



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:35 PM UTC

PDB ID : 3K2B / pdb_00003k2b
Title : Crystal structure of photosynthetic A4 isoform glyceraldehyde-3-phosphate dehydrogenase complexed with NAD, from Arabidopsis thaliana
Authors : Fermani, S.; Falini, G.; Thumiger, A.; Sparla, F.; Marri, L.; Trost, P.
Deposited on : 2009-09-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

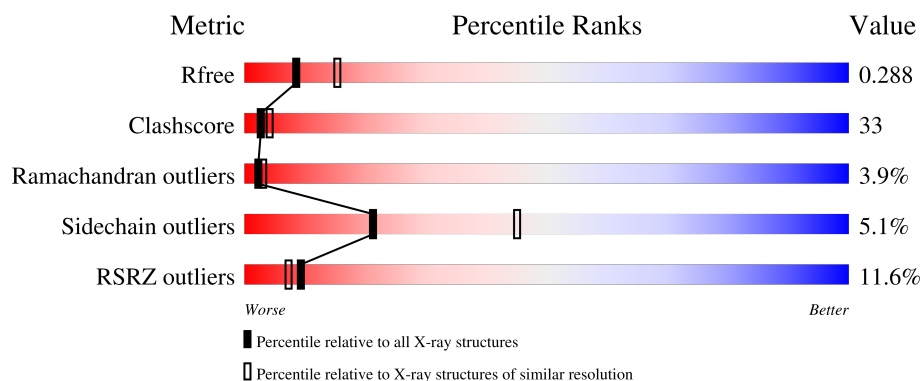
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	
1	E	337	

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Mol	Chain	Length	Quality of chain
1	F	337	29%33%56%11%
1	G	337	18%40%50%10%
1	H	337	14%38%52%9%
1	O	337	64%33%
1	Q	337	58%36%5%

2 Entry composition

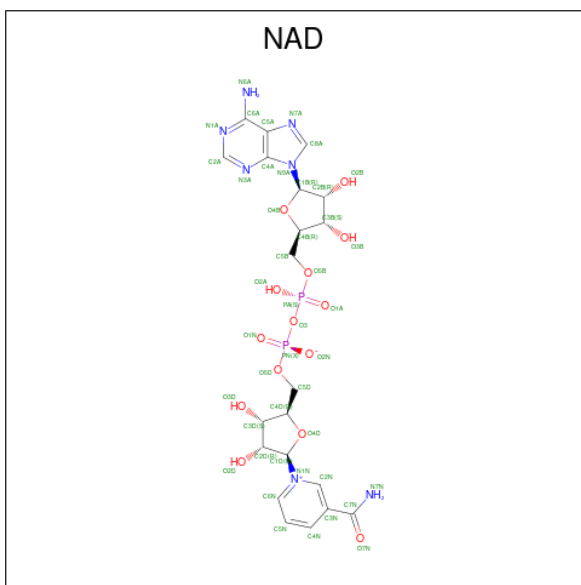
There are 4 unique types of molecules in this entry. The entry contains 27072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 A, chloroplastic.

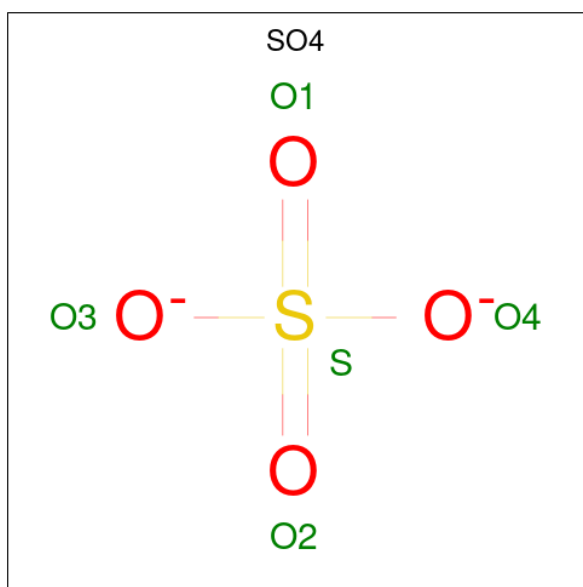
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	B	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	C	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	D	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	E	336	Total	C	N	O	S	0	0	0
			2547	1609	443	486	9			
1	F	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	G	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	H	335	Total	C	N	O	S	0	0	0
			2542	1606	442	485	9			
1	O	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	Q	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	G	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	H	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	84	Total	O	0	0
			84	84		
4	C	94	Total	O	0	0
			94	94		
4	D	85	Total	O	0	0
			85	85		
4	E	79	Total	O	0	0
			79	79		
4	F	65	Total	O	0	0
			65	65		
4	G	81	Total	O	0	0
			81	81		
4	H	56	Total	O	0	0
			56	56		
4	O	129	Total	O	0	0
			129	129		

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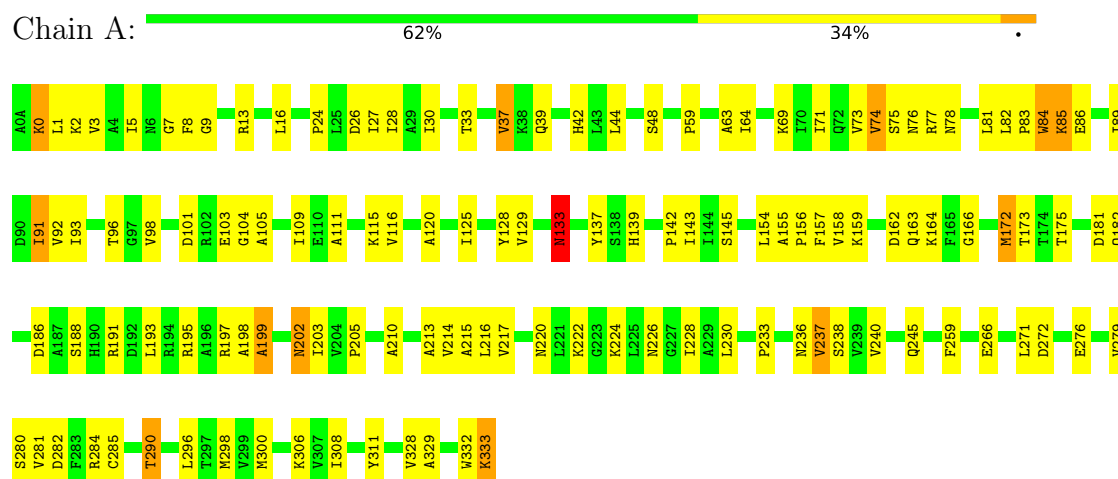
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	100	Total 100	O 100	0	0

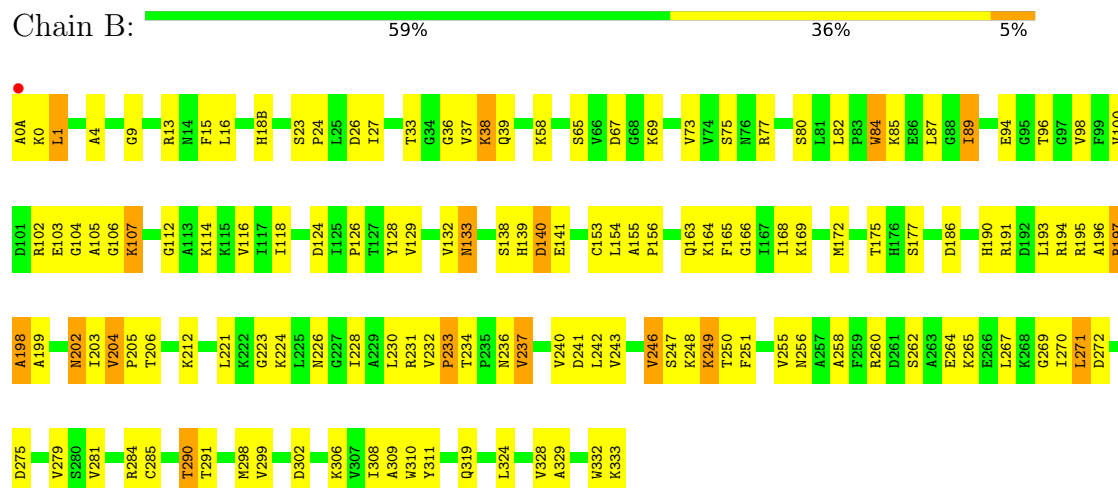
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 A, chloroplastic

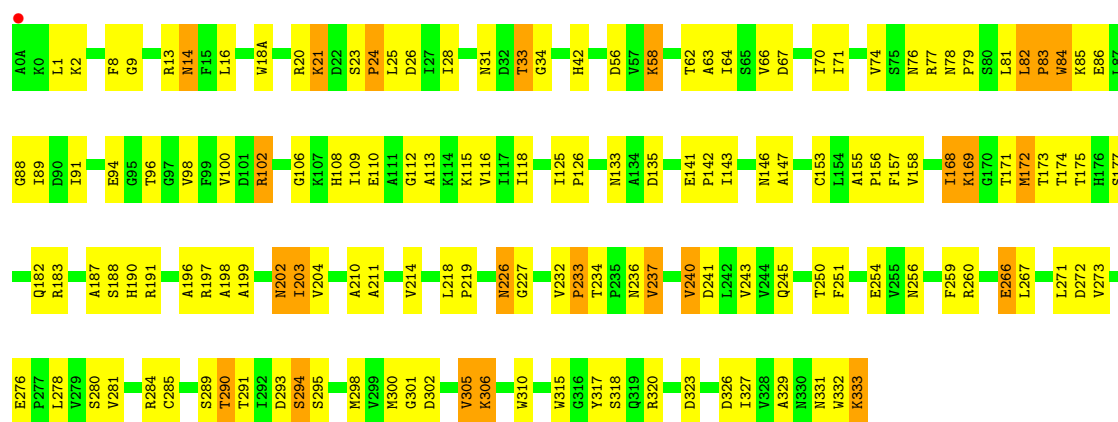


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

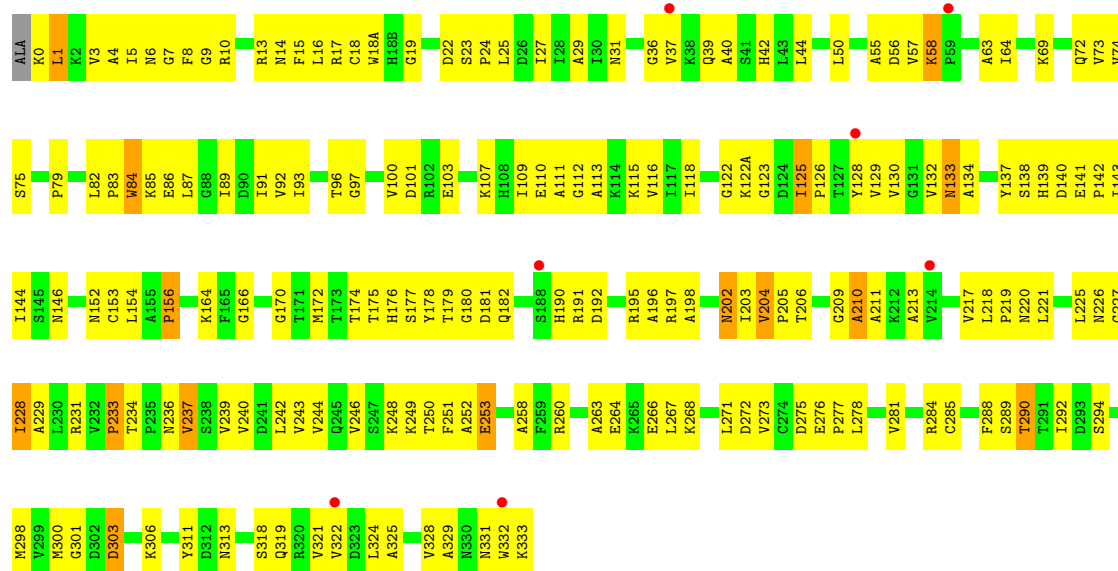
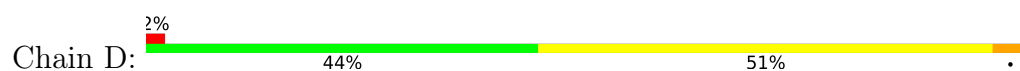


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

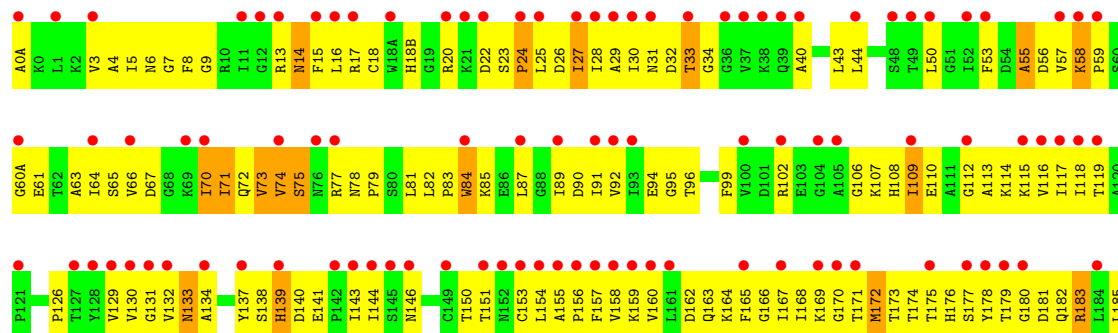


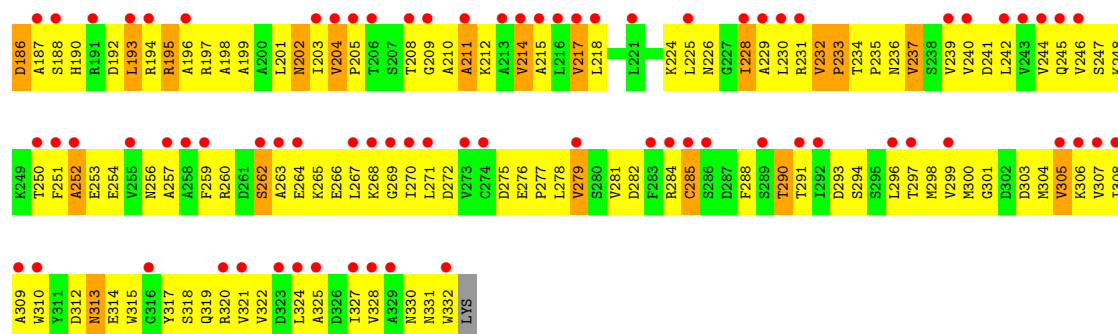


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

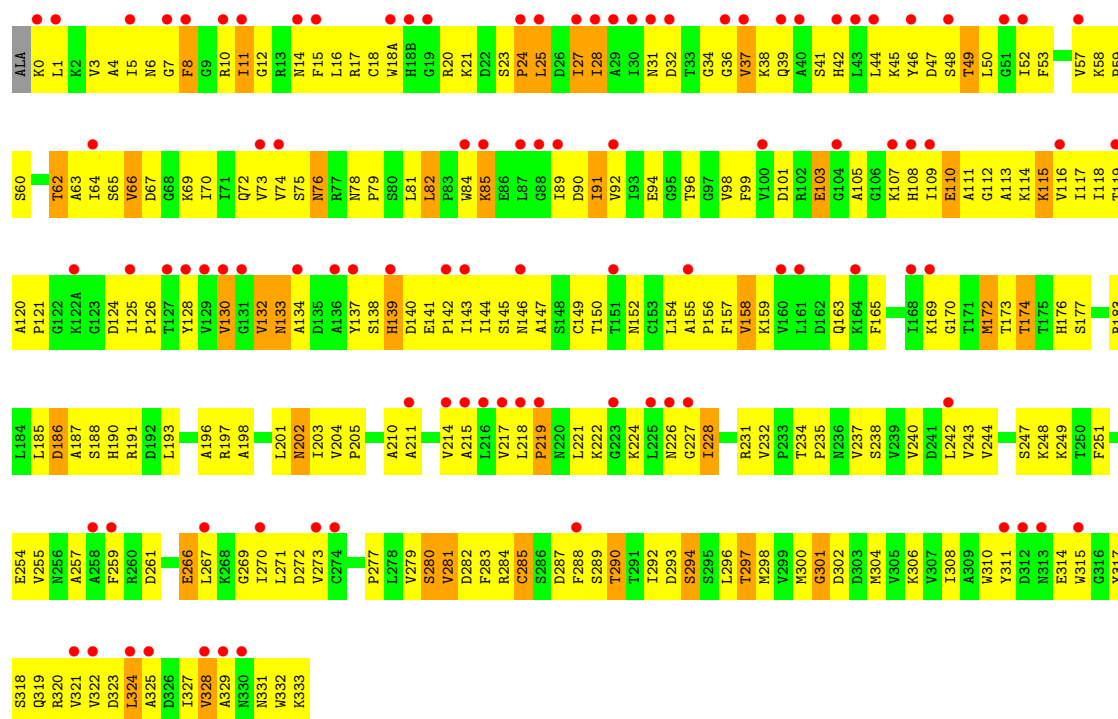


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

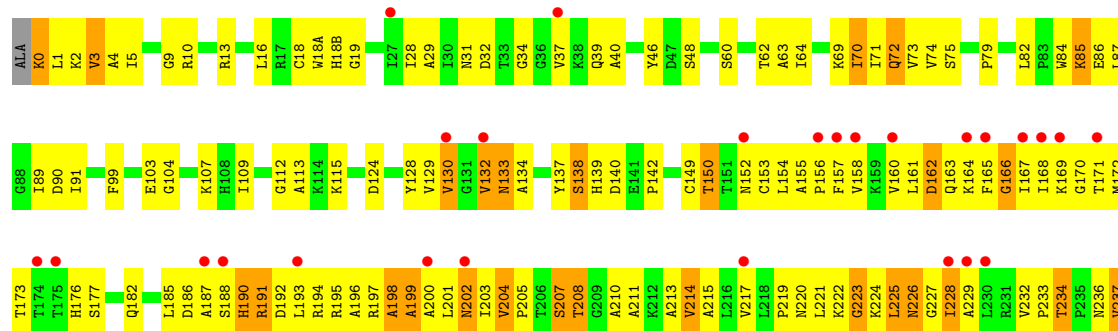
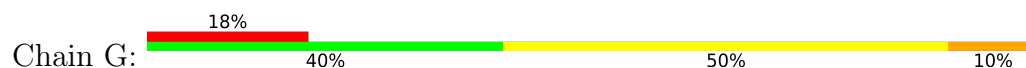


