88
3	P	401	NAD	C4D-O4D-C1D	-2.12	107.98	109.92

There are no chirality outliers.

All (356) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	401	NAD	C5B-O5B-PA-O1A
3	O	401	NAD	C5B-O5B-PA-O3
3	O	401	NAD	C5D-O5D-PN-O3
3	O	401	NAD	C5D-O5D-PN-O1N
3	O	401	NAD	C5D-O5D-PN-O2N
3	O	401	NAD	O4D-C1D-N1N-C2N
3	O	401	NAD	C2N-C3N-C7N-O7N
3	O	401	NAD	C2N-C3N-C7N-N7N
3	P	401	NAD	C5B-O5B-PA-O1A
3	P	401	NAD	C5B-O5B-PA-O2A
3	P	401	NAD	C5B-O5B-PA-O3
3	P	401	NAD	C5D-O5D-PN-O3
3	P	401	NAD	C5D-O5D-PN-O1N
3	P	401	NAD	C5D-O5D-PN-O2N
3	Q	401	NAD	C5B-O5B-PA-O1A
3	Q	401	NAD	PN-O3-PA-O5B
3	Q	401	NAD	C5D-O5D-PN-O3
3	Q	401	NAD	C5D-O5D-PN-O1N
3	Q	401	NAD	C5D-O5D-PN-O2N
3	R	401	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	R	401	NAD	C5B-O5B-PA-O3
3	R	401	NAD	C5D-O5D-PN-O3
3	R	401	NAD	C5D-O5D-PN-O1N
3	R	401	NAD	O4D-C1D-N1N-C2N
3	R	401	NAD	O4D-C1D-N1N-C6N
3	R	401	NAD	C2D-C1D-N1N-C2N
3	R	401	NAD	C2D-C1D-N1N-C6N
3	R	401	NAD	C2N-C3N-C7N-N7N
3	A	401	NAD	C5B-O5B-PA-O1A
3	A	401	NAD	C5B-O5B-PA-O3
3	A	401	NAD	C5D-O5D-PN-O3
3	A	401	NAD	C5D-O5D-PN-O1N
3	A	401	NAD	C5D-O5D-PN-O2N
3	A	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	C2N-C3N-C7N-O7N
3	A	401	NAD	C2N-C3N-C7N-N7N
3	A	401	NAD	C4N-C3N-C7N-N7N
3	B	401	NAD	C5B-O5B-PA-O2A
3	B	401	NAD	C5B-O5B-PA-O3
3	B	401	NAD	C5D-O5D-PN-O3
3	B	401	NAD	C5D-O5D-PN-O1N
3	B	401	NAD	C5D-O5D-PN-O2N
3	C	401	NAD	C5B-O5B-PA-O1A
3	C	401	NAD	C5B-O5B-PA-O3
3	C	401	NAD	C5D-O5D-PN-O3
3	C	401	NAD	C5D-O5D-PN-O1N
3	C	401	NAD	C5D-O5D-PN-O2N
3	C	401	NAD	O4D-C1D-N1N-C2N
3	C	401	NAD	C2N-C3N-C7N-N7N
3	D	401	NAD	C5B-O5B-PA-O2A
3	D	401	NAD	C5B-O5B-PA-O3
3	D	401	NAD	C5D-O5D-PN-O3
3	D	401	NAD	C5D-O5D-PN-O1N
3	D	401	NAD	O4D-C1D-N1N-C2N
3	D	401	NAD	O4D-C1D-N1N-C6N
3	D	401	NAD	C2D-C1D-N1N-C2N
3	D	401	NAD	C2D-C1D-N1N-C6N
3	D	401	NAD	C2N-C3N-C7N-N7N
3	G	401	NAD	C5B-O5B-PA-O1A
3	G	401	NAD	C5B-O5B-PA-O3
3	G	401	NAD	C5D-O5D-PN-O3
3	G	401	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
3	G	401	NAD	C5D-O5D-PN-O2N
3	G	401	NAD	O4D-C1D-N1N-C2N
3	G	401	NAD	C2N-C3N-C7N-O7N
3	G	401	NAD	C2N-C3N-C7N-N7N
3	H	401	NAD	C5B-O5B-PA-O2A
3	H	401	NAD	C5B-O5B-PA-O3
3	H	401	NAD	PN-O3-PA-O5B
3	H	401	NAD	C5D-O5D-PN-O3
3	H	401	NAD	C5D-O5D-PN-O1N
3	H	401	NAD	C5D-O5D-PN-O2N
3	E	401	NAD	C5B-O5B-PA-O1A
3	E	401	NAD	C5B-O5B-PA-O3
3	E	401	NAD	C5D-O5D-PN-O3
3	E	401	NAD	C5D-O5D-PN-O1N
3	E	401	NAD	C5D-O5D-PN-O2N
3	E	401	NAD	O4D-C1D-N1N-C2N
3	E	401	NAD	C2N-C3N-C7N-N7N
3	F	401	NAD	C5B-O5B-PA-O2A
3	F	401	NAD	C5B-O5B-PA-O3
3	F	401	NAD	C5D-O5D-PN-O3
3	F	401	NAD	C5D-O5D-PN-O1N
3	F	401	NAD	O4D-C1D-N1N-C2N
3	F	401	NAD	O4D-C1D-N1N-C6N
3	F	401	NAD	C2D-C1D-N1N-C2N
3	F	401	NAD	C2D-C1D-N1N-C6N
3	F	401	NAD	C2N-C3N-C7N-N7N
3	I	401	NAD	C5B-O5B-PA-O1A
3	I	401	NAD	C5B-O5B-PA-O3
3	I	401	NAD	C5D-O5D-PN-O3
3	I	401	NAD	C5D-O5D-PN-O1N
3	I	401	NAD	C5D-O5D-PN-O2N
3	I	401	NAD	O4D-C1D-N1N-C2N
3	I	401	NAD	C2N-C3N-C7N-O7N
3	I	401	NAD	C2N-C3N-C7N-N7N
3	J	400	NAD	C5B-O5B-PA-O2A
3	J	400	NAD	C5B-O5B-PA-O3
3	J	400	NAD	PN-O3-PA-O5B
3	J	400	NAD	C5D-O5D-PN-O3
3	J	400	NAD	C5D-O5D-PN-O1N
3	J	400	NAD	C5D-O5D-PN-O2N
3	K	401	NAD	C5B-O5B-PA-O1A
3	K	401	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
3	K	401	NAD	C5D-O5D-PN-O3
3	K	401	NAD	C5D-O5D-PN-O1N
3	K	401	NAD	C5D-O5D-PN-O2N
3	K	401	NAD	O4D-C1D-N1N-C2N
3	K	401	NAD	C2N-C3N-C7N-N7N
3	L	401	NAD	C5B-O5B-PA-O2A
3	L	401	NAD	C5B-O5B-PA-O3
3	L	401	NAD	C5D-O5D-PN-O3
3	L	401	NAD	C5D-O5D-PN-O1N
3	L	401	NAD	O4D-C1D-N1N-C2N
3	L	401	NAD	O4D-C1D-N1N-C6N
3	L	401	NAD	C2D-C1D-N1N-C2N
3	L	401	NAD	C2D-C1D-N1N-C6N
3	L	401	NAD	C2N-C3N-C7N-N7N
3	M	401	NAD	C5B-O5B-PA-O1A
3	M	401	NAD	C5B-O5B-PA-O3
3	M	401	NAD	C5D-O5D-PN-O3
3	M	401	NAD	C5D-O5D-PN-O1N
3	M	401	NAD	C5D-O5D-PN-O2N
3	M	401	NAD	O4D-C1D-N1N-C2N
3	M	401	NAD	C2N-C3N-C7N-O7N
3	M	401	NAD	C2N-C3N-C7N-N7N
3	N	401	NAD	C5B-O5B-PA-O2A
3	N	401	NAD	C5B-O5B-PA-O3
3	N	401	NAD	PN-O3-PA-O5B
3	N	401	NAD	C5D-O5D-PN-O3
3	N	401	NAD	C5D-O5D-PN-O1N
3	N	401	NAD	C5D-O5D-PN-O2N
3	S	401	NAD	C5B-O5B-PA-O1A
3	S	401	NAD	C5B-O5B-PA-O3
3	S	401	NAD	C5D-O5D-PN-O3
3	S	401	NAD	C5D-O5D-PN-O1N
3	S	401	NAD	C5D-O5D-PN-O2N
3	S	401	NAD	O4D-C1D-N1N-C2N
3	S	401	NAD	C2N-C3N-C7N-N7N
3	T	401	NAD	C5B-O5B-PA-O2A
3	T	401	NAD	C5B-O5B-PA-O3
3	T	401	NAD	C5D-O5D-PN-O3
3	T	401	NAD	C5D-O5D-PN-O1N
3	T	401	NAD	O4D-C1D-N1N-C2N
3	T	401	NAD	O4D-C1D-N1N-C6N
3	T	401	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	T	401	NAD	C2D-C1D-N1N-C6N
3	T	401	NAD	C2N-C3N-C7N-N7N
3	O	401	NAD	C4N-C3N-C7N-O7N
3	O	401	NAD	C4N-C3N-C7N-N7N
3	A	401	NAD	C4N-C3N-C7N-O7N
3	G	401	NAD	C4N-C3N-C7N-O7N
3	G	401	NAD	C4N-C3N-C7N-N7N
3	I	401	NAD	C4N-C3N-C7N-O7N
3	I	401	NAD	C4N-C3N-C7N-N7N
3	M	401	NAD	C4N-C3N-C7N-O7N
3	M	401	NAD	C4N-C3N-C7N-N7N
3	C	401	NAD	C4N-C3N-C7N-N7N
3	S	401	NAD	C4N-C3N-C7N-N7N
3	C	401	NAD	C4N-C3N-C7N-O7N
3	E	401	NAD	C4N-C3N-C7N-N7N
3	F	401	NAD	C4N-C3N-C7N-N7N
3	K	401	NAD	C4N-C3N-C7N-O7N
3	K	401	NAD	C4N-C3N-C7N-N7N
3	L	401	NAD	C4N-C3N-C7N-N7N
3	S	401	NAD	C4N-C3N-C7N-O7N
3	T	401	NAD	C4N-C3N-C7N-N7N
3	R	401	NAD	C4N-C3N-C7N-N7N
3	D	401	NAD	C4N-C3N-C7N-N7N
3	E	401	NAD	C4N-C3N-C7N-O7N
3	R	401	NAD	C2N-C3N-C7N-O7N
3	C	401	NAD	C2N-C3N-C7N-O7N
3	D	401	NAD	C2N-C3N-C7N-O7N
3	E	401	NAD	C2N-C3N-C7N-O7N
3	F	401	NAD	C2N-C3N-C7N-O7N
3	K	401	NAD	C2N-C3N-C7N-O7N
3	L	401	NAD	C2N-C3N-C7N-O7N
3	S	401	NAD	C2N-C3N-C7N-O7N
3	T	401	NAD	C2N-C3N-C7N-O7N
3	F	401	NAD	C4N-C3N-C7N-O7N
3	L	401	NAD	C4N-C3N-C7N-O7N
3	T	401	NAD	C4N-C3N-C7N-O7N
3	R	401	NAD	C4N-C3N-C7N-O7N
3	D	401	NAD	C4N-C3N-C7N-O7N
3	L	401	NAD	C3D-C4D-C5D-O5D
3	P	401	NAD	C2N-C3N-C7N-O7N
3	P	401	NAD	C2N-C3N-C7N-N7N
3	H	401	NAD	C2N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
3	J	400	NAD	C2N-C3N-C7N-O7N
3	J	400	NAD	C2N-C3N-C7N-N7N
3	N	401	NAD	C2N-C3N-C7N-O7N
3	P	401	NAD	C4N-C3N-C7N-N7N
3	N	401	NAD	C2N-C3N-C7N-N7N
3	J	400	NAD	C4N-C3N-C7N-N7N
3	R	401	NAD	O4B-C4B-C5B-O5B
3	R	401	NAD	O4D-C4D-C5D-O5D
3	R	401	NAD	C3D-C4D-C5D-O5D
3	B	401	NAD	O4B-C4B-C5B-O5B
3	D	401	NAD	O4B-C4B-C5B-O5B
3	D	401	NAD	O4D-C4D-C5D-O5D
3	D	401	NAD	C3D-C4D-C5D-O5D
3	H	401	NAD	O4B-C4B-C5B-O5B
3	F	401	NAD	O4B-C4B-C5B-O5B
3	F	401	NAD	O4D-C4D-C5D-O5D
3	F	401	NAD	C3D-C4D-C5D-O5D
3	L	401	NAD	O4B-C4B-C5B-O5B
3	L	401	NAD	O4D-C4D-C5D-O5D
3	N	401	NAD	O4B-C4B-C5B-O5B
3	T	401	NAD	O4B-C4B-C5B-O5B
3	T	401	NAD	O4D-C4D-C5D-O5D
3	T	401	NAD	C3D-C4D-C5D-O5D
3	P	401	NAD	C4N-C3N-C7N-O7N
3	H	401	NAD	C4N-C3N-C7N-N7N
3	N	401	NAD	C4N-C3N-C7N-N7N
3	H	401	NAD	C2N-C3N-C7N-N7N
3	J	400	NAD	C4N-C3N-C7N-O7N
3	N	401	NAD	C4N-C3N-C7N-O7N
3	B	401	NAD	C2N-C3N-C7N-O7N
3	B	401	NAD	C2N-C3N-C7N-N7N
3	B	401	NAD	C4N-C3N-C7N-N7N
3	H	401	NAD	C4N-C3N-C7N-O7N
3	R	401	NAD	C3B-C4B-C5B-O5B
3	B	401	NAD	C3B-C4B-C5B-O5B
3	D	401	NAD	C3B-C4B-C5B-O5B
3	H	401	NAD	C3B-C4B-C5B-O5B
3	F	401	NAD	C3B-C4B-C5B-O5B
3	J	400	NAD	O4B-C4B-C5B-O5B
3	J	400	NAD	C3B-C4B-C5B-O5B
3	L	401	NAD	C3B-C4B-C5B-O5B
3	N	401	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	T	401	NAD	C3B-C4B-C5B-O5B
3	B	401	NAD	C4N-C3N-C7N-O7N
3	P	401	NAD	O4B-C4B-C5B-O5B
3	P	401	NAD	C3B-C4B-C5B-O5B
3	A	401	NAD	O4D-C4D-C5D-O5D
3	G	401	NAD	O4D-C4D-C5D-O5D
3	M	401	NAD	O4D-C4D-C5D-O5D
3	O	401	NAD	O4D-C4D-C5D-O5D
3	C	401	NAD	O4D-C4D-C5D-O5D
3	E	401	NAD	O4D-C4D-C5D-O5D
3	I	401	NAD	O4D-C4D-C5D-O5D
3	K	401	NAD	O4D-C4D-C5D-O5D
3	S	401	NAD	O4D-C4D-C5D-O5D
3	Q	401	NAD	O4B-C4B-C5B-O5B
3	C	401	NAD	O4B-C4B-C5B-O5B
3	E	401	NAD	O4B-C4B-C5B-O5B
3	K	401	NAD	O4B-C4B-C5B-O5B
3	S	401	NAD	O4B-C4B-C5B-O5B
3	O	401	NAD	C3D-C4D-C5D-O5D
3	A	401	NAD	C3D-C4D-C5D-O5D
3	C	401	NAD	C3D-C4D-C5D-O5D
3	G	401	NAD	C3D-C4D-C5D-O5D
3	I	401	NAD	C3D-C4D-C5D-O5D
3	M	401	NAD	C3D-C4D-C5D-O5D
3	O	401	NAD	PA-O3-PN-O1N
3	A	401	NAD	PA-O3-PN-O1N
3	G	401	NAD	PA-O3-PN-O1N
3	I	401	NAD	PA-O3-PN-O1N
3	M	401	NAD	PA-O3-PN-O1N
3	O	401	NAD	O4B-C4B-C5B-O5B
3	Q	401	NAD	C3B-C4B-C5B-O5B
3	A	401	NAD	O4B-C4B-C5B-O5B
3	C	401	NAD	C3B-C4B-C5B-O5B
3	G	401	NAD	O4B-C4B-C5B-O5B
3	E	401	NAD	C3B-C4B-C5B-O5B
3	I	401	NAD	O4B-C4B-C5B-O5B
3	K	401	NAD	C3B-C4B-C5B-O5B
3	M	401	NAD	O4B-C4B-C5B-O5B
3	S	401	NAD	C3B-C4B-C5B-O5B
3	E	401	NAD	C3D-C4D-C5D-O5D
3	K	401	NAD	C3D-C4D-C5D-O5D
3	S	401	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	O	401	NAD	PN-O3-PA-O5B
3	P	401	NAD	PN-O3-PA-O5B
3	R	401	NAD	PN-O3-PA-O5B
3	R	401	NAD	PA-O3-PN-O5D
3	A	401	NAD	PN-O3-PA-O5B
3	B	401	NAD	PN-O3-PA-O5B
3	C	401	NAD	PN-O3-PA-O5B
3	D	401	NAD	PN-O3-PA-O5B
3	D	401	NAD	PA-O3-PN-O5D
3	G	401	NAD	PN-O3-PA-O5B
3	E	401	NAD	PN-O3-PA-O5B
3	F	401	NAD	PN-O3-PA-O5B
3	F	401	NAD	PA-O3-PN-O5D
3	I	401	NAD	PN-O3-PA-O5B
3	K	401	NAD	PN-O3-PA-O5B
3	L	401	NAD	PN-O3-PA-O5B
3	L	401	NAD	PA-O3-PN-O5D
3	M	401	NAD	PN-O3-PA-O5B
3	S	401	NAD	PN-O3-PA-O5B
3	T	401	NAD	PN-O3-PA-O5B
3	T	401	NAD	PA-O3-PN-O5D
3	O	401	NAD	C3B-C4B-C5B-O5B
3	A	401	NAD	C3B-C4B-C5B-O5B
3	G	401	NAD	C3B-C4B-C5B-O5B
3	I	401	NAD	C3B-C4B-C5B-O5B
3	M	401	NAD	C3B-C4B-C5B-O5B
3	O	401	NAD	C5B-O5B-PA-O2A
3	Q	401	NAD	C5B-O5B-PA-O3
3	A	401	NAD	C5B-O5B-PA-O2A
3	C	401	NAD	C5B-O5B-PA-O2A
3	G	401	NAD	C5B-O5B-PA-O2A
3	E	401	NAD	C5B-O5B-PA-O2A
3	I	401	NAD	C5B-O5B-PA-O2A
3	K	401	NAD	C5B-O5B-PA-O2A
3	M	401	NAD	C5B-O5B-PA-O2A
3	S	401	NAD	C5B-O5B-PA-O2A
3	O	401	NAD	PA-O3-PN-O2N
3	A	401	NAD	PA-O3-PN-O2N
3	C	401	NAD	PA-O3-PN-O1N
3	G	401	NAD	PA-O3-PN-O2N
3	E	401	NAD	PA-O3-PN-O1N
3	I	401	NAD	PA-O3-PN-O2N