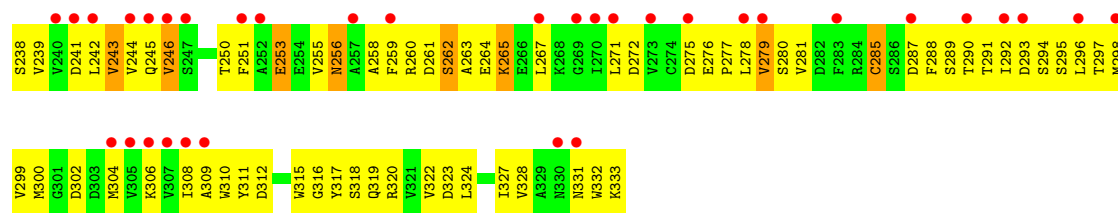


● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

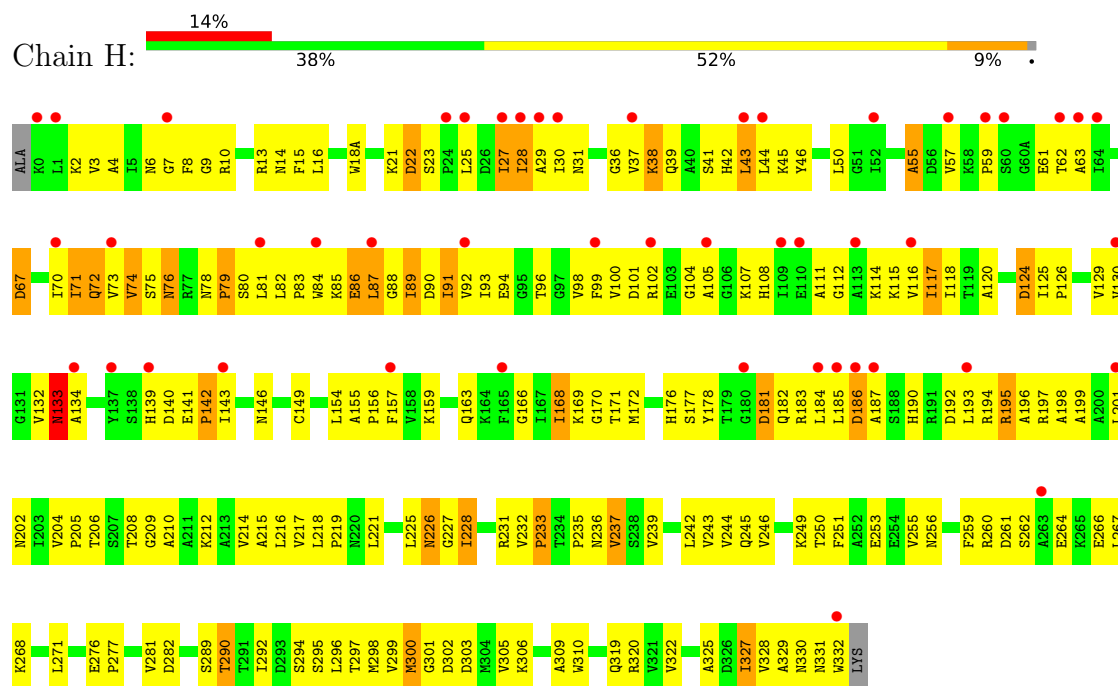


● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

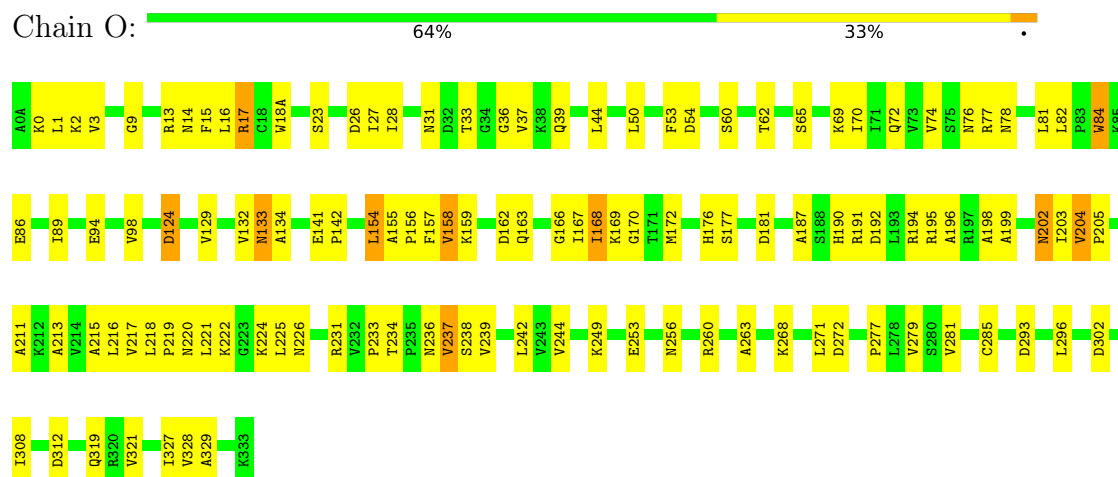




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.74Å 188.62Å 314.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.22 – 2.60 94.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (94.22-2.60) 95.9 (94.22-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.62Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.237 , 0.289 0.237 , 0.288	Depositor DCC
R_{free} test set	6671 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27072	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.48	0/2601	0.97	9/3530 (0.3%)
1	B	0.48	0/2601	0.99	9/3530 (0.3%)
1	C	0.46	0/2601	1.01	18/3530 (0.5%)
1	D	0.43	0/2596	1.01	10/3523 (0.3%)
1	E	0.44	0/2591	0.97	11/3519 (0.3%)
1	F	0.39	0/2596	0.96	12/3523 (0.3%)
1	G	0.43	0/2596	0.94	4/3523 (0.1%)
1	H	0.37	0/2586	0.89	3/3512 (0.1%)
1	O	0.57	0/2601	1.06	15/3530 (0.4%)
1	Q	0.54	1/2596 (0.0%)	1.03	13/3523 (0.4%)
All	All	0.46	1/25965 (0.0%)	0.99	104/35243 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	240	VAL	CA-CB	5.17	1.60	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	VAL	N-CA-C	11.02	118.46	107.55
1	D	24	PRO	N-CA-C	-8.85	105.47	114.68
1	Q	203	ILE	N-CA-C	-8.77	95.18	107.99
1	C	204	VAL	N-CA-C	8.69	116.90	107.60
1	F	204	VAL	N-CA-C	8.42	115.22	107.56
1	O	203	ILE	N-CA-C	-8.34	95.82	107.99
1	E	204	VAL	N-CA-C	8.24	117.12	107.73
1	O	204	VAL	N-CA-C	8.22	116.40	107.60
1	A	203	ILE	N-CA-C	-8.14	95.99	107.80
1	D	203	ILE	N-CA-C	-7.92	95.71	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ILE	N-CA-C	-7.88	96.37	107.80
1	O	37	VAL	N-CA-C	7.76	118.30	110.23
1	C	202	ASN	N-CA-C	7.69	121.09	109.41
1	C	203	ILE	N-CA-C	-7.49	96.35	107.51
1	F	158	VAL	N-CA-C	-7.17	102.53	112.50
1	F	301	GLY	N-CA-C	-7.16	105.17	115.27
1	Q	202	ASN	N-CA-C	7.09	120.18	109.41
1	E	232	VAL	CA-C-N	7.07	128.68	119.84
1	E	232	VAL	C-N-CA	7.07	128.68	119.84
1	C	24	PRO	N-CA-C	-7.04	107.36	114.68
1	D	202	ASN	N-CA-C	6.90	119.90	109.41
1	O	319	GLN	N-CA-C	-6.83	103.28	111.69
1	O	44	LEU	N-CA-C	-6.83	103.96	112.90
1	Q	199	ALA	N-CA-C	6.81	119.54	111.71
1	C	266	GLU	N-CA-C	6.64	118.17	111.07
1	F	110	GLU	N-CA-C	-6.61	105.96	112.97
1	O	98	VAL	N-CA-C	6.58	118.61	111.77
1	O	202	ASN	N-CA-C	6.50	119.30	109.41
1	Q	164	LYS	N-CA-C	6.47	121.26	113.23
1	C	102	ARG	N-CA-C	6.36	118.74	111.11
1	B	232	VAL	CA-C-N	6.33	127.75	119.84
1	B	232	VAL	C-N-CA	6.33	127.75	119.84
1	Q	44	LEU	N-CA-C	-6.32	105.72	113.50
1	G	204	VAL	N-CA-C	6.31	115.12	107.61
1	E	141	GLU	CA-C-N	6.30	126.21	119.28
1	E	141	GLU	C-N-CA	6.30	126.21	119.28
1	C	158	VAL	N-CA-C	-6.16	103.18	111.44
1	G	34	GLY	N-CA-C	6.16	115.81	110.21
1	Q	234	THR	CA-C-N	6.12	126.24	119.87
1	Q	234	THR	C-N-CA	6.12	126.24	119.87
1	E	214	VAL	N-CA-C	-6.12	105.33	112.98
1	O	168	ILE	N-CA-C	-6.11	105.77	111.45
1	B	199	ALA	N-CA-C	6.09	117.58	111.07
1	C	199	ALA	N-CA-C	6.09	118.42	111.11
1	E	211	ALA	N-CA-C	-6.05	105.73	113.23
1	F	203	ILE	N-CA-C	-5.92	97.88	106.88
1	O	199	ALA	N-CA-C	5.91	118.20	111.11
1	B	204	VAL	N-CA-C	5.89	113.90	107.60
1	G	262	SER	N-CA-C	-5.89	104.21	111.33
1	F	247	SER	N-CA-C	-5.82	106.08	112.72
1	C	315	TRP	N-CA-C	5.82	117.31	110.97
1	A	224	LYS	N-CA-C	5.79	120.34	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	SER	N-CA-C	5.76	117.14	109.83
1	D	324	LEU	N-CA-C	-5.74	106.12	113.01
1	A	158	VAL	N-CA-C	-5.74	103.75	111.44
1	A	202	ASN	N-CA-C	5.72	117.48	108.96
1	O	158	VAL	N-CA-C	-5.72	103.78	111.44
1	E	195	ARG	N-CA-C	-5.68	106.31	113.18
1	B	202	ASN	N-CA-C	5.67	117.23	109.18
1	Q	158	VAL	N-CA-C	-5.62	104.06	111.09
1	A	199	ALA	N-CA-C	5.58	117.36	111.28
1	H	168	ILE	N-CA-C	-5.57	106.27	111.45
1	D	176	HIS	N-CA-C	5.55	118.53	109.59
1	C	227	GLY	N-CA-C	5.49	119.55	110.55
1	H	327	ILE	N-CA-C	-5.47	105.20	110.72
1	F	202	ASN	N-CA-C	5.42	117.22	109.14
1	A	24	PRO	N-CA-C	-5.42	107.58	114.35
1	B	89	ILE	N-CA-C	5.40	116.66	109.37
1	Q	190	HIS	N-CA-C	-5.37	100.58	108.79
1	C	232	VAL	N-CA-C	5.37	113.80	107.84
1	Q	3	VAL	N-CA-C	5.34	117.08	108.85
1	F	82	LEU	CA-C-N	5.34	126.51	119.84
1	F	82	LEU	C-N-CA	5.34	126.51	119.84
1	O	14	ASN	N-CA-C	-5.33	105.37	111.07
1	F	324	LEU	N-CA-C	-5.31	106.06	112.54
1	E	96	THR	N-CA-C	-5.30	106.99	113.50
1	O	233	PRO	N-CA-C	5.29	123.37	112.47
1	D	325	ALA	N-CA-C	-5.26	105.14	112.45
1	G	5	ILE	CB-CA-C	-5.25	106.23	111.80
1	C	141	GLU	CA-C-N	5.25	124.58	118.85
1	C	141	GLU	C-N-CA	5.25	124.58	118.85
1	F	328	VAL	N-CA-C	-5.25	105.67	113.39
1	D	303	ASP	N-CA-C	5.23	118.78	111.56
1	O	62	THR	N-CA-C	5.23	117.57	110.88
1	Q	172	MET	N-CA-C	5.21	117.16	108.99
1	A	44	LEU	N-CA-C	-5.20	106.09	112.90
1	C	305	VAL	N-CA-C	5.18	116.43	108.71
1	A	42	HIS	N-CA-C	5.16	116.91	111.28
1	C	175	THR	N-CA-C	-5.15	99.36	108.23
1	O	234	THR	N-CA-C	-5.15	102.23	110.10
1	E	262	SER	N-CA-C	-5.14	105.59	111.14
1	O	36	GLY	N-CA-C	5.12	120.81	112.61
1	C	82	LEU	CA-C-N	5.12	126.24	119.84
1	C	82	LEU	C-N-CA	5.12	126.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	THR	N-CA-C	-5.12	99.43	108.23
1	F	172	MET	N-CA-C	5.10	117.71	108.69
1	B	175	THR	N-CA-C	-5.08	100.79	108.67
1	B	197	ARG	N-CA-C	5.08	117.89	109.46
1	E	305	VAL	N-CA-C	5.05	115.85	108.53
1	H	177	SER	N-CA-C	-5.03	103.76	110.55
1	D	29	ALA	N-CA-C	5.02	116.68	108.55
1	C	168	ILE	N-CA-C	-5.02	105.70	110.42
1	Q	82	LEU	CA-C-N	5.01	126.10	119.84
1	Q	82	LEU	C-N-CA	5.01	126.10	119.84

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	2557	0	2598	130	0
1	B	2557	0	2598	124	0
1	C	2557	0	2598	132	0
1	D	2552	0	2593	179	1
1	E	2547	0	2585	364	0
1	F	2552	0	2593	276	0
1	G	2552	0	2593	264	0
1	H	2542	0	2580	259	0
1	O	2557	0	2598	102	0
1	Q	2552	0	2593	126	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	3	0
2	E	44	0	26	5	0
2	F	44	0	26	2	0
2	G	44	0	26	1	0
2	H	44	0	26	2	0
2	O	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	44	0	26	0	0
3	A	35	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
3	E	20	0	0	3	0
3	F	15	0	0	0	0
3	G	25	0	0	0	0
3	H	15	0	0	0	0
3	O	30	0	0	0	0
3	Q	25	0	0	0	0
4	A	109	0	0	1	0
4	B	84	0	0	1	0
4	C	94	0	0	4	0
4	D	85	0	0	6	0
4	E	79	0	0	9	0
4	F	65	0	0	1	0
4	G	81	0	0	4	0
4	H	56	0	0	0	0
4	O	129	0	0	2	0
4	Q	100	0	0	4	0
All	All	27072	0	26189	1753	1

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 33.

All (1753) 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:A:154:LEU:HD22	1:A:172:MET:HE3	1.39	1.05
1:Q:191:ARG:HB3	1:Q:191:ARG:HH11	1.22	1.04
1:G:63:ALA:HB1	1:G:70:ILE:HD11	1.34	1.04
1:E:17:ARG:HA	1:E:17:ARG:HE	1.18	1.03
1:F:90:ASP:HA	1:F:114:LYS:HD3	1.41	1.03
1:D:139:HIS:HB3	1:D:333:LYS:HE2	1.40	1.02
1:F:126:PRO:HG2	1:F:141:GLU:HG2	1.42	1.01
1:G:221:LEU:HD21	1:G:225:LEU:HD11	1.46	0.98
1:O:17:ARG:NH1	1:O:53:PHE:HB2	1.79	0.98
1:H:72:GLN:NE2	1:H:72:GLN:H	1.62	0.97
1:G:161:LEU:HB2	1:G:167:ILE:HD11	1.51	0.93
1:Q:38:LYS:HE3	1:Q:38:LYS:H	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:ARG:HH21	1:G:277:PRO:HA	1.34	0.91
1:E:226:ASN:HB3	1:G:300:MET:HE2	1.49	0.91
1:G:256:ASN:HD21	1:G:297:THR:HG21	1.35	0.91
1:E:126:PRO:HB2	1:E:144:ILE:HG22	1.53	0.90
1:D:85:LYS:HG3	1:D:112:GLY:HA2	1.51	0.90
1:E:70:ILE:HD13	1:E:70:ILE:H	1.35	0.90
1:A:202:ASN:HD21	1:C:281:VAL:HG12	1.37	0.89
1:E:117:ILE:HG22	1:E:144:ILE:HD11	1.52	0.89
1:E:304:MET:HE1	1:G:245:GLN:HB2	1.53	0.88
1:F:202:ASN:HD22	1:H:281:VAL:H	1.23	0.87
1:F:85:LYS:HG2	1:F:112:GLY:HA2	1.57	0.86
1:F:96:THR:OG1	1:F:98:VAL:HG22	1.76	0.86
1:E:154:LEU:HD21	1:E:172:MET:HG3	1.58	0.86
1:G:251:PHE:O	1:G:255:VAL:HG23	1.77	0.85
1:G:2:LYS:HD2	1:G:28:ILE:HG21	1.58	0.85
1:F:317:TYR:O	1:F:321:VAL:HG23	1.77	0.84
1:E:133:ASN:H	1:E:133:ASN:HD22	1.22	0.84
1:H:190:HIS:HB3	1:H:196:ALA:HB2	1.59	0.84
1:C:333:LYS:HE2	4:C:423:HOH:O	1.76	0.83
1:F:298:MET:HE3	1:F:306:LYS:HD3	1.61	0.83
1:E:176:HIS:O	1:E:231:ARG:HA	1.78	0.82
1:E:139:HIS:CE1	1:E:332:TRP:HA	2.14	0.82
1:Q:191:ARG:HB3	1:Q:191:ARG:NH1	1.94	0.82
1:B:139:HIS:NE2	1:B:333:LYS:HD3	1.95	0.81
1:F:130:VAL:HB	1:F:320:ARG:HD3	1.61	0.81
1:F:328:VAL:O	1:F:332:TRP:HB2	1.80	0.81
1:F:31:ASN:HB2	1:F:74:VAL:HG13	1.61	0.81
1:H:96:THR:OG1	1:H:98:VAL:HG22	1.81	0.81
1:D:172:MET:HE3	1:D:211:ALA:HB2	1.61	0.80
1:E:17:ARG:HA	1:E:17:ARG:NE	1.96	0.80
1:C:156:PRO:HB2	1:C:290:THR:HG21	1.63	0.80
1:D:129:VAL:HG23	1:D:217:VAL:HG11	1.63	0.80
1:E:232:VAL:HG21	1:G:203:ILE:HD11	1.61	0.80
1:D:264:GLU:HA	1:D:268:LYS:HE3	1.62	0.80
1:H:170:GLY:HA3	1:H:244:VAL:HG12	1.64	0.80
1:H:228:ILE:H	1:H:228:ILE:HD13	1.47	0.80
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.63	0.79
1:G:294:SER:O	1:G:297:THR:HG22	1.81	0.79
1:H:129:VAL:H	1:H:133:ASN:HD21	1.27	0.79
1:H:86:GLU:O	1:H:87:LEU:HB2	1.81	0.79
1:O:281:VAL:HB	1:Q:202:ASN:HD21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:0:LYS:O	1:Q:0:LYS:HD2	1.84	0.78
1:E:203:ILE:HD11	1:G:232:VAL:HG21	1.64	0.78
1:E:262:SER:HB3	1:E:267:LEU:HD12	1.65	0.78
1:G:211:ALA:CB	1:G:226:ASN:HA	2.14	0.78
1:H:195:ARG:HH21	1:H:206:THR:HG21	1.49	0.78
1:B:163:GLN:HE21	1:B:164:LYS:NZ	1.82	0.77
1:E:133:ASN:HD22	1:E:133:ASN:N	1.78	0.77
1:E:277:PRO:HA	1:G:194:ARG:HE	1.50	0.77
1:Q:159:LYS:HG2	1:Q:163:GLN:HE21	1.47	0.77
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.18	0.77
1:F:315:TRP:O	1:F:319:GLN:HG2	1.83	0.77
1:D:91:ILE:HA	1:D:115:LYS:O	1.85	0.77
1:E:72:GLN:HG3	1:E:73:VAL:H	1.50	0.77
1:B:226:ASN:ND2	1:D:298:MET:SD	2.58	0.77
1:E:171:THR:HB	1:G:300:MET:HG2	1.64	0.77
1:E:0(A):ALA:HB1	1:E:26:ASP:HB2	1.65	0.77
1:G:154:LEU:HD22	1:G:172:MET:HE2	1.67	0.77
1:H:130:VAL:HA	1:H:134:ALA:HB2	1.67	0.77
1:E:169:LYS:HE3	1:G:304:MET:HB2	1.66	0.76
1:F:79:PRO:HA	1:F:82:LEU:HD12	1.65	0.76
1:E:165:PHE:HD1	1:E:248:LYS:HD2	1.50	0.76
1:Q:138:SER:HB3	1:Q:141:GLU:OE2	1.83	0.76
1:B:154:LEU:HD21	1:B:172:MET:HE2	1.67	0.76
1:E:64:ILE:HG23	1:E:73:VAL:HG21	1.67	0.76
1:A:156:PRO:HB2	1:A:290:THR:HG21	1.66	0.75
1:A:85:LYS:N	1:A:85:LYS:HE3	2.02	0.75
1:E:167:ILE:HG23	1:E:244:VAL:HB	1.68	0.75
1:Q:78:ASN:HB3	1:Q:81:LEU:HD12	1.69	0.75
1:F:243:VAL:HG11	1:H:171:THR:HG21	1.69	0.75
1:G:293:ASP:OD1	1:G:296:LEU:HG	1.87	0.75
1:B:153:CYS:HA	1:B:290:THR:HG22	1.67	0.75
1:E:194:ARG:HG2	1:G:277:PRO:O	1.86	0.75
1:F:284:ARG:O	1:F:285:CYS:HB2	1.87	0.75
1:H:38:LYS:H	1:H:38:LYS:HD2	1.51	0.75
1:F:85:LYS:HG2	1:F:112:GLY:CA	2.17	0.75
1:E:58:LYS:HB2	1:E:59:PRO:HD2	1.69	0.74
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.67	0.74
1:E:194:ARG:HE	1:G:277:PRO:C	1.95	0.74
1:B:233:PRO:HB2	1:D:233:PRO:HB2	1.67	0.74
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.88	0.74
1:E:256:ASN:HD21	1:E:297:THR:HB	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG13	1:A:71:ILE:HD11	1.67	0.74
1:O:281:VAL:HB	1:Q:202:ASN:ND2	2.01	0.74
1:D:91:ILE:HG22	1:D:115:LYS:HB3	1.69	0.73
1:H:156:PRO:HB2	1:H:290:THR:HG21	1.69	0.73
1:C:76:ASN:HD22	1:C:77:ARG:N	1.85	0.73
1:H:81:LEU:HD12	1:H:81:LEU:H	1.53	0.73
1:B:271:LEU:HD13	1:B:272:ASP:N	2.03	0.73
1:F:78:ASN:HB3	1:F:81:LEU:HD13	1.69	0.73
1:E:279:VAL:CG1	1:G:204:VAL:HG22	2.18	0.73
1:G:129:VAL:H	1:G:133:ASN:HD21	1.35	0.73
1:H:168:ILE:HD12	1:H:245:GLN:HG2	1.69	0.73
1:A:33:THR:HG22	1:A:77:ARG:HG2	1.69	0.73
1:E:156:PRO:HB2	1:E:290:THR:HG21	1.71	0.73
1:F:60:SER:H	1:F:64:ILE:HA	1.54	0.73
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.23	0.73
1:F:228:ILE:H	1:F:228:ILE:HD13	1.54	0.73
1:E:217:VAL:HG23	1:E:218:LEU:HG	1.71	0.73
1:H:183:ARG:HG2	1:H:196:ALA:HA	1.71	0.73
1:E:194:ARG:NH2	1:G:277:PRO:HA	2.03	0.73
1:H:70:ILE:HG22	1:H:71:ILE:H	1.53	0.73
1:E:7:GLY:HA2	2:E:335:NAD:H1B	1.70	0.72
1:F:267:LEU:HD22	1:F:270:ILE:HG21	1.68	0.72
1:F:222:LYS:HG2	1:F:224:LYS:HE2	1.71	0.72
1:D:153:CYS:HA	1:D:290:THR:HG22	1.72	0.72
1:G:130:VAL:HA	1:G:134:ALA:HB2	1.71	0.72
1:E:20:ARG:NH2	1:E:322:VAL:HB	2.03	0.72
1:F:16:LEU:HD22	1:F:44:LEU:HD11	1.71	0.72
1:F:249:LYS:HG2	1:F:302:ASP:HB3	1.71	0.72
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.70	0.72
1:G:193:LEU:H	1:G:193:LEU:HD22	1.54	0.72
1:B:105:ALA:HB1	1:B:116:VAL:HG11	1.71	0.71
1:D:0:LYS:HD2	4:D:363:HOH:O	1.90	0.71
1:E:194:ARG:HD3	1:E:205:PRO:HG2	1.73	0.71
1:D:74:VAL:HG22	1:D:75:SER:H	1.54	0.71
1:E:3:VAL:HG21	1:E:25:LEU:HD22	1.72	0.71
1:E:235:PRO:HB3	1:H:201:LEU:HD11	1.72	0.71
1:A:300:MET:HE3	1:C:226:ASN:HB3	1.71	0.71
1:G:62:THR:HG22	1:Q:62:THR:HG22	1.73	0.71
1:E:186:ASP:HB2	1:H:10:ARG:NH1	2.06	0.70
1:E:195:ARG:HH22	1:E:231:ARG:NH2	1.89	0.70
1:F:21:LYS:N	1:F:21:LYS:HD2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:HIS:CD2	1:B:333:LYS:HD3	2.25	0.70
1:G:241:ASP:OD1	1:G:308:ILE:HD11	1.91	0.70
1:A:271:LEU:HD12	1:A:272:ASP:H	1.57	0.70
1:G:186:ASP:OD1	1:G:197:ARG:HA	1.92	0.70
1:G:296:LEU:O	1:G:298:MET:HE2	1.91	0.70
1:H:4:ALA:HB2	1:H:89:ILE:HD12	1.72	0.70
1:E:178:TYR:HA	1:E:182:GLN:OE1	1.92	0.70
1:G:154:LEU:CD2	1:G:172:MET:HE2	2.20	0.70
1:A:27:ILE:HG22	1:A:71:ILE:HD12	1.74	0.70
1:A:48:SER:HA	1:B:281:VAL:HG11	1.73	0.70
1:D:83:PRO:HB3	1:H:72:GLN:OE1	1.92	0.70
1:E:119:THR:HG22	1:E:321:VAL:HG11	1.74	0.70
1:F:318:SER:O	1:F:322:VAL:HG23	1.92	0.70
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.27	0.70
1:E:157:PHE:HE1	1:E:307:VAL:HG21	1.56	0.70
1:B:281:VAL:HG12	1:D:202:ASN:HD21	1.57	0.70
1:F:11:ILE:O	1:F:11:ILE:HD13	1.92	0.70
1:H:37:VAL:HG21	1:H:62:THR:HA	1.74	0.70
1:H:181:ASP:HB3	1:H:195:ARG:HD3	1.74	0.70
1:Q:4:ALA:HB2	1:Q:89:ILE:HD12	1.74	0.70
1:E:192:ASP:HB3	1:E:195:ARG:HB2	1.73	0.69
1:F:222:LYS:HG2	1:F:224:LYS:CE	2.21	0.69
1:F:228:ILE:HG21	1:H:296:LEU:HD22	1.74	0.69
1:H:72:GLN:H	1:H:72:GLN:HE21	1.37	0.69
1:G:256:ASN:HD22	1:G:256:ASN:N	1.89	0.69
1:F:75:SER:O	1:F:76:ASN:HB2	1.91	0.69
1:F:300:MET:HG2	1:H:226:ASN:ND2	2.07	0.69
1:E:194:ARG:HH12	1:G:296:LEU:HD21	1.57	0.69
1:G:0:LYS:HZ2	1:G:0:LYS:HB3	1.57	0.69
1:B:212:LYS:HE3	4:B:785:HOH:O	1.91	0.69
1:D:18:CYS:HB3	1:D:319:GLN:OE1	1.92	0.69
1:G:256:ASN:HB3	1:G:260:ARG:NH1	2.07	0.69
1:A:3:VAL:HG22	1:A:91:ILE:HG23	1.72	0.69
1:A:228:ILE:C	1:A:228:ILE:HD12	2.18	0.69
1:F:126:PRO:HB2	1:F:144:ILE:HG22	1.74	0.69
1:H:45:LYS:HB2	1:H:57:VAL:HB	1.74	0.69
1:O:202:ASN:HD21	1:Q:281:VAL:HB	1.57	0.69
1:E:63:ALA:HA	1:E:73:VAL:HG23	1.74	0.69
1:E:204:VAL:HG22	1:G:279:VAL:HG11	1.75	0.69
1:F:21:LYS:HD2	1:F:21:LYS:H	1.59	0.69
1:F:133:ASN:HD21	1:F:217:VAL:HG12	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ASP:O	1:F:327:ILE:HG13	1.92	0.69
1:O:159:LYS:O	1:O:163:GLN:HG3	1.92	0.69
1:A:281:VAL:CG1	1:C:202:ASN:HD21	2.06	0.68
1:E:114:LYS:HB2	1:E:332:TRP:HH2	1.57	0.68
1:F:31:ASN:HB2	1:F:74:VAL:CG1	2.23	0.68
1:G:170:GLY:HA2	1:G:243:VAL:O	1.92	0.68
1:G:18(A):TRP:C	1:G:19:GLY:H	1.99	0.68
1:E:154:LEU:O	1:E:158:VAL:HG23	1.94	0.68
1:F:202:ASN:HD21	1:H:281:VAL:HB	1.58	0.68
1:A:300:MET:HE3	1:C:226:ASN:CB	2.22	0.68
1:E:183:ARG:HD3	1:E:190:HIS:HB2	1.76	0.68
1:G:256:ASN:ND2	1:G:297:THR:HG21	2.08	0.68
1:A:202:ASN:HD21	1:C:281:VAL:CG1	2.05	0.68
1:A:281:VAL:H	1:C:202:ASN:ND2	1.92	0.68
1:C:115:LYS:HE2	1:C:142:PRO:HA	1.76	0.68
1:E:55:ALA:O	1:E:57:VAL:HG23	1.94	0.68
1:Q:169:LYS:HE3	1:Q:245:GLN:NE2	2.09	0.68
1:E:134:ALA:HB3	4:E:490:HOH:O	1.93	0.67
1:A:281:VAL:HG12	1:C:202:ASN:HD21	1.59	0.67
1:D:172:MET:O	1:D:227:GLY:HA3	1.94	0.67
1:E:304:MET:CE	1:G:245:GLN:HB2	2.23	0.67
1:G:0:LYS:HB3	1:G:0:LYS:NZ	2.09	0.67
1:Q:85:LYS:HB2	1:Q:112:GLY:HA3	1.75	0.67
1:A:78:ASN:ND2	1:A:81:LEU:HG	2.08	0.67
1:E:240:VAL:HG23	1:E:309:ALA:HB3	1.76	0.67
1:H:159:LYS:HE3	1:H:218:LEU:HD21	1.77	0.67
1:E:31:ASN:HA	1:E:74:VAL:CG2	2.24	0.67
1:F:5:ILE:HD13	1:F:8:PHE:HD1	1.59	0.67
1:F:272:ASP:HB2	1:F:288:PHE:CD2	2.30	0.67
1:B:240:VAL:HG22	1:B:309:ALA:HB3	1.75	0.67
1:E:293:ASP:OD1	1:E:296:LEU:HG	1.93	0.67
1:F:210:ALA:O	1:F:214:VAL:HG23	1.94	0.67
1:Q:206:THR:HG22	1:Q:229:ALA:HB3	1.77	0.67
1:F:133:ASN:ND2	1:F:217:VAL:HG12	2.10	0.67
1:F:154:LEU:HD22	1:F:172:MET:HE2	1.77	0.67
1:E:194:ARG:HE	1:G:277:PRO:CA	2.07	0.67
1:E:300:MET:HE1	1:G:171:THR:OG1	1.94	0.67
1:E:5:ILE:CD1	1:E:27:ILE:HD12	2.25	0.67
1:A:226:ASN:HD22	1:C:300:MET:HE2	1.58	0.67
1:F:222:LYS:H	1:F:224:LYS:HE3	1.57	0.67
1:G:262:SER:HB3	1:G:267:LEU:HG	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ASN:O	1:F:289:SER:HB3	1.96	0.66
1:B:38:LYS:H	1:B:38:LYS:HD2	1.60	0.66
1:G:162:ASP:HA	1:G:167:ILE:HG13	1.75	0.66
1:E:25:LEU:HD11	1:E:325:ALA:HB3	1.76	0.66
1:Q:154:LEU:O	1:Q:158:VAL:HG23	1.95	0.66
1:A:105:ALA:HB1	1:A:116:VAL:HG11	1.77	0.66
1:E:242:LEU:HB3	1:E:307:VAL:CG2	2.26	0.66
1:E:279:VAL:HG22	1:E:282:ASP:OD2	1.94	0.66
1:F:202:ASN:ND2	1:H:281:VAL:HB	2.11	0.66
1:C:58:LYS:HE2	4:C:378:HOH:O	1.96	0.66
1:D:83:PRO:O	1:D:87:LEU:HD23	1.94	0.66
1:E:126:PRO:HD2	1:E:143:ILE:O	1.95	0.66
1:E:132:VAL:HG21	1:E:155:ALA:HB1	1.77	0.66
1:F:125:ILE:HD12	1:F:125:ILE:H	1.61	0.66
1:D:109:ILE:HA	1:D:113:ALA:O	1.95	0.66
1:D:116:VAL:HB	1:D:143:ILE:HD12	1.78	0.66
1:F:169:LYS:HD2	1:H:301:GLY:HA3	1.77	0.66
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.76	0.66
1:F:280:SER:HB3	1:F:310:TRP:HZ3	1.61	0.66
1:E:299:VAL:HG22	1:E:305:VAL:HG22	1.76	0.66
1:F:114:LYS:N	1:F:114:LYS:HD2	2.11	0.66
1:G:187:ALA:O	1:G:196:ALA:HB1	1.95	0.66
1:F:266:GLU:HG3	4:F:578:HOH:O	1.96	0.66
1:G:168:ILE:HG22	1:G:169:LYS:HG3	1.77	0.65
1:B:38:LYS:HD2	1:B:38:LYS:N	2.10	0.65
1:F:176:HIS:O	1:F:231:ARG:HA	1.95	0.65
1:G:294:SER:C	1:G:296:LEU:H	2.03	0.65
1:H:129:VAL:HG23	1:H:217:VAL:HG11	1.78	0.65
1:A:202:ASN:ND2	1:C:281:VAL:HG12	2.11	0.65
1:E:279:VAL:HG12	1:G:204:VAL:HG22	1.76	0.65
1:B:33:THR:HG21	1:B:77:ARG:HD3	1.79	0.65
1:E:5:ILE:HD12	1:E:27:ILE:HD12	1.77	0.65
1:E:13:ARG:HH11	1:E:13:ARG:HG3	1.62	0.65
1:E:297:THR:HG23	1:E:306:LYS:O	1.96	0.65
1:H:204:VAL:HB	1:H:231:ARG:HB2	1.79	0.65
1:F:226:ASN:HB3	1:H:300:MET:SD	2.37	0.65
1:B:193:LEU:HD13	1:C:42:HIS:CG	2.31	0.65
1:B:80:SER:OG	1:B:107:LYS:HG2	1.97	0.65
1:E:210:ALA:O	1:E:214:VAL:HG23	1.97	0.65
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.79	0.65
1:G:285:CYS:HA	1:G:315:TRP:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:124:ASP:CG	1:O:124:ASP:O	2.40	0.65
1:E:151:THR:HG23	1:E:214:VAL:HG22	1.79	0.65
1:E:170:GLY:N	1:E:224:LYS:O	2.30	0.65
1:F:226:ASN:ND2	1:H:298:MET:SD	2.70	0.65
1:A:1:LEU:HD22	1:A:329:ALA:CB	2.27	0.65
1:F:118:ILE:H	1:F:118:ILE:HD12	1.61	0.65
1:G:208:THR:C	1:G:210:ALA:H	2.05	0.64
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.78	0.64
1:A:64:ILE:HG13	1:A:71:ILE:HG23	1.78	0.64
1:F:188:SER:HB2	1:G:39:GLN:OE1	1.96	0.64
1:H:182:GLN:HE22	1:H:231:ARG:HB3	1.61	0.64
1:B:168:ILE:HD11	1:B:247:SER:HB3	1.79	0.64
1:F:281:VAL:HB	1:H:202:ASN:HB3	1.79	0.64
1:H:236:ASN:O	1:H:237:VAL:HB	1.96	0.64
1:F:89:ILE:O	1:F:113:ALA:HA	1.97	0.64
1:F:296:LEU:HD22	1:H:228:ILE:HG21	1.79	0.64
1:H:91:ILE:HD13	1:H:91:ILE:C	2.23	0.64
1:D:133:ASN:C	1:D:133:ASN:HD22	2.05	0.64
1:G:130:VAL:CG2	1:G:320:ARG:HD3	2.28	0.64
1:G:221:LEU:HD21	1:G:225:LEU:CD1	2.25	0.64
1:H:239:VAL:HG23	1:H:309:ALA:O	1.97	0.64
1:F:187:ALA:O	1:F:196:ALA:HB1	1.97	0.64
1:F:280:SER:HB3	1:F:310:TRP:CZ3	2.33	0.64
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.32	0.64
1:D:284:ARG:O	1:D:285:CYS:HB2	1.95	0.64
1:H:251:PHE:HE2	1:H:253:GLU:HB2	1.61	0.64
1:E:165:PHE:CD1	1:E:248:LYS:HD2	2.33	0.64
1:E:183:ARG:HH11	1:E:183:ARG:HA	1.62	0.64
1:E:277:PRO:CA	1:G:194:ARG:HE	2.10	0.64
1:E:328:VAL:O	1:E:332:TRP:HB2	1.97	0.64
1:G:260:ARG:O	1:G:263:ALA:HB3	1.98	0.64
1:E:79:PRO:HB2	1:E:107:LYS:HB2	1.79	0.64
1:G:64:ILE:O	1:G:70:ILE:HD12	1.98	0.64
1:G:124:ASP:HB2	4:G:634:HOH:O	1.97	0.64
1:H:78:ASN:HB3	1:H:81:LEU:HD13	1.79	0.64
1:H:129:VAL:CG2	1:H:217:VAL:HG11	2.26	0.64
1:F:324:LEU:O	1:F:328:VAL:HG23	1.97	0.63
1:B:132:VAL:HG21	1:B:155:ALA:HB1	1.80	0.63
1:D:74:VAL:HG22	1:D:75:SER:N	2.12	0.63
1:E:176:HIS:N	1:E:230:LEU:O	2.28	0.63
1:E:250:THR:OG1	1:E:254:GLU:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:CYS:HA	1:F:315:TRP:CD1	2.33	0.63
1:B:4:ALA:HB2	1:B:89:ILE:HG12	1.80	0.63
1:E:109:ILE:O	1:E:109:ILE:HD13	1.98	0.63
1:F:59:PRO:HA	1:F:64:ILE:HA	1.81	0.63
1:G:221:LEU:HD11	1:G:225:LEU:HD21	1.79	0.63
1:H:251:PHE:CE2	1:H:253:GLU:HB2	2.34	0.63
1:E:293:ASP:CG	1:E:296:LEU:HG	2.23	0.63
1:F:145:SER:C	1:F:147:ALA:H	2.06	0.63
1:O:78:ASN:ND2	1:O:81:LEU:HG	2.12	0.63
1:B:269:GLY:C	1:B:270:ILE:HD12	2.24	0.63
1:F:118:ILE:HD12	1:F:118:ILE:N	2.12	0.63
1:H:70:ILE:HG22	1:H:71:ILE:N	2.12	0.63
1:H:299:VAL:HG22	1:H:305:VAL:HG22	1.81	0.63
1:C:77:ARG:O	1:C:79:PRO:HD3	1.99	0.63
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.13	0.63
1:G:130:VAL:HA	1:G:134:ALA:CB	2.28	0.63
1:D:272:ASP:HB2	1:D:288:PHE:CD2	2.33	0.63
1:E:72:GLN:HG3	1:E:73:VAL:N	2.13	0.63
1:E:79:PRO:HB2	1:E:107:LYS:CB	2.28	0.63
1:F:11:ILE:HD12	1:F:119:THR:HG21	1.80	0.63
1:O:17:ARG:HH11	1:O:53:PHE:HB2	1.61	0.63
1:O:172:MET:HE3	1:O:211:ALA:HB2	1.81	0.63
1:O:202:ASN:HD21	1:Q:281:VAL:CG1	2.12	0.63
1:D:125:ILE:HD12	1:D:126:PRO:HD2	1.80	0.63
1:G:150:THR:HG23	1:G:311:TYR:OH	1.99	0.63
1:G:192:ASP:CG	1:G:195:ARG:HG3	2.24	0.63
1:F:64:ILE:O	1:F:70:ILE:HG23	1.99	0.63
1:G:166:GLY:O	1:G:246:VAL:HA	1.98	0.63
1:O:204:VAL:HB	1:O:231:ARG:HB2	1.81	0.63
1:B:281:VAL:H	1:D:202:ASN:ND2	1.97	0.62
1:E:74:VAL:O	1:E:75:SER:HB2	1.98	0.62
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.81	0.62
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.80	0.62
1:G:171:THR:O	1:G:242:LEU:HB2	2.00	0.62
1:F:27:ILE:N	1:F:27:ILE:HD12	2.15	0.62
1:C:26:ASP:O	1:C:28:ILE:HG23	1.99	0.62
1:E:28:ILE:HA	1:E:71:ILE:HG12	1.82	0.62
1:H:183:ARG:HE	1:H:187:ALA:HB3	1.62	0.62
1:A:306:LYS:HD2	1:C:171:THR:OG1	2.00	0.62
1:B:15:PHE:HE2	1:B:27:ILE:HD11	1.64	0.62
1:O:33:THR:CG2	1:O:77:ARG:HG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HD13	1:A:91:ILE:C	2.25	0.62
1:O:134:ALA:HB3	4:O:401:HOH:O	1.97	0.62
1:A:173:THR:HG23	1:A:228:ILE:HD11	1.82	0.62
1:D:318:SER:O	1:D:322:VAL:HG23	2.00	0.62
1:E:119:THR:CG2	1:E:321:VAL:HG11	2.29	0.62
1:E:270:ILE:HD11	4:E:491:HOH:O	1.99	0.62
1:G:259:PHE:CD2	1:G:292:ILE:HG21	2.34	0.62
1:O:202:ASN:ND2	1:Q:281:VAL:HB	2.14	0.62
1:Q:8:PHE:N	1:Q:32:ASP:OD2	2.31	0.62
1:E:183:ARG:CZ	1:E:187:ALA:HB3	2.30	0.62
1:E:208:THR:HG23	1:E:208:THR:O	1.99	0.62
1:B:281:VAL:H	1:D:202:ASN:HD22	1.48	0.62
1:Q:272:ASP:O	1:Q:291:THR:HA	1.99	0.62
1:B:262:SER:HB3	1:B:267:LEU:HD12	1.82	0.61
1:E:263:ALA:O	1:E:268:LYS:HA	1.99	0.61
1:F:108:HIS:O	1:F:111:ALA:HB3	1.99	0.61
1:G:239:VAL:HG23	1:G:309:ALA:O	1.99	0.61
1:A:281:VAL:H	1:C:202:ASN:HD22	1.47	0.61
1:E:174:THR:HB	1:E:240:VAL:HG12	1.81	0.61
1:E:260:ARG:HD2	4:E:538:HOH:O	2.01	0.61
1:D:138:SER:O	1:D:141:GLU:HG2	2.01	0.61
1:F:16:LEU:HD23	1:F:16:LEU:C	2.24	0.61
1:O:202:ASN:HD22	1:Q:281:VAL:H	1.46	0.61
1:E:84:TRP:CE3	1:E:89:ILE:HG13	2.35	0.61
1:H:84:TRP:HA	1:H:89:ILE:HG13	1.81	0.61
1:H:85:LYS:HB2	1:H:111:ALA:O	2.01	0.61
1:C:62:THR:HG22	1:C:62:THR:O	2.00	0.61
1:E:117:ILE:O	1:E:117:ILE:HG13	2.00	0.61
1:F:138:SER:HA	1:F:331:ASN:OD1	2.01	0.61
1:G:18:CYS:SG	1:G:319:GLN:HG2	2.41	0.61
1:G:221:LEU:HD11	1:G:225:LEU:CD2	2.30	0.61
1:E:264:GLU:HG3	4:E:535:HOH:O	2.00	0.61
1:F:38:LYS:HG3	1:F:39:GLN:N	2.16	0.61
1:F:279:VAL:O	1:F:281:VAL:N	2.34	0.61
1:H:21:LYS:O	1:H:22:ASP:C	2.44	0.61
1:C:250:THR:OG1	1:C:251:PHE:N	2.34	0.61
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.36	0.61
1:H:176:HIS:HB3	1:H:231:ARG:HD3	1.83	0.61
1:H:192:ASP:HB3	1:H:195:ARG:HB3	1.83	0.61
1:F:159:LYS:HB2	1:F:218:LEU:HD11	1.82	0.61
1:G:225:LEU:O	1:G:226:ASN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:O	1:D:300:MET:HE2	2.01	0.60
1:E:265:LYS:HB2	1:E:266:GLU:OE1	2.00	0.60
1:F:6:ASN:OD1	1:F:31:ASN:ND2	2.34	0.60
1:O:224:LYS:O	1:O:225:LEU:HD23	2.01	0.60
1:D:133:ASN:C	1:D:133:ASN:ND2	2.58	0.60
1:H:31:ASN:OD1	1:H:74:VAL:HG23	2.01	0.60
1:A:298:MET:SD	1:C:226:ASN:OD1	2.59	0.60
1:E:209:GLY:HA3	1:E:212:LYS:HE2	1.84	0.60
1:E:270:ILE:HG13	4:E:828:HOH:O	2.00	0.60
1:G:177:SER:HB3	1:G:234:THR:O	2.01	0.60
1:A:142:PRO:HB2	1:A:143:ILE:HD12	1.82	0.60
1:E:186:ASP:O	1:H:13:ARG:NH2	2.35	0.60
1:G:162:ASP:CA	1:G:167:ILE:HG13	2.31	0.60
1:H:38:LYS:H	1:H:38:LYS:CD	2.12	0.60
1:O:202:ASN:HD21	1:Q:281:VAL:CB	2.15	0.60
1:A:226:ASN:ND2	1:C:300:MET:HE2	2.15	0.60
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.83	0.60
1:E:6:ASN:ND2	1:E:108:HIS:HE1	1.99	0.60
1:F:251:PHE:CZ	1:F:254:GLU:HB2	2.37	0.60
1:O:281:VAL:CB	1:Q:202:ASN:HD21	2.14	0.60
1:E:94:GLU:OE1	1:E:99:PHE:HB2	2.00	0.60
1:F:126:PRO:CG	1:F:141:GLU:HG2	2.26	0.60
1:F:243:VAL:HG22	1:F:306:LYS:HG3	1.82	0.60
1:H:194:ARG:C	1:H:196:ALA:H	2.10	0.60
1:A:5:ILE:HD11	1:A:27:ILE:HD13	1.84	0.60
1:B:281:VAL:CG1	1:D:202:ASN:HD21	2.14	0.60
1:E:320:ARG:NE	1:E:320:ARG:HA	2.17	0.60
1:Q:31:ASN:OD1	1:Q:74:VAL:HG23	2.01	0.60
1:E:226:ASN:HD22	1:G:300:MET:HE1	1.67	0.60
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.30	0.60
1:H:133:ASN:HD22	1:H:133:ASN:N	1.99	0.60
1:H:264:GLU:HA	1:H:268:LYS:HG3	1.84	0.60
1:F:14:ASN:ND2	1:F:314:GLU:HG2	2.17	0.59
1:H:27:ILE:O	1:H:28:ILE:HB	2.02	0.59
1:H:256:ASN:O	1:H:260:ARG:HG3	2.02	0.59
1:Q:183:ARG:NH1	4:Q:463:HOH:O	2.27	0.59
1:F:186:ASP:HA	1:F:196:ALA:O	2.02	0.59
1:F:277:PRO:HB2	1:H:194:ARG:HG3	1.84	0.59
1:O:192:ASP:CG	1:O:195:ARG:HG3	2.27	0.59
1:E:31:ASN:HA	1:E:74:VAL:HG22	1.83	0.59
1:A:245:GLN:HE22	1:C:245:GLN:NE2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:C	1:A:333:LYS:HE2	2.27	0.59
1:E:157:PHE:CE1	1:E:307:VAL:HG21	2.37	0.59
1:C:56:ASP:O	1:C:66:VAL:HA	2.02	0.59
1:E:18:CYS:O	1:E:20:ARG:HG2	2.02	0.59
1:E:190:HIS:HB3	1:E:196:ALA:HB2	1.85	0.59
1:E:194:ARG:HH11	1:E:205:PRO:HG2	1.67	0.59
1:F:149:CYS:HB3	2:F:335:NAD:H5N	1.84	0.59
1:F:267:LEU:HD22	1:F:270:ILE:CG2	2.33	0.59
1:G:168:ILE:HG22	1:G:169:LYS:HE3	1.84	0.59
1:H:294:SER:C	1:H:296:LEU:H	2.09	0.59
1:O:129:VAL:H	1:O:133:ASN:HD21	1.48	0.59
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.83	0.59
1:A:245:GLN:HE22	1:C:245:GLN:HE22	1.51	0.59
1:A:271:LEU:HD12	1:A:272:ASP:N	2.17	0.59
1:D:154:LEU:HD22	1:D:172:MET:HE2	1.85	0.59
1:D:164:LYS:HD2	1:D:258:ALA:HB1	1.85	0.59
1:E:195:ARG:NH2	1:E:231:ARG:NH2	2.51	0.59
1:A:281:VAL:CB	1:C:202:ASN:HD21	2.16	0.59
1:F:271:LEU:HD13	1:F:290:THR:HG23	1.84	0.59
1:Q:2:LYS:HE2	4:Q:451:HOH:O	2.02	0.59
1:E:44:LEU:O	1:E:53:PHE:HD1	1.86	0.59
1:E:202:ASN:HD22	1:G:281:VAL:CG1	2.16	0.59
1:F:6:ASN:O	1:F:96:THR:HG23	2.03	0.59
1:F:271:LEU:HD13	1:F:290:THR:CG2	2.32	0.59
1:G:205:PRO:HA	1:G:229:ALA:O	2.03	0.59
1:E:3:VAL:CG2	1:E:25:LEU:HD22	2.32	0.59
1:E:109:ILE:HA	1:E:113:ALA:O	2.03	0.59
1:E:117:ILE:HG22	1:E:144:ILE:CD1	2.31	0.59
1:F:183:ARG:NE	1:F:187:ALA:HB3	2.18	0.59
1:F:243:VAL:CG1	1:H:171:THR:HG21	2.33	0.59
1:E:169:LYS:HE2	1:E:245:GLN:CD	2.27	0.58
1:E:318:SER:O	1:E:322:VAL:HG23	2.03	0.58
1:C:241:ASP:OD1	1:C:306:LYS:HE3	2.03	0.58
1:E:157:PHE:HB2	1:E:259:PHE:CE1	2.37	0.58
1:E:159:LYS:O	1:E:163:GLN:HG3	2.03	0.58
1:E:199:ALA:HB2	1:H:184:LEU:HD21	1.85	0.58
1:E:279:VAL:HG22	1:G:197:ARG:NH1	2.18	0.58
1:F:271:LEU:HD11	1:F:292:ILE:HD11	1.84	0.58
1:H:108:HIS:HB2	1:H:116:VAL:HG21	1.85	0.58
1:E:228:ILE:HD13	1:E:228:ILE:H	1.68	0.58
1:G:172:MET:O	1:G:227:GLY:HA3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:VAL:HG22	1:G:306:LYS:HE2	1.85	0.58
1:Q:276:GLU:HB2	1:Q:278:LEU:HG	1.86	0.58
1:G:228:ILE:HD13	1:G:228:ILE:H	1.69	0.58
1:O:1:LEU:CD1	1:O:329:ALA:HA	2.34	0.58
1:O:277:PRO:HA	1:Q:194:ARG:NH2	2.19	0.58
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.01	0.58
1:E:115:LYS:HD2	1:E:328:VAL:HG11	1.86	0.58
1:E:228:ILE:HG23	1:G:298:MET:HE1	1.85	0.58
1:F:115:LYS:HD2	1:F:332:TRP:HZ3	1.68	0.58
1:F:154:LEU:HG	1:F:158:VAL:HG21	1.84	0.58
1:C:210:ALA:O	1:C:214:VAL:HG23	2.03	0.58
1:F:140:ASP:O	1:F:142:PRO:HD3	2.03	0.58
1:H:27:ILE:HG22	1:H:28:ILE:H	1.68	0.58
1:F:202:ASN:HD21	1:H:281:VAL:CG1	2.17	0.58
1:F:235:PRO:HB3	1:G:201:LEU:HD11	1.86	0.58
1:H:195:ARG:HH21	1:H:206:THR:CG2	2.15	0.58
1:E:183:ARG:NE	1:E:187:ALA:HB3	2.19	0.58
1:E:267:LEU:HD13	1:E:271:LEU:HD23	1.86	0.58
1:G:251:PHE:HA	1:G:299:VAL:HG21	1.86	0.58
1:H:328:VAL:O	1:H:332:TRP:HB2	2.03	0.58
1:O:33:THR:HG22	1:O:77:ARG:HG2	1.86	0.58
1:Q:123:GLY:O	1:Q:125:ILE:N	2.32	0.58
1:E:298:MET:SD	1:G:226:ASN:ND2	2.74	0.57
1:E:277:PRO:HG2	1:F:42:HIS:CE1	2.39	0.57
1:F:205:PRO:HG2	1:H:310:TRP:HZ2	1.68	0.57
1:G:294:SER:O	1:G:296:LEU:N	2.37	0.57
1:O:168:ILE:HG22	1:O:169:LYS:HG2	1.86	0.57
1:E:193:LEU:HB3	1:H:42:HIS:CD2	2.39	0.57
1:F:0:LYS:HD2	1:F:24:PRO:HA	1.85	0.57
1:G:157:PHE:O	1:G:161:LEU:HG	2.05	0.57
1:A:271:LEU:HD13	1:A:290:THR:OG1	2.04	0.57
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.86	0.57
1:E:71:ILE:HD13	1:E:72:GLN:N	2.19	0.57
1:H:38:LYS:HD2	1:H:38:LYS:N	2.19	0.57
1:D:3:VAL:HG21	1:D:25:LEU:HD22	1.86	0.57
1:D:58:LYS:NZ	1:D:58:LYS:HB3	2.20	0.57
1:E:160:VAL:O	1:E:164:LYS:HB2	2.05	0.57
1:E:203:ILE:HA	1:E:231:ARG:O	2.04	0.57
1:G:264:GLU:O	1:G:264:GLU:HG2	2.04	0.57
1:H:134:ALA:HB1	1:H:327:ILE:CD1	2.35	0.57
1:G:153:CYS:O	1:G:156:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:LEU:HD11	1:G:292:ILE:HG12	1.86	0.57
1:E:74:VAL:HG23	1:E:75:SER:N	2.18	0.57
1:F:255:VAL:C	1:F:257:ALA:H	2.10	0.57
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.53	0.57
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.05	0.57
1:D:82:LEU:HD13	1:D:84:TRP:CZ2	2.39	0.57
1:D:220:ASN:C	1:D:221:LEU:HD22	2.30	0.57
1:E:15:PHE:CE1	1:E:322:VAL:HG22	2.40	0.57
1:E:205:PRO:HA	1:E:229:ALA:O	2.05	0.57
1:H:83:PRO:HB2	1:H:86:GLU:CG	2.34	0.57
1:H:246:VAL:HG22	1:H:303:ASP:O	2.05	0.57
1:Q:190:HIS:HB3	1:Q:196:ALA:HB2	1.87	0.57
1:A:115:LYS:HD2	1:A:332:TRP:CZ3	2.39	0.57
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.38	0.57
1:C:172:MET:HG2	1:C:173:THR:N	2.20	0.57
1:D:4:ALA:HB2	1:D:89:ILE:HG12	1.87	0.57
1:E:24:PRO:HG2	1:E:330:ASN:HD21	1.70	0.57
1:B:38:LYS:H	1:B:38:LYS:CD	2.13	0.56
1:B:255:VAL:O	1:B:258:ALA:HB3	2.05	0.56
1:E:33:THR:O	1:E:33:THR:HG22	2.05	0.56
1:F:37:VAL:N	1:F:73:VAL:HG11	2.20	0.56
1:H:330:ASN:C	1:H:332:TRP:H	2.13	0.56
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.06	0.56
1:E:13:ARG:HG3	1:E:13:ARG:NH1	2.20	0.56
1:F:156:PRO:O	1:F:159:LYS:HB3	2.05	0.56
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.70	0.56
1:B:256:ASN:HB3	1:B:260:ARG:HH12	1.68	0.56
1:E:272:ASP:HB2	1:E:288:PHE:CD2	2.40	0.56
1:F:304:MET:HB2	1:H:169:LYS:NZ	2.19	0.56
1:G:185:LEU:HA	1:G:198:ALA:HB2	1.87	0.56
1:A:281:VAL:HG12	1:C:202:ASN:ND2	2.20	0.56
1:F:279:VAL:HG12	1:H:204:VAL:HA	1.88	0.56
1:H:91:ILE:HA	1:H:115:LYS:O	2.06	0.56
1:E:64:ILE:O	1:E:70:ILE:HA	2.06	0.56
1:E:279:VAL:HG11	1:G:204:VAL:HG22	1.85	0.56
1:O:236:ASN:O	1:O:237:VAL:HB	2.04	0.56
1:C:21:LYS:HE3	1:C:21:LYS:H	1.70	0.56
1:C:243:VAL:HG22	1:C:306:LYS:HG2	1.88	0.56
1:G:28:ILE:HD11	1:G:89:ILE:CD1	2.35	0.56
1:H:132:VAL:O	1:H:133:ASN:HB3	2.05	0.56
1:Q:84:TRP:CE3	1:Q:89:ILE:HG13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:169:LYS:HE3	1:Q:245:GLN:HE22	1.69	0.56
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.40	0.56
1:B:15:PHE:CE2	1:B:27:ILE:HD11	2.40	0.56
1:D:209:GLY:O	1:D:211:ALA:N	2.39	0.56
1:A:103:GLU:HB2	1:G:253:GLU:OE1	2.05	0.56
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.41	0.56
1:B:193:LEU:HD13	1:C:42:HIS:CD2	2.41	0.56
1:E:279:VAL:CG2	1:E:281:VAL:HG12	2.36	0.56
1:F:202:ASN:HD21	1:H:281:VAL:CB	2.17	0.56
1:A:210:ALA:O	1:A:214:VAL:HG23	2.05	0.56
1:C:266:GLU:HG2	1:C:267:LEU:N	2.19	0.56
1:D:292:ILE:N	1:D:292:ILE:HD12	2.19	0.56
1:E:158:VAL:HG11	1:E:225:LEU:HD11	1.87	0.56
1:E:171:THR:HG23	1:G:306:LYS:HE3	1.88	0.56
1:F:172:MET:O	1:F:227:GLY:HA3	2.06	0.55
1:D:246:VAL:O	1:D:303:ASP:HB2	2.05	0.55
1:E:4:ALA:HB3	1:E:92:VAL:HG22	1.89	0.55
1:E:25:LEU:HD11	1:E:325:ALA:CB	2.36	0.55
1:E:241:ASP:OD1	1:E:306:LYS:HE2	2.06	0.55
1:F:37:VAL:H	1:F:73:VAL:HG11	1.71	0.55
1:G:192:ASP:OD1	1:G:195:ARG:HG3	2.07	0.55
1:H:18(A):TRP:CD1	1:H:23:SER:HG	2.24	0.55
1:B:177:SER:HB3	1:B:234:THR:O	2.07	0.55
1:F:115:LYS:HD2	1:F:332:TRP:CZ3	2.41	0.55
1:G:222:LYS:O	1:G:224:LYS:N	2.39	0.55
1:D:75:SER:HB3	1:H:61:GLU:HB3	1.87	0.55
1:E:183:ARG:HB3	1:E:187:ALA:HB3	1.88	0.55
1:F:157:PHE:HB2	1:F:259:PHE:CE1	2.41	0.55
1:F:170:GLY:HA3	1:F:244:VAL:HG12	1.88	0.55
1:H:9:GLY:HA2	1:H:13:ARG:HH12	1.72	0.55
1:H:102:ARG:NE	1:H:124:ASP:OD1	2.40	0.55
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.05	0.55
1:C:76:ASN:HD22	1:C:76:ASN:C	2.13	0.55