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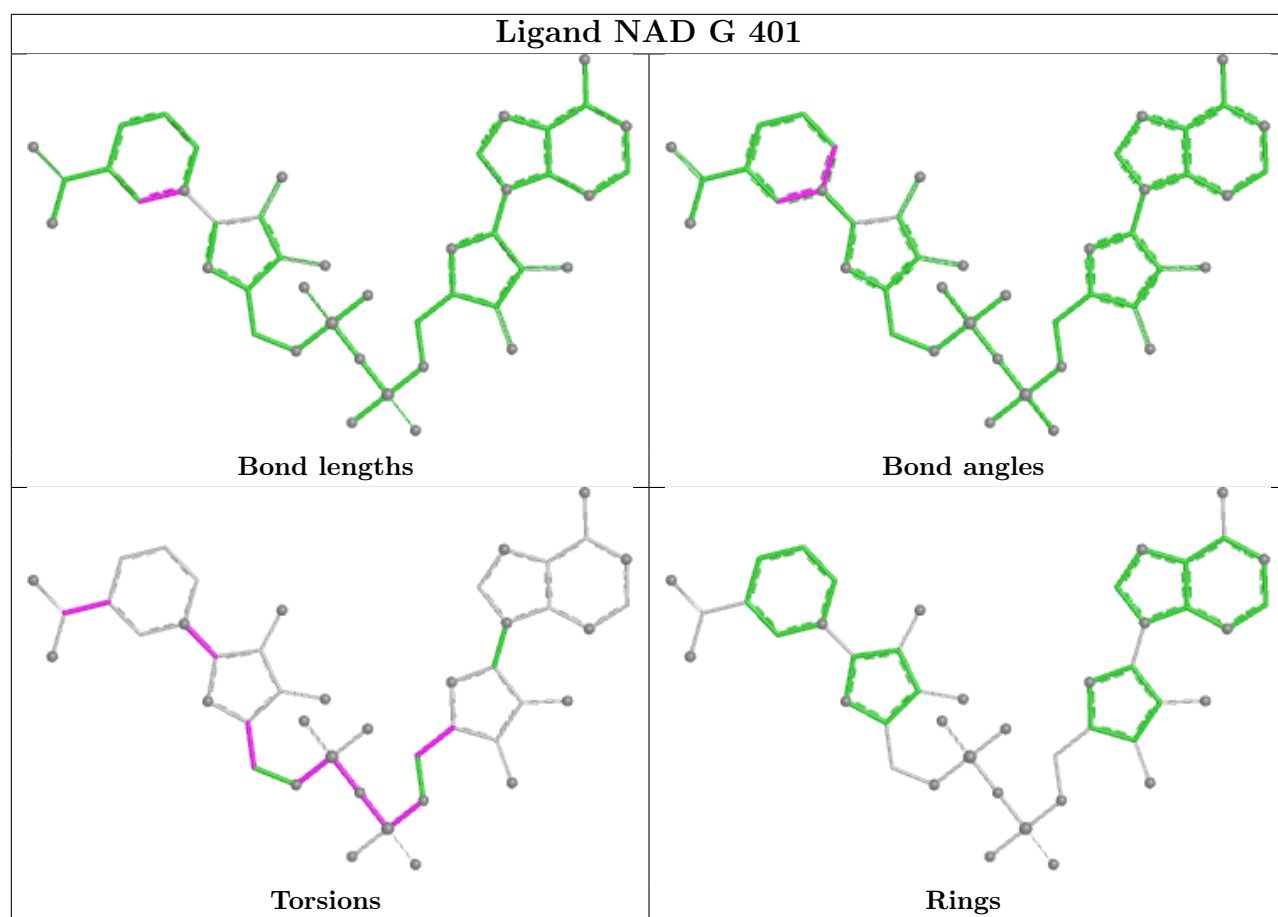
Mol	Chain	Res	Type	Atoms
3	K	401	NAD	PA-O3-PN-O1N
3	M	401	NAD	PA-O3-PN-O2N
3	S	401	NAD	PA-O3-PN-O1N
3	P	401	NAD	C4B-C5B-O5B-PA
3	R	401	NAD	C4B-C5B-O5B-PA
3	D	401	NAD	C4B-C5B-O5B-PA
3	T	401	NAD	C4B-C5B-O5B-PA
3	O	401	NAD	O4D-C1D-N1N-C6N
3	A	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	C	401	NAD	O4D-C1D-N1N-C6N
3	G	401	NAD	O4D-C1D-N1N-C6N
3	E	401	NAD	O4D-C1D-N1N-C6N
3	I	401	NAD	O4D-C1D-N1N-C6N
3	K	401	NAD	O4D-C1D-N1N-C6N
3	M	401	NAD	O4D-C1D-N1N-C6N
3	S	401	NAD	O4D-C1D-N1N-C6N
3	F	401	NAD	C4B-C5B-O5B-PA
3	L	401	NAD	C4B-C5B-O5B-PA
3	J	400	NAD	C4B-C5B-O5B-PA
3	Q	401	NAD	PA-O3-PN-O2N
3	R	401	NAD	PN-O3-PA-O2A
3	C	401	NAD	PA-O3-PN-O2N
3	D	401	NAD	PN-O3-PA-O2A
3	H	401	NAD	PN-O3-PA-O1A
3	E	401	NAD	PA-O3-PN-O2N
3	F	401	NAD	PN-O3-PA-O2A
3	K	401	NAD	PA-O3-PN-O2N
3	L	401	NAD	PN-O3-PA-O2A
3	N	401	NAD	PN-O3-PA-O1A
3	S	401	NAD	PA-O3-PN-O2N
3	T	401	NAD	PN-O3-PA-O2A
3	Q	401	NAD	C4N-C3N-C7N-N7N
3	B	401	NAD	C4B-C5B-O5B-PA
3	H	401	NAD	C4B-C5B-O5B-PA
3	N	401	NAD	C4B-C5B-O5B-PA
3	C	401	NAD	C4D-C5D-O5D-PN
3	P	401	NAD	PN-O3-PA-O1A
3	B	401	NAD	PN-O3-PA-O1A
3	B	401	NAD	PN-O3-PA-O2A
3	J	400	NAD	PN-O3-PA-O1A
3	N	401	NAD	PN-O3-PA-O2A

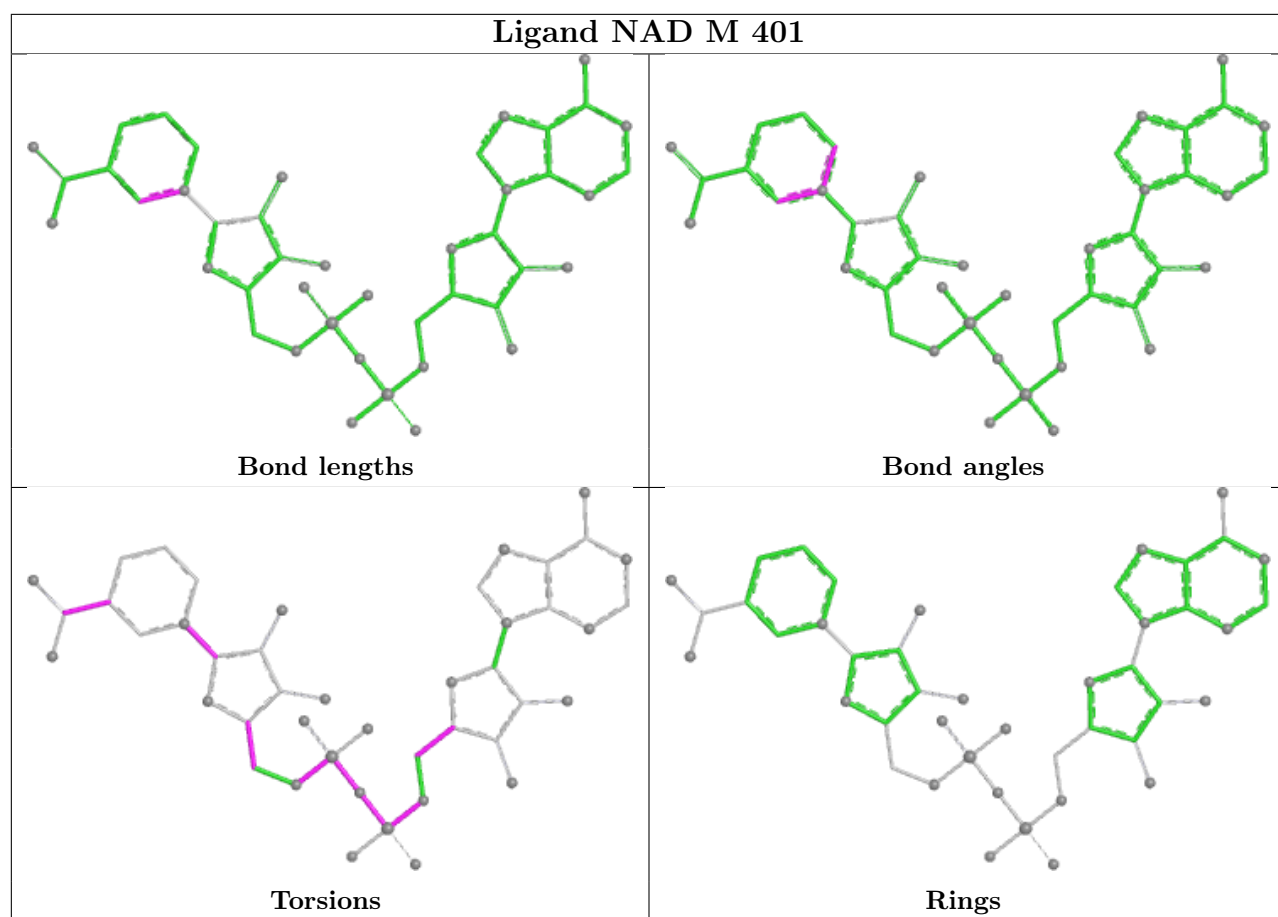
There are no ring outliers.

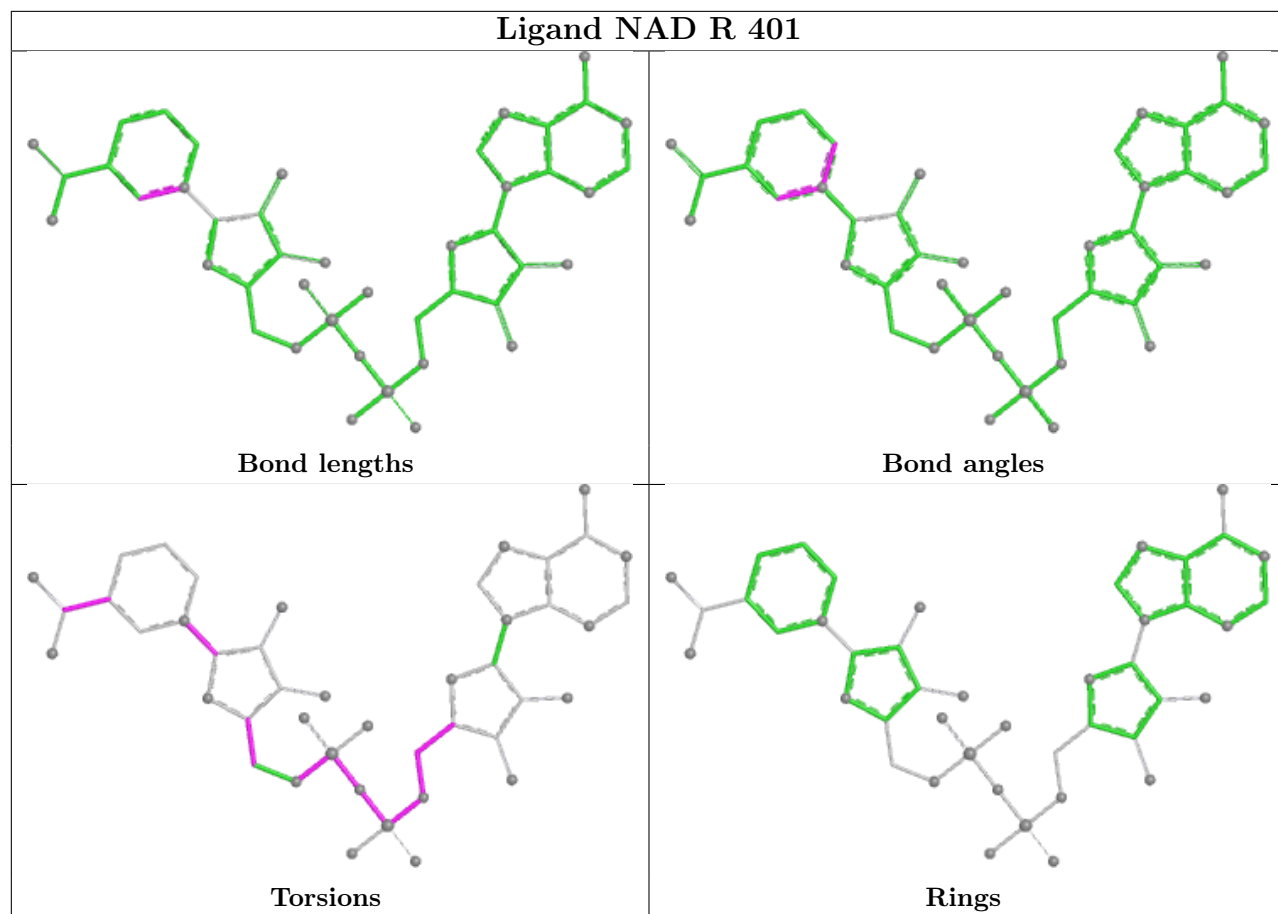
15 monomers are involved in 15 short contacts:

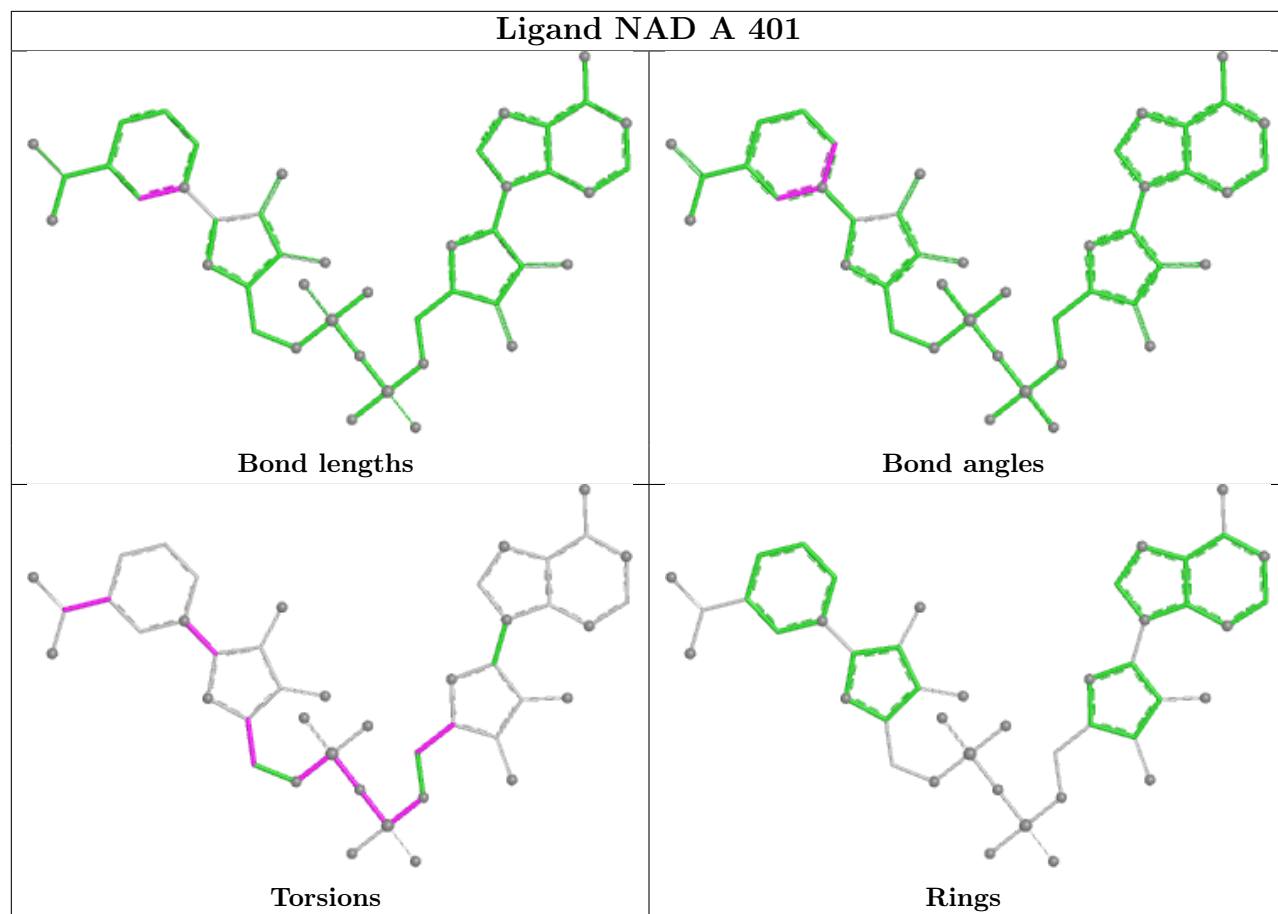
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	NAD	1	0
3	M	401	NAD	1	0
3	R	401	NAD	1	0
3	A	401	NAD	1	0
3	S	401	NAD	1	0
3	T	401	NAD	1	0
3	E	401	NAD	1	0
3	F	401	NAD	1	0
3	O	401	NAD	1	0
3	D	401	NAD	1	0
3	Q	401	NAD	1	0
3	L	401	NAD	1	0
3	K	401	NAD	1	0
3	C	401	NAD	1	0
3	I	401	NAD	1	0

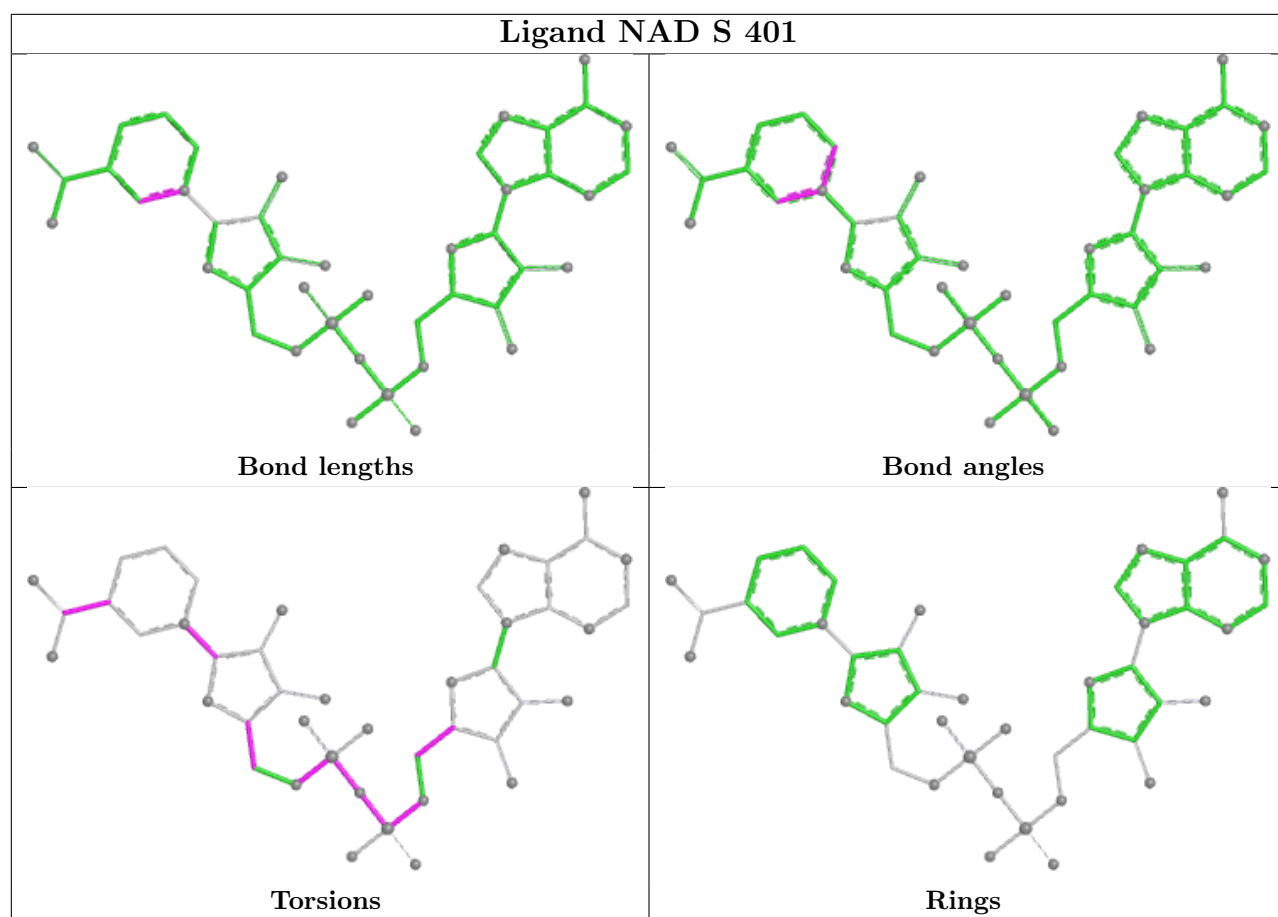
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