1:D:37:VAL:HG22	1:D:73:VAL:HB	1.89	0.55
1:D:79:PRO:HA	1:D:82:LEU:HD12	1.88	0.55
1:E:119:THR:HG22	1:E:321:VAL:CG1	2.36	0.55
1:E:202:ASN:HD22	1:G:281:VAL:HG12	1.72	0.55
1:E:85:LYS:N	1:E:112:GLY:HA3	2.21	0.55
1:E:257:ALA:HB2	4:E:537:HOH:O	2.07	0.55
1:E:276:GLU:OE2	1:E:277:PRO:HD2	2.06	0.55
1:G:168:ILE:C	1:G:169:LYS:HG3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLN:HE22	1:D:231:ARG:HB3	1.72	0.55
1:E:256:ASN:HD21	1:E:297:THR:CB	2.19	0.55
1:G:193:LEU:H	1:G:193:LEU:CD2	2.20	0.55
1:H:2:LYS:HD2	1:H:88:GLY:CA	2.37	0.55
1:H:28:ILE:C	1:H:71:ILE:HG13	2.32	0.55
1:H:132:VAL:O	1:H:132:VAL:HG12	2.06	0.55
1:H:181:ASP:CB	1:H:195:ARG:HD3	2.36	0.55
1:A:85:LYS:HE3	1:A:85:LYS:H	1.71	0.55
1:D:91:ILE:CG2	1:D:115:LYS:HB3	2.35	0.55
1:D:266:GLU:HG2	1:D:267:LEU:HG	1.89	0.55
1:H:266:GLU:HG2	1:H:267:LEU:HG	1.89	0.55
1:O:213:ALA:O	1:O:216:LEU:HB2	2.07	0.55
1:B:240:VAL:CG2	1:B:309:ALA:HB3	2.37	0.55
1:D:84:TRP:HB2	1:D:112:GLY:HA3	1.89	0.55
1:E:179:THR:HG22	1:E:180:GLY:N	2.22	0.55
1:F:301:GLY:HA3	1:H:169:LYS:HD2	1.89	0.55
1:G:194:ARG:HH11	1:G:205:PRO:HB2	1.72	0.55
1:H:90:ASP:O	1:H:114:LYS:HB2	2.07	0.55
1:O:162:ASP:OD2	1:O:220:ASN:ND2	2.40	0.55
1:Q:317:TYR:O	1:Q:320:ARG:HB2	2.07	0.55
1:B:193:LEU:HB3	1:C:42:HIS:CD2	2.42	0.55
1:C:243:VAL:HA	1:C:305:VAL:O	2.06	0.55
1:D:129:VAL:CG2	1:D:217:VAL:HG11	2.35	0.55
1:F:300:MET:O	1:F:300:MET:HE3	2.07	0.55
1:H:125:ILE:HD12	1:H:125:ILE:N	2.23	0.55
1:Q:78:ASN:OD1	1:Q:80:SER:HB2	2.07	0.55
1:E:210:ALA:HB2	3:E:337:SO4:O4	2.06	0.54
1:G:271:LEU:HD13	1:G:290:THR:HG23	1.89	0.54
1:A:129:VAL:H	1:A:133:ASN:ND2	2.05	0.54
1:C:85:LYS:N	1:C:112:GLY:HA3	2.22	0.54
1:C:272:ASP:O	1:C:291:THR:HA	2.07	0.54
1:E:172:MET:HG2	1:E:173:THR:N	2.23	0.54
1:O:202:ASN:ND2	1:Q:281:VAL:H	2.04	0.54
1:Q:135:ASP:OD2	1:Q:135:ASP:N	2.36	0.54
1:Q:160:VAL:HG13	1:Q:164:LYS:HE3	1.89	0.54
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.42	0.54
1:E:166:GLY:O	1:E:246:VAL:HA	2.07	0.54
1:F:169:LYS:CD	1:H:301:GLY:HA3	2.37	0.54
1:H:130:VAL:HG21	1:H:320:ARG:HD3	1.90	0.54
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.42	0.54
1:D:313:ASN:O	2:D:335:NAD:H4N	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:LEU:HD12	1:E:308:ILE:HG21	1.90	0.54
1:E:312:ASP:CG	1:E:315:TRP:HB3	2.32	0.54
1:A:2:LYS:HG2	1:A:28:ILE:HD13	1.90	0.54
1:A:9:GLY:HA3	2:A:335:NAD:O5B	2.08	0.54
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.72	0.54
1:A:226:ASN:ND2	1:C:300:MET:HB2	2.22	0.54
1:E:14:ASN:HB3	1:E:318:SER:OG	2.08	0.54
1:E:70:ILE:HD13	1:E:70:ILE:N	2.16	0.54
1:E:87:LEU:N	1:E:87:LEU:HD12	2.22	0.54
1:G:201:LEU:O	1:G:233:PRO:HG2	2.07	0.54
1:H:194:ARG:HD3	1:H:205:PRO:O	2.07	0.54
1:A:91:ILE:HD11	1:A:93:ILE:HD13	1.89	0.54
1:E:17:ARG:HH11	1:E:18(B):HIS:HB3	1.72	0.54
1:Q:133:ASN:HD22	1:Q:133:ASN:H	1.55	0.54
1:B:271:LEU:HD22	1:B:290:THR:OG1	2.07	0.54
1:C:76:ASN:ND2	1:C:78:ASN:H	2.06	0.54
1:F:310:TRP:HZ2	1:H:205:PRO:HG2	1.72	0.54
1:G:176:HIS:HA	1:G:238:SER:OG	2.08	0.54
1:G:256:ASN:N	1:G:256:ASN:ND2	2.54	0.54
1:E:138:SER:O	1:E:140:ASP:N	2.41	0.54
1:E:151:THR:HG23	1:E:214:VAL:CG2	2.37	0.54
1:E:209:GLY:O	1:E:212:LYS:HG2	2.07	0.54
1:F:28:ILE:HG22	1:F:89:ILE:HD11	1.90	0.54
1:F:38:LYS:HG3	1:F:39:GLN:H	1.72	0.54
1:G:161:LEU:O	1:G:165:PHE:HB2	2.08	0.54
1:A:30:ILE:HG13	1:A:71:ILE:CD1	2.35	0.54
1:D:152:ASN:O	1:D:289:SER:HB3	2.08	0.54
1:E:58:LYS:CG	1:E:65:SER:HB3	2.38	0.54
1:O:84:TRP:HA	1:O:84:TRP:HE3	1.73	0.54
1:B:242:LEU:O	1:B:306:LYS:HA	2.08	0.53
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.43	0.53
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.72	0.53
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.38	0.53
1:G:90:ASP:HB3	1:G:332:TRP:CH2	2.43	0.53
1:H:15:PHE:CE2	1:H:93:ILE:HG13	2.44	0.53
1:Q:90:ASP:HA	1:Q:114:LYS:HG2	1.90	0.53
1:B:251:PHE:C	1:B:299:VAL:HG21	2.34	0.53
1:E:252:ALA:HB1	1:E:298:MET:HA	1.90	0.53
1:F:202:ASN:ND2	1:H:281:VAL:H	1.98	0.53
1:F:228:ILE:H	1:F:228:ILE:CD1	2.21	0.53
1:G:291:THR:CG2	1:G:310:TRP:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:192:ASP:OD2	1:O:195:ARG:HG3	2.08	0.53
1:A:281:VAL:HB	1:C:202:ASN:HD21	1.72	0.53
1:C:115:LYS:HG3	1:C:142:PRO:O	2.08	0.53
1:E:77:ARG:CZ	1:E:77:ARG:HB3	2.38	0.53
1:E:199:ALA:HB3	1:H:184:LEU:HD11	1.90	0.53
1:E:279:VAL:HB	1:G:203:ILE:O	2.08	0.53
1:E:304:MET:HE2	1:G:304:MET:HE2	1.89	0.53
1:Q:38:LYS:H	1:Q:38:LYS:CE	2.16	0.53
1:C:1:LEU:HD23	1:C:91:ILE:HD11	1.89	0.53
1:E:211:ALA:CB	1:E:226:ASN:HA	2.39	0.53
1:F:126:PRO:HD2	1:F:143:ILE:O	2.07	0.53
1:F:296:LEU:O	1:F:298:MET:HG3	2.08	0.53
1:G:18(A):TRP:C	1:G:19:GLY:N	2.64	0.53
1:H:105:ALA:HB3	1:H:143:ILE:HD13	1.91	0.53
1:O:277:PRO:HA	1:Q:194:ARG:CZ	2.38	0.53
1:C:70:ILE:N	1:C:70:ILE:HD12	2.24	0.53
1:G:188:SER:O	1:G:190:HIS:HB2	2.07	0.53
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.91	0.53
1:A:191:ARG:HH11	1:A:191:ARG:HB2	1.73	0.53
1:D:263:ALA:O	1:D:268:LYS:HA	2.09	0.53
1:E:32:ASP:C	1:E:34:GLY:H	2.17	0.53
1:E:130:VAL:HA	1:E:134:ALA:HB2	1.91	0.53
1:E:317:TYR:O	1:E:321:VAL:HG23	2.09	0.53
1:F:120:ALA:O	1:F:145:SER:HB2	2.08	0.53
1:F:176:HIS:HA	1:F:238:SER:HB3	1.91	0.53
1:G:13:ARG:HH11	1:G:13:ARG:HG3	1.73	0.53
1:G:152:ASN:O	1:G:289:SER:HB3	2.09	0.53
1:O:162:ASP:HB2	1:O:167:ILE:HD12	1.91	0.53
1:C:289:SER:OG	1:C:320:ARG:HD2	2.09	0.53
1:E:153:CYS:O	1:E:156:PRO:HD2	2.08	0.53
1:E:208:THR:C	1:E:210:ALA:H	2.15	0.53
1:E:270:ILE:HG22	1:E:270:ILE:O	2.07	0.53
1:A:101:ASP:OD1	1:A:103:GLU:HG3	2.09	0.53
1:F:279:VAL:HG12	1:H:205:PRO:CD	2.39	0.53
1:G:138:SER:HB2	1:G:140:ASP:OD2	2.09	0.53
1:H:81:LEU:HD12	1:H:81:LEU:N	2.21	0.53
1:O:133:ASN:HD22	1:O:133:ASN:H	1.55	0.53
1:B:223:GLY:O	1:D:300:MET:HE1	2.09	0.53
1:E:242:LEU:HB3	1:E:307:VAL:HG23	1.91	0.53
1:G:31:ASN:OD1	1:G:74:VAL:HG23	2.09	0.53
1:G:79:PRO:HA	1:G:82:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:18(A):TRP:CD2	1:O:27:ILE:HD13	2.44	0.53
1:D:79:PRO:HB2	1:D:107:LYS:HB2	1.90	0.53
1:D:236:ASN:O	1:D:237:VAL:HB	2.09	0.53
1:E:18:CYS:HB3	1:E:319:GLN:CD	2.34	0.53
1:H:25:LEU:HD11	1:H:325:ALA:HB1	1.91	0.53
1:H:83:PRO:O	1:H:86:GLU:HG2	2.09	0.53
1:H:125:ILE:HD12	1:H:125:ILE:H	1.72	0.53
1:D:251:PHE:CE2	1:D:253:GLU:HG2	2.44	0.52
1:F:198:ALA:HB1	1:F:201:LEU:HG	1.91	0.52
1:F:301:GLY:HA3	1:H:169:LYS:CD	2.39	0.52
1:H:94:GLU:OE2	1:H:99:PHE:HD2	1.92	0.52
1:H:186:ASP:OD2	1:H:197:ARG:NE	2.42	0.52
1:H:250:THR:OG1	1:H:251:PHE:N	2.42	0.52
1:B:163:GLN:HE21	1:B:164:LYS:HZ2	1.53	0.52
1:B:205:PRO:HA	1:B:230:LEU:HD23	1.92	0.52
1:E:58:LYS:HG3	1:E:65:SER:HB3	1.90	0.52
1:H:242:LEU:HD12	1:H:243:VAL:H	1.74	0.52
1:C:1:LEU:HD21	1:C:332:TRP:CE3	2.45	0.52
1:E:162:ASP:HA	1:E:167:ILE:HG13	1.91	0.52
1:E:204:VAL:HG22	1:G:279:VAL:CG1	2.40	0.52
1:F:18(A):TRP:HA	1:F:20:ARG:HG2	1.90	0.52
1:G:16:LEU:HD23	1:G:16:LEU:O	2.09	0.52
1:H:83:PRO:HB2	1:H:86:GLU:HG3	1.89	0.52
1:C:21:LYS:H	1:C:21:LYS:CE	2.23	0.52
1:E:129:VAL:HG21	1:E:217:VAL:HG11	1.91	0.52
1:E:192:ASP:OD2	1:E:195:ARG:HD2	2.10	0.52
1:G:236:ASN:O	1:G:237:VAL:HB	2.09	0.52
1:H:115:LYS:HE2	1:H:332:TRP:HZ3	1.74	0.52
1:A:16:LEU:HD23	1:A:16:LEU:O	2.10	0.52
1:B:87:LEU:HB2	1:B:89:ILE:HD13	1.91	0.52
1:C:23:SER:C	1:C:25:LEU:H	2.16	0.52
1:E:79:PRO:HA	1:E:82:LEU:HG	1.90	0.52
1:E:185:LEU:HA	1:E:198:ALA:HB2	1.91	0.52
1:E:236:ASN:CG	1:E:237:VAL:H	2.17	0.52
1:F:60:SER:N	1:F:64:ILE:HA	2.24	0.52
1:F:296:LEU:HD13	1:F:308:ILE:HG13	1.91	0.52
1:G:294:SER:C	1:G:296:LEU:N	2.68	0.52
1:H:294:SER:O	1:H:296:LEU:N	2.41	0.52
1:O:133:ASN:HD22	1:O:133:ASN:N	2.08	0.52
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	1.92	0.52
1:Q:219:PRO:O	1:Q:222:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:NH1	1:B:102:ARG:HG2	2.24	0.52
1:G:160:VAL:CG1	1:G:258:ALA:HB1	2.40	0.52
1:G:276:GLU:HB3	1:G:277:PRO:HD2	1.91	0.52
1:H:134:ALA:HB1	1:H:327:ILE:HD13	1.91	0.52
1:Q:156:PRO:HB2	1:Q:290:THR:HG21	1.92	0.52
1:E:183:ARG:HG2	1:E:196:ALA:HA	1.91	0.52
1:E:279:VAL:HG22	1:G:197:ARG:HH12	1.75	0.52
1:H:129:VAL:N	1:H:133:ASN:HD21	2.04	0.52
1:O:129:VAL:H	1:O:133:ASN:ND2	2.08	0.52
1:O:226:ASN:HB2	1:Q:300:MET:CE	2.40	0.52
1:Q:128:TYR:HA	1:Q:133:ASN:HD21	1.75	0.52
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.36	0.52
1:C:271:LEU:HD12	1:C:290:THR:HG23	1.92	0.52
1:E:181:ASP:OD2	1:E:195:ARG:NH1	2.43	0.52
1:F:186:ASP:OD1	1:F:197:ARG:HA	2.09	0.52
1:F:243:VAL:HG11	1:H:171:THR:CG2	2.39	0.52
1:B:310:TRP:HZ2	1:D:205:PRO:HG2	1.74	0.52
1:C:64:ILE:CD1	1:C:66:VAL:HG23	2.40	0.52
1:D:4:ALA:HB3	1:D:92:VAL:HG22	1.92	0.52
1:D:218:LEU:HB3	1:D:221:LEU:HD23	1.92	0.52
1:E:115:LYS:HD2	1:E:328:VAL:CG1	2.40	0.52
1:F:306:LYS:HD2	1:H:171:THR:OG1	2.09	0.52
1:G:137:TYR:CE2	1:G:328:VAL:HA	2.44	0.52
1:G:168:ILE:CG2	1:G:169:LYS:HE3	2.40	0.52
1:G:197:ARG:O	1:G:199:ALA:N	2.43	0.52
1:G:243:VAL:CG2	1:G:306:LYS:HE2	2.40	0.52
1:H:192:ASP:C	1:H:194:ARG:H	2.16	0.52
1:Q:28:ILE:HD12	1:Q:28:ILE:C	2.35	0.52
1:Q:84:TRP:HA	1:Q:84:TRP:HE3	1.75	0.52
1:B:9:GLY:HA3	2:B:335:NAD:O5B	2.10	0.51
1:G:161:LEU:HD13	1:G:244:VAL:HG21	1.91	0.51
1:G:243:VAL:HG13	1:G:306:LYS:HB2	1.92	0.51
1:D:130:VAL:HA	1:D:134:ALA:HB2	1.90	0.51
1:E:171:THR:CG2	1:G:306:LYS:HE3	2.41	0.51
1:F:128:TYR:HA	1:F:133:ASN:HD21	1.76	0.51
1:G:296:LEU:HD13	1:G:308:ILE:HG21	1.93	0.51
1:H:72:GLN:NE2	1:H:72:GLN:N	2.46	0.51
1:A:133:ASN:ND2	1:A:133:ASN:C	2.67	0.51
1:D:89:ILE:O	1:D:113:ALA:HA	2.10	0.51
1:D:101:ASP:CB	1:D:122(A):LYS:HB2	2.40	0.51
1:D:175:THR:HB	1:D:239:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:SER:C	1:E:140:ASP:H	2.17	0.51
1:F:4:ALA:HB3	1:F:89:ILE:HG21	1.92	0.51
1:G:208:THR:C	1:G:210:ALA:N	2.68	0.51
1:H:14:ASN:OD1	1:H:50:LEU:HD11	2.11	0.51
1:O:154:LEU:HD22	1:O:172:MET:HE2	1.91	0.51
1:Q:1:LEU:HG	1:Q:1:LEU:O	2.10	0.51
1:Q:86:GLU:OE2	1:Q:86:GLU:N	2.44	0.51
1:E:202:ASN:CB	1:G:280:SER:OG	2.58	0.51
1:H:81:LEU:H	1:H:81:LEU:CD1	2.21	0.51
1:H:264:GLU:O	1:H:268:LYS:HD2	2.11	0.51
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.92	0.51
1:D:79:PRO:HA	1:D:82:LEU:CD1	2.40	0.51
1:E:175:THR:HB	1:E:239:VAL:HG12	1.92	0.51
1:E:203:ILE:HD11	1:G:232:VAL:CG2	2.36	0.51
1:E:253:GLU:HG3	3:E:334:SO4:O3	2.10	0.51
1:E:320:ARG:HA	1:E:320:ARG:HE	1.75	0.51
1:F:79:PRO:HB3	1:F:108:HIS:CE1	2.46	0.51
1:F:255:VAL:C	1:F:257:ALA:N	2.68	0.51
1:H:92:VAL:HG11	1:H:108:HIS:CE1	2.46	0.51
1:H:242:LEU:HD12	1:H:243:VAL:N	2.26	0.51
1:Q:84:TRP:CE3	1:Q:84:TRP:HA	2.46	0.51
1:Q:271:LEU:C	1:Q:271:LEU:HD23	2.35	0.51
1:A:83:PRO:HA	1:A:85:LYS:HE2	1.93	0.51
1:B:37:VAL:HG22	1:B:73:VAL:HB	1.93	0.51
1:D:271:LEU:HD11	1:D:292:ILE:HD11	1.93	0.51
1:F:174:THR:HB	1:F:240:VAL:HG12	1.92	0.51
1:G:137:TYR:OH	1:G:328:VAL:HG13	2.11	0.51
1:O:0:LYS:NZ	1:O:23:SER:O	2.44	0.51
1:A:172:MET:HG2	1:A:173:THR:N	2.25	0.51
1:A:280:SER:HB3	1:C:203:ILE:HB	1.93	0.51
1:B:221:LEU:HA	1:B:224:LYS:HD2	1.91	0.51
1:B:324:LEU:O	1:B:328:VAL:HG23	2.11	0.51
1:D:170:GLY:O	1:D:225:LEU:HA	2.11	0.51
1:E:27:ILE:HD11	1:E:30:ILE:CG1	2.40	0.51
1:F:279:VAL:HG12	1:H:205:PRO:HD2	1.92	0.51
1:G:99:PHE:HB3	1:G:104:GLY:O	2.11	0.51
1:H:72:GLN:HE21	1:H:72:GLN:N	2.07	0.51
1:H:289:SER:OG	1:H:320:ARG:NH1	2.43	0.51
1:A:193:LEU:HD13	1:D:42:HIS:CG	2.46	0.51
1:B:114:LYS:HD2	1:B:332:TRP:HZ2	1.76	0.51
1:E:43:LEU:HD11	1:H:187:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LEU:C	1:E:158:VAL:HG23	2.36	0.51
1:F:218:LEU:N	1:F:219:PRO:HD3	2.26	0.51
1:G:130:VAL:HG21	1:G:320:ARG:HD3	1.92	0.51
1:Q:191:ARG:HG2	1:Q:192:ASP:N	2.26	0.51
1:A:74:VAL:HG23	1:A:75:SER:N	2.26	0.51
1:C:64:ILE:HD11	1:C:71:ILE:HD12	1.93	0.51
1:C:76:ASN:OD1	1:C:81:LEU:HB2	2.11	0.51
1:C:301:GLY:O	1:C:302:ASP:HB2	2.10	0.51
1:D:16:LEU:HD23	1:D:16:LEU:O	2.11	0.51
1:E:199:ALA:CB	1:H:184:LEU:HD21	2.40	0.51
1:F:174:THR:HA	1:F:240:VAL:HA	1.93	0.51
1:O:253:GLU:H	1:O:253:GLU:CD	2.19	0.51
1:A:78:ASN:HD22	1:A:81:LEU:HG	1.76	0.51
1:A:271:LEU:HD12	1:A:290:THR:O	2.11	0.51
1:E:32:ASP:OD2	1:E:40:ALA:HB2	2.11	0.51
1:E:272:ASP:HB2	1:E:288:PHE:CG	2.46	0.51
1:F:157:PHE:HB2	1:F:259:PHE:HE1	1.76	0.51
1:B:0(A):ALA:HB3	1:B:23:SER:O	2.11	0.50
1:E:89:ILE:HG21	1:E:92:VAL:HG22	1.93	0.50
1:E:212:LYS:O	1:E:215:ALA:HB3	2.10	0.50
1:G:85:LYS:HG3	1:G:86:GLU:N	2.26	0.50
1:O:17:ARG:HD2	1:O:53:PHE:CD1	2.46	0.50
1:Q:1:LEU:HD23	1:Q:91:ILE:HD11	1.93	0.50
1:B:84:TRP:HA	1:B:84:TRP:CE3	2.46	0.50
1:B:224:LYS:C	1:D:300:MET:HE2	2.37	0.50
1:C:9:GLY:O	1:C:13:ARG:HG3	2.11	0.50
1:E:267:LEU:HD13	1:E:271:LEU:CD2	2.41	0.50
1:F:60:SER:OG	1:F:70:ILE:HD13	2.12	0.50
1:F:287:ASP:OD1	1:F:319:GLN:NE2	2.44	0.50
1:A:143:ILE:HD12	1:A:143:ILE:N	2.27	0.50
1:G:129:VAL:H	1:G:133:ASN:ND2	2.07	0.50
1:O:279:VAL:HG11	1:Q:204:VAL:HG22	1.93	0.50
1:Q:107:LYS:O	1:Q:110:GLU:HB2	2.10	0.50
1:D:103:GLU:OE1	1:D:103:GLU:N	2.41	0.50
1:E:15:PHE:CD1	1:E:322:VAL:HG22	2.47	0.50
1:F:169:LYS:HA	1:F:224:LYS:HB3	1.92	0.50
1:F:232:VAL:HG11	1:H:232:VAL:HG11	1.93	0.50
1:G:162:ASP:C	1:G:164:LYS:H	2.19	0.50
1:O:9:GLY:O	1:O:13:ARG:HG3	2.12	0.50
1:A:226:ASN:HB2	1:C:298:MET:HE2	1.93	0.50
1:E:79:PRO:HA	1:E:82:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:SER:O	1:H:76:ASN:HB2	2.11	0.50
1:H:129:VAL:H	1:H:133:ASN:ND2	2.03	0.50
1:O:26:ASP:OD1	1:O:69:LYS:HE2	2.11	0.50
1:A:1:LEU:HD22	1:A:329:ALA:HB2	1.94	0.50
1:E:194:ARG:NH1	1:E:205:PRO:HG2	2.26	0.50
1:F:315:TRP:NE1	1:F:319:GLN:HE21	2.10	0.50
1:G:226:ASN:ND2	1:G:227:GLY:H	2.09	0.50
1:G:256:ASN:HB3	1:G:260:ARG:HH11	1.75	0.50
1:H:8:PHE:CE1	1:H:16:LEU:HD12	2.46	0.50
1:H:88:GLY:O	1:H:89:ILE:C	2.55	0.50
1:B:169:LYS:CD	1:D:301:GLY:HA3	2.42	0.50
1:C:187:ALA:O	1:C:196:ALA:HB1	2.11	0.50
1:F:23:SER:C	1:F:25:LEU:H	2.20	0.50
1:H:3:VAL:HG23	1:H:91:ILE:O	2.11	0.50
1:D:97:GLY:HA2	2:D:335:NAD:O3D	2.12	0.50
1:G:278:LEU:HD21	1:H:46:TYR:CZ	2.46	0.50
1:H:185:LEU:O	1:H:186:ASP:C	2.55	0.50
1:O:1:LEU:HD11	1:O:329:ALA:HA	1.94	0.50
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.43	0.50
1:A:156:PRO:HB2	1:A:290:THR:CG2	2.39	0.50
1:E:146:ASN:ND2	1:E:324:LEU:HD22	2.27	0.50
1:F:150:THR:O	1:F:150:THR:HG22	2.12	0.50
1:F:155:ALA:HB3	1:F:156:PRO:HD3	1.92	0.50
1:G:182:GLN:HB3	1:G:199:ALA:HB2	1.93	0.50
1:A:245:GLN:NE2	1:C:245:GLN:HE22	2.08	0.49
1:B:39:GLN:NE2	1:C:190:HIS:H	2.09	0.49
1:B:194:ARG:CZ	1:D:277:PRO:HA	2.41	0.49
1:D:206:THR:HG23	1:D:229:ALA:HB3	1.93	0.49
1:F:177:SER:HB3	1:F:234:THR:O	2.12	0.49
1:G:3:VAL:HG22	1:G:91:ILE:HB	1.93	0.49
1:G:109:ILE:CD1	1:G:142:PRO:HB2	2.41	0.49
1:H:55:ALA:HB1	1:H:67:ASP:OD1	2.11	0.49
1:O:219:PRO:O	1:O:222:LYS:HG2	2.12	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.12	0.49
1:A:245:GLN:NE2	1:C:245:GLN:NE2	2.60	0.49
1:C:62:THR:O	1:C:63:ALA:HB2	2.11	0.49
1:D:204:VAL:HB	1:D:231:ARG:HB2	1.94	0.49
1:E:277:PRO:HA	1:G:194:ARG:NE	2.23	0.49
1:F:4:ALA:O	1:F:92:VAL:HG13	2.13	0.49
1:F:159:LYS:O	1:F:163:GLN:HB2	2.13	0.49
1:H:63:ALA:HA	1:H:73:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.47	0.49
1:H:91:ILE:HD11	1:H:117:ILE:CG2	2.42	0.49
1:H:228:ILE:H	1:H:228:ILE:CD1	2.22	0.49
1:O:226:ASN:HB2	1:Q:300:MET:HE2	1.93	0.49
1:O:281:VAL:H	1:Q:202:ASN:HD22	1.59	0.49
1:Q:151:THR:OG1	1:Q:210:ALA:HA	2.13	0.49
1:B:228:ILE:HG23	1:D:298:MET:HE2	1.93	0.49
1:C:251:PHE:CZ	1:C:254:GLU:HB2	2.47	0.49
1:E:30:ILE:O	1:E:74:VAL:HG22	2.12	0.49
1:E:77:ARG:HB3	1:E:77:ARG:NH1	2.28	0.49
1:E:109:ILE:HG12	1:E:113:ALA:O	2.12	0.49
1:E:129:VAL:HB	1:E:133:ASN:HD21	1.77	0.49
1:F:133:ASN:HD22	1:F:133:ASN:N	2.10	0.49
1:F:185:LEU:O	1:F:186:ASP:C	2.55	0.49
1:F:240:VAL:HG23	1:F:240:VAL:O	2.12	0.49
1:G:210:ALA:O	1:G:214:VAL:HG23	2.12	0.49
1:H:84:TRP:HA	1:H:84:TRP:CE3	2.47	0.49
1:H:319:GLN:OE1	1:H:319:GLN:HA	2.12	0.49
1:O:33:THR:HG22	1:O:77:ARG:CG	2.42	0.49
1:H:2:LYS:HD2	1:H:88:GLY:HA2	1.94	0.49
1:H:139:HIS:C	1:H:141:GLU:H	2.20	0.49
1:B:248:LYS:O	1:B:249:LYS:C	2.55	0.49
1:C:1:LEU:HD22	1:C:329:ALA:CB	2.42	0.49
1:C:256:ASN:OD1	1:C:294:SER:HB2	2.12	0.49
1:E:211:ALA:HB1	1:E:226:ASN:HA	1.95	0.49
1:E:260:ARG:HB3	4:E:534:HOH:O	2.11	0.49
1:G:158:VAL:HG13	1:G:167:ILE:CD1	2.43	0.49
1:Q:190:HIS:CB	1:Q:196:ALA:HB2	2.42	0.49
1:B:85:LYS:HB2	1:B:112:GLY:HA3	1.94	0.49
1:B:250:THR:OG1	1:B:251:PHE:N	2.43	0.49
1:E:6:ASN:ND2	1:E:108:HIS:CE1	2.80	0.49
1:E:202:ASN:HB2	1:G:280:SER:OG	2.12	0.49
1:G:13:ARG:HG3	1:G:13:ARG:NH1	2.27	0.49
1:H:6:ASN:ND2	1:H:96:THR:HG21	2.27	0.49
1:H:157:PHE:HE1	1:H:242:LEU:HD23	1.76	0.49
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.94	0.49
1:O:221:LEU:HA	1:O:224:LYS:HD2	1.93	0.49
1:Q:109:ILE:HA	1:Q:113:ALA:O	2.12	0.49
1:Q:239:VAL:HG23	1:Q:309:ALA:O	2.12	0.49
1:C:1:LEU:HD23	1:C:91:ILE:CD1	2.42	0.49
1:E:16:LEU:HD13	1:E:44:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:PRO:O	1:E:82:LEU:HG	2.13	0.49
1:E:139:HIS:CG	1:E:139:HIS:O	2.66	0.49
1:F:32:ASP:OD2	2:F:335:NAD:H1B	2.13	0.49
1:Q:137:TYR:CZ	1:Q:328:VAL:HG22	2.48	0.49
1:Q:191:ARG:H	1:Q:191:ARG:CZ	2.26	0.49
1:B:0(A):ALA:N	1:B:26:ASP:HB2	2.28	0.49
1:D:123:GLY:O	1:D:125:ILE:HG22	2.12	0.49
1:E:16:LEU:O	1:E:16:LEU:HD23	2.12	0.49
1:E:70:ILE:H	1:E:70:ILE:CD1	2.15	0.49
1:E:172:MET:HA	1:E:242:LEU:HA	1.95	0.49
1:E:232:VAL:O	1:E:234:THR:N	2.38	0.49
1:F:228:ILE:HG21	1:H:296:LEU:CD2	2.43	0.49
1:F:292:ILE:HG22	1:F:293:ASP:N	2.27	0.49
1:H:182:GLN:HE22	1:H:231:ARG:CB	2.26	0.49
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.78	0.49
1:C:84:TRP:HA	1:C:84:TRP:CE3	2.48	0.49
1:C:260:ARG:HG2	1:C:273:VAL:HG21	1.95	0.49
1:D:85:LYS:HG3	1:D:112:GLY:CA	2.33	0.49
1:D:107:LYS:HA	1:D:110:GLU:HB3	1.95	0.49
1:E:171:THR:HB	1:G:300:MET:CG	2.39	0.49
1:F:193:LEU:HD12	1:H:277:PRO:HG3	1.95	0.49
1:H:142:PRO:HG2	1:H:143:ILE:H	1.78	0.49
1:A:173:THR:HG23	1:A:228:ILE:CD1	2.43	0.49
1:C:109:ILE:CD1	1:C:142:PRO:HB2	2.42	0.49
1:E:252:ALA:HB2	4:E:545:HOH:O	2.12	0.49
1:G:2:LYS:HE3	1:G:87:LEU:O	2.13	0.49
1:G:168:ILE:HB	1:G:245:GLN:O	2.12	0.49
1:O:242:LEU:HD11	1:O:244:VAL:HG13	1.94	0.49
1:O:281:VAL:CG1	1:Q:202:ASN:HD21	2.25	0.49
1:A:188:SER:HA	1:D:39:GLN:OE1	2.13	0.48
1:C:16:LEU:HD23	1:C:16:LEU:C	2.38	0.48
1:C:108:HIS:HB2	1:C:116:VAL:HG21	1.95	0.48
1:C:317:TYR:O	1:C:320:ARG:HB2	2.13	0.48
1:D:190:HIS:HB3	1:D:196:ALA:HB2	1.95	0.48
1:F:152:ASN:O	1:F:156:PRO:HG2	2.13	0.48
1:A:101:ASP:OD1	1:A:104:GLY:N	2.40	0.48
1:C:323:ASP:O	1:C:327:ILE:HG13	2.14	0.48
1:D:260:ARG:O	1:D:263:ALA:HB3	2.13	0.48
1:F:202:ASN:ND2	1:H:281:VAL:CB	2.76	0.48
1:H:126:PRO:HG2	1:H:141:GLU:OE2	2.13	0.48
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:NH1	4:A:770:HOH:O	2.45	0.48
1:C:168:ILE:HG22	1:C:169:LYS:HD3	1.95	0.48
1:D:44:LEU:HD23	1:D:57:VAL:CG1	2.44	0.48
1:D:84:TRP:HA	1:D:89:ILE:HD13	1.94	0.48
1:D:292:ILE:HD12	1:D:292:ILE:H	1.78	0.48
1:E:299:VAL:CG2	1:E:305:VAL:HG22	2.42	0.48
1:F:118:ILE:H	1:F:118:ILE:CD1	2.26	0.48
1:F:327:ILE:O	1:F:327:ILE:HG22	2.14	0.48
1:H:84:TRP:HA	1:H:84:TRP:HE3	1.78	0.48
1:H:242:LEU:O	1:H:306:LYS:HA	2.14	0.48
1:B:36:GLY:HA3	1:B:38:LYS:HE3	1.94	0.48
1:C:182:GLN:HB3	4:C:396:HOH:O	2.12	0.48
1:C:329:ALA:O	1:C:332:TRP:HB2	2.14	0.48
1:D:93:ILE:HD12	1:D:93:ILE:N	2.28	0.48
1:D:248:LYS:O	1:D:249:LYS:C	2.56	0.48
1:D:253:GLU:H	1:D:253:GLU:CD	2.21	0.48
1:D:272:ASP:OD2	1:D:273:VAL:N	2.46	0.48
1:F:17:ARG:HD3	1:F:50:LEU:HD12	1.95	0.48
1:G:79:PRO:HB2	1:G:107:LYS:HB2	1.95	0.48
1:H:249:LYS:HA	1:H:302:ASP:O	2.13	0.48
1:A:64:ILE:CG1	1:A:71:ILE:HG23	2.42	0.48
1:B:270:ILE:HD12	1:B:270:ILE:N	2.27	0.48
1:E:90:ASP:OD1	1:E:114:LYS:HD2	2.14	0.48
1:G:194:ARG:HD3	1:G:205:PRO:HD2	1.94	0.48
1:B:126:PRO:HG2	1:B:141:GLU:HG2	1.95	0.48
1:C:177:SER:HB2	1:C:237:VAL:O	2.14	0.48
1:D:132:VAL:HG13	1:D:218:LEU:HD21	1.96	0.48
1:E:169:LYS:HE2	1:E:245:GLN:OE1	2.13	0.48
1:E:251:PHE:CE1	1:E:254:GLU:HB2	2.49	0.48
1:F:132:VAL:HG13	1:F:218:LEU:HD21	1.95	0.48
1:G:318:SER:O	1:G:322:VAL:HG23	2.13	0.48
1:H:7:GLY:CA	1:H:96:THR:HG22	2.44	0.48
1:H:16:LEU:O	1:H:16:LEU:HD23	2.13	0.48
1:O:1:LEU:HD12	1:O:329:ALA:CB	2.44	0.48
1:O:15:PHE:CE1	1:O:321:VAL:HG12	2.48	0.48
1:A:85:LYS:HZ2	1:A:86:GLU:HB3	1.78	0.48
1:A:296:LEU:HB3	1:A:308:ILE:HD12	1.96	0.48
1:B:251:PHE:O	1:B:255:VAL:HG23	2.14	0.48
1:C:31:ASN:HB2	1:C:74:VAL:HG23	1.95	0.48
1:D:103:GLU:CD	1:D:103:GLU:H	2.19	0.48
1:D:209:GLY:O	1:D:210:ALA:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ALA:O	1:H:43:LEU:HD11	2.14	0.48
1:G:48:SER:HA	1:H:281:VAL:HG11	1.96	0.48
1:G:130:VAL:HG23	1:G:320:ARG:HD3	1.96	0.48
1:D:84:TRP:HB3	1:D:113:ALA:H	1.79	0.48
1:H:79:PRO:HB2	1:H:107:LYS:HB3	1.95	0.48
1:A:64:ILE:HG13	1:A:71:ILE:CG2	2.43	0.48
1:G:191:ARG:HG3	1:G:192:ASP:N	2.29	0.48
1:B:228:ILE:HG23	1:D:298:MET:CE	2.44	0.48
1:C:109:ILE:HA	1:C:113:ALA:O	2.14	0.48
1:E:14:ASN:OD1	1:E:315:TRP:HA	2.13	0.48
1:E:71:ILE:HD13	1:E:72:GLN:O	2.14	0.48
1:E:279:VAL:HG23	1:E:281:VAL:HG12	1.95	0.48
1:F:144:ILE:HD12	1:F:324:LEU:HD21	1.95	0.48
1:G:250:THR:OG1	1:G:251:PHE:N	2.46	0.48
1:H:28:ILE:HG23	1:H:29:ALA:N	2.29	0.48
1:H:178:TYR:HA	1:H:182:GLN:OE1	2.13	0.48
1:A:133:ASN:C	1:A:133:ASN:HD22	2.22	0.47
1:C:280:SER:HA	1:C:310:TRP:CZ3	2.48	0.47
1:D:14:ASN:OD1	1:D:50:LEU:HD11	2.14	0.47
1:D:44:LEU:HA	4:D:341:HOH:O	2.13	0.47
1:F:59:PRO:HA	1:F:64:ILE:HG22	1.95	0.47
1:H:38:LYS:HG2	1:H:39:GLN:N	2.29	0.47
1:H:132:VAL:HG21	1:H:155:ALA:HB1	1.96	0.47
1:H:149:CYS:HB3	2:H:335:NAD:C5N	2.44	0.47
1:C:236:ASN:O	1:C:237:VAL:HB	2.14	0.47
1:C:284:ARG:O	1:C:285:CYS:HB2	2.14	0.47
1:D:87:LEU:HB2	1:D:89:ILE:CD1	2.44	0.47
1:E:83:PRO:O	1:E:87:LEU:HD13	2.14	0.47
1:F:280:SER:OG	1:H:202:ASN:HB2	2.14	0.47
1:G:153:CYS:C	1:G:156:PRO:HD2	2.39	0.47
1:G:194:ARG:O	1:G:204:VAL:HG11	2.15	0.47
1:G:194:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:G:299:VAL:HG11	4:G:872:HOH:O	2.13	0.47
1:O:293:ASP:HB3	1:O:296:LEU:HD12	1.96	0.47
1:D:85:LYS:CG	1:D:112:GLY:HA2	2.33	0.47
1:E:58:LYS:HB2	1:E:59:PRO:CD	2.39	0.47
1:E:226:ASN:HD22	1:G:300:MET:CE	2.26	0.47
1:F:62:THR:O	1:F:63:ALA:HB2	2.14	0.47
1:F:321:VAL:O	1:F:325:ALA:HB2	2.14	0.47
1:G:128:TYR:CZ	1:G:137:TYR:HA	2.49	0.47
1:G:312:ASP:HB3	1:G:316:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:GLY:HA3	2:O:335:NAD:O5B	2.14	0.47
1:Q:115:LYS:HG3	1:Q:142:PRO:O	2.14	0.47
1:C:331:ASN:O	1:C:333:LYS:HD3	2.15	0.47
1:D:126:PRO:HB2	1:D:144:ILE:HG22	1.95	0.47
1:E:115:LYS:HE3	1:E:137:TYR:OH	2.14	0.47
1:E:300:MET:SD	1:G:170:GLY:O	2.72	0.47
1:F:90:ASP:HA	1:F:114:LYS:CD	2.28	0.47
1:F:296:LEU:O	1:F:297:THR:C	2.56	0.47
1:G:198:ALA:O	1:G:200:ALA:N	2.48	0.47
1:G:261:ASP:O	1:G:262:SER:C	2.57	0.47
1:O:253:GLU:CD	1:O:253:GLU:N	2.72	0.47
1:Q:126:PRO:HD2	1:Q:143:ILE:O	2.14	0.47
1:B:102:ARG:O	1:B:106:GLY:N	2.47	0.47
1:B:194:ARG:NH1	1:D:278:LEU:O	2.47	0.47
1:E:115:LYS:HE3	1:E:328:VAL:HG13	1.96	0.47
1:F:240:VAL:HG13	1:F:311:TYR:CE1	2.49	0.47
1:G:62:THR:CG2	1:Q:62:THR:HG22	2.44	0.47
1:G:239:VAL:HB	1:G:310:TRP:CE3	2.49	0.47
1:H:15:PHE:CE1	1:H:322:VAL:HG22	2.49	0.47
1:Q:44:LEU:HD12	1:Q:44:LEU:O	2.15	0.47
1:A:63:ALA:HA	1:A:73:VAL:HG23	1.96	0.47
1:B:195:ARG:HH21	1:B:206:THR:HG21	1.79	0.47
1:D:64:ILE:HG23	1:D:73:VAL:HG21	1.96	0.47
1:E:5:ILE:HD12	1:E:27:ILE:CD1	2.43	0.47
1:E:190:HIS:N	1:H:39:GLN:OE1	2.47	0.47
1:E:194:ARG:CG	1:G:277:PRO:O	2.60	0.47
1:E:284:ARG:O	1:E:285:CYS:HB2	2.14	0.47
1:H:154:LEU:O	1:H:155:ALA:C	2.58	0.47
1:A:142:PRO:C	1:A:143:ILE:HD12	2.40	0.47
1:B:102:ARG:HG2	1:B:102:ARG:HH11	1.79	0.47
1:B:165:PHE:HB3	1:B:246:VAL:HG11	1.96	0.47
1:D:0:LYS:O	1:D:1:LEU:HB2	2.15	0.47
1:D:177:SER:HB3	1:D:234:THR:O	2.14	0.47
1:E:58:LYS:HB3	1:E:58:LYS:HZ2	1.79	0.47
1:E:185:LEU:O	1:E:186:ASP:C	2.57	0.47
1:F:4:ALA:HB3	1:F:92:VAL:HG22	1.96	0.47
1:F:132:VAL:C	1:F:134:ALA:H	2.23	0.47
1:G:133:ASN:HD22	1:G:133:ASN:N	2.13	0.47
1:H:228:ILE:HD13	1:H:228:ILE:N	2.24	0.47
1:O:28:ILE:HD11	1:O:89:ILE:HD13	1.97	0.47
1:Q:130:VAL:HA	1:Q:134:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:272:ASP:HB2	1:Q:288:PHE:CD2	2.49	0.47
1:Q:284:ARG:O	1:Q:285:CYS:HB2	2.15	0.47
1:A:197:ARG:O	1:A:198:ALA:C	2.57	0.47
1:B:186:ASP:HA	1:B:196:ALA:O	2.15	0.47
1:B:240:VAL:HG13	1:B:311:TYR:CE1	2.49	0.47
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.49	0.47
1:E:84:TRP:C	1:E:112:GLY:HA3	2.40	0.47
1:O:187:ALA:O	1:O:196:ALA:HB1	2.15	0.47
1:D:134:ALA:HB3	4:D:396:HOH:O	2.15	0.47
1:F:298:MET:CE	1:H:228:ILE:HG23	2.45	0.47
1:G:260:ARG:NH2	1:G:275:ASP:OD1	2.47	0.47
1:H:8:PHE:HE1	1:H:16:LEU:HD12	1.80	0.47
1:B:279:VAL:HG22	1:D:197:ARG:NH1	2.29	0.47
1:C:84:TRP:HA	1:C:84:TRP:HE3	1.79	0.47
1:C:241:ASP:OD1	1:C:306:LYS:CE	2.63	0.47
1:E:226:ASN:CB	1:G:300:MET:HE2	2.34	0.47
1:O:169:LYS:HD2	1:Q:300:MET:HG3	1.97	0.47
1:Q:183:ARG:HG3	1:Q:196:ALA:HA	1.97	0.47
1:A:120:ALA:O	1:A:145:SER:OG	2.29	0.46
1:A:226:ASN:HD21	1:C:300:MET:HB2	1.80	0.46
1:A:284:ARG:O	1:A:285:CYS:HB2	2.14	0.46
1:B:202:ASN:OD1	1:D:281:VAL:HB	2.16	0.46
1:C:153:CYS:SG	1:C:240:VAL:HG13	2.55	0.46
1:E:117:ILE:CG2	1:E:144:ILE:HD11	2.36	0.46
1:F:107:LYS:HA	1:F:110:GLU:HG2	1.96	0.46
1:F:177:SER:O	1:F:231:ARG:HD2	2.15	0.46
1:H:146:ASN:OD1	1:H:146:ASN:O	2.32	0.46
1:Q:18:CYS:HB3	1:Q:319:GLN:OE1	2.15	0.46
1:B:284:ARG:O	1:B:285:CYS:HB2	2.13	0.46
1:E:108:HIS:HB2	1:E:116:VAL:HG21	1.97	0.46
1:G:85:LYS:N	1:G:112:GLY:HA3	2.31	0.46
1:H:149:CYS:HB3	2:H:335:NAD:H5N	1.96	0.46
1:H:256:ASN:ND2	1:H:297:THR:OG1	2.31	0.46
1:B:133:ASN:HD22	1:B:133:ASN:H	1.61	0.46
1:E:169:LYS:HE3	1:G:304:MET:CB	2.43	0.46
1:E:179:THR:HG22	1:E:180:GLY:H	1.80	0.46
1:E:179:THR:OG1	1:E:231:ARG:NH1	2.49	0.46
1:F:85:LYS:HD2	1:F:85:LYS:HA	1.78	0.46
1:F:301:GLY:O	1:F:302:ASP:HB2	2.15	0.46
1:F:322:VAL:O	1:F:325:ALA:HB3	2.15	0.46
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HD13	1:A:92:VAL:N	2.31	0.46
1:B:140:ASP:OD2	1:B:140:ASP:N	2.45	0.46
1:D:15:PHE:CE1	1:D:322:VAL:HG22	2.50	0.46
1:D:139:HIS:CB	1:D:333:LYS:HE2	2.27	0.46
1:E:79:PRO:HB2	1:E:107:LYS:HB3	1.96	0.46
1:E:251:PHE:CZ	1:E:254:GLU:HB2	2.50	0.46
1:F:65:SER:HA	1:F:70:ILE:HA	1.97	0.46
1:O:271:LEU:HD23	1:O:271:LEU:C	2.40	0.46
1:Q:194:ARG:HD2	1:Q:205:PRO:O	2.15	0.46
1:C:211:ALA:HB1	1:C:226:ASN:N	2.31	0.46
1:D:37:VAL:O	1:D:40:ALA:HB3	2.15	0.46
1:F:108:HIS:HB2	1:F:116:VAL:HG21	1.97	0.46
1:G:4:ALA:HB2	1:G:89:ILE:HD12	1.97	0.46
1:G:172:MET:HB2	1:G:242:LEU:CB	2.45	0.46
1:A:159:LYS:NZ	1:A:163:GLN:HE22	2.13	0.46
1:B:191:ARG:NH1	1:B:191:ARG:HB2	2.30	0.46
1:C:33:THR:HG21	1:C:77:ARG:CZ	2.45	0.46
1:E:178:TYR:CB	1:E:199:ALA:HB1	2.46	0.46
1:E:202:ASN:ND2	1:G:281:VAL:CG1	2.78	0.46
1:G:39:GLN:O	1:G:40:ALA:C	2.57	0.46
1:G:84:TRP:HA	1:G:84:TRP:CE3	2.50	0.46
1:C:320:ARG:NE	1:C:320:ARG:HA	2.30	0.46
1:E:284:ARG:O	1:E:285:CYS:CB	2.63	0.46
1:F:15:PHE:CE1	1:F:322:VAL:HG22	2.50	0.46
1:F:18:CYS:SG	1:F:319:GLN:OE1	2.74	0.46
1:F:36:GLY:O	1:F:37:VAL:C	2.58	0.46
1:F:45:LYS:HD3	1:F:57:VAL:HB	1.97	0.46
1:H:132:VAL:O	1:H:133:ASN:CB	2.63	0.46
1:O:215:ALA:HB1	1:O:222:LYS:HD3	1.97	0.46
1:O:285:CYS:N	1:O:312:ASP:OD2	2.45	0.46
1:E:260:ARG:HD3	4:E:534:HOH:O	2.15	0.46
1:F:27:ILE:N	1:F:27:ILE:CD1	2.77	0.46
1:F:90:ASP:O	1:F:115:LYS:N	2.41	0.46
1:H:36:GLY:C	1:H:38:LYS:HD2	2.40	0.46
1:O:2:LYS:HD2	1:O:28:ILE:HD13	1.97	0.46
1:Q:271:LEU:HD23	1:Q:272:ASP:N	2.31	0.46
1:E:183:ARG:CG	1:E:196:ALA:HA	2.46	0.46
1:H:210:ALA:O	1:H:214:VAL:HG23	2.16	0.46
1:O:327:ILE:O	1:O:328:VAL:C	2.59	0.46
1:A:84:TRP:CE3	1:A:84:TRP:HA	2.52	0.45
1:A:228:ILE:C	1:A:228:ILE:CD1	2.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:HE3	1:C:226:ASN:HB2	1.97	0.45
1:B:154:LEU:O	1:B:155:ALA:C	2.57	0.45
1:B:163:GLN:NE2	1:B:164:LYS:NZ	2.58	0.45
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.97	0.45
1:D:322:VAL:O	1:D:322:VAL:HG12	2.16	0.45
1:E:133:ASN:H	1:E:133:ASN:ND2	2.01	0.45
1:F:66:VAL:O	1:F:67:ASP:HB2	2.16	0.45
1:F:154:LEU:HD11	1:F:242:LEU:HD13	1.98	0.45
1:G:28:ILE:C	1:G:71:ILE:HG23	2.41	0.45
1:G:228:ILE:HD13	1:G:228:ILE:N	2.30	0.45
1:H:130:VAL:CG2	1:H:320:ARG:HD3	2.46	0.45
1:Q:9:GLY:O	1:Q:10:ARG:C	2.59	0.45
1:C:14:ASN:HB3	1:C:318:SER:OG	2.16	0.45
1:D:83:PRO:HB2	1:D:87:LEU:HD23	1.98	0.45
1:D:101:ASP:HB3	1:D:122(A):LYS:HB2	1.98	0.45
1:D:228:ILE:HD13	1:D:228:ILE:H	1.80	0.45
1:D:242:LEU:HG	1:D:244:VAL:HG13	1.98	0.45
1:E:17:ARG:HE	1:E:17:ARG:CA	2.05	0.45
1:E:63:ALA:HB2	1:E:72:GLN:OE1	2.15	0.45
1:E:235:PRO:HG2	1:E:236:ASN:H	1.81	0.45
1:F:81:LEU:N	1:F:81:LEU:HD12	2.30	0.45
1:F:109:ILE:CD1	1:F:142:PRO:HB3	2.45	0.45
1:F:139:HIS:CD2	1:F:333:LYS:HG2	2.51	0.45
1:F:145:SER:O	1:F:147:ALA:N	2.49	0.45
1:G:242:LEU:HD23	1:G:242:LEU:H	1.82	0.45
1:G:291:THR:O	1:G:291:THR:HG23	2.16	0.45
1:H:4:ALA:HB3	1:H:92:VAL:HG22	1.98	0.45
1:H:194:ARG:C	1:H:196:ALA:N	2.75	0.45
1:H:208:THR:HG23	1:H:208:THR:O	2.16	0.45
1:A:213:ALA:O	1:A:216:LEU:HB2	2.17	0.45
1:A:296:LEU:O	1:A:298:MET:HG3	2.16	0.45
1:B:172:MET:HE3	1:B:172:MET:HB3	1.82	0.45
1:C:82:LEU:HA	1:C:83:PRO:HD3	1.79	0.45
1:D:210:ALA:O	1:D:213:ALA:HB3	2.17	0.45
1:E:246:VAL:O	1:E:303:ASP:HB2	2.16	0.45
1:F:235:PRO:HB3	1:G:201:LEU:HD21	1.97	0.45
1:G:291:THR:HG22	1:G:310:TRP:O	2.15	0.45
1:H:105:ALA:HB1	1:H:116:VAL:HG11	1.98	0.45
1:A:215:ALA:HB2	1:A:222:LYS:HA	1.98	0.45
1:B:38:LYS:N	1:B:38:LYS:CD	2.77	0.45
1:F:145:SER:C	1:F:147:ALA:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:PRO:O	1:H:80:SER:C	2.59	0.45
1:O:279:VAL:CG1	1:Q:204:VAL:HG22	2.46	0.45
1:Q:183:ARG:CG	1:Q:196:ALA:HA	2.46	0.45
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.98	0.45
1:B:319:GLN:OE1	1:B:319:GLN:HA	2.16	0.45
1:D:3:VAL:CG1	1:D:93:ILE:HD13	2.45	0.45
1:D:10:ARG:HG2	4:D:377:HOH:O	2.16	0.45
1:D:181:ASP:OD1	1:D:195:ARG:NE	2.50	0.45
1:E:70:ILE:O	1:E:70:ILE:HG12	2.15	0.45
1:E:109:ILE:HD13	1:E:109:ILE:C	2.42	0.45
1:E:290:THR:HA	1:E:310:TRP:O	2.17	0.45
1:F:27:ILE:CD1	1:F:27:ILE:H	2.30	0.45
1:F:47:ASP:OD1	1:F:48:SER:N	2.49	0.45
1:G:193:LEU:HD22	1:G:193:LEU:N	2.26	0.45
1:G:267:LEU:HD12	1:G:271:LEU:HD22	1.99	0.45
1:A:279:VAL:HG23	1:A:281:VAL:HG12	1.99	0.45
1:C:126:PRO:HD2	1:C:143:ILE:O	2.17	0.45
1:D:18(A):TRP:CE3	1:D:27:ILE:HD12	2.51	0.45
1:D:27:ILE:O	1:D:69:LYS:HE3	2.16	0.45
1:E:186:ASP:HB2	1:H:10:ARG:HH12	1.82	0.45
1:F:31:ASN:ND2	1:F:82:LEU:HD11	2.31	0.45
1:F:84:TRP:HA	1:F:84:TRP:CE3	2.52	0.45
1:F:101:ASP:OD1	1:F:103:GLU:HB3	2.16	0.45
1:F:119:THR:O	1:F:120:ALA:HB2	2.16	0.45
1:H:294:SER:C	1:H:296:LEU:N	2.74	0.45
1:O:176:HIS:HA	1:O:238:SER:HB3	1.99	0.45
1:Q:178:TYR:CE1	1:Q:235:PRO:HA	2.52	0.45
1:A:129:VAL:H	1:A:133:ASN:HD21	1.65	0.45
1:C:2:LYS:HD3	1:C:28:ILE:HD13	1.98	0.45
1:C:293:ASP:O	1:C:295:SER:N	2.49	0.45
1:E:102:ARG:O	1:E:106:GLY:N	2.50	0.45
1:F:137:TYR:CE2	1:F:328:VAL:HA	2.52	0.45
1:F:271:LEU:HA	1:F:290:THR:HG23	1.99	0.45
1:A:159:LYS:O	1:A:163:GLN:HB2	2.17	0.45
1:D:44:LEU:HD23	1:D:57:VAL:HG11	1.99	0.45
1:E:7:GLY:HA2	2:E:335:NAD:C1B	2.42	0.45
1:E:66:VAL:O	1:E:67:ASP:HB2	2.16	0.45
1:E:194:ARG:NH1	1:G:296:LEU:HD21	2.30	0.45
1:F:52:ILE:HG22	1:F:53:PHE:N	2.31	0.45
1:H:329:ALA:O	1:H:332:TRP:HB3	2.16	0.45
1:O:154:LEU:CD2	1:O:172:MET:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:218:LEU:HB3	1:O:221:LEU:HD23	1.99	0.45
1:Q:69:LYS:HD3	4:Q:618:HOH:O	2.15	0.45
1:B:271:LEU:HD13	1:B:272:ASP:H	1.76	0.45
1:E:9:GLY:N	2:E:335:NAD:H4B	2.31	0.45
1:E:23:SER:C	1:E:25:LEU:H	2.25	0.45
1:E:31:ASN:HA	1:E:74:VAL:HG23	1.98	0.45
1:E:132:VAL:HG13	1:E:218:LEU:HD21	1.99	0.45
1:G:28:ILE:HD11	1:G:89:ILE:HD13	1.98	0.45
1:H:3:VAL:HG13	1:H:27:ILE:HA	1.99	0.45
1:H:192:ASP:OD1	1:H:194:ARG:HB2	2.16	0.45
1:H:218:LEU:HB3	1:H:221:LEU:HD23	1.99	0.45
1:O:263:ALA:O	1:O:268:LYS:HA	2.17	0.45
1:A:109:ILE:C	1:A:111:ALA:N	2.73	0.45
1:B:241:ASP:HA	1:B:308:ILE:HD13	1.99	0.45
1:D:58:LYS:HB3	1:D:58:LYS:HZ3	1.82	0.45
1:D:74:VAL:CG2	1:D:75:SER:H	2.28	0.45
1:D:116:VAL:HB	1:D:143:ILE:CD1	2.47	0.45
1:E:278:LEU:HD21	1:F:46:TYR:CE2	2.52	0.45
1:F:48:SER:O	1:F:49:THR:OG1	2.31	0.45
1:F:132:VAL:HG11	1:F:218:LEU:HG	1.98	0.45
1:G:32:ASP:OD1	2:G:335:NAD:H1B	2.17	0.45
1:G:46:TYR:HB3	1:H:282:ASP:OD1	2.17	0.45
1:G:79:PRO:HB2	1:G:107:LYS:CB	2.47	0.45
1:G:287:ASP:OD1	1:G:319:GLN:HG3	2.16	0.45
1:H:92:VAL:HB	1:H:116:VAL:HG22	1.99	0.45
1:H:132:VAL:HG13	1:H:218:LEU:HD21	1.98	0.45
1:Q:1:LEU:HD22	1:Q:329:ALA:CB	2.47	0.45
1:Q:212:LYS:HB3	4:Q:459:HOH:O	2.15	0.45
1:A:215:ALA:CB	1:A:222:LYS:HA	2.47	0.44
1:D:112:GLY:O	1:D:113:ALA:C	2.59	0.44
1:E:173:THR:HG23	1:E:228:ILE:HD11	1.99	0.44
1:F:190:HIS:HB3	1:F:196:ALA:HB2	1.99	0.44
1:F:249:LYS:HZ2	1:F:302:ASP:CG	2.24	0.44
1:G:204:VAL:HA	1:G:205:PRO:HD3	1.83	0.44
1:H:133:ASN:N	1:H:133:ASN:ND2	2.65	0.44
1:H:176:HIS:HB3	1:H:231:ARG:CD	2.46	0.44
1:H:276:GLU:HB3	1:H:277:PRO:HD2	1.98	0.44
1:O:54:ASP:HB3	4:O:425:HOH:O	2.16	0.44
1:O:157:PHE:HE1	1:O:242:LEU:HD23	1.83	0.44
1:Q:133:ASN:HD22	1:Q:133:ASN:N	2.13	0.44
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PRO:HA	1:A:85:LYS:CE	2.47	0.44
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.00	0.44
1:D:146:ASN:HD22	1:D:321:VAL:HG22	1.81	0.44
1:D:191:ARG:NE	4:D:338:HOH:O	2.47	0.44
1:E:7:GLY:HA3	1:E:95:GLY:C	2.43	0.44
1:E:28:ILE:HG12	1:E:28:ILE:O	2.17	0.44
1:E:178:TYR:CA	1:E:182:GLN:OE1	2.63	0.44
1:F:132:VAL:HG12	1:F:133:ASN:N	2.31	0.44
1:F:215:ALA:O	1:F:219:PRO:HG3	2.18	0.44
1:F:251:PHE:CE1	1:F:254:GLU:HB2	2.52	0.44
1:G:75:SER:HB2	1:Q:61:GLU:HG2	1.99	0.44
1:G:172:MET:HA	1:G:242:LEU:HA	2.00	0.44
1:H:292:ILE:HD13	1:H:309:ALA:HB2	1.99	0.44
1:O:70:ILE:HD12	1:O:70:ILE:N	2.31	0.44
1:A:33:THR:CG2	1:A:77:ARG:HG2	2.44	0.44
1:B:298:MET:SD	1:D:226:ASN:ND2	2.90	0.44
1:D:13:ARG:HD2	4:D:341:HOH:O	2.17	0.44
1:D:197:ARG:HD2	1:D:197:ARG:N	2.32	0.44
1:E:327:ILE:HG23	3:E:338:SO4:O3	2.18	0.44
1:F:84:TRP:HA	1:F:84:TRP:HE3	1.82	0.44
1:G:9:GLY:O	1:G:10:ARG:C	2.58	0.44
1:G:185:LEU:HA	1:G:198:ALA:CB	2.47	0.44
1:G:278:LEU:HD22	1:H:46:TYR:CD2	2.52	0.44
1:H:157:PHE:CE1	1:H:242:LEU:HD23	2.53	0.44
1:Q:1:LEU:O	1:Q:90:ASP:HB2	2.17	0.44
1:Q:191:ARG:NH1	1:Q:191:ARG:CB	2.75	0.44
1:B:138:SER:C	1:B:140:ASP:H	2.26	0.44
1:D:228:ILE:H	1:D:228:ILE:CD1	2.30	0.44
1:E:203:ILE:CD1	1:G:232:VAL:HG21	2.42	0.44
1:E:251:PHE:O	1:E:253:GLU:N	2.51	0.44
1:F:98:VAL:HG23	1:F:99:PHE:CD1	2.52	0.44
1:H:170:GLY:H	1:H:225:LEU:HD23	1.83	0.44
1:H:226:ASN:OD1	1:H:227:GLY:N	2.51	0.44
1:O:157:PHE:CE1	1:O:242:LEU:HD23	2.53	0.44
1:B:272:ASP:O	1:B:291:THR:HA	2.17	0.44
1:D:17:ARG:HD3	1:D:50:LEU:HD13	2.00	0.44
1:D:221:LEU:HD22	1:D:221:LEU:N	2.33	0.44
1:D:329:ALA:O	1:D:332:TRP:HB2	2.18	0.44
1:E:50:LEU:HB2	1:E:53:PHE:CZ	2.52	0.44
1:E:170:GLY:O	1:E:225:LEU:HA	2.18	0.44
1:E:173:THR:HG23	1:E:228:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ARG:NH1	1:G:279:VAL:HG22	2.33	0.44
1:A:137:TYR:CZ	1:A:328:VAL:HG22	2.52	0.44
1:A:205:PRO:HA	1:A:230:LEU:HD23	1.98	0.44
1:C:276:GLU:HB2	1:C:278:LEU:HG	1.99	0.44
1:D:122:GLY:C	1:D:125:ILE:HG21	2.43	0.44
1:E:60(A):GLY:O	1:E:61:GLU:HG2	2.17	0.44
1:F:18:CYS:SG	1:F:319:GLN:CD	3.01	0.44
1:H:208:THR:C	1:H:210:ALA:H	2.26	0.44
1:Q:3:VAL:HG12	1:Q:4:ALA:N	2.33	0.44
1:A:84:TRP:HA	1:A:84:TRP:HE3	1.82	0.44
1:B:133:ASN:HD22	1:B:133:ASN:N	2.15	0.44
1:C:146:ASN:O	1:C:147:ALA:HB3	2.17	0.44
1:D:133:ASN:OD1	1:D:217:VAL:HA	2.18	0.44
1:E:106:GLY:O	1:E:110:GLU:HG3	2.18	0.44
1:F:154:LEU:HD23	1:F:214:VAL:HG21	2.00	0.44
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.81	0.44
1:Q:255:VAL:O	1:Q:258:ALA:HB3	2.18	0.44
1:A:0:LYS:HG2	1:A:26:ASP:HB2	2.00	0.44
1:E:194:ARG:HE	1:G:277:PRO:HA	1.82	0.44
1:F:74:VAL:HG22	1:F:75:SER:N	2.32	0.44
1:G:37:VAL:HG21	1:G:62:THR:HA	2.00	0.44
1:G:251:PHE:CA	1:G:299:VAL:HG21	2.46	0.44
1:H:182:GLN:HB3	1:H:199:ALA:HB2	1.99	0.44
1:H:192:ASP:C	1:H:194:ARG:N	2.75	0.44
1:B:154:LEU:CD2	1:B:172:MET:HE2	2.44	0.44
1:C:56:ASP:N	1:C:67:ASP:OD1	2.35	0.44
1:D:175:THR:HB	1:D:239:VAL:HG13	2.00	0.44
1:E:8:PHE:CZ	1:E:13:ARG:HG2	2.53	0.44
1:E:138:SER:C	1:E:140:ASP:N	2.75	0.44
1:E:158:VAL:O	1:E:158:VAL:HG12	2.18	0.44
1:E:201:LEU:HD11	1:H:235:PRO:HB3	1.99	0.44
1:F:259:PHE:HB3	1:F:273:VAL:HG21	1.98	0.44
1:G:211:ALA:HB1	1:G:226:ASN:CA	2.44	0.44
1:G:222:LYS:HG2	1:G:223:GLY:N	2.32	0.44
1:H:2:LYS:HD2	1:H:88:GLY:HA3	1.99	0.44
1:H:30:ILE:HG13	1:H:71:ILE:HD11	2.00	0.44
1:Q:1:LEU:HD22	1:Q:329:ALA:HA	1.99	0.44
1:Q:125:ILE:HG23	1:Q:143:ILE:O	2.17	0.44
1:Q:174:THR:O	1:Q:174:THR:HG23	2.18	0.44
1:D:276:GLU:HB2	1:D:278:LEU:HG	2.00	0.43
1:E:106:GLY:O	1:E:109:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LYS:CE	1:G:193:LEU:HD21	2.48	0.43
1:F:280:SER:C	1:F:282:ASP:N	2.76	0.43
1:G:16:LEU:HD23	1:G:16:LEU:C	2.43	0.43
1:G:162:ASP:O	1:G:164:LYS:N	2.49	0.43
1:O:158:VAL:HG13	1:O:167:ILE:CD1	2.48	0.43
1:Q:206:THR:HG23	1:Q:207:SER:O	2.17	0.43
1:C:64:ILE:C	1:C:64:ILE:HD12	2.43	0.43
1:E:77:ARG:NH1	1:E:77:ARG:CB	2.81	0.43
1:E:153:CYS:SG	1:E:240:VAL:HG21	2.58	0.43
1:E:172:MET:HE1	1:E:208:THR:HG21	2.00	0.43
1:F:279:VAL:O	1:F:279:VAL:HG23	2.17	0.43
1:H:70:ILE:CG2	1:H:71:ILE:H	2.27	0.43
1:O:2:LYS:CD	1:O:28:ILE:HD13	2.48	0.43
1:O:236:ASN:O	1:O:237:VAL:CB	2.66	0.43
1:Q:172:MET:HE1	1:Q:211:ALA:HB2	1.99	0.43
1:A:76:ASN:ND2	1:A:81:LEU:HB2	2.34	0.43
1:C:76:ASN:C	1:C:76:ASN:ND2	2.76	0.43
1:E:192:ASP:C	1:E:194:ARG:H	2.26	0.43
1:F:10:ARG:HH11	1:G:186:ASP:HB2	1.84	0.43
1:F:279:VAL:CG1	1:H:204:VAL:HA	2.47	0.43
1:F:301:GLY:HA3	1:H:169:LYS:CE	2.48	0.43
1:A:109:ILE:HD12	1:A:109:ILE:N	2.33	0.43
1:A:233:PRO:HB2	1:C:233:PRO:HB2	2.00	0.43
1:B:256:ASN:HB3	1:B:260:ARG:NH1	2.32	0.43
1:E:228:ILE:HD13	1:E:228:ILE:N	2.32	0.43
1:E:266:GLU:HG2	1:E:267:LEU:N	2.33	0.43
1:E:277:PRO:HA	1:G:194:ARG:HH21	1.82	0.43
1:F:125:ILE:CG2	1:F:143:ILE:HG22	2.48	0.43
1:F:277:PRO:HG3	1:H:193:LEU:HD12	2.00	0.43
1:G:1:LEU:HD21	1:G:332:TRP:CE3	2.54	0.43
1:G:167:ILE:O	1:G:167:ILE:HG22	2.18	0.43
1:G:327:ILE:HG23	1:G:331:ASN:HD22	1.83	0.43
1:H:79:PRO:HB2	1:H:107:LYS:CB	2.47	0.43
1:B:9:GLY:O	1:B:13:ARG:HG3	2.17	0.43
1:D:109:ILE:C	1:D:111:ALA:H	2.27	0.43
1:D:174:THR:HG23	1:D:174:THR:O	2.19	0.43
1:E:177:SER:OG	1:E:237:VAL:O	2.36	0.43
1:G:64:ILE:HG23	1:G:73:VAL:HG21	2.01	0.43
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.53	0.43
1:A:39:GLN:NE2	1:D:190:HIS:O	2.44	0.43
1:A:101:ASP:HA	1:A:125:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ALA:HB1	1:E:67:ASP:OD1	2.19	0.43
1:E:312:ASP:O	1:E:314:GLU:N	2.51	0.43
1:H:23:SER:C	1:H:25:LEU:H	2.25	0.43
1:H:61:GLU:O	1:H:61:GLU:HG3	2.19	0.43
1:E:139:HIS:CG	1:E:331:ASN:O	2.72	0.43
1:E:236:ASN:CG	1:E:237:VAL:N	2.77	0.43
1:F:228:ILE:HG22	1:H:298:MET:HE3	2.00	0.43
1:F:304:MET:HB2	1:H:169:LYS:HZ2	1.82	0.43
1:G:69:LYS:HE3	1:G:71:ILE:HD11	2.00	0.43
1:H:37:VAL:HG22	1:H:73:VAL:HB	2.01	0.43
1:B:251:PHE:N	1:B:251:PHE:CD1	2.87	0.43
1:D:250:THR:OG1	1:D:251:PHE:N	2.52	0.43
1:E:79:PRO:HA	1:E:82:LEU:HD11	1.99	0.43
1:E:277:PRO:C	1:G:194:ARG:HE	2.26	0.43
1:F:1:LEU:HD22	1:F:329:ALA:HB2	2.01	0.43
1:F:235:PRO:CB	1:G:201:LEU:HD11	2.48	0.43
1:O:33:THR:HG21	1:O:77:ARG:HG2	1.99	0.43
1:B:33:THR:HA	1:B:75:SER:OG	2.19	0.43
1:D:84:TRP:CB	1:D:112:GLY:HA3	2.48	0.43
1:D:100:VAL:HA	1:D:118:ILE:HD13	2.00	0.43
1:E:9:GLY:CA	2:E:335:NAD:H4B	2.48	0.43
1:F:105:ALA:HB3	1:F:143:ILE:HD13	2.01	0.43
1:G:158:VAL:HG11	1:G:221:LEU:CD2	2.49	0.43
1:G:219:PRO:O	1:G:221:LEU:N	2.52	0.43
1:H:23:SER:O	1:H:25:LEU:N	2.43	0.43
1:O:17:ARG:NH2	1:O:50:LEU:HB3	2.34	0.43
1:A:238:SER:HB2	1:A:311:TYR:CE1	2.53	0.43
1:B:236:ASN:O	1:B:237:VAL:HB	2.18	0.43
1:C:183:ARG:NH1	1:C:188:SER:O	2.52	0.43
1:D:72:GLN:HE22	1:H:83:PRO:HG3	1.84	0.43
1:F:300:MET:HE3	1:F:304:MET:HB3	2.01	0.43
1:G:0:LYS:HG3	4:G:597:HOH:O	2.17	0.43
1:G:18(A):TRP:O	1:G:19:GLY:N	2.52	0.43
1:G:28:ILE:HD11	1:G:89:ILE:HD11	1.99	0.43
1:H:3:VAL:O	1:H:28:ILE:HG22	2.19	0.43
1:H:36:GLY:HA3	1:H:38:LYS:CD	2.49	0.43
1:H:261:ASP:OD1	1:H:262:SER:N	2.52	0.43
1:O:202:ASN:HD21	1:Q:281:VAL:HG12	1.82	0.43
1:Q:162:ASP:HB2	1:Q:167:ILE:HD12	2.01	0.43
1:A:37:VAL:CG1	1:A:59:PRO:HB3	2.49	0.42
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:HB2	1:A:111:ALA:O	2.19	0.42
1:B:18(B):HIS:HE1	1:B:67:ASP:OD2	2.01	0.42
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.19	0.42
1:B:240:VAL:O	1:B:240:VAL:HG23	2.19	0.42
1:C:174:THR:HG23	1:C:174:THR:O	2.19	0.42
1:D:179:THR:O	1:D:181:ASP:N	2.52	0.42
1:F:173:THR:OG1	1:F:228:ILE:HD11	2.19	0.42
1:G:164:LYS:O	1:G:164:LYS:HG2	2.19	0.42
1:H:70:ILE:CG2	1:H:71:ILE:N	2.81	0.42
1:H:195:ARG:NH2	1:H:206:THR:HG21	2.27	0.42
1:A:191:ARG:HB2	1:A:191:ARG:NH1	2.34	0.42
1:E:32:ASP:C	1:E:34:GLY:N	2.76	0.42
1:E:78:ASN:HB3	1:E:81:LEU:HG	1.99	0.42
1:H:209:GLY:HA3	1:H:212:LYS:HE2	2.01	0.42
1:O:249:LYS:HB3	1:O:302:ASP:HB3	2.00	0.42
1:Q:31:ASN:HA	1:Q:74:VAL:O	2.19	0.42
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.19	0.42
1:B:163:GLN:HE21	1:B:164:LYS:CE	2.32	0.42
1:C:24:PRO:HD2	1:C:326:ASP:OD1	2.19	0.42
1:C:28:ILE:HD11	1:C:89:ILE:HD13	2.01	0.42
1:D:156:PRO:HB2	1:D:290:THR:HG21	2.01	0.42
1:E:29:ALA:HB1	1:E:84:TRP:HZ3	1.85	0.42
1:E:150:THR:HB	1:E:210:ALA:CB	2.49	0.42
1:E:242:LEU:HD21	1:E:244:VAL:HG13	2.00	0.42
1:F:37:VAL:HG12	1:F:38:LYS:N	2.34	0.42
1:F:126:PRO:HB3	1:F:128:TYR:OH	2.18	0.42
1:F:154:LEU:O	1:F:158:VAL:HG23	2.19	0.42
1:F:234:THR:HG22	1:H:233:PRO:HG2	2.00	0.42
1:A:162:ASP:OD2	1:A:220:ASN:ND2	2.39	0.42
1:C:241:ASP:OD2	1:C:306:LYS:HE2	2.19	0.42
1:D:16:LEU:HD23	1:D:16:LEU:C	2.44	0.42
1:D:86:GLU:H	1:D:86:GLU:CD	2.28	0.42
1:D:178:TYR:HB2	1:D:182:GLN:OE1	2.18	0.42
1:E:159:LYS:HB2	1:E:218:LEU:HD11	2.01	0.42
1:E:269:GLY:HA2	1:E:288:PHE:CE1	2.54	0.42
1:F:58:LYS:O	1:F:65:SER:N	2.52	0.42
1:G:236:ASN:O	1:G:237:VAL:CB	2.67	0.42
1:H:171:THR:HG23	1:H:243:VAL:HB	2.01	0.42
1:D:7:GLY:HA3	1:D:96:THR:HG22	2.01	0.42
1:D:15:PHE:CD1	1:D:322:VAL:HG22	2.54	0.42
1:D:72:GLN:NE2	1:H:83:PRO:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:GLU:CA	1:D:268:LYS:HE3	2.43	0.42
1:E:79:PRO:HA	1:E:82:LEU:CG	2.49	0.42
1:E:157:PHE:C	1:E:159:LYS:H	2.27	0.42
1:E:252:ALA:HA	1:E:299:VAL:HG23	2.02	0.42
1:F:11:ILE:HD13	1:F:11:ILE:C	2.43	0.42
1:F:27:ILE:HD12	1:F:27:ILE:H	1.82	0.42
1:F:293:ASP:O	1:F:294:SER:C	2.63	0.42
1:O:132:VAL:HG21	1:O:155:ALA:HB1	2.01	0.42
1:Q:16:LEU:HD23	1:Q:16:LEU:O	2.19	0.42
1:Q:241:ASP:HA	1:Q:308:ILE:HD13	2.01	0.42
1:A:1:LEU:HD21	1:A:332:TRP:CE3	2.54	0.42
1:B:260:ARG:NH2	1:B:275:ASP:OD1	2.52	0.42
1:D:153:CYS:SG	1:D:290:THR:HB	2.59	0.42
1:D:240:VAL:HG13	1:D:311:TYR:HE1	1.82	0.42
1:E:188:SER:HA	1:H:39:GLN:OE1	2.19	0.42
1:E:194:ARG:NH1	1:E:205:PRO:CG	2.83	0.42
1:E:202:ASN:OD1	1:E:202:ASN:N	2.52	0.42
1:F:41:SER:OG	1:F:59:PRO:HD3	2.20	0.42
1:F:222:LYS:HG2	1:F:224:LYS:HE3	1.98	0.42
1:G:157:PHE:HZ	1:G:242:LEU:HD22	1.85	0.42
1:G:256:ASN:HD21	1:G:297:THR:CG2	2.18	0.42
1:O:205:PRO:HG2	1:Q:310:TRP:HZ2	1.85	0.42
1:B:129:VAL:H	1:B:133:ASN:ND2	2.18	0.42
1:B:243:VAL:HG11	1:D:243:VAL:HG11	2.00	0.42
1:D:192:ASP:HB3	1:D:195:ARG:HB2	2.01	0.42
1:E:239:VAL:HG22	1:E:240:VAL:H	1.83	0.42
1:H:251:PHE:O	1:H:255:VAL:HG23	2.19	0.42
1:O:194:ARG:HD2	1:O:205:PRO:O	2.18	0.42
1:A:182:GLN:HB3	1:A:199:ALA:HB2	2.00	0.42
1:B:65:SER:HA	1:B:69:LYS:O	2.20	0.42
1:B:191:ARG:HB2	1:B:191:ARG:HH11	1.84	0.42
1:B:197:ARG:O	1:B:198:ALA:C	2.63	0.42
1:C:177:SER:OG	1:C:234:THR:O	2.34	0.42
1:D:128:TYR:HA	1:D:133:ASN:HD21	1.85	0.42
1:E:183:ARG:CZ	1:E:187:ALA:CB	2.96	0.42
1:F:156:PRO:HB2	1:F:290:THR:HG21	2.01	0.42
1:G:291:THR:CG2	1:G:291:THR:O	2.67	0.42
1:O:60:SER:HB2	1:O:65:SER:HB2	2.02	0.42
1:Q:79:PRO:HA	1:Q:82:LEU:HG	2.00	0.42
1:A:139:HIS:CE1	1:A:333:LYS:HG2	2.55	0.42
1:B:0(A):ALA:H1	1:B:26:ASP:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:SER:HA	1:B:24:PRO:HD3	1.78	0.42
1:C:21:LYS:H	1:C:21:LYS:HZ2	1.67	0.42
1:C:218:LEU:O	1:C:219:PRO:C	2.63	0.42
1:C:237:VAL:CG2	1:C:284:ARG:HD3	2.50	0.42
1:D:79:PRO:HB2	1:D:107:LYS:CB	2.50	0.42
1:E:31:ASN:ND2	2:E:335:NAD:H2A	2.34	0.42
1:E:137:TYR:CZ	1:E:139:HIS:HA	2.55	0.42
1:E:162:ASP:HB2	1:E:167:ILE:HD12	2.01	0.42
1:H:84:TRP:HD1	1:H:111:ALA:HB3	1.85	0.42
1:C:106:GLY:O	1:C:110:GLU:HG3	2.19	0.42
1:D:63:ALA:HB2	1:D:72:GLN:HA	2.02	0.42
1:E:129:VAL:HB	1:E:133:ASN:ND2	2.34	0.42
1:E:291:THR:HB	1:E:310:TRP:HB2	2.02	0.42
1:H:6:ASN:HD22	1:H:96:THR:HG21	1.85	0.42
1:G:213:ALA:O	1:G:215:ALA:N	2.53	0.41
1:G:222:LYS:C	1:G:224:LYS:H	2.27	0.41
1:G:255:VAL:HG12	1:G:259:PHE:CE2	2.56	0.41
1:O:170:GLY:HA3	1:O:244:VAL:HG12	2.02	0.41
1:O:256:ASN:O	1:O:260:ARG:HG3	2.20	0.41
1:A:116:VAL:HB	1:A:143:ILE:HG13	2.02	0.41
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.54	0.41
1:C:156:PRO:HB2	1:C:290:THR:CG2	2.43	0.41
1:C:271:LEU:HG	1:C:272:ASP:N	2.35	0.41
1:E:154:LEU:CD1	1:E:240:VAL:HG11	2.50	0.41
1:E:185:LEU:O	1:E:187:ALA:N	2.53	0.41
1:E:324:LEU:HD12	1:E:327:ILE:HD12	2.01	0.41
1:F:4:ALA:HB2	1:F:89:ILE:HD12	2.03	0.41
1:F:37:VAL:HG22	1:F:63:ALA:H	1.85	0.41
1:F:85:LYS:O	1:F:85:LYS:HE3	2.20	0.41
1:F:118:ILE:HD11	1:F:143:ILE:HG23	2.02	0.41
1:F:218:LEU:O	1:F:221:LEU:HD23	2.20	0.41
1:O:76:ASN:HB3	1:O:82:LEU:CD2	2.50	0.41
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.56	0.41
1:O:191:ARG:HG3	1:O:191:ARG:HH11	1.82	0.41
1:A:129:VAL:HG23	1:A:217:VAL:HG11	2.02	0.41
1:D:109:ILE:HG13	1:D:116:VAL:HG23	2.01	0.41
1:F:34:GLY:HA2	1:F:39:GLN:NE2	2.35	0.41
1:G:320:ARG:NE	1:G:323:ASP:OD2	2.50	0.41
1:H:44:LEU:HB3	1:H:57:VAL:HG11	2.02	0.41
1:H:83:PRO:HB2	1:H:86:GLU:HG2	2.03	0.41
1:H:330:ASN:C	1:H:332:TRP:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:110:GLU:C	1:Q:112:GLY:H	2.28	0.41
1:Q:221:LEU:HD12	1:Q:225:LEU:HD11	2.01	0.41
1:B:100:VAL:O	1:B:118:ILE:HD13	2.20	0.41
1:D:138:SER:C	1:D:140:ASP:N	2.77	0.41
1:E:30:ILE:CD1	1:E:71:ILE:HD12	2.50	0.41
1:E:239:VAL:HG22	1:E:240:VAL:N	2.36	0.41
1:F:17:ARG:HD3	1:F:50:LEU:CD1	2.50	0.41
1:F:202:ASN:HD21	1:H:281:VAL:HG12	1.85	0.41
1:G:170:GLY:CA	1:G:243:VAL:O	2.67	0.41
1:G:291:THR:HG22	1:G:310:TRP:HB2	2.01	0.41
1:H:115:LYS:HE2	1:H:115:LYS:HB2	1.97	0.41
1:Q:175:THR:CG2	1:Q:232:VAL:HG11	2.50	0.41
1:B:39:GLN:HE22	1:C:188:SER:HB2	1.86	0.41
1:B:165:PHE:CB	1:B:246:VAL:HG11	2.51	0.41
1:B:262:SER:HB3	1:B:267:LEU:HB2	2.02	0.41
1:C:2:LYS:HD3	1:C:28:ILE:CD1	2.50	0.41
1:F:79:PRO:HA	1:F:82:LEU:CD1	2.43	0.41
1:F:138:SER:O	1:F:139:HIS:HB3	2.19	0.41
1:F:310:TRP:CZ2	1:H:205:PRO:HG2	2.55	0.41
1:G:190:HIS:O	1:G:191:ARG:C	2.63	0.41
1:G:302:ASP:HB3	4:G:651:HOH:O	2.20	0.41
1:H:216:LEU:N	1:H:216:LEU:HD12	2.35	0.41
1:C:77:ARG:NH2	4:C:364:HOH:O	2.45	0.41
1:D:6:ASN:OD1	1:D:31:ASN:ND2	2.40	0.41
1:F:117:ILE:HD11	1:F:328:VAL:HG21	2.03	0.41
1:F:319:GLN:OE1	1:F:319:GLN:HA	2.20	0.41
1:G:109:ILE:HA	1:G:113:ALA:O	2.20	0.41
1:H:100:VAL:HG23	1:H:101:ASP:N	2.36	0.41
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.51	0.41
1:B:221:LEU:HD22	1:B:221:LEU:N	2.35	0.41
1:C:96:THR:HB	1:C:98:VAL:HG22	2.02	0.41
1:D:328:VAL:O	1:D:329:ALA:C	2.64	0.41
1:E:131:GLY:HA3	1:E:270:ILE:HG21	2.03	0.41
1:E:209:GLY:C	1:E:212:LYS:HG2	2.45	0.41
1:F:28:ILE:O	1:F:72:GLN:HB2	2.20	0.41
1:F:114:LYS:N	1:F:114:LYS:CD	2.82	0.41
1:F:114:LYS:HB2	1:F:332:TRP:HH2	1.85	0.41
1:F:128:TYR:OH	1:F:141:GLU:OE2	2.39	0.41
1:F:269:GLY:HA2	1:F:288:PHE:CE2	2.56	0.41
1:G:177:SER:CB	1:G:234:THR:O	2.66	0.41
1:A:96:THR:OG1	1:A:98:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASP:CG	1:C:197:ARG:HH12	2.27	0.41
1:C:102:ARG:HB2	1:C:125:ILE:HD11	2.01	0.41
1:E:214:VAL:O	1:E:214:VAL:HG12	2.20	0.41
1:E:301:GLY:C	1:E:303:ASP:H	2.28	0.41
1:F:78:ASN:CB	1:F:81:LEU:HD13	2.44	0.41
1:G:171:THR:O	1:G:242:LEU:HA	2.19	0.41
1:G:324:LEU:O	1:G:327:ILE:HB	2.21	0.41
1:H:76:ASN:HB3	1:H:82:LEU:HD23	2.03	0.41
1:H:118:ILE:HG22	1:H:120:ALA:H	1.86	0.41
1:H:271:LEU:HD12	1:H:290:THR:O	2.21	0.41
1:O:192:ASP:OD1	1:O:192:ASP:C	2.64	0.41
1:B:153:CYS:O	1:B:290:THR:HG21	2.21	0.41
1:C:8:PHE:O	1:C:13:ARG:NH1	2.51	0.41
1:C:332:TRP:C	1:C:333:LYS:HD3	2.46	0.41
1:D:9:GLY:HA3	2:D:335:NAD:O5B	2.21	0.41
1:D:89:ILE:N	1:D:89:ILE:HD12	2.36	0.41
1:E:168:ILE:HD11	1:E:247:SER:HB3	2.02	0.41
1:E:300:MET:HE1	1:G:171:THR:CB	2.51	0.41
1:F:5:ILE:HD11	1:F:12:GLY:CA	2.51	0.41
1:F:17:ARG:NH2	1:F:53:PHE:HA	2.36	0.41
1:F:259:PHE:C	1:F:261:ASP:N	2.78	0.41
1:F:267:LEU:HD13	1:F:271:LEU:HB2	2.03	0.41
1:F:282:ASP:OD2	1:H:197:ARG:NH1	2.50	0.41
1:F:333:LYS:OXT	1:F:333:LYS:HG3	2.21	0.41
1:G:29:ALA:HA	1:G:72:GLN:O	2.21	0.41
1:G:207:SER:O	1:G:208:THR:HB	2.20	0.41
1:G:317:TYR:O	1:G:320:ARG:HB2	2.21	0.41
1:H:38:LYS:CD	1:H:38:LYS:N	2.82	0.41
1:H:41:SER:O	1:H:57:VAL:HG12	2.21	0.41
1:H:85:LYS:CG	1:H:112:GLY:HA3	2.50	0.41
1:H:197:ARG:O	1:H:198:ALA:C	2.63	0.41
1:O:141:GLU:HA	1:O:142:PRO:HD2	1.92	0.41
1:O:190:HIS:HB3	1:O:196:ALA:HB2	2.02	0.41
1:O:271:LEU:HD23	1:O:272:ASP:N	2.36	0.41
1:Q:90:ASP:HA	1:Q:114:LYS:CG	2.51	0.41
1:Q:142:PRO:O	1:Q:143:ILE:HD13	2.21	0.41
1:Q:293:ASP:O	1:Q:294:SER:C	2.64	0.41
1:A:76:ASN:HD21	1:A:78:ASN:HB3	1.86	0.41
1:C:2:LYS:HD2	1:C:88:GLY:O	2.21	0.41
1:C:100:VAL:HA	1:C:118:ILE:HD13	2.03	0.41
1:D:5:ILE:HD11	1:D:27:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18(A):TRP:C	1:D:19:GLY:N	2.78	0.41
1:D:137:TYR:CE2	1:D:328:VAL:HA	2.56	0.41
1:D:243:VAL:HG22	1:D:306:LYS:HE3	2.02	0.41
1:E:32:ASP:CG	1:E:40:ALA:HB2	2.46	0.41
1:G:132:VAL:HG12	1:G:133:ASN:N	2.36	0.41
1:G:219:PRO:C	1:G:221:LEU:N	2.78	0.41
1:G:265:LYS:HD2	1:G:265:LYS:HA	1.83	0.41
1:G:272:ASP:HB2	1:G:288:PHE:CD1	2.56	0.41
1:H:215:ALA:O	1:H:219:PRO:HA	2.21	0.41
1:O:239:VAL:CG2	1:O:308:ILE:HG23	2.51	0.41
1:B:202:ASN:O	1:B:233:PRO:HD3	2.21	0.40
1:E:178:TYR:HB2	1:E:199:ALA:HB1	2.02	0.40
1:E:275:ASP:HA	1:E:294:SER:OG	2.20	0.40
1:F:31:ASN:CB	1:F:74:VAL:HG13	2.43	0.40
1:F:48:SER:OG	1:G:202:ASN:ND2	2.54	0.40
1:F:165:PHE:HD1	1:F:248:LYS:HB3	1.86	0.40
1:F:283:PHE:CD2	1:F:283:PHE:N	2.89	0.40
1:G:173:THR:O	1:G:241:ASP:N	2.54	0.40
1:G:293:ASP:CG	1:G:296:LEU:HG	2.44	0.40
1:H:41:SER:CB	1:H:59:PRO:HG3	2.50	0.40
1:Q:115:LYS:HE3	1:Q:115:LYS:HB2	1.82	0.40
1:A:139:HIS:ND1	1:A:333:LYS:HB3	2.36	0.40
1:B:264:GLU:O	1:B:265:LYS:HD3	2.21	0.40
1:C:64:ILE:HD13	1:C:66:VAL:HG23	2.04	0.40
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.56	0.40
1:D:137:TYR:CZ	1:D:328:VAL:HG22	2.57	0.40
1:E:146:ASN:O	1:E:146:ASN:OD1	2.39	0.40
1:F:139:HIS:HB2	1:F:331:ASN:O	2.22	0.40
1:G:208:THR:O	1:G:210:ALA:N	2.54	0.40
1:Q:235:PRO:O	1:Q:236:ASN:HB2	2.20	0.40
1:C:333:LYS:HD2	1:C:333:LYS:HA	1.81	0.40
1:D:142:PRO:O	1:D:143:ILE:HD13	2.21	0.40
1:D:275:ASP:HA	1:D:294:SER:OG	2.21	0.40
1:E:94:GLU:HB3	1:E:118:ILE:HG23	2.04	0.40
1:E:176:HIS:CE1	1:E:313:ASN:HD22	2.40	0.40
1:E:179:THR:C	1:E:181:ASP:N	2.78	0.40
1:G:18(A):TRP:HH2	1:G:69:LYS:HE2	1.85	0.40
1:H:76:ASN:HB3	1:H:82:LEU:CD2	2.51	0.40
1:O:31:ASN:HB2	1:O:74:VAL:HG22	2.03	0.40
1:O:293:ASP:OD1	1:O:296:LEU:HG	2.21	0.40
1:A:7:GLY:C	1:A:9:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG22	1:C:197:ARG:NH1	2.36	0.40
1:B:1:LEU:HD22	1:B:329:ALA:HA	2.03	0.40
1:D:172:MET:CE	1:D:211:ALA:HB2	2.43	0.40
1:E:252:ALA:CB	1:E:298:MET:HA	2.49	0.40
1:E:275:ASP:HB3	1:E:294:SER:OG	2.21	0.40
1:F:3:VAL:HG22	1:F:91:ILE:HG23	2.01	0.40
1:F:16:LEU:HD23	1:F:16:LEU:O	2.21	0.40
1:G:232:VAL:HG23	1:G:234:THR:OG1	2.21	0.40
1:H:239:VAL:O	1:H:239:VAL:HG13	2.22	0.40
1:Q:267:LEU:O	1:Q:268:LYS:C	2.63	0.40
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.90	0.40
1:D:146:ASN:HD22	1:D:321:VAL:CG2	2.34	0.40
1:E:27:ILE:HD11	1:E:30:ILE:HG12	2.03	0.40
1:E:108:HIS:C	1:E:113:ALA:HB3	2.47	0.40
1:E:242:LEU:HD21	1:E:244:VAL:CG1	2.51	0.40
1:F:91:ILE:HD11	1:F:117:ILE:HD12	2.03	0.40
1:F:240:VAL:O	1:F:240:VAL:CG2	2.70	0.40
1:H:154:LEU:HD21	1:H:172:MET:HG3	2.04	0.40
1:Q:122(A):LYS:HA	1:Q:122(A):LYS:HD3	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASN:OD1	1:D:331:ASN:OD1[3_656]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	335/337 (99%)	292 (87%)	36 (11%)	7 (2%)	5 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	4	9
1	C	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	4	9
1	D	334/337 (99%)	269 (80%)	52 (16%)	13 (4%)	2	3
1	E	334/337 (99%)	260 (78%)	57 (17%)	17 (5%)	1	2
1	F	334/337 (99%)	244 (73%)	67 (20%)	23 (7%)	1	1
1	G	334/337 (99%)	257 (77%)	55 (16%)	22 (7%)	1	1
1	H	333/337 (99%)	248 (74%)	61 (18%)	24 (7%)	1	1
1	O	335/337 (99%)	308 (92%)	24 (7%)	3 (1%)	14	30
1	Q	334/337 (99%)	298 (89%)	31 (9%)	5 (2%)	8	18
All	All	3343/3370 (99%)	2762 (83%)	451 (14%)	130 (4%)	2	3