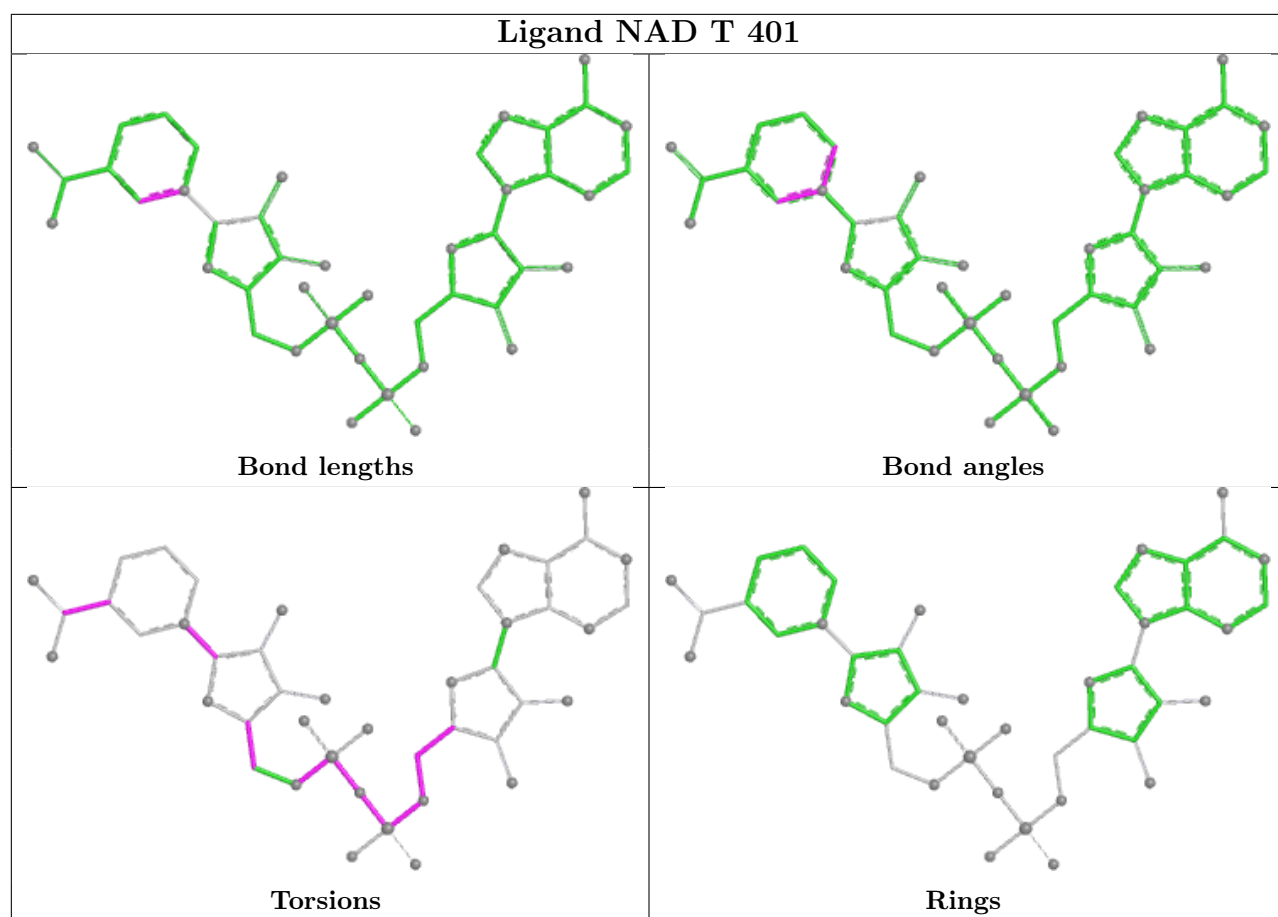


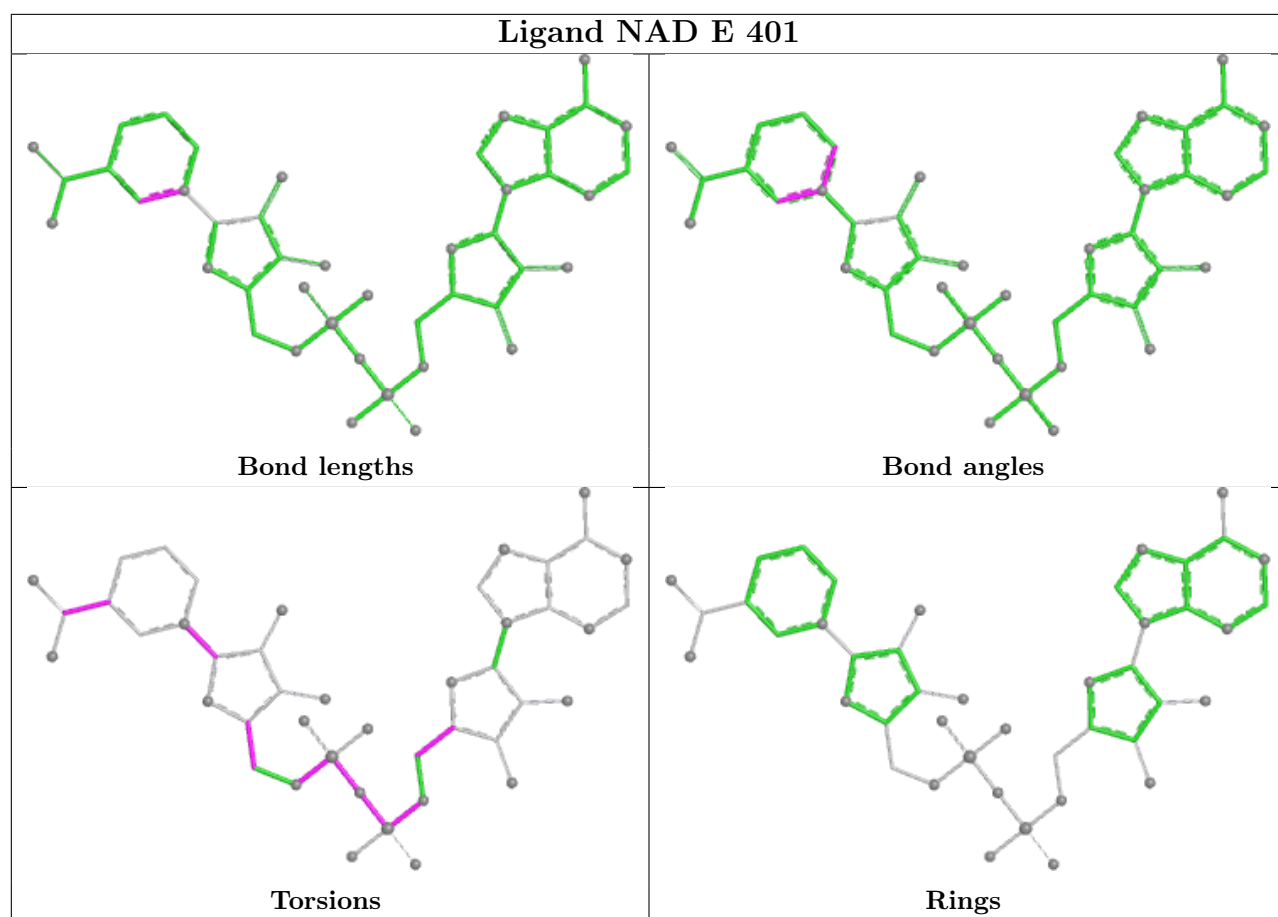


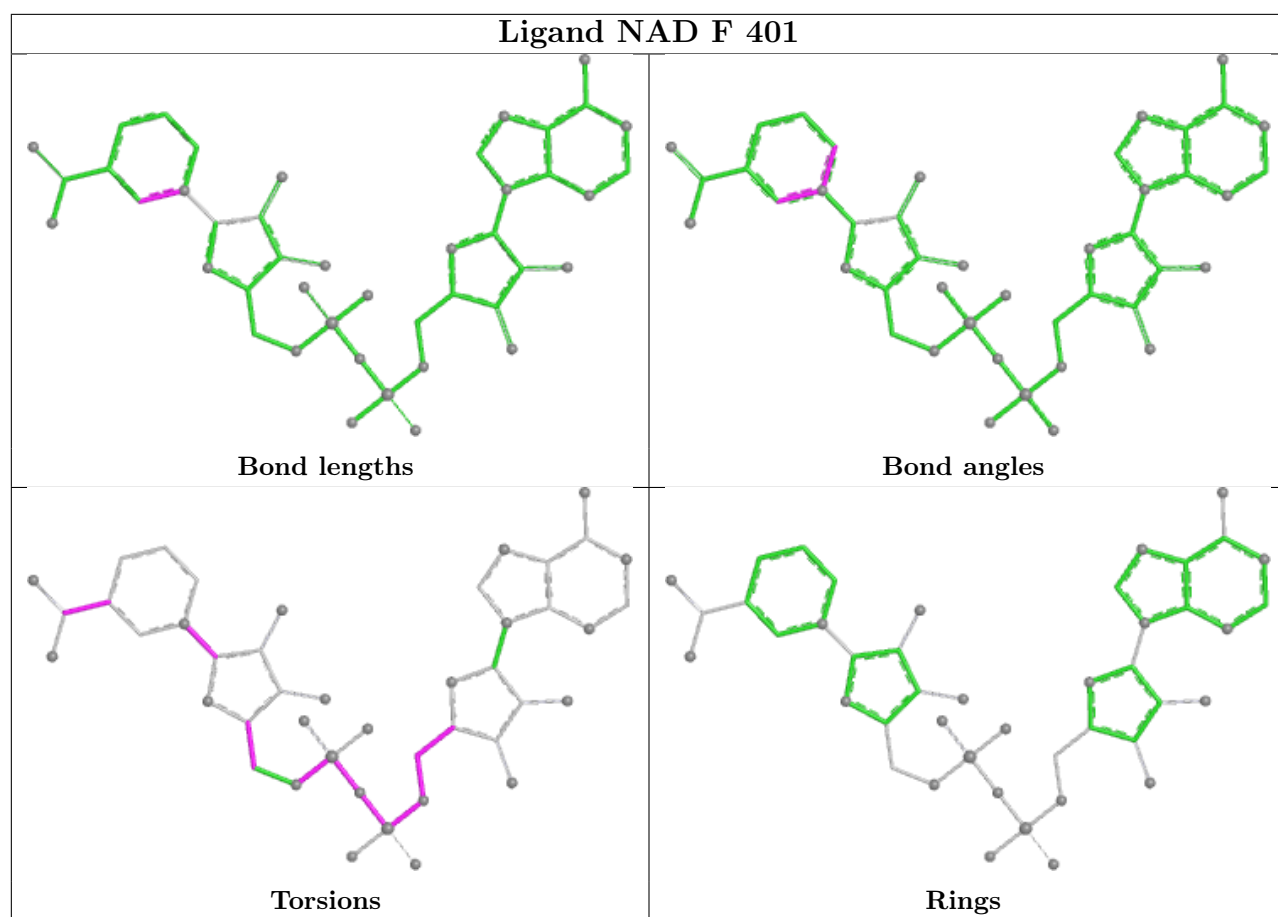


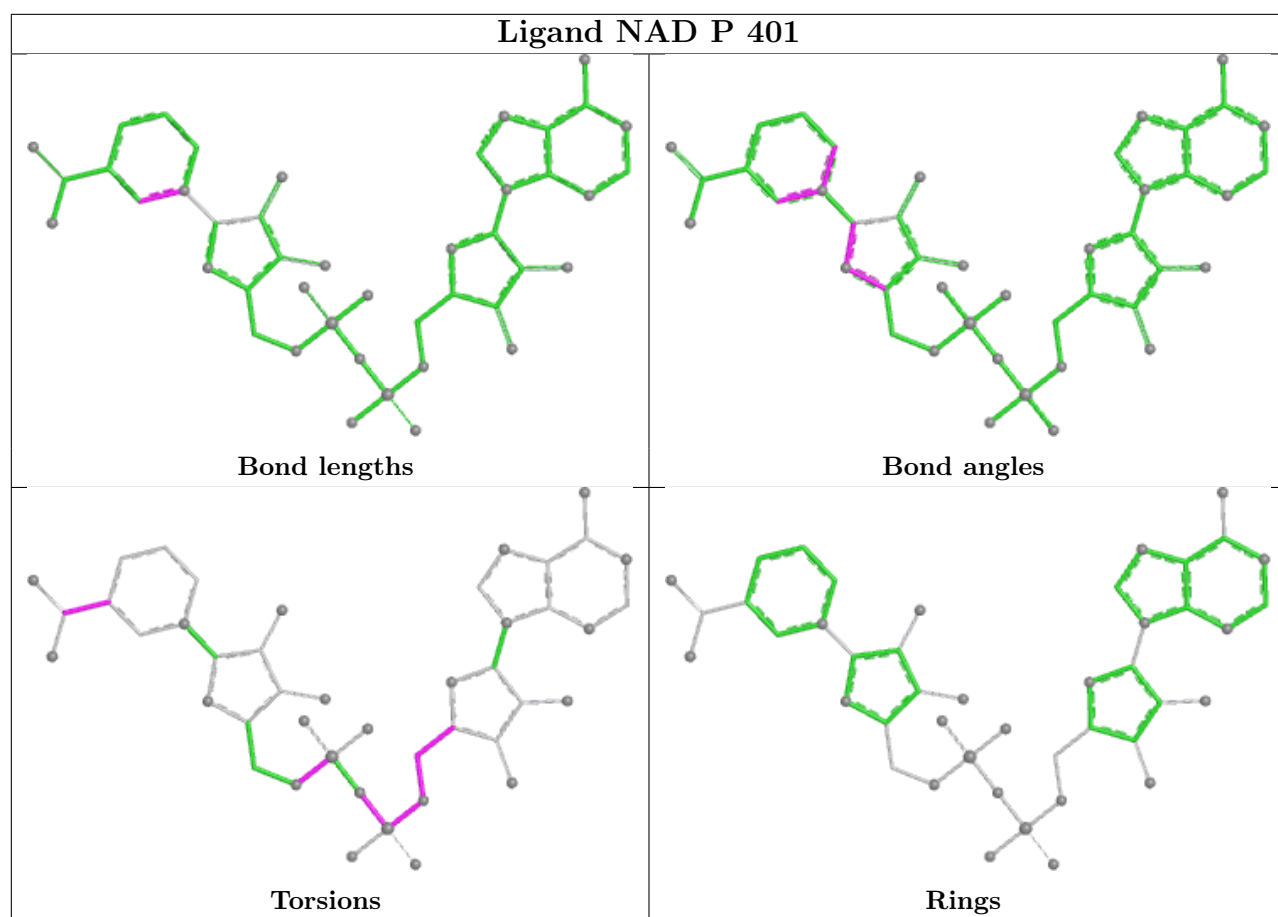


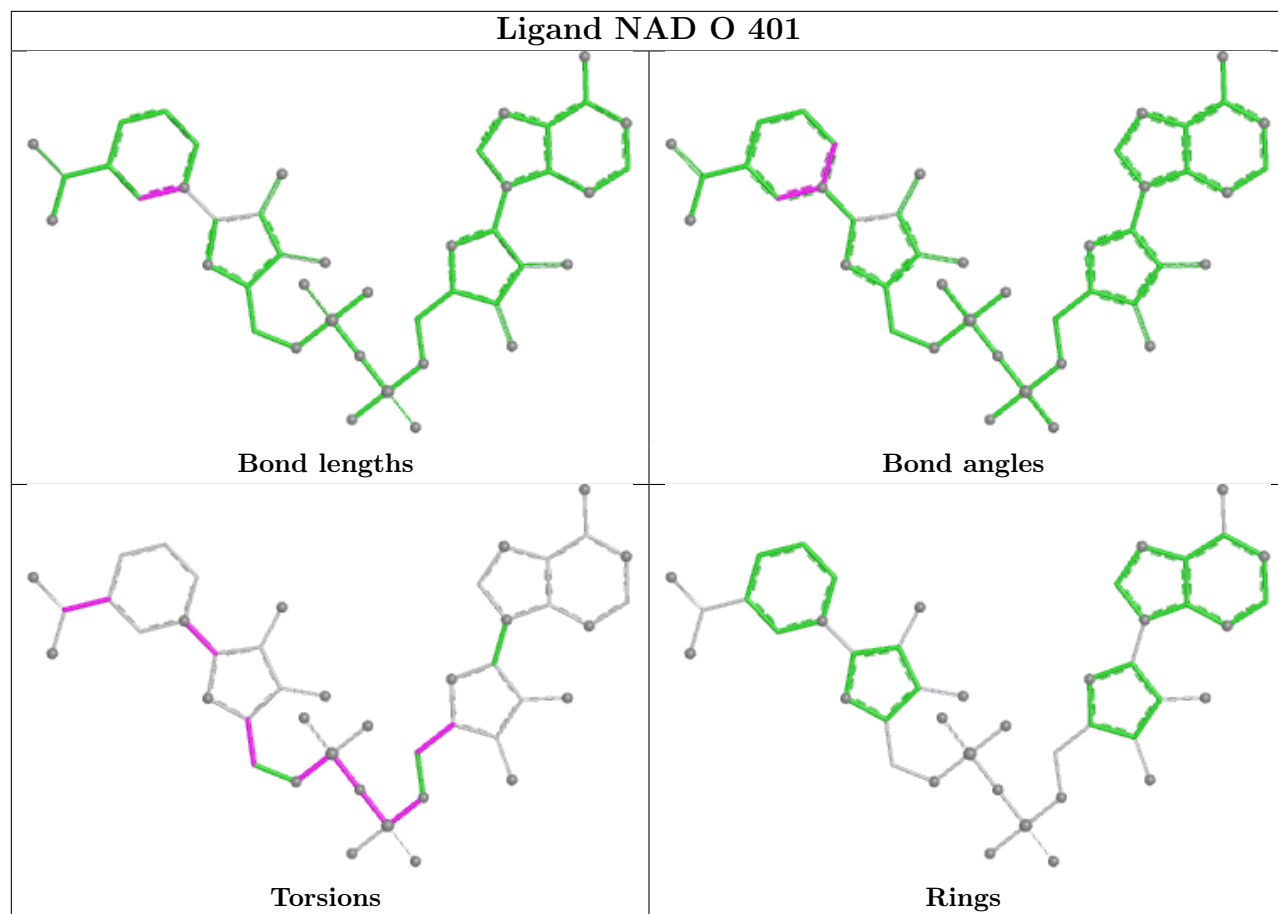


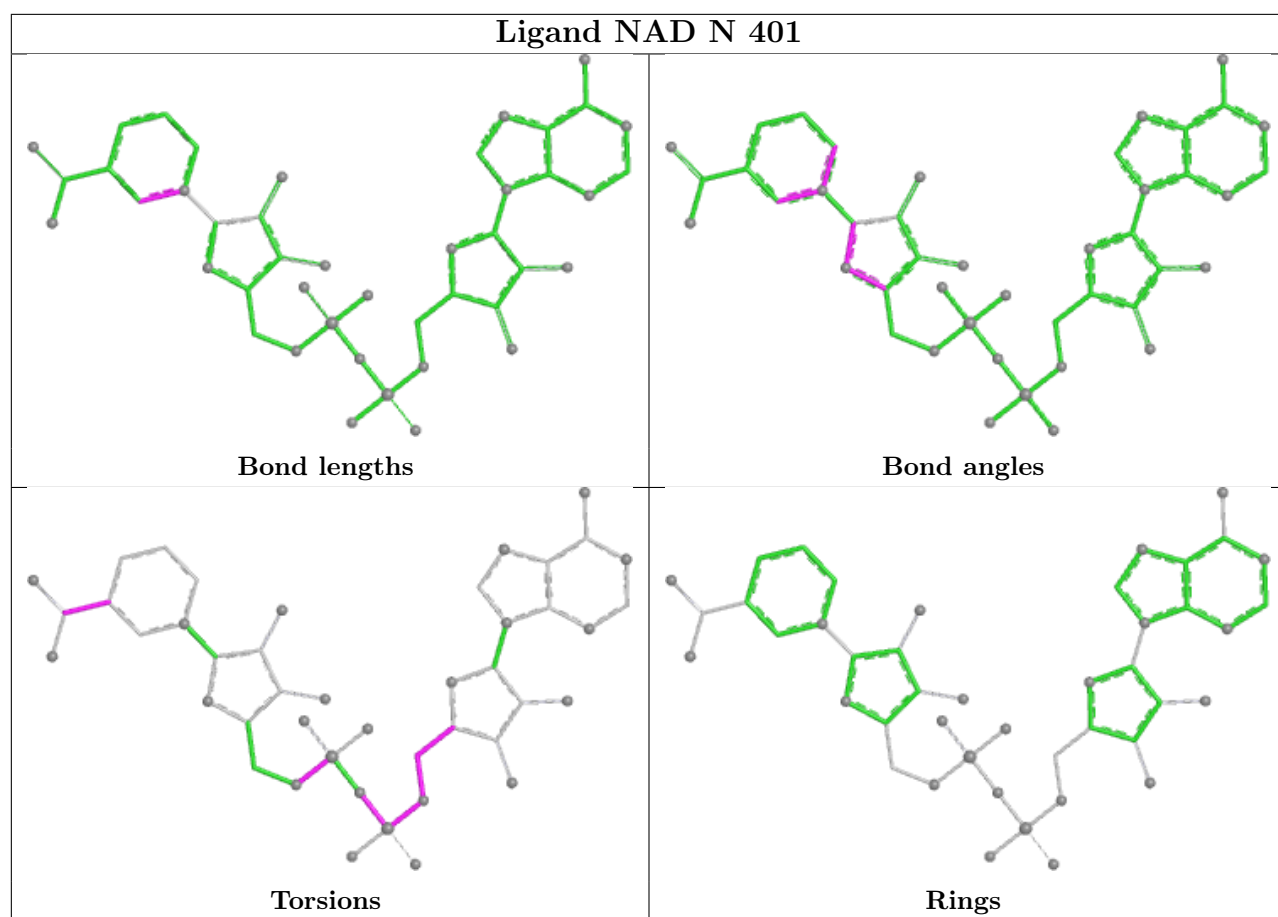


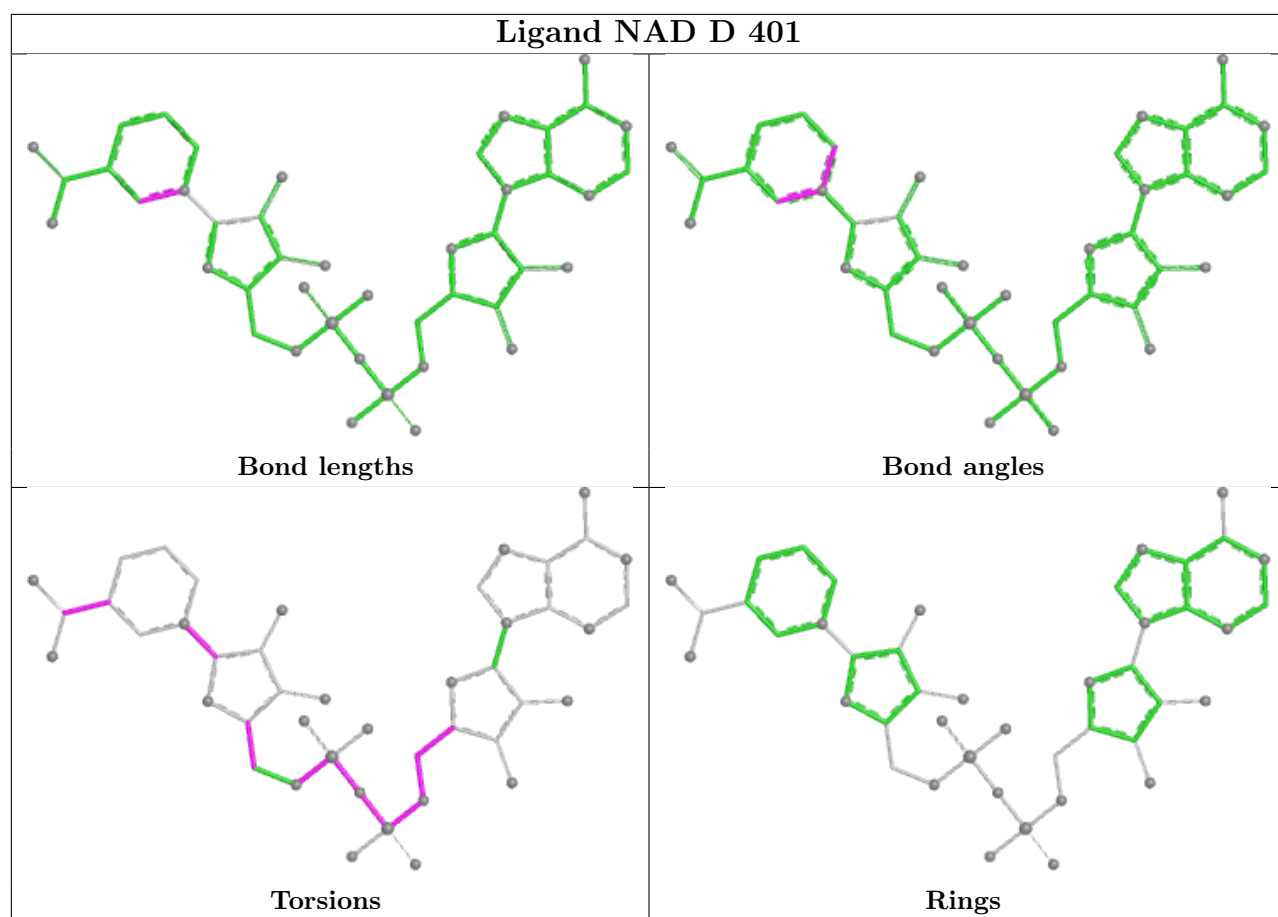


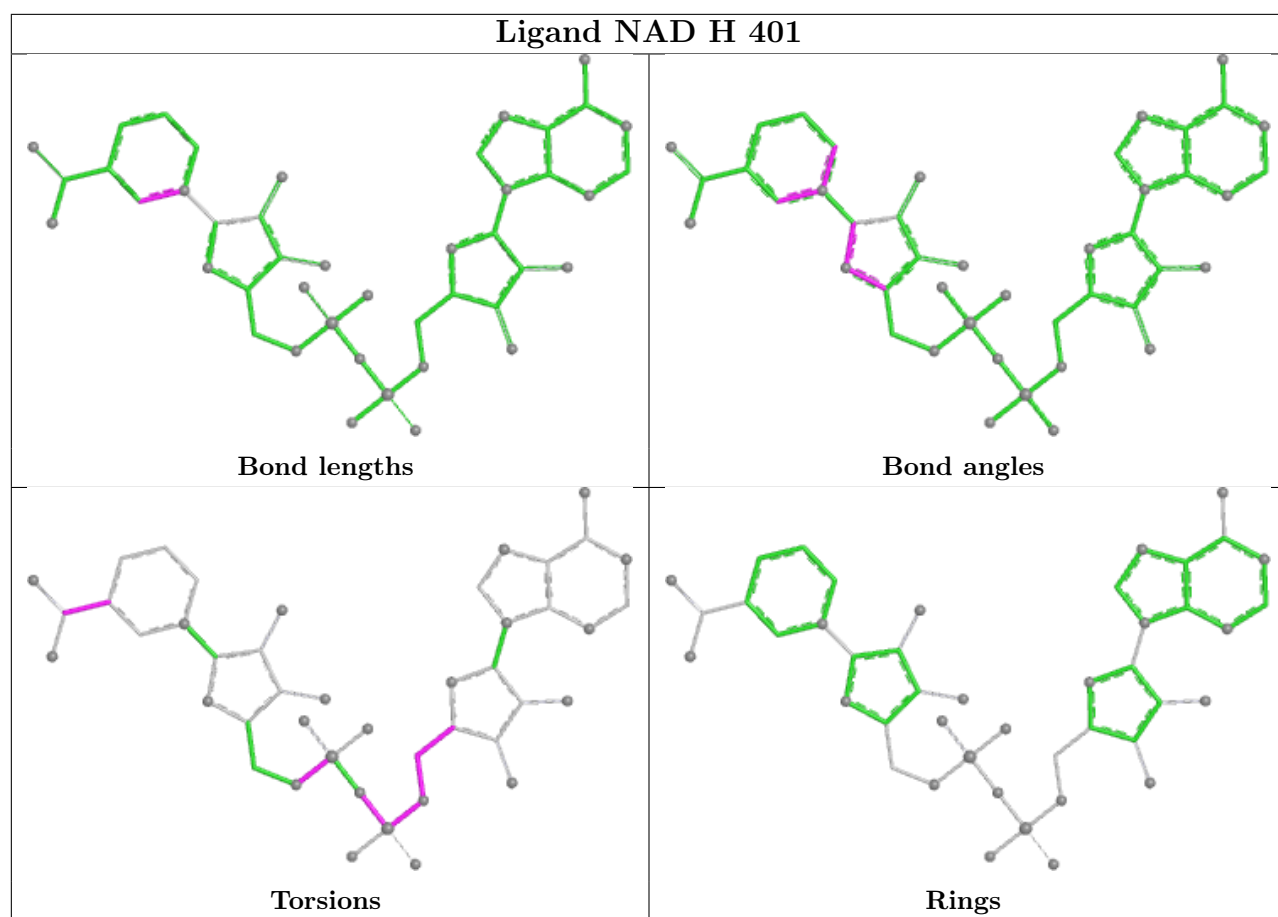


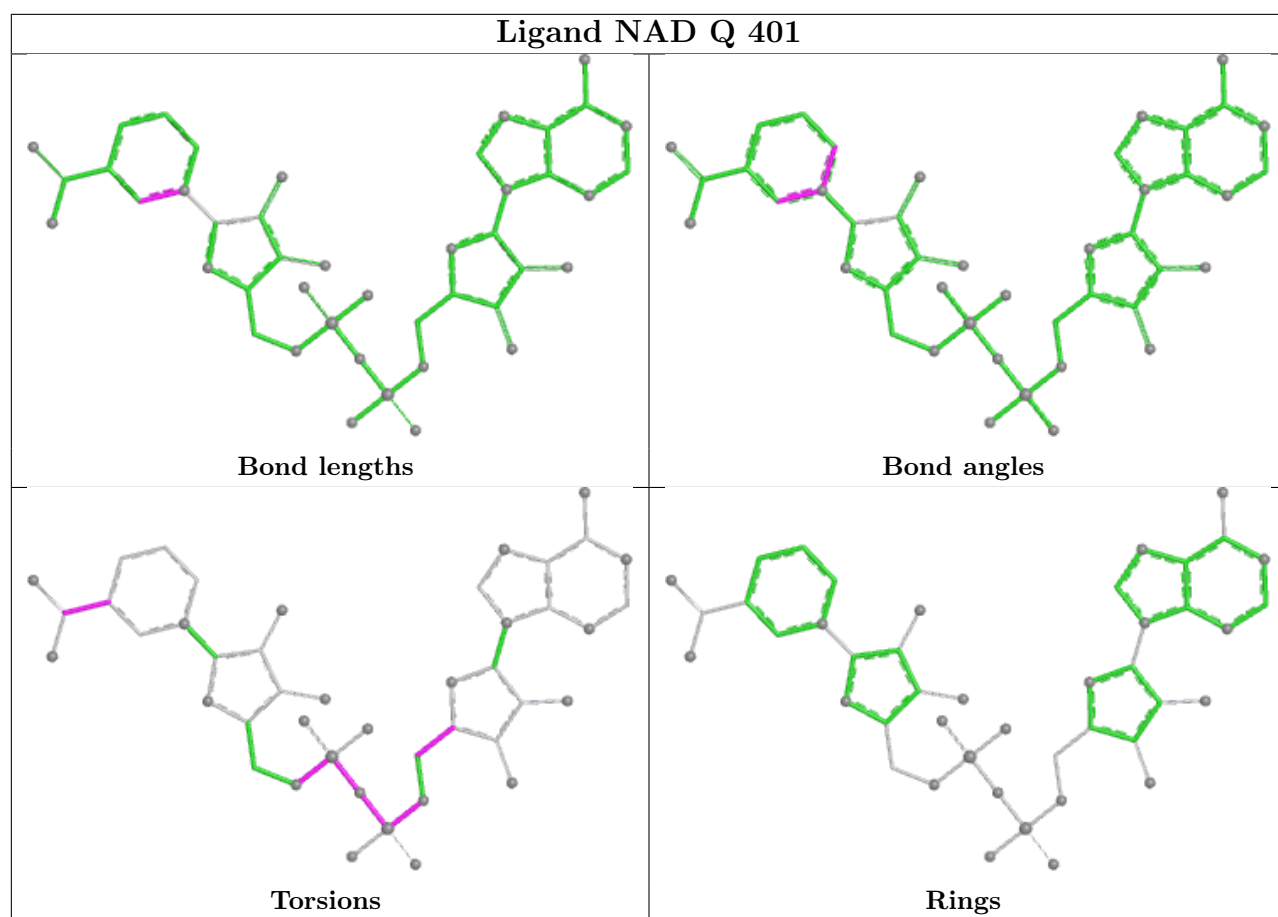