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	SER
1	D	1	LEU
1	D	210	ALA
1	E	75	SER
1	E	237	VAL
1	E	313	ASN
1	F	37	VAL
1	F	76	ASN
1	F	280	SER
1	G	198	ALA
1	G	202	ASN
1	G	208	THR
1	G	225	LEU
1	G	295	SER
1	H	27	ILE
1	H	28	ILE
1	H	71	ILE
1	H	87	LEU
1	H	89	ILE
1	H	133	ASN
1	Q	2	LYS
1	Q	124	ASP
1	A	237	VAL
1	B	0	LYS
1	B	166	GLY

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Mol	Chain	Res	Type
1	B	237	VAL
1	B	302	ASP
1	C	237	VAL
1	D	36	GLY
1	D	166	GLY
1	D	180	GLY
1	D	237	VAL
1	E	55	ALA
1	E	74	VAL
1	E	139	HIS
1	E	186	ASP
1	E	233	PRO
1	E	252	ALA
1	F	49	THR
1	F	69	LYS
1	F	130	VAL
1	F	146	ASN
1	F	266	GLU
1	F	297	THR
1	G	132	VAL
1	G	163	GLN
1	G	166	GLY
1	G	199	ALA
1	G	220	ASN
1	G	223	GLY
1	G	226	ASN
1	G	237	VAL
1	H	22	ASP
1	H	104	GLY
1	H	186	ASP
1	H	237	VAL
1	H	295	SER
1	O	237	VAL
1	Q	302	ASP
1	A	8	PHE
1	A	133	ASN
1	B	233	PRO
1	C	33	THR
1	C	34	GLY
1	C	198	ALA
1	D	55	ALA
1	E	56	ASP