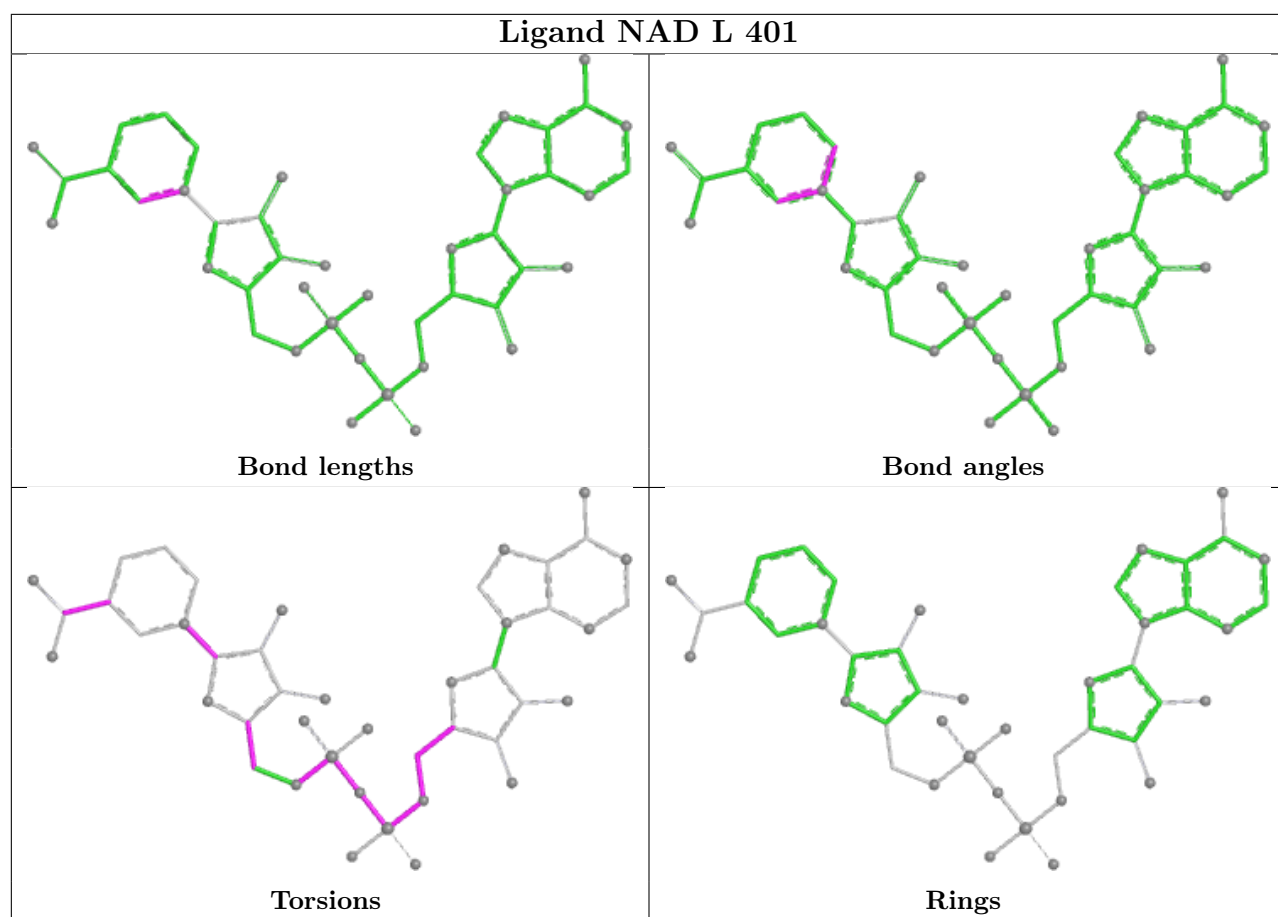


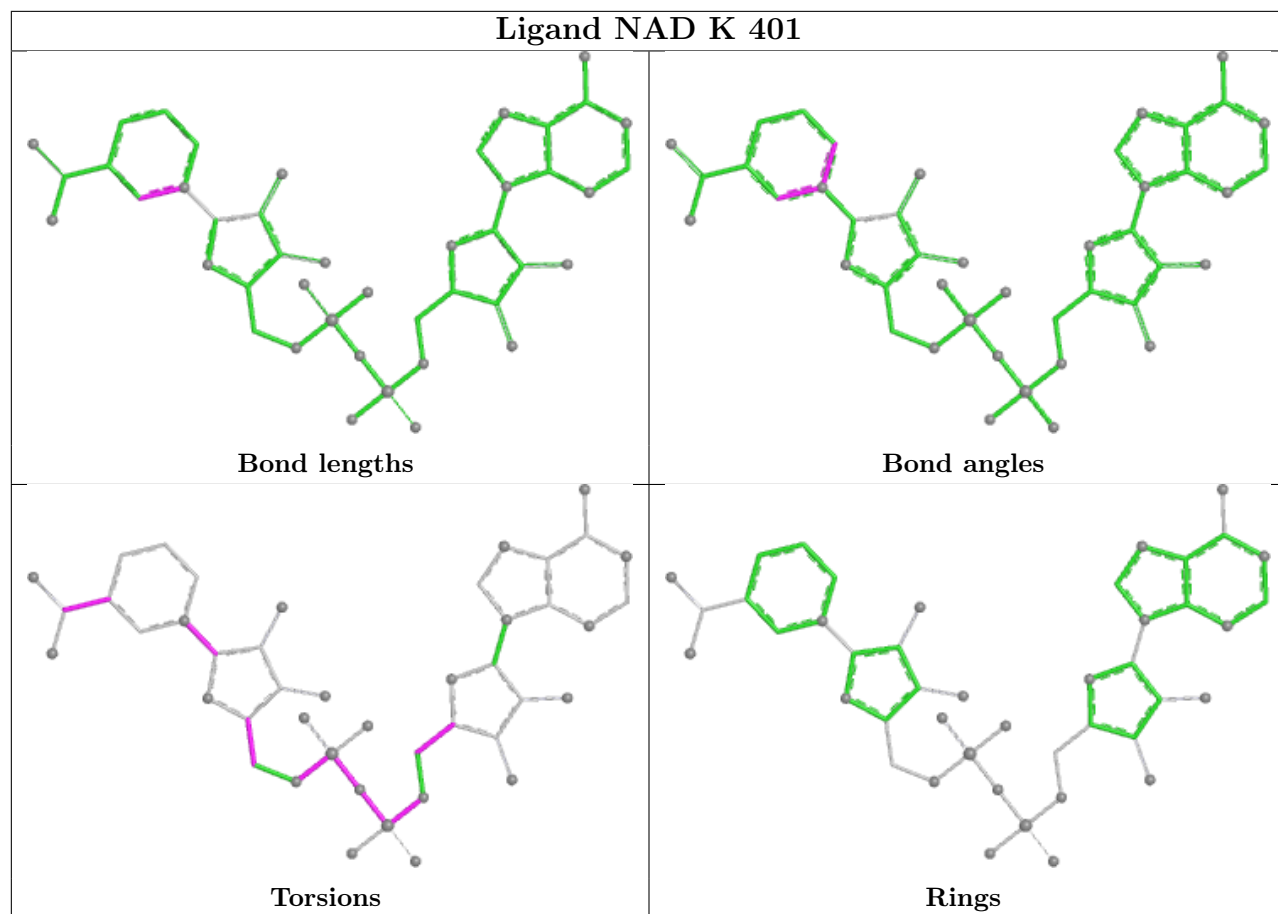


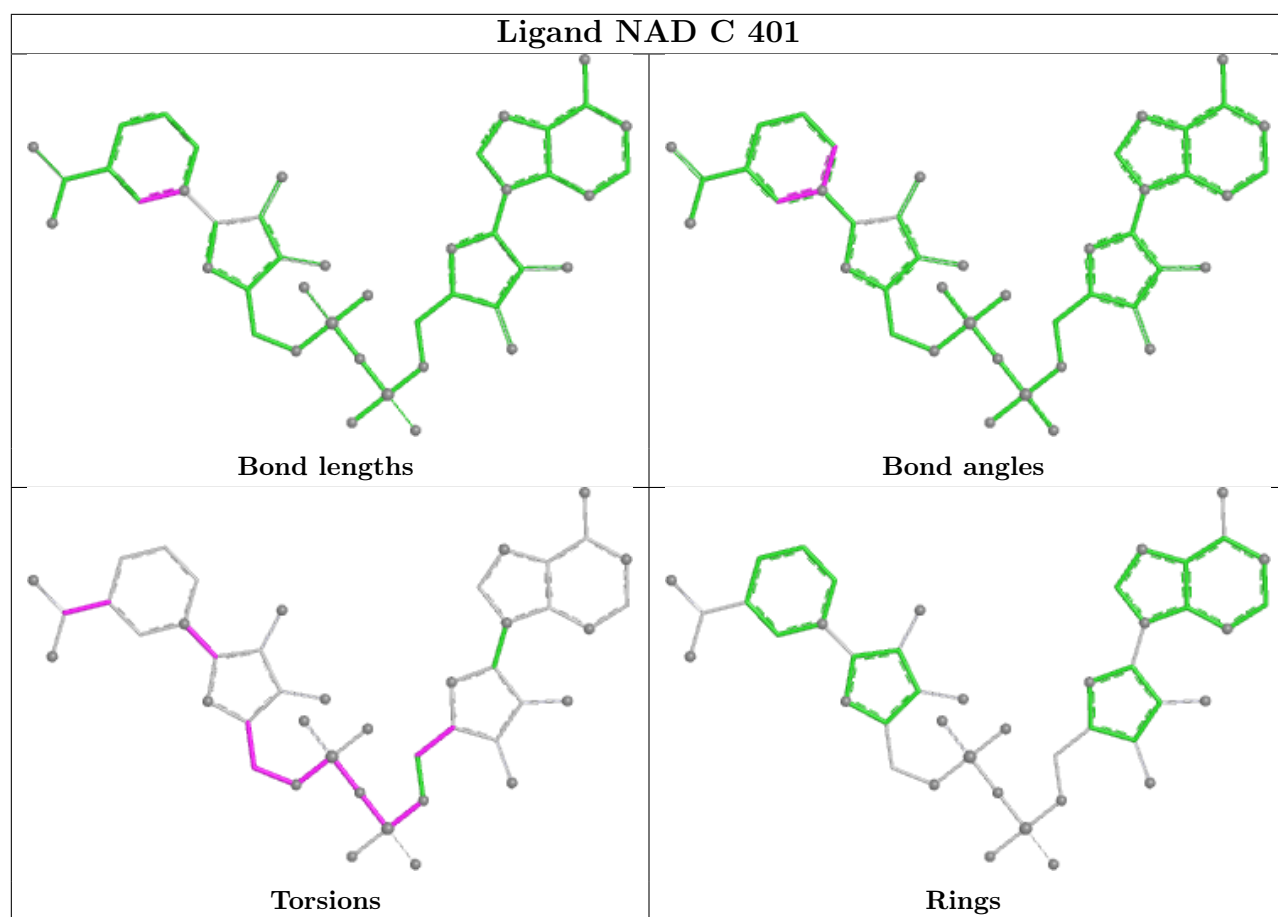


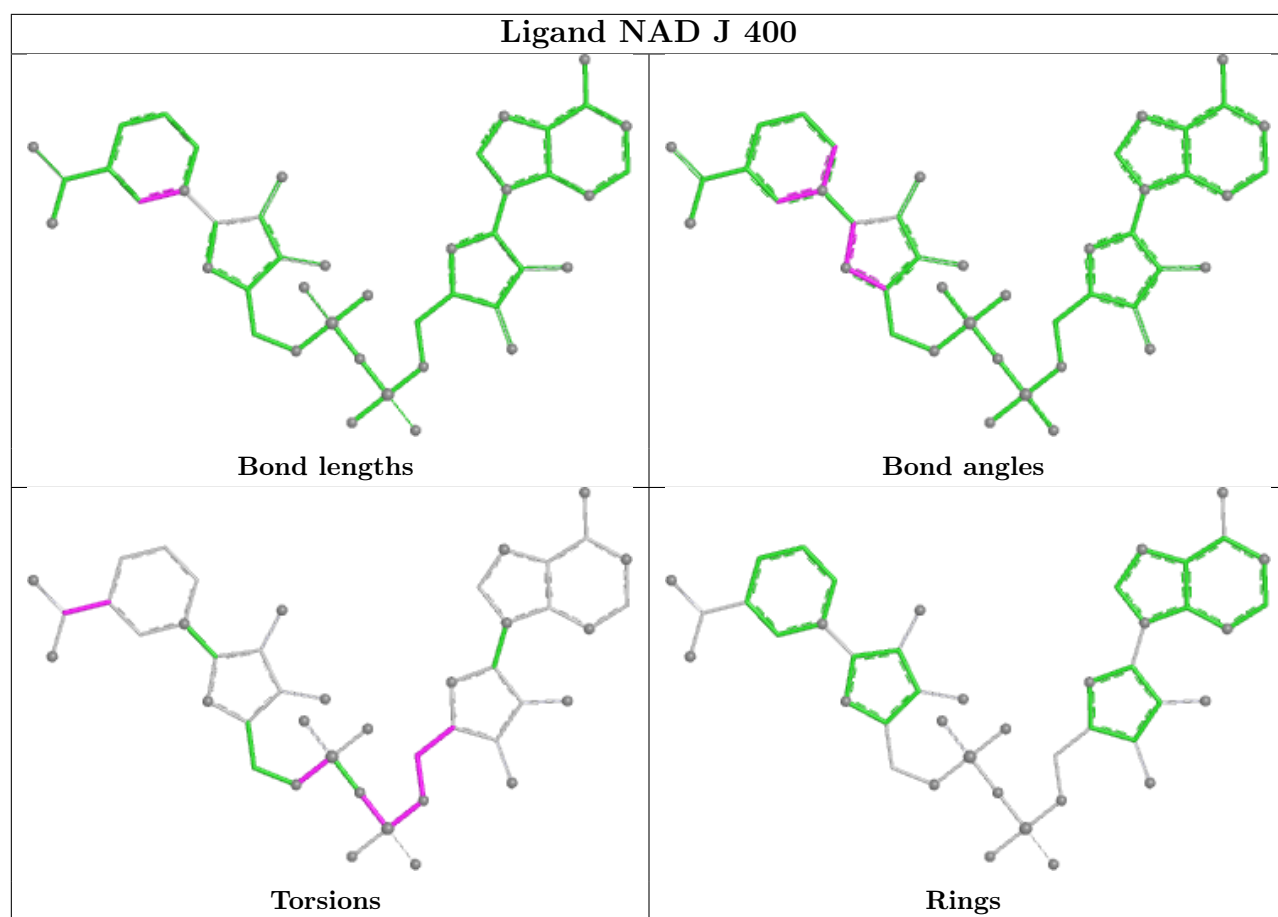


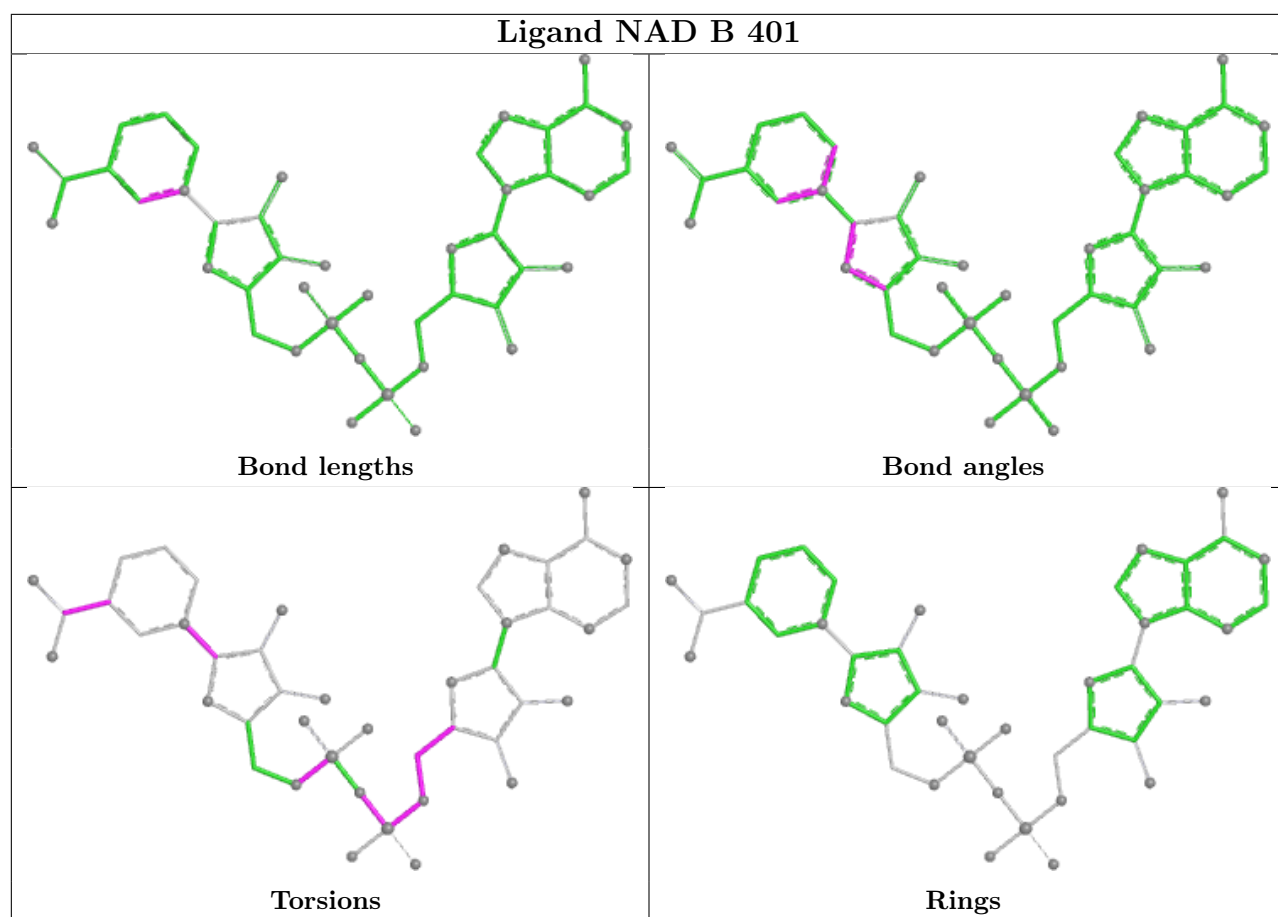


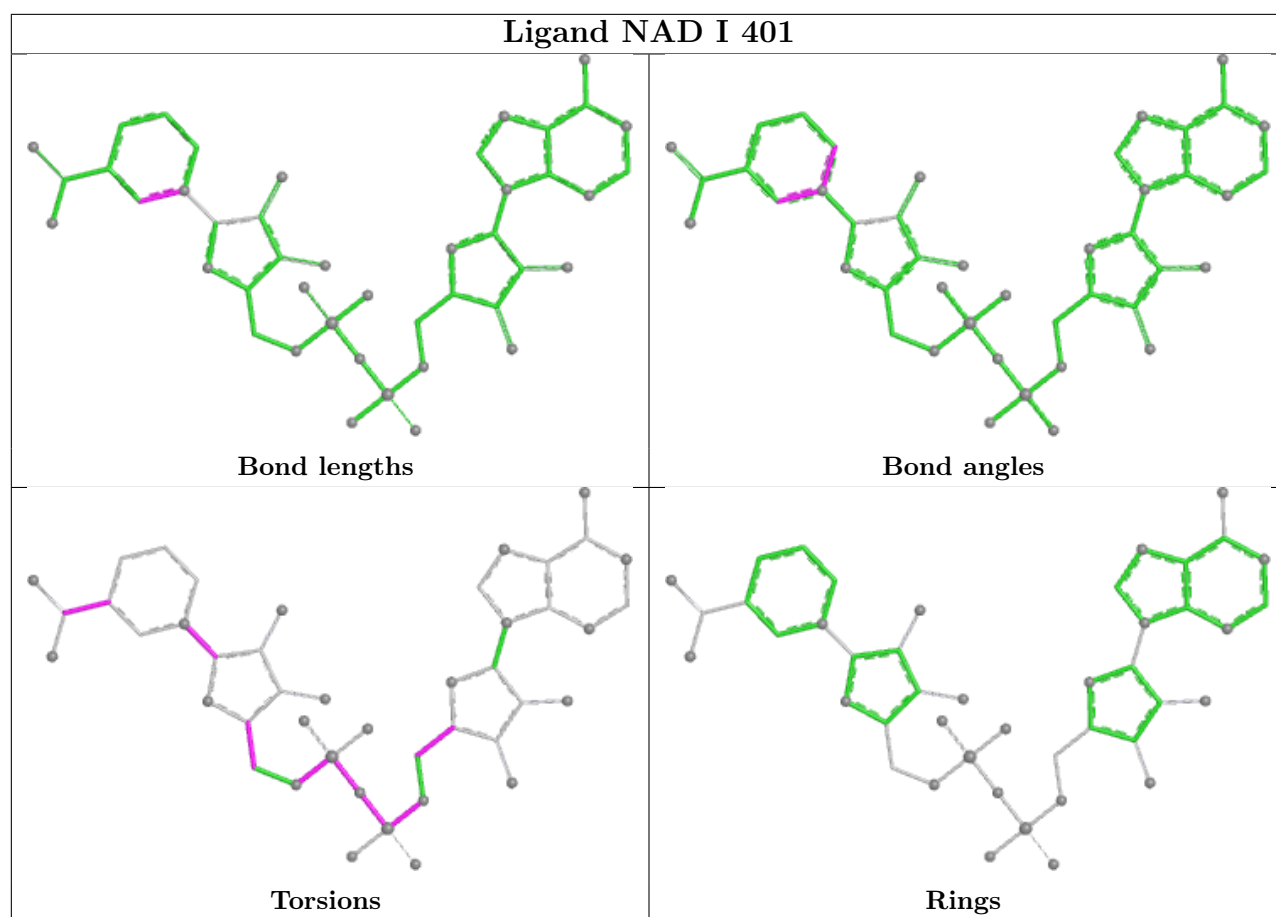












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13828. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

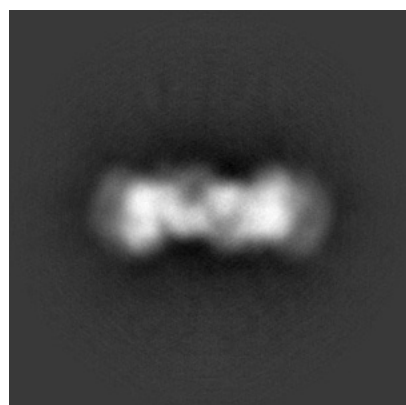


Y

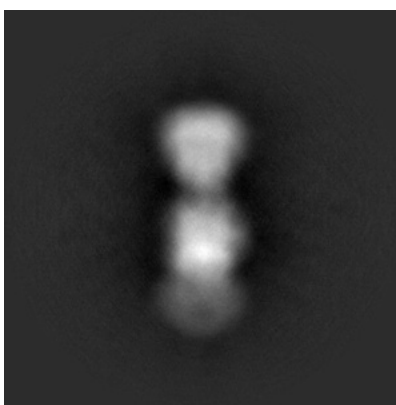


Z

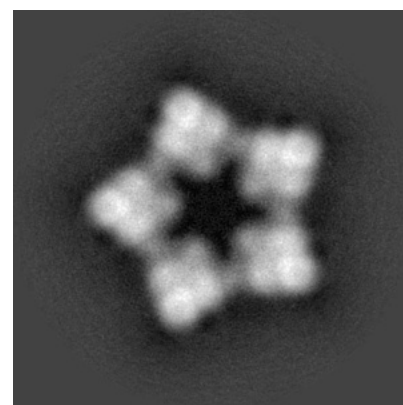
6.1.2 Raw map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

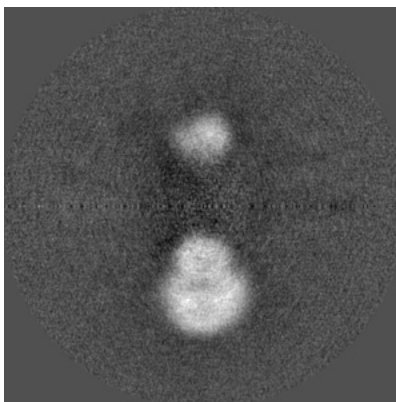


Z Index: 150

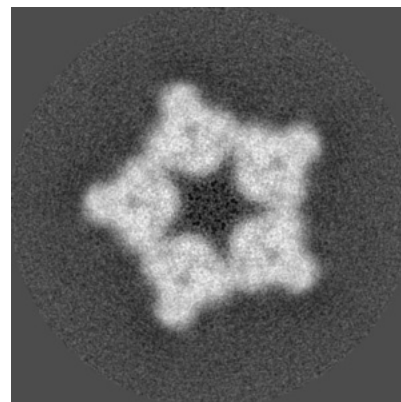
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 118