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Mol	Chain	Res	Type
1	F	8	PHE
1	F	132	VAL
1	F	211	ALA
1	F	237	VAL
1	G	18(B)	HIS
1	G	214	VAL
1	G	285	CYS
1	H	43	LEU
1	H	76	ASN
1	H	140	ASP
1	Q	237	VAL
1	B	198	ALA
1	B	249	LYS
1	C	133	ASN
1	D	233	PRO
1	D	252	ALA
1	E	22	ASP
1	E	33	THR
1	E	73	VAL
1	E	193	LEU
1	E	285	CYS
1	F	186	ASP
1	F	285	CYS
1	F	294	SER
1	G	60	SER
1	G	162	ASP
1	G	190	HIS
1	G	207	SER
1	G	246	VAL
1	H	55	ALA
1	H	195	ARG
1	H	226	ASN
1	H	233	PRO
1	O	198	ALA
1	D	22	ASP
1	D	198	ALA
1	F	103	GLU
1	F	139	HIS
1	G	139	HIS
1	H	163	GLN
1	H	166	GLY
1	H	331	ASN

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Mol	Chain	Res	Type
1	O	166	GLY
1	A	0	LYS
1	A	186	ASP
1	F	7	GLY
1	F	24	PRO
1	H	79	PRO
1	E	24	PRO
1	E	279	VAL
1	F	66	VAL
1	B	104	GLY
1	C	83	PRO
1	D	219	PRO
1	F	281	VAL
1	A	166	GLY
1	C	233	PRO
1	D	156	PRO
1	F	219	PRO
1	H	74	VAL
1	A	37	VAL
1	H	142	PRO
1	Q	34	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	279/279 (100%)	266 (95%)	13 (5%)	23	48
1	B	279/279 (100%)	265 (95%)	14 (5%)	22	46
1	C	279/279 (100%)	264 (95%)	15 (5%)	20	42
1	D	279/279 (100%)	270 (97%)	9 (3%)	34	62
1	E	278/279 (100%)	262 (94%)	16 (6%)	18	39
1	F	279/279 (100%)	263 (94%)	16 (6%)	18	40
1	G	279/279 (100%)	258 (92%)	21 (8%)	12	28
1	H	278/279 (100%)	266 (96%)	12 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	279/279 (100%)	267 (96%)	12 (4%)	26	51
1	Q	279/279 (100%)	265 (95%)	14 (5%)	22	46
All	All	2788/2790 (100%)	2646 (95%)	142 (5%)	21	45

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	74	VAL
1	A	84	TRP
1	A	85	LYS
1	A	91	ILE
1	A	133	ASN
1	A	164	LYS
1	A	172	MET
1	A	240	VAL
1	A	266	GLU
1	A	276	GLU
1	A	290	THR
1	A	333	LYS
1	B	1	LEU
1	B	16	LEU
1	B	38	LYS
1	B	58	LYS
1	B	84	TRP
1	B	94	GLU
1	B	103	GLU
1	B	107	LYS
1	B	124	ASP
1	B	133	ASN
1	B	140	ASP
1	B	246	VAL
1	B	271	LEU
1	B	290	THR
1	C	14	ASN
1	C	21	LYS
1	C	58	LYS
1	C	84	TRP
1	C	86	GLU
1	C	94	GLU
1	C	135	ASP

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Mol	Chain	Res	Type
1	C	169	LYS
1	C	172	MET
1	C	191	ARG
1	C	226	ASN
1	C	240	VAL
1	C	290	THR
1	C	306	LYS
1	C	333	LYS
1	D	8	PHE
1	D	56	ASP
1	D	58	LYS
1	D	84	TRP
1	D	125	ILE
1	D	133	ASN
1	D	228	ILE
1	D	253	GLU
1	D	290	THR
1	E	14	ASN
1	E	27	ILE
1	E	58	LYS
1	E	70	ILE
1	E	71	ILE
1	E	84	TRP
1	E	91	ILE
1	E	109	ILE
1	E	133	ASN
1	E	172	MET
1	E	183	ARG
1	E	202	ASN
1	E	217	VAL
1	E	228	ILE
1	E	233	PRO
1	E	290	THR
1	F	11	ILE
1	F	25	LEU
1	F	27	ILE
1	F	28	ILE
1	F	62	THR
1	F	85	LYS
1	F	91	ILE
1	F	94	GLU
1	F	115	LYS

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Mol	Chain	Res	Type
1	F	121	PRO
1	F	124	ASP
1	F	133	ASN
1	F	174	THR
1	F	191	ARG
1	F	228	ILE
1	F	290	THR
1	G	0	LYS
1	G	3	VAL
1	G	70	ILE
1	G	72	GLN
1	G	85	LYS
1	G	103	GLU
1	G	115	LYS
1	G	130	VAL
1	G	133	ASN
1	G	138	SER
1	G	149	CYS
1	G	150	THR
1	G	191	ARG
1	G	228	ILE
1	G	234	THR
1	G	243	VAL
1	G	253	GLU
1	G	256	ASN
1	G	265	LYS
1	G	279	VAL
1	G	333	LYS
1	H	38	LYS
1	H	67	ASP
1	H	72	GLN
1	H	86	GLU
1	H	91	ILE
1	H	117	ILE
1	H	124	ASP
1	H	133	ASN
1	H	181	ASP
1	H	228	ILE
1	H	290	THR
1	H	300	MET
1	O	3	VAL
1	O	16	LEU

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Mol	Chain	Res	Type
1	O	17	ARG
1	O	39	GLN
1	O	72	GLN
1	O	84	TRP
1	O	86	GLU
1	O	94	GLU
1	O	124	ASP
1	O	133	ASN
1	O	154	LEU
1	O	177	SER
1	Q	38	LYS
1	Q	56	ASP
1	Q	84	TRP
1	Q	94	GLU
1	Q	103	GLU
1	Q	114	LYS
1	Q	133	ASN
1	Q	135	ASP
1	Q	140	ASP
1	Q	172	MET
1	Q	191	ARG
1	Q	240	VAL
1	Q	276	GLU
1	Q	290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	ASN
1	A	133	ASN
1	A	163	GLN
1	A	202	ASN
1	A	226	ASN
1	A	236	ASN
1	A	245	GLN
1	A	256	ASN
1	A	330	ASN
1	B	18(B)	HIS
1	B	39	GLN
1	B	133	ASN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	226	ASN
1	B	236	ASN
1	B	245	GLN
1	B	256	ASN
1	B	330	ASN
1	C	39	GLN
1	C	42	HIS
1	C	76	ASN
1	C	133	ASN
1	C	152	ASN
1	C	202	ASN
1	C	245	GLN
1	C	256	ASN
1	C	330	ASN
1	D	72	GLN
1	D	133	ASN
1	D	139	HIS
1	D	146	ASN
1	D	202	ASN
1	D	245	GLN
1	D	256	ASN
1	D	330	ASN
1	E	18(B)	HIS
1	E	39	GLN
1	E	42	HIS
1	E	108	HIS
1	E	133	ASN
1	E	146	ASN
1	E	163	GLN
1	E	202	ASN
1	E	226	ASN
1	E	245	GLN
1	E	256	ASN
1	E	330	ASN
1	E	331	ASN
1	F	14	ASN
1	F	31	ASN
1	F	42	HIS
1	F	133	ASN
1	F	139	HIS
1	F	152	ASN
1	F	202	ASN

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Mol	Chain	Res	Type
1	F	256	ASN
1	F	330	ASN
1	G	72	GLN
1	G	133	ASN
1	G	202	ASN
1	G	236	ASN
1	G	256	ASN
1	G	330	ASN
1	G	331	ASN
1	H	72	GLN
1	H	76	ASN
1	H	133	ASN
1	H	152	ASN
1	H	202	ASN
1	H	220	ASN
1	H	245	GLN
1	H	256	ASN
1	H	330	ASN
1	O	14	ASN
1	O	18(B)	HIS
1	O	72	GLN
1	O	78	ASN
1	O	133	ASN
1	O	152	ASN
1	O	202	ASN
1	O	256	ASN
1	Q	133	ASN
1	Q	146	ASN
1	Q	163	GLN
1	Q	202	ASN
1	Q	245	GLN
1	Q	256	ASN
1	Q	330	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

55 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	SO4	Q	339	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	C	334	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	C	337	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	C	336	-	4,4,4	0.39	0	6,6,6	0.16	0
3	SO4	E	338	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	A	337	-	4,4,4	0.42	0	6,6,6	0.12	0
3	SO4	G	337	-	4,4,4	0.39	0	6,6,6	0.07	0
3	SO4	C	338	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	A	340	-	4,4,4	0.35	0	6,6,6	0.13	0
3	SO4	G	334	-	4,4,4	0.41	0	6,6,6	0.10	0
3	SO4	F	337	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	B	338	-	4,4,4	0.38	0	6,6,6	0.11	0
2	NAD	D	335	-	46,48,48	1.87	10 (21%)	64,73,73	1.77	13 (20%)
3	SO4	B	334	-	4,4,4	0.41	0	6,6,6	0.07	0
3	SO4	O	339	-	4,4,4	0.40	0	6,6,6	0.12	0
3	SO4	D	337	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	339	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	B	336	-	4,4,4	0.38	0	6,6,6	0.13	0
2	NAD	O	335	-	46,48,48	1.66	7 (15%)	64,73,73	1.80	13 (20%)
3	SO4	A	338	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	O	340	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	A	334	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	F	336	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	G	338	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	O	336	-	4,4,4	0.38	0	6,6,6	0.12	0
2	NAD	E	335	-	46,48,48	1.80	9 (19%)	64,73,73	1.86	15 (23%)
3	SO4	Q	336	-	4,4,4	0.43	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	335	-	46,48,48	2.09	9 (19%)	64,73,73	1.72	11 (17%)
3	SO4	E	336	-	4,4,4	0.41	0	6,6,6	0.06	0
3	SO4	Q	334	-	4,4,4	0.36	0	6,6,6	0.12	0
3	SO4	F	334	-	4,4,4	0.34	0	6,6,6	0.10	0
2	NAD	G	335	-	46,48,48	1.81	9 (19%)	64,73,73	1.81	14 (21%)
3	SO4	E	334	-	4,4,4	0.37	0	6,6,6	0.16	0
3	SO4	H	334	-	4,4,4	0.38	0	6,6,6	0.11	0
2	NAD	B	335	-	46,48,48	1.74	9 (19%)	64,73,73	1.77	11 (17%)
3	SO4	A	341	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	H	336	-	4,4,4	0.42	0	6,6,6	0.10	0
3	SO4	H	337	-	4,4,4	0.39	0	6,6,6	0.07	0
3	SO4	B	337	-	4,4,4	0.35	0	6,6,6	0.14	0
2	NAD	A	335	-	46,48,48	1.87	9 (19%)	64,73,73	1.81	13 (20%)
3	SO4	O	337	-	4,4,4	0.39	0	6,6,6	0.13	0
3	SO4	Q	337	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	G	336	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	D	336	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	A	336	-	4,4,4	0.35	0	6,6,6	0.11	0
3	SO4	G	339	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	E	337	-	4,4,4	0.36	0	6,6,6	0.07	0
2	NAD	F	335	-	46,48,48	1.77	10 (21%)	64,73,73	1.79	12 (18%)
3	SO4	Q	338	-	4,4,4	0.34	0	6,6,6	0.15	0
3	SO4	O	338	-	4,4,4	0.38	0	6,6,6	0.05	0
2	NAD	Q	335	-	46,48,48	1.99	11 (23%)	64,73,73	1.71	13 (20%)
3	SO4	O	334	-	4,4,4	0.37	0	6,6,6	0.16	0
3	SO4	B	339	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	D	334	-	4,4,4	0.37	0	6,6,6	0.15	0
2	NAD	H	335	-	46,48,48	1.85	9 (19%)	64,73,73	1.80	14 (21%)

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
2	NAD	D	335	-	-	8/30/62/62	0/5/5/5
2	NAD	G	335	-	-	11/30/62/62	0/5/5/5
2	NAD	F	335	-	-	11/30/62/62	0/5/5/5
2	NAD	O	335	-	-	5/30/62/62	0/5/5/5
2	NAD	B	335	-	-	7/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	Q	335	-	-	10/30/62/62	0/5/5/5
2	NAD	E	335	-	-	14/30/62/62	0/5/5/5
2	NAD	A	335	-	-	10/30/62/62	0/5/5/5
2	NAD	C	335	-	-	6/30/62/62	0/5/5/5
2	NAD	H	335	-	-	10/30/62/62	0/5/5/5