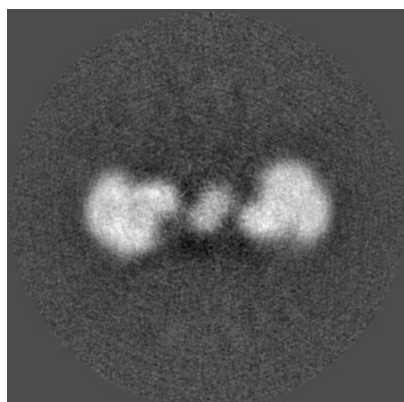


Y Index: 102

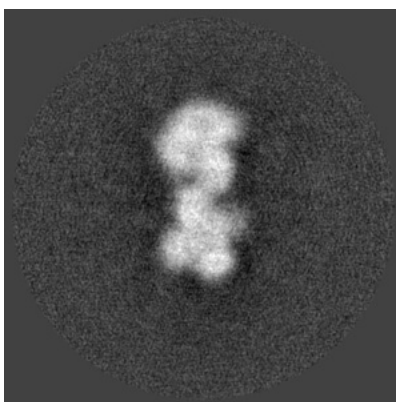


Z Index: 149

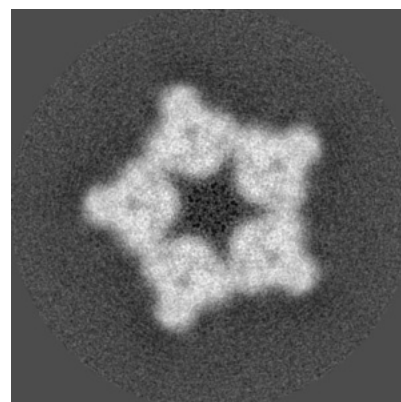
6.3.2 Raw map



X Index: 122



Y Index: 102

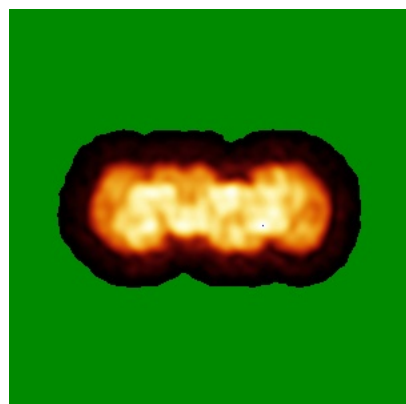


Z Index: 150

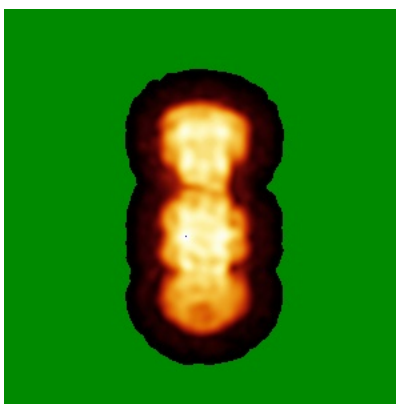
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

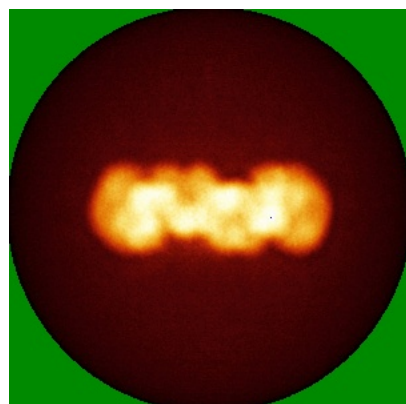


Y

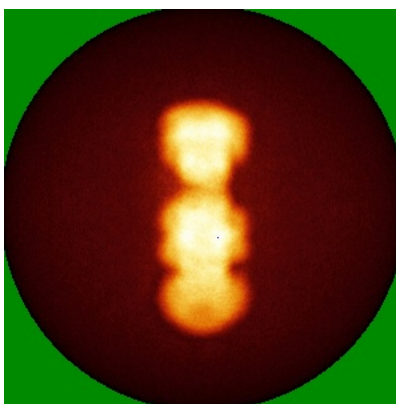


Z

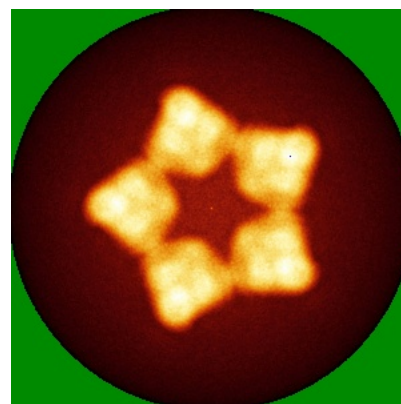
6.4.2 Raw map



X



Y

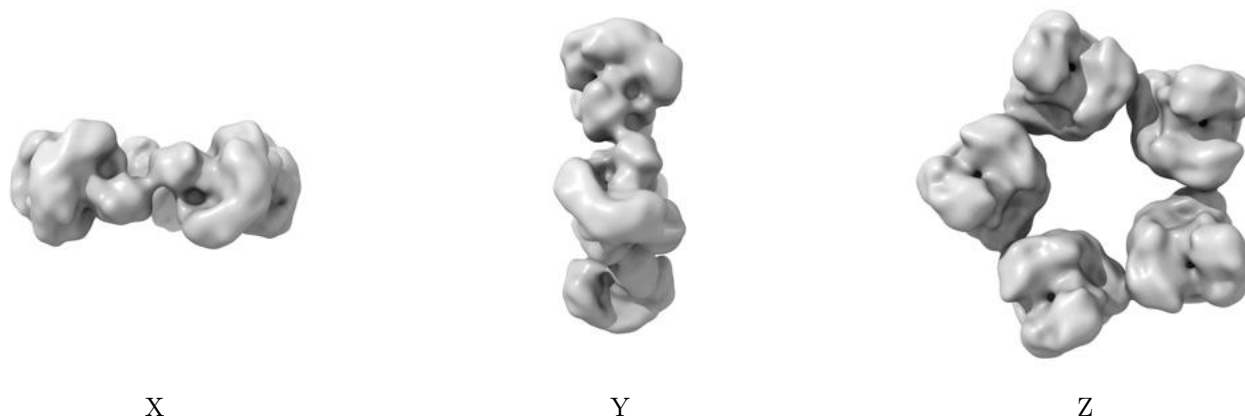


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

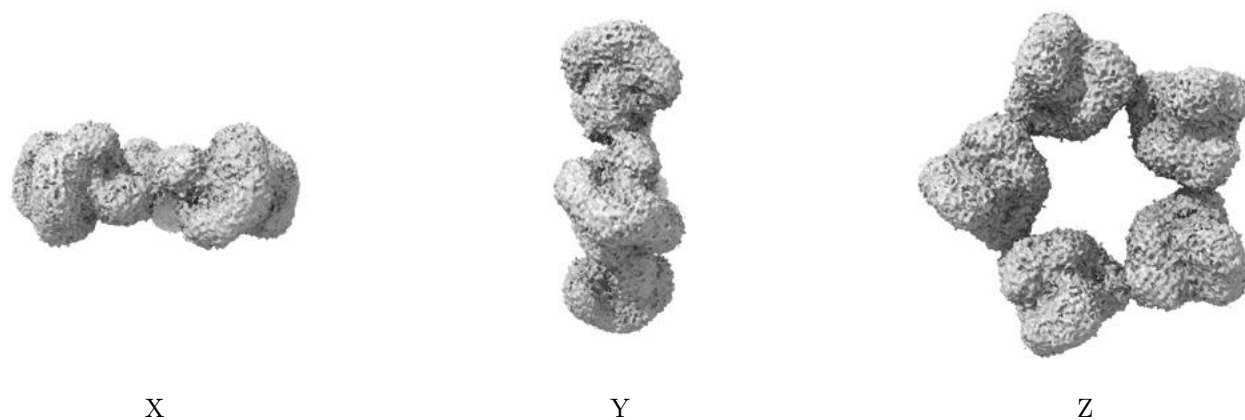
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

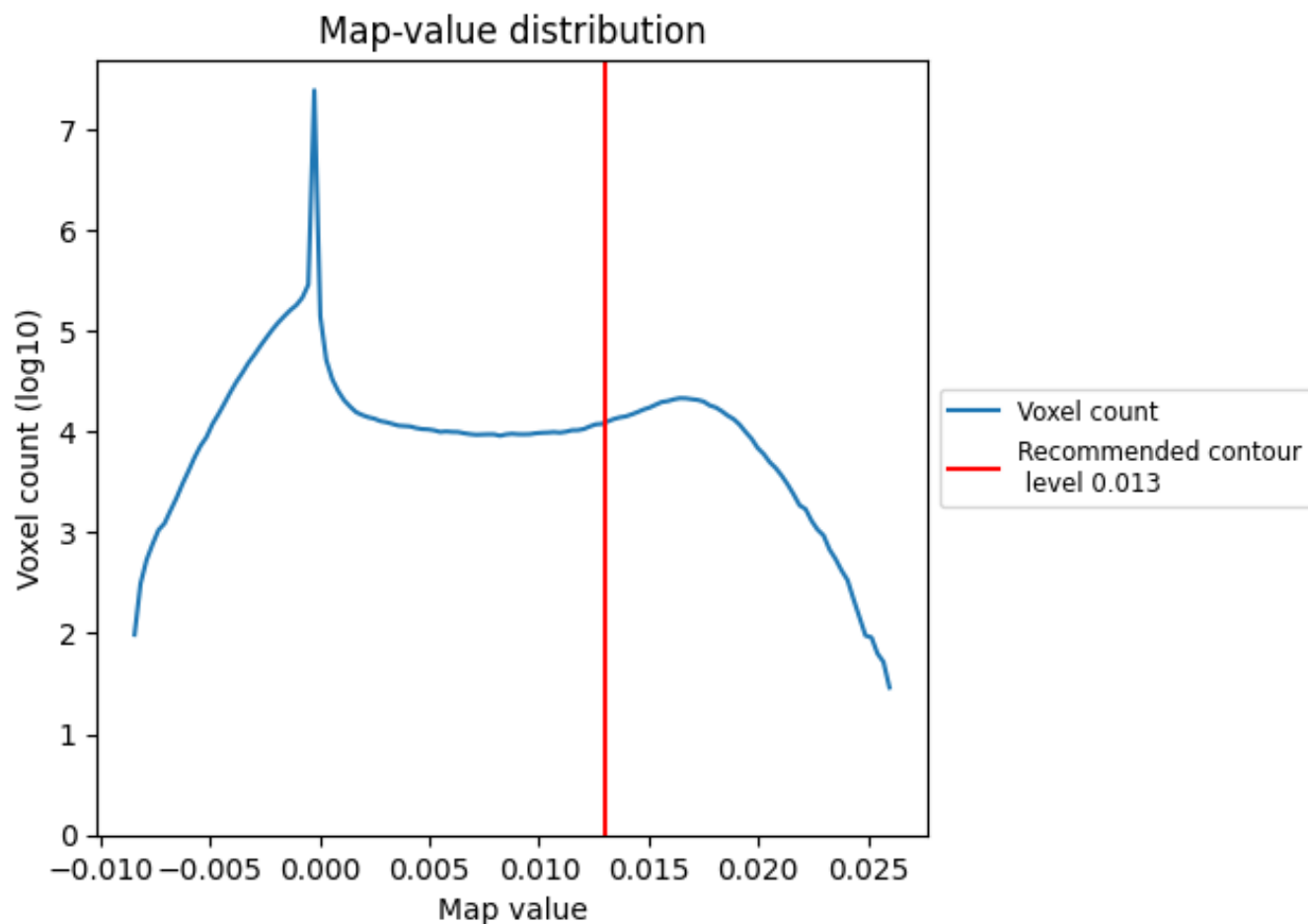
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

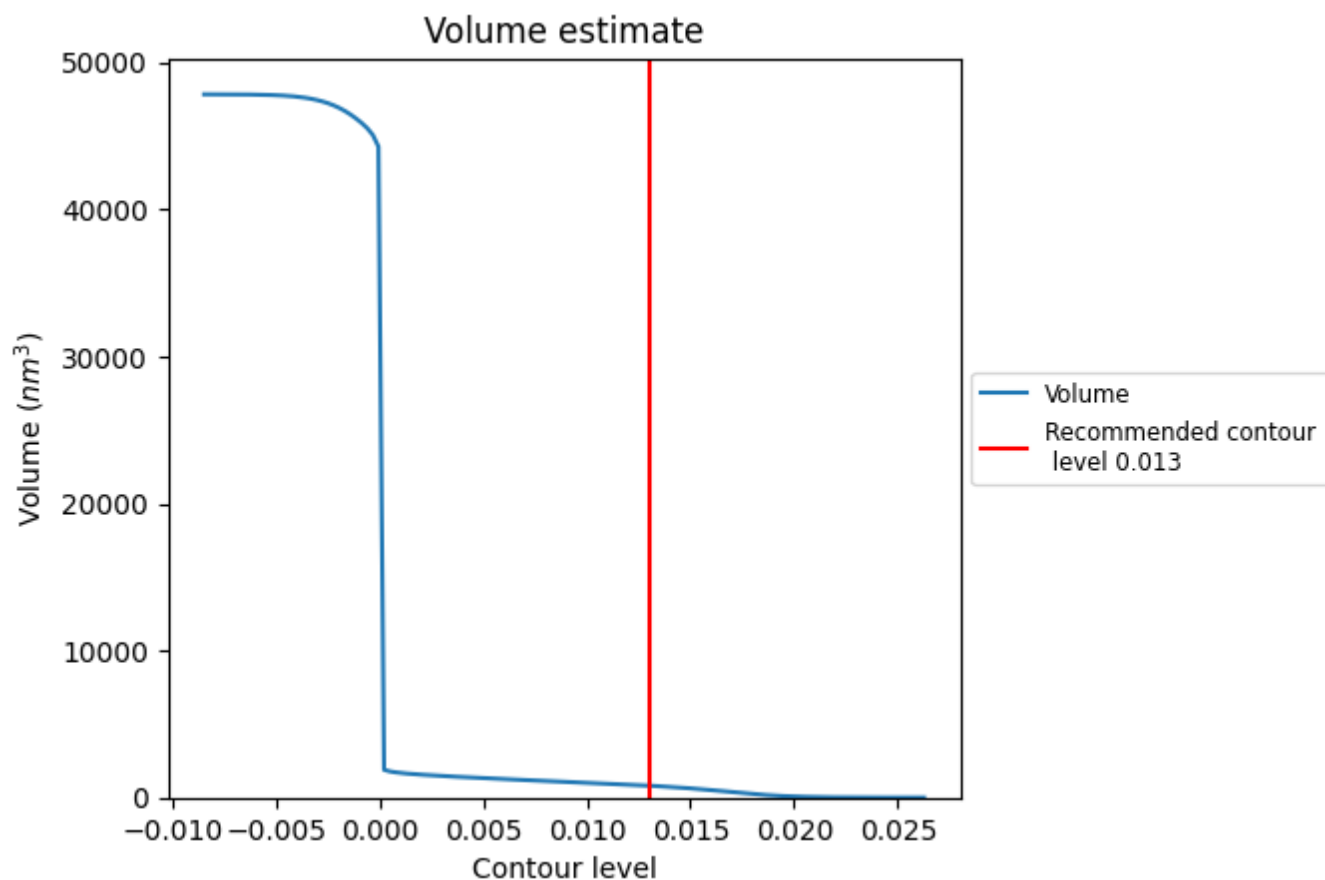
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

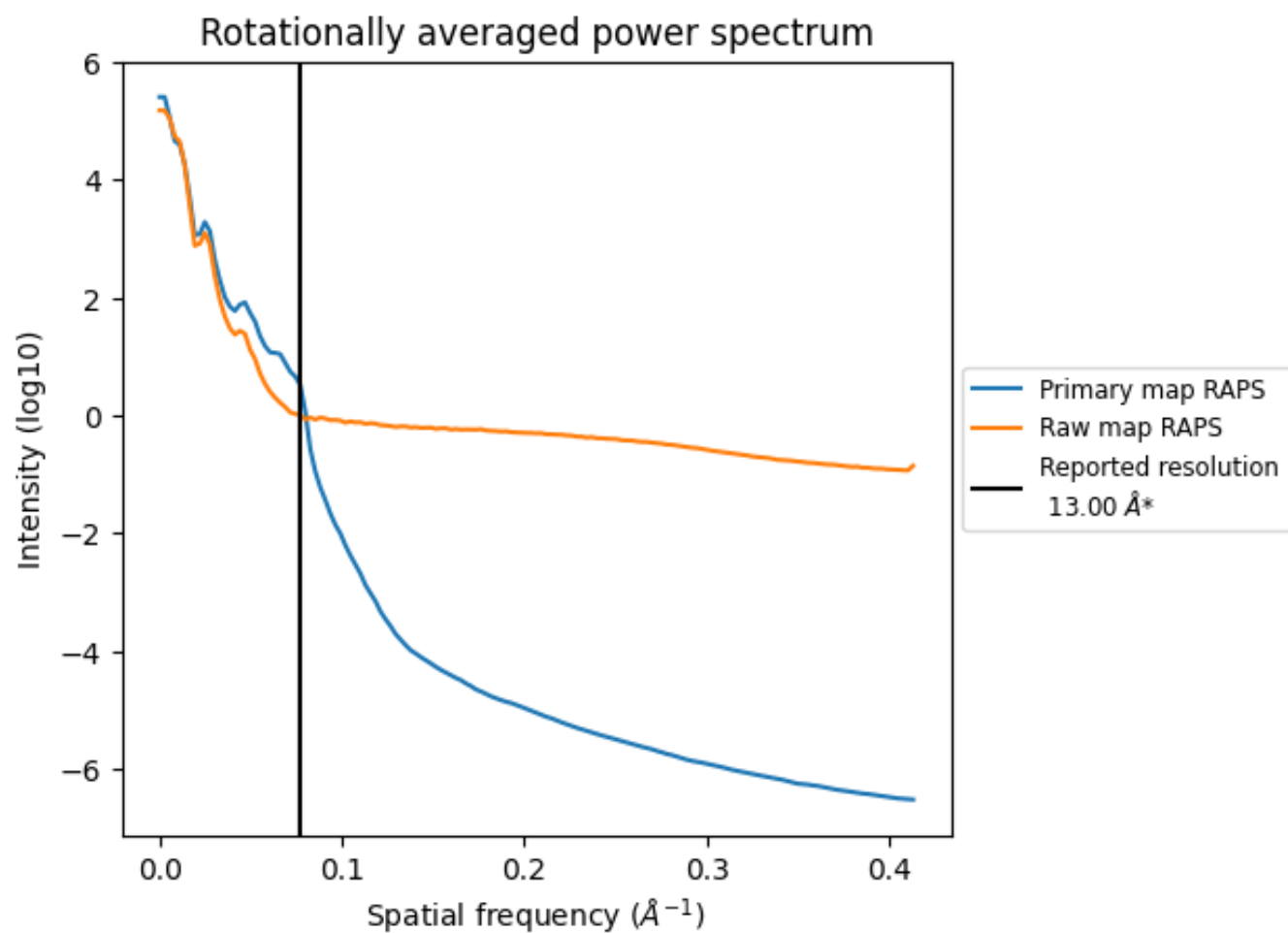
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm³; this corresponds to an approximate mass of 732 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

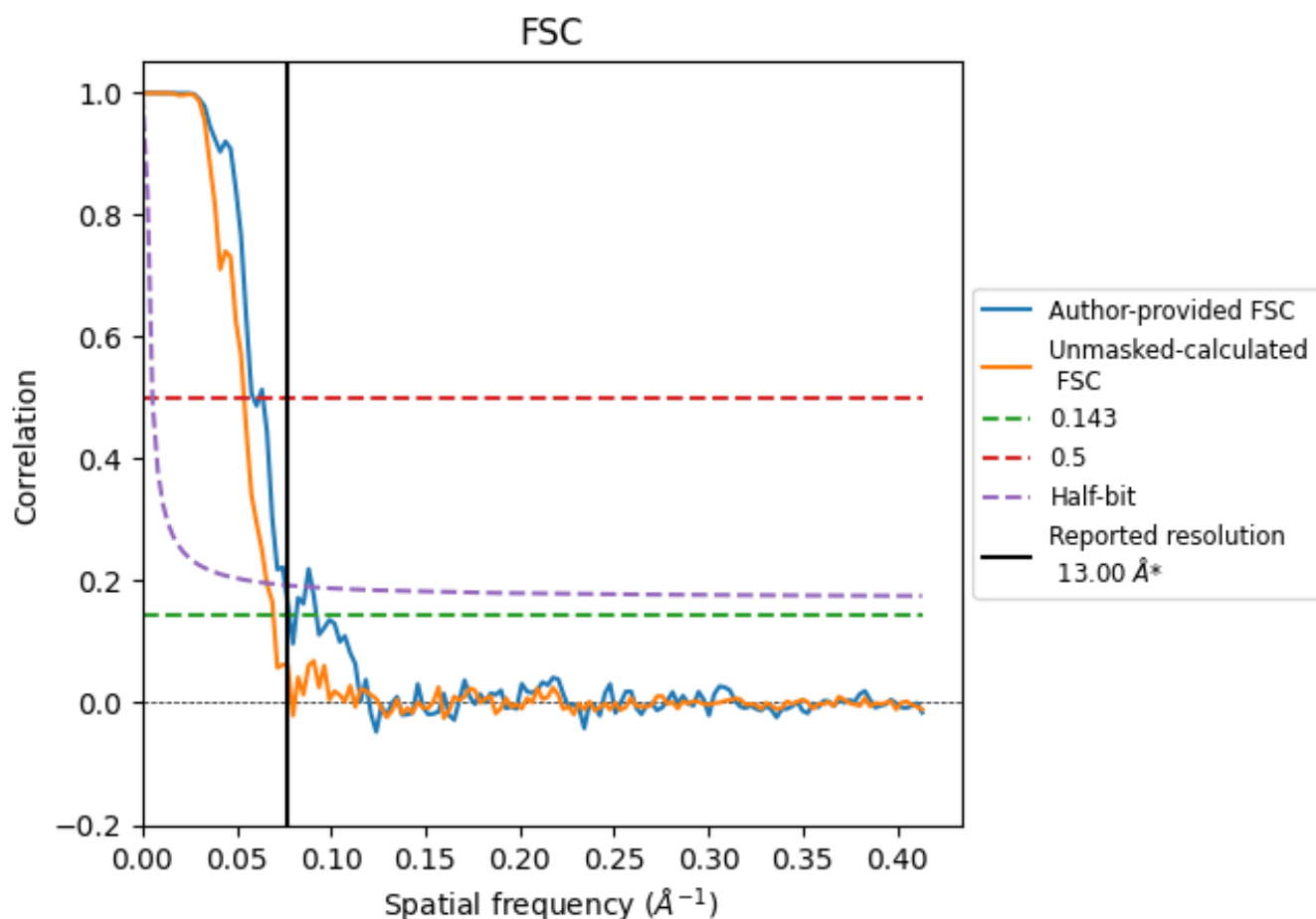


*Reported resolution corresponds to spatial frequency of 0.077 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.077 Å⁻¹

8.2 Resolution estimates [i](#)

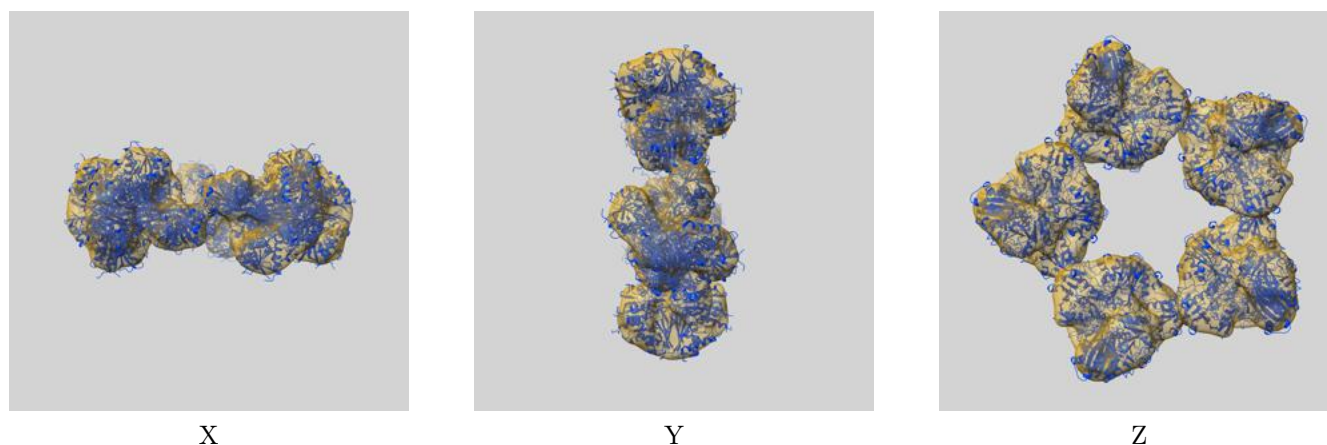
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.00	-	-
Author-provided FSC curve	12.82	17.01	13.19
Unmasked-calculated*	14.39	18.52	15.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.39 differs from the reported value 13.0 by more than 10 %

9 Map-model fit [i](#)

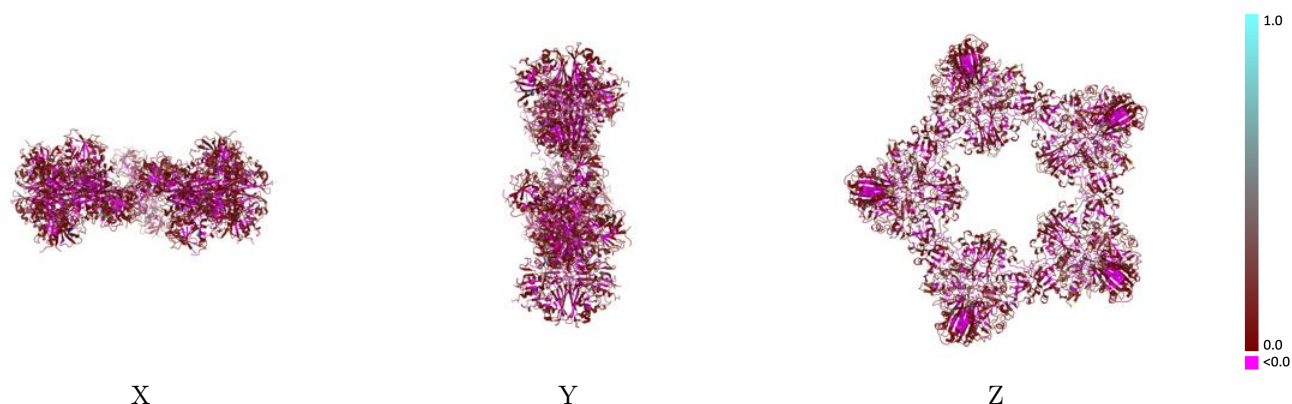
This section contains information regarding the fit between EMDB map EMD-13828 and PDB model 7Q57. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



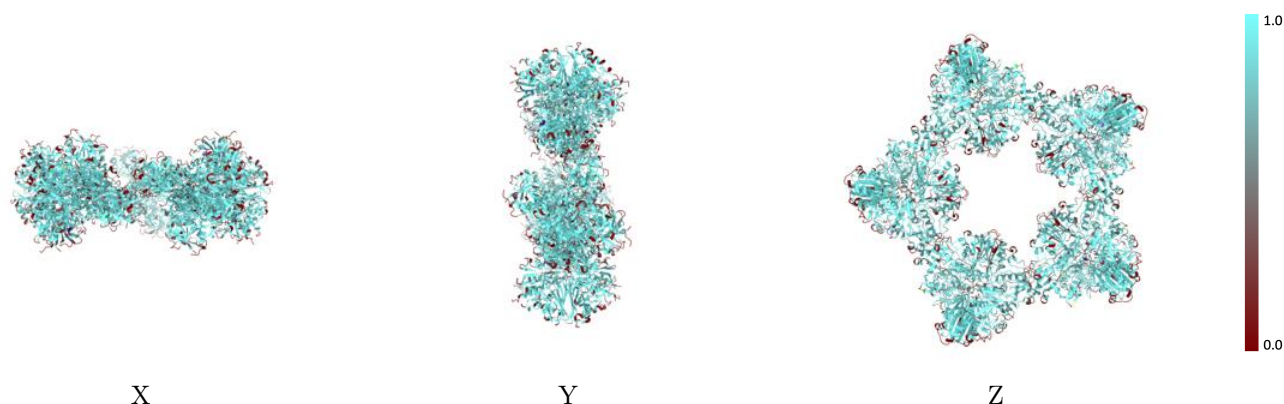
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



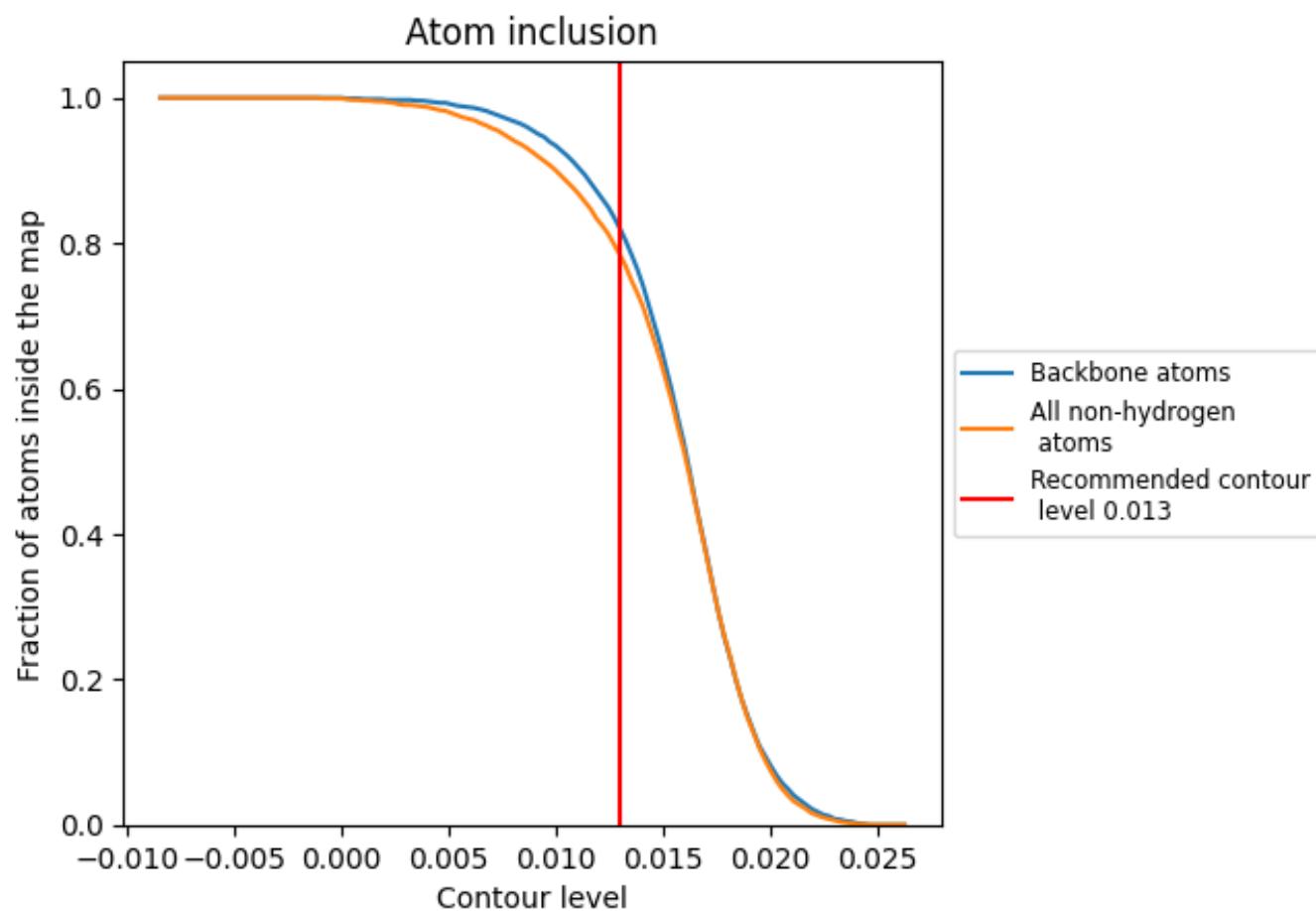
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.0690
A	0.7950	0.0710
B	0.7860	0.0660
C	0.7650	0.0670
D	0.7880	0.0670
E	0.7910	0.0710
F	0.7880	0.0670
G	0.7670	0.0690
H	0.7840	0.0680
I	0.7950	0.0730
J	0.7850	0.0670
K	0.7670	0.0690
L	0.7870	0.0670
M	0.7670	0.0700
N	0.7860	0.0660
O	0.7950	0.0730
P	0.7840	0.0660
Q	0.7720	0.0680
R	0.7830	0.0670
S	0.7930	0.0740
T	0.7920	0.0650

1.0

0.0

<0.0