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	335	NAD	PN-O3	-6.34	1.52	1.59
2	A	335	NAD	PN-O3	-5.92	1.53	1.59
2	Q	335	NAD	PN-O3	-5.80	1.53	1.59
2	C	335	NAD	PA-O3	-5.44	1.53	1.59
2	B	335	NAD	PN-O3	-5.11	1.54	1.59
2	D	335	NAD	PA-O3	-5.06	1.54	1.59
2	O	335	NAD	PN-O3	-5.05	1.54	1.59
2	F	335	NAD	C3N-C7N	5.04	1.58	1.50
2	A	335	NAD	PA-O3	-5.01	1.54	1.59
2	Q	335	NAD	PA-O3	-4.96	1.54	1.59
2	G	335	NAD	C3N-C7N	4.95	1.58	1.50
2	D	335	NAD	PN-O3	-4.93	1.54	1.59
2	C	335	NAD	C2N-N1N	4.88	1.40	1.35
2	H	335	NAD	C3N-C7N	4.84	1.57	1.50
2	C	335	NAD	C3N-C7N	4.78	1.57	1.50
2	Q	335	NAD	C3N-C7N	4.77	1.57	1.50
2	O	335	NAD	PA-O3	-4.72	1.54	1.59
2	H	335	NAD	PN-O3	-4.55	1.54	1.59
2	D	335	NAD	C3N-C7N	4.50	1.57	1.50
2	G	335	NAD	C2N-N1N	4.43	1.39	1.35
2	E	335	NAD	PN-O3	-4.40	1.54	1.59
2	E	335	NAD	C3N-C7N	4.34	1.57	1.50
2	H	335	NAD	C2N-N1N	4.32	1.39	1.35
2	D	335	NAD	C6N-N1N	4.32	1.45	1.35
2	F	335	NAD	C6N-N1N	4.28	1.45	1.35
2	E	335	NAD	C2N-N1N	4.27	1.39	1.35
2	F	335	NAD	C2N-N1N	4.18	1.39	1.35
2	B	335	NAD	C6N-N1N	4.17	1.44	1.35
2	E	335	NAD	C6N-N1N	4.15	1.44	1.35
2	Q	335	NAD	C6N-N1N	4.14	1.44	1.35
2	G	335	NAD	PN-O3	-4.13	1.55	1.59
2	H	335	NAD	C6N-N1N	4.10	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	NAD	PA-O3	-4.03	1.55	1.59
2	H	335	NAD	PA-O3	-4.02	1.55	1.59
2	C	335	NAD	C6N-N1N	4.01	1.44	1.35
2	E	335	NAD	PA-O3	-4.01	1.55	1.59
2	G	335	NAD	C6N-N1N	3.99	1.44	1.35
2	Q	335	NAD	C2N-N1N	3.98	1.39	1.35
2	F	335	NAD	PN-O3	-3.98	1.55	1.59
2	A	335	NAD	C6N-N1N	3.95	1.44	1.35
2	O	335	NAD	C6N-N1N	3.79	1.44	1.35
2	A	335	NAD	C2N-N1N	3.79	1.39	1.35
2	Q	335	NAD	C4N-C3N	3.76	1.45	1.39
2	C	335	NAD	C4N-C3N	3.73	1.45	1.39
2	G	335	NAD	PA-O3	-3.72	1.55	1.59
2	F	335	NAD	C4N-C3N	3.66	1.45	1.39
2	D	335	NAD	C4N-C3N	3.51	1.44	1.39
2	O	335	NAD	C3N-C7N	3.50	1.55	1.50
2	B	335	NAD	C2N-N1N	3.47	1.38	1.35
2	B	335	NAD	C3N-C7N	3.35	1.55	1.50
2	E	335	NAD	C4N-C3N	3.27	1.44	1.39
2	A	335	NAD	C4N-C3N	3.26	1.44	1.39
2	D	335	NAD	C2N-N1N	3.21	1.38	1.35
2	F	335	NAD	PA-O3	-3.10	1.56	1.59
2	H	335	NAD	C4N-C3N	3.10	1.44	1.39
2	G	335	NAD	C4N-C3N	3.01	1.44	1.39
2	O	335	NAD	C4N-C3N	2.97	1.43	1.39
2	B	335	NAD	C4N-C3N	2.87	1.43	1.39
2	A	335	NAD	C3N-C7N	2.75	1.54	1.50
2	Q	335	NAD	C4A-N3A	2.74	1.39	1.34
2	G	335	NAD	C4A-N3A	2.71	1.39	1.34
2	D	335	NAD	C4A-N3A	2.68	1.39	1.34
2	A	335	NAD	C5N-C4N	2.66	1.43	1.38
2	E	335	NAD	C4A-N3A	2.49	1.39	1.34
2	H	335	NAD	C4A-N3A	2.46	1.39	1.34
2	A	335	NAD	C4A-N3A	2.43	1.39	1.34
2	F	335	NAD	C4A-N3A	2.38	1.38	1.34
2	E	335	NAD	C5N-C4N	2.34	1.42	1.38
2	B	335	NAD	O5B-C5B	2.31	1.53	1.44
2	F	335	NAD	C5N-C4N	2.28	1.42	1.38
2	B	335	NAD	C4A-N3A	2.28	1.38	1.34
2	H	335	NAD	O5B-C5B	2.28	1.53	1.44
2	E	335	NAD	O5B-C5B	2.27	1.53	1.44
2	C	335	NAD	O3D-C3D	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	335	NAD	O5B-C5B	2.23	1.53	1.44
2	O	335	NAD	C5N-C4N	2.23	1.42	1.38
2	O	335	NAD	C2N-N1N	2.23	1.37	1.35
2	Q	335	NAD	C5N-C4N	2.23	1.42	1.38
2	B	335	NAD	C5N-C4N	2.22	1.42	1.38
2	F	335	NAD	O5B-C5B	2.17	1.52	1.44
2	C	335	NAD	O5B-C5B	2.15	1.52	1.44
2	H	335	NAD	C5N-C4N	2.15	1.42	1.38
2	A	335	NAD	C7N-N7N	-2.12	1.29	1.33
2	D	335	NAD	O3D-C3D	2.07	1.48	1.43
2	Q	335	NAD	C7N-N7N	-2.07	1.29	1.33
2	D	335	NAD	O5B-C5B	2.05	1.52	1.44
2	C	335	NAD	C4A-N3A	2.04	1.38	1.34
2	G	335	NAD	O5B-C5B	2.04	1.52	1.44
2	G	335	NAD	C5N-C4N	2.04	1.42	1.38
2	D	335	NAD	C5N-C4N	2.04	1.42	1.38
2	F	335	NAD	C2A-N1A	2.01	1.37	1.33
2	Q	335	NAD	O3D-C3D	2.00	1.47	1.43

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	NAD	C5N-C6N-N1N	-5.89	112.35	120.38
2	C	335	NAD	C6N-N1N-C2N	5.88	126.88	121.88
2	A	335	NAD	C6N-N1N-C2N	5.84	126.84	121.88
2	B	335	NAD	C5N-C6N-N1N	-5.80	112.48	120.38
2	O	335	NAD	C5N-C6N-N1N	-5.69	112.63	120.38
2	D	335	NAD	C5N-C6N-N1N	-5.66	112.66	120.38
2	G	335	NAD	C5N-C6N-N1N	-5.66	112.66	120.38
2	F	335	NAD	C6N-N1N-C2N	5.63	126.67	121.88
2	Q	335	NAD	C5N-C6N-N1N	-5.62	112.72	120.38
2	E	335	NAD	C5N-C6N-N1N	-5.60	112.74	120.38
2	F	335	NAD	C5N-C6N-N1N	-5.59	112.76	120.38
2	Q	335	NAD	C6N-N1N-C2N	5.59	126.63	121.88
2	H	335	NAD	C5N-C6N-N1N	-5.51	112.87	120.38
2	C	335	NAD	C5N-C6N-N1N	-5.47	112.92	120.38
2	D	335	NAD	C6N-N1N-C2N	5.43	126.50	121.88
2	E	335	NAD	C6N-N1N-C2N	5.43	126.49	121.88
2	O	335	NAD	C6N-N1N-C2N	5.38	126.45	121.88
2	G	335	NAD	C6N-N1N-C2N	5.26	126.35	121.88
2	B	335	NAD	C6N-N1N-C2N	5.06	126.18	121.88
2	H	335	NAD	C6N-N1N-C2N	5.03	126.16	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	335	NAD	C6N-C5N-C4N	4.20	125.51	119.45
2	H	335	NAD	C6N-C5N-C4N	4.19	125.49	119.45
2	G	335	NAD	C6N-C5N-C4N	4.16	125.45	119.45
2	O	335	NAD	C5N-C4N-C3N	-4.13	116.31	120.36
2	H	335	NAD	C4N-C3N-C7N	-4.06	109.99	121.06
2	E	335	NAD	C4N-C3N-C7N	-4.06	110.01	121.06
2	A	335	NAD	C6N-C5N-C4N	4.06	125.30	119.45
2	E	335	NAD	C6N-C5N-C4N	4.04	125.27	119.45
2	F	335	NAD	C6N-C5N-C4N	3.96	125.16	119.45
2	Q	335	NAD	C6N-C5N-C4N	3.93	125.12	119.45
2	C	335	NAD	C4N-C3N-C7N	-3.93	110.36	121.06
2	B	335	NAD	C5N-C4N-C3N	-3.92	116.51	120.36
2	D	335	NAD	C6N-C5N-C4N	3.92	125.10	119.45
2	O	335	NAD	C6N-C5N-C4N	3.90	125.07	119.45
2	G	335	NAD	C4N-C3N-C7N	-3.83	110.64	121.06
2	A	335	NAD	C5N-C4N-C3N	-3.81	116.62	120.36
2	C	335	NAD	C6N-C5N-C4N	3.72	124.81	119.45
2	H	335	NAD	C3N-C7N-N7N	3.71	122.31	117.74
2	F	335	NAD	C4N-C3N-C7N	-3.67	111.07	121.06
2	H	335	NAD	C5N-C4N-C3N	-3.58	116.84	120.36
2	E	335	NAD	C5N-C4N-C3N	-3.58	116.85	120.36
2	A	335	NAD	C4N-C3N-C7N	-3.56	111.35	121.06
2	B	335	NAD	C4N-C3N-C7N	-3.56	111.36	121.06
2	G	335	NAD	C3N-C7N-N7N	3.49	122.04	117.74
2	E	335	NAD	C3N-C7N-N7N	3.49	122.04	117.74
2	D	335	NAD	C4N-C3N-C7N	-3.48	111.58	121.06
2	D	335	NAD	C5N-C4N-C3N	-3.47	116.95	120.36
2	O	335	NAD	C4N-C3N-C7N	-3.45	111.65	121.06
2	Q	335	NAD	C4N-C3N-C7N	-3.45	111.66	121.06
2	F	335	NAD	C3N-C7N-N7N	3.39	121.92	117.74
2	Q	335	NAD	C5N-C4N-C3N	-3.37	117.05	120.36
2	G	335	NAD	C5N-C4N-C3N	-3.25	117.17	120.36
2	F	335	NAD	C5N-C4N-C3N	-3.15	117.27	120.36
2	H	335	NAD	C2N-C3N-C7N	3.13	128.51	119.46
2	C	335	NAD	C2N-C3N-C7N	3.08	128.36	119.46
2	E	335	NAD	C2N-C3N-C7N	3.07	128.31	119.46
2	B	335	NAD	C2N-C3N-C4N	3.04	121.80	118.26
2	O	335	NAD	C2N-C3N-C4N	3.04	121.79	118.26
2	G	335	NAD	C2N-C3N-C7N	3.01	128.16	119.46
2	C	335	NAD	C6N-N1N-C1D	-3.01	113.82	119.73
2	B	335	NAD	O3D-C3D-C4D	-2.99	102.50	111.08
2	E	335	NAD	C2N-C3N-C4N	2.94	121.68	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	335	NAD	O4B-C1B-N9A	-2.90	102.52	108.09
2	A	335	NAD	C2N-C3N-C4N	2.89	121.62	118.26
2	F	335	NAD	C2N-C3N-C7N	2.88	127.78	119.46
2	B	335	NAD	C3N-C7N-N7N	2.85	121.24	117.74
2	H	335	NAD	C2N-C3N-C4N	2.79	121.50	118.26
2	H	335	NAD	C4D-O4D-C1D	2.76	112.46	109.92
2	C	335	NAD	O3D-C3D-C4D	-2.76	103.14	111.08
2	C	335	NAD	C5N-C4N-C3N	-2.76	117.65	120.36
2	D	335	NAD	C2N-C3N-C4N	2.75	121.46	118.26
2	O	335	NAD	C3N-C7N-N7N	2.75	121.13	117.74
2	G	335	NAD	C6N-N1N-C1D	-2.74	114.35	119.73
2	H	335	NAD	C6N-N1N-C1D	-2.74	114.35	119.73
2	F	335	NAD	C6N-N1N-C1D	-2.74	114.36	119.73
2	E	335	NAD	C2B-C3B-C4B	2.74	107.89	102.61
2	O	335	NAD	O2A-PA-O3	2.73	114.66	107.27
2	G	335	NAD	O2A-PA-O3	2.71	114.61	107.27
2	D	335	NAD	C3N-C7N-N7N	2.68	121.04	117.74
2	E	335	NAD	C6N-N1N-C1D	-2.68	114.46	119.73
2	A	335	NAD	C3N-C7N-N7N	2.67	121.03	117.74
2	A	335	NAD	O5B-C5B-C4B	-2.65	99.98	108.99
2	Q	335	NAD	C2N-C3N-C7N	2.64	127.07	119.46
2	A	335	NAD	C2N-C3N-C7N	2.62	127.03	119.46
2	G	335	NAD	C4D-O4D-C1D	2.62	112.32	109.92
2	Q	335	NAD	C3N-C7N-N7N	2.60	120.94	117.74
2	D	335	NAD	C2N-C3N-C7N	2.60	126.96	119.46
2	C	335	NAD	C2N-C3N-C4N	2.59	121.27	118.26
2	C	335	NAD	C3N-C7N-N7N	2.59	120.92	117.74
2	Q	335	NAD	C2N-C3N-C4N	2.59	121.27	118.26
2	G	335	NAD	O3D-C3D-C4D	-2.58	103.68	111.08
2	B	335	NAD	C2N-C3N-C7N	2.56	126.85	119.46
2	E	335	NAD	O3D-C3D-C4D	-2.56	103.74	111.08
2	O	335	NAD	O3D-C3D-C4D	-2.54	103.78	111.08
2	G	335	NAD	C2N-C3N-C4N	2.53	121.20	118.26
2	E	335	NAD	O2A-PA-O3	2.52	114.09	107.27
2	F	335	NAD	O2A-PA-O3	2.49	114.00	107.27
2	F	335	NAD	C2N-C3N-C4N	2.48	121.15	118.26
2	O	335	NAD	C2N-C3N-C7N	2.46	126.56	119.46
2	O	335	NAD	O5B-C5B-C4B	-2.45	100.64	108.99
2	Q	335	NAD	C6N-N1N-C1D	-2.45	114.93	119.73
2	Q	335	NAD	O3D-C3D-C4D	-2.43	104.10	111.08
2	D	335	NAD	C6N-N1N-C1D	-2.42	114.99	119.73
2	A	335	NAD	O2A-PA-O3	2.39	113.73	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	335	NAD	O2A-PA-O3	2.38	113.70	107.27
2	A	335	NAD	O3D-C3D-C4D	-2.36	104.30	111.08
2	F	335	NAD	O3D-C3D-C4D	-2.36	104.30	111.08
2	G	335	NAD	O3-PN-O1N	-2.36	103.62	110.70
2	A	335	NAD	C6N-N1N-C1D	-2.34	115.13	119.73
2	A	335	NAD	O3-PN-O1N	-2.34	103.66	110.70
2	B	335	NAD	O2A-PA-O3	2.34	113.60	107.27
2	E	335	NAD	O7N-C7N-C3N	-2.33	116.75	119.60
2	H	335	NAD	O4B-C1B-N9A	-2.29	103.69	108.09
2	H	335	NAD	O7N-C7N-C3N	-2.28	116.81	119.60
2	G	335	NAD	O5B-C5B-C4B	-2.28	101.24	108.99
2	D	335	NAD	O4B-C1B-N9A	-2.25	103.77	108.09
2	D	335	NAD	C4D-O4D-C1D	2.25	111.98	109.92
2	H	335	NAD	O3D-C3D-C4D	-2.23	104.68	111.08
2	F	335	NAD	O5B-C5B-C4B	-2.19	101.52	108.99
2	D	335	NAD	O2A-PA-O3	2.19	113.19	107.27
2	Q	335	NAD	O4B-C1B-N9A	-2.17	103.92	108.09
2	E	335	NAD	C4D-O4D-C1D	2.16	111.90	109.92
2	D	335	NAD	O3D-C3D-C4D	-2.14	104.93	111.08
2	B	335	NAD	C6N-N1N-C1D	-2.14	115.52	119.73
2	C	335	NAD	O5B-C5B-C4B	-2.11	101.80	108.99
2	E	335	NAD	O4B-C1B-N9A	-2.05	104.16	108.09
2	O	335	NAD	O7N-C7N-C3N	-2.04	117.10	119.60
2	Q	335	NAD	O2A-PA-O3	2.03	112.75	107.27
2	Q	335	NAD	O3-PN-O1N	-2.01	104.67	110.70

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	335	NAD	O4D-C1D-N1N-C2N
2	A	335	NAD	O4D-C1D-N1N-C6N
2	A	335	NAD	C2D-C1D-N1N-C2N
2	A	335	NAD	C2D-C1D-N1N-C6N
2	B	335	NAD	O4D-C1D-N1N-C2N
2	B	335	NAD	O4D-C1D-N1N-C6N
2	B	335	NAD	C2D-C1D-N1N-C2N
2	B	335	NAD	C2D-C1D-N1N-C6N
2	C	335	NAD	O4D-C1D-N1N-C2N
2	C	335	NAD	O4D-C1D-N1N-C6N
2	C	335	NAD	C2D-C1D-N1N-C2N
2	C	335	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	D	335	NAD	C5B-O5B-PA-O1A
2	D	335	NAD	C5B-O5B-PA-O3
2	D	335	NAD	O4D-C1D-N1N-C2N
2	E	335	NAD	C5B-O5B-PA-O2A
2	E	335	NAD	C5B-O5B-PA-O3
2	E	335	NAD	O4D-C1D-N1N-C2N
2	E	335	NAD	O4D-C1D-N1N-C6N
2	E	335	NAD	C2D-C1D-N1N-C2N
2	E	335	NAD	C2D-C1D-N1N-C6N
2	E	335	NAD	C2N-C3N-C7N-O7N
2	E	335	NAD	C2N-C3N-C7N-N7N
2	F	335	NAD	C5B-O5B-PA-O1A
2	F	335	NAD	C5B-O5B-PA-O3
2	F	335	NAD	O4D-C1D-N1N-C2N
2	G	335	NAD	C5B-O5B-PA-O1A
2	G	335	NAD	C5B-O5B-PA-O3
2	G	335	NAD	O4D-C1D-N1N-C2N
2	G	335	NAD	O4D-C1D-N1N-C6N
2	H	335	NAD	O4D-C1D-N1N-C2N
2	H	335	NAD	O4D-C1D-N1N-C6N
2	O	335	NAD	O4D-C1D-N1N-C2N
2	O	335	NAD	O4D-C1D-N1N-C6N
2	O	335	NAD	C2D-C1D-N1N-C2N
2	O	335	NAD	C2D-C1D-N1N-C6N
2	Q	335	NAD	O4D-C1D-N1N-C2N
2	Q	335	NAD	O4D-C1D-N1N-C6N
2	Q	335	NAD	C2D-C1D-N1N-C2N
2	Q	335	NAD	C2D-C1D-N1N-C6N
2	E	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	C4N-C3N-C7N-N7N
2	E	335	NAD	C3B-C4B-C5B-O5B
2	H	335	NAD	C2N-C3N-C7N-O7N
2	H	335	NAD	C2N-C3N-C7N-N7N
2	H	335	NAD	C4N-C3N-C7N-N7N
2	H	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	O4B-C4B-C5B-O5B
2	G	335	NAD	O4B-C4B-C5B-O5B
2	A	335	NAD	PN-O3-PA-O1A
2	Q	335	NAD	O4B-C4B-C5B-O5B
2	F	335	NAD	PN-O3-PA-O5B
2	F	335	NAD	O4D-C4D-C5D-O5D
2	F	335	NAD	PA-O3-PN-O2N

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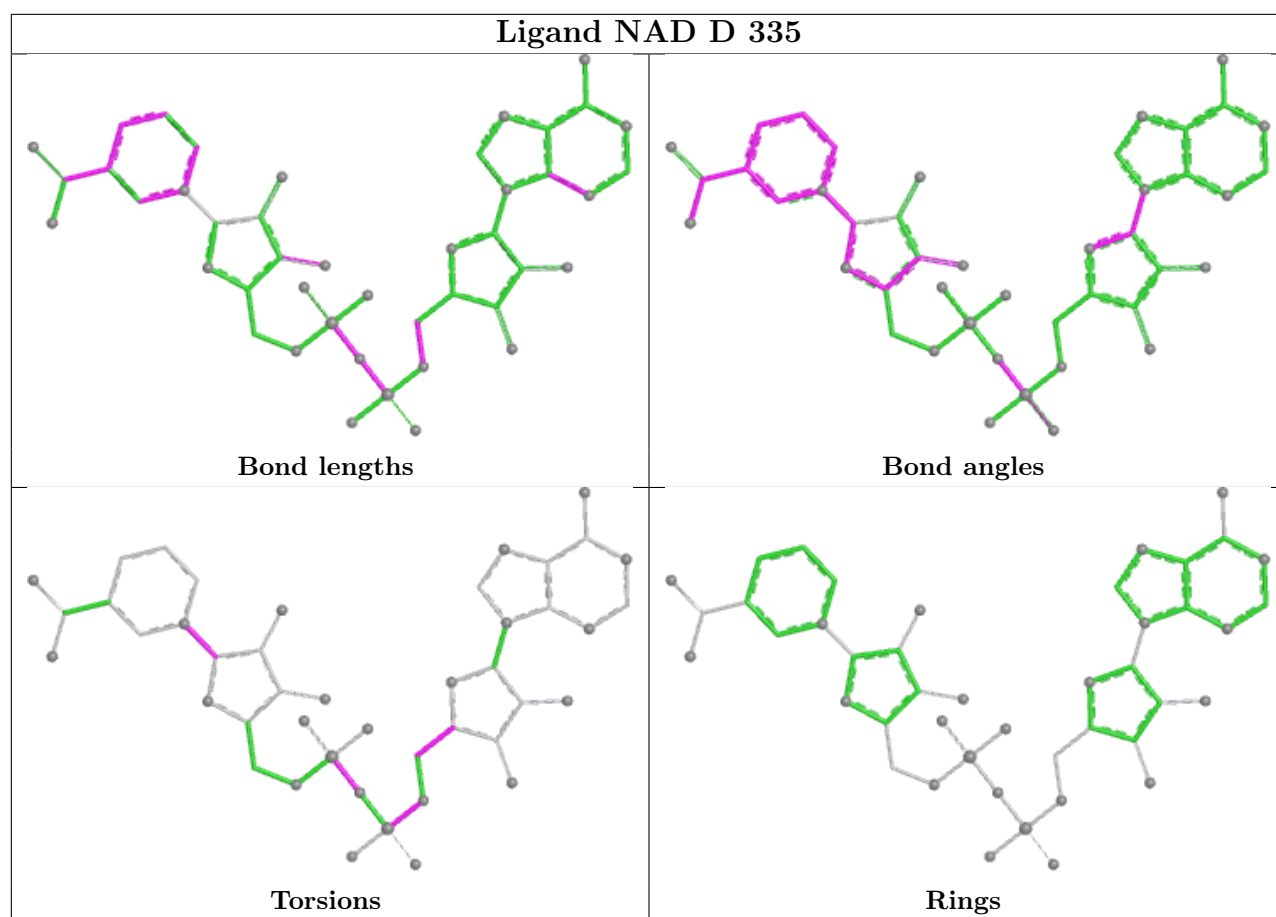
Mol	Chain	Res	Type	Atoms
2	C	335	NAD	O4B-C4B-C5B-O5B
2	D	335	NAD	C5B-O5B-PA-O2A
2	F	335	NAD	C5B-O5B-PA-O2A
2	G	335	NAD	C5B-O5B-PA-O2A
2	H	335	NAD	C5B-O5B-PA-O2A
2	H	335	NAD	C5B-O5B-PA-O3
2	Q	335	NAD	C5B-O5B-PA-O2A
2	Q	335	NAD	C5B-O5B-PA-O3
2	A	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	PN-O3-PA-O2A
2	D	335	NAD	O4B-C4B-C5B-O5B
2	A	335	NAD	C4N-C3N-C7N-N7N
2	G	335	NAD	C2D-C1D-N1N-C2N
2	G	335	NAD	C2D-C1D-N1N-C6N
2	H	335	NAD	C2D-C1D-N1N-C2N
2	H	335	NAD	C2D-C1D-N1N-C6N
2	B	335	NAD	O4B-C4B-C5B-O5B
2	D	335	NAD	O4D-C1D-N1N-C6N
2	F	335	NAD	C3D-C4D-C5D-O5D
2	F	335	NAD	O4D-C1D-N1N-C6N
2	D	335	NAD	PA-O3-PN-O2N
2	Q	335	NAD	PA-O3-PN-O2N
2	F	335	NAD	C4B-C5B-O5B-PA
2	A	335	NAD	PN-O3-PA-O2A
2	B	335	NAD	PA-O3-PN-O2N
2	C	335	NAD	PA-O3-PN-O2N
2	D	335	NAD	PA-O3-PN-O1N
2	G	335	NAD	PA-O3-PN-O1N
2	G	335	NAD	PA-O3-PN-O2N
2	F	335	NAD	O4B-C4B-C5B-O5B
2	G	335	NAD	C3B-C4B-C5B-O5B
2	O	335	NAD	O4B-C4B-C5B-O5B
2	A	335	NAD	C2N-C3N-C7N-O7N
2	Q	335	NAD	C3B-C4B-C5B-O5B
2	A	335	NAD	C2N-C3N-C7N-N7N
2	B	335	NAD	PA-O3-PN-O1N
2	E	335	NAD	PN-O3-PA-O1A
2	Q	335	NAD	PA-O3-PN-O1N

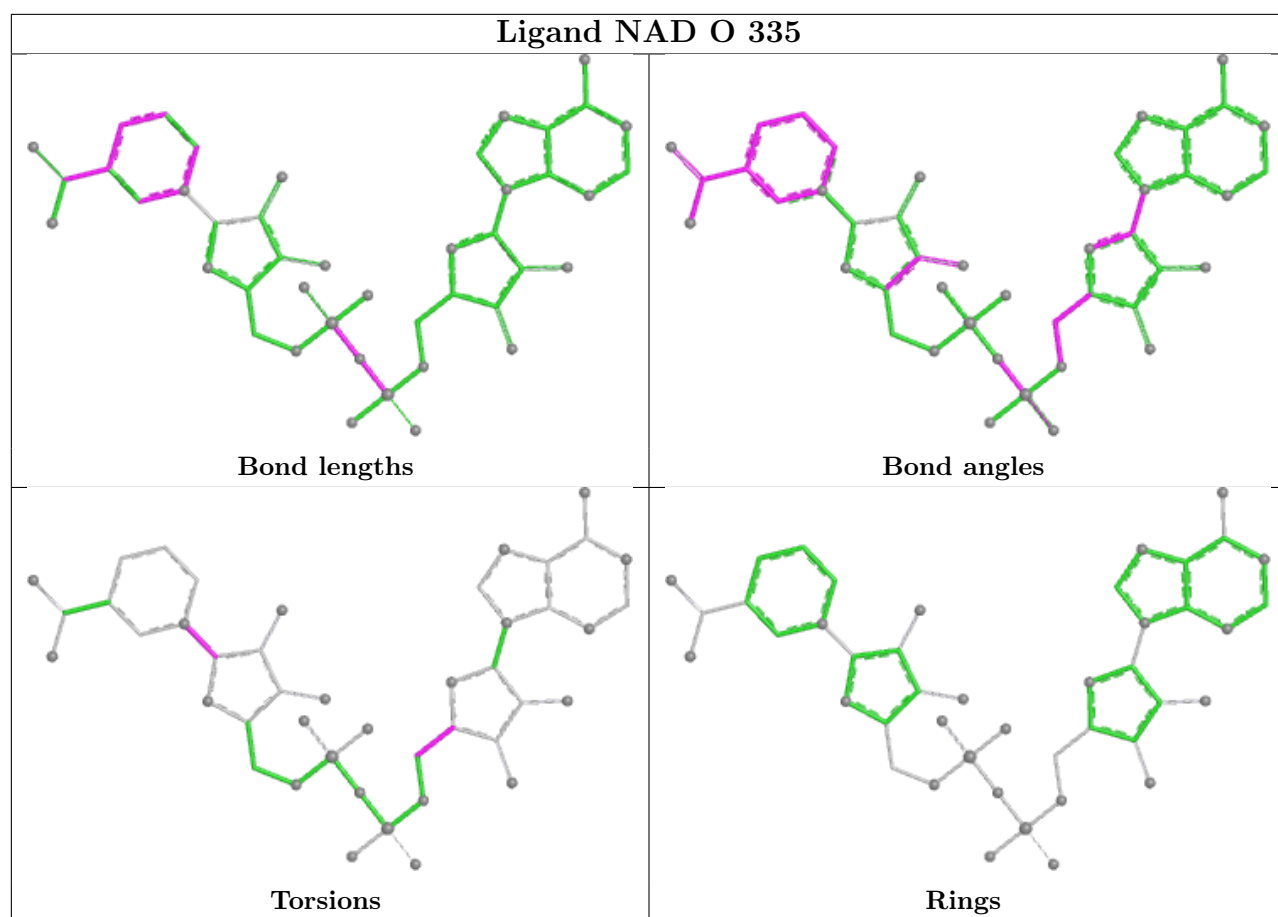
There are no ring outliers.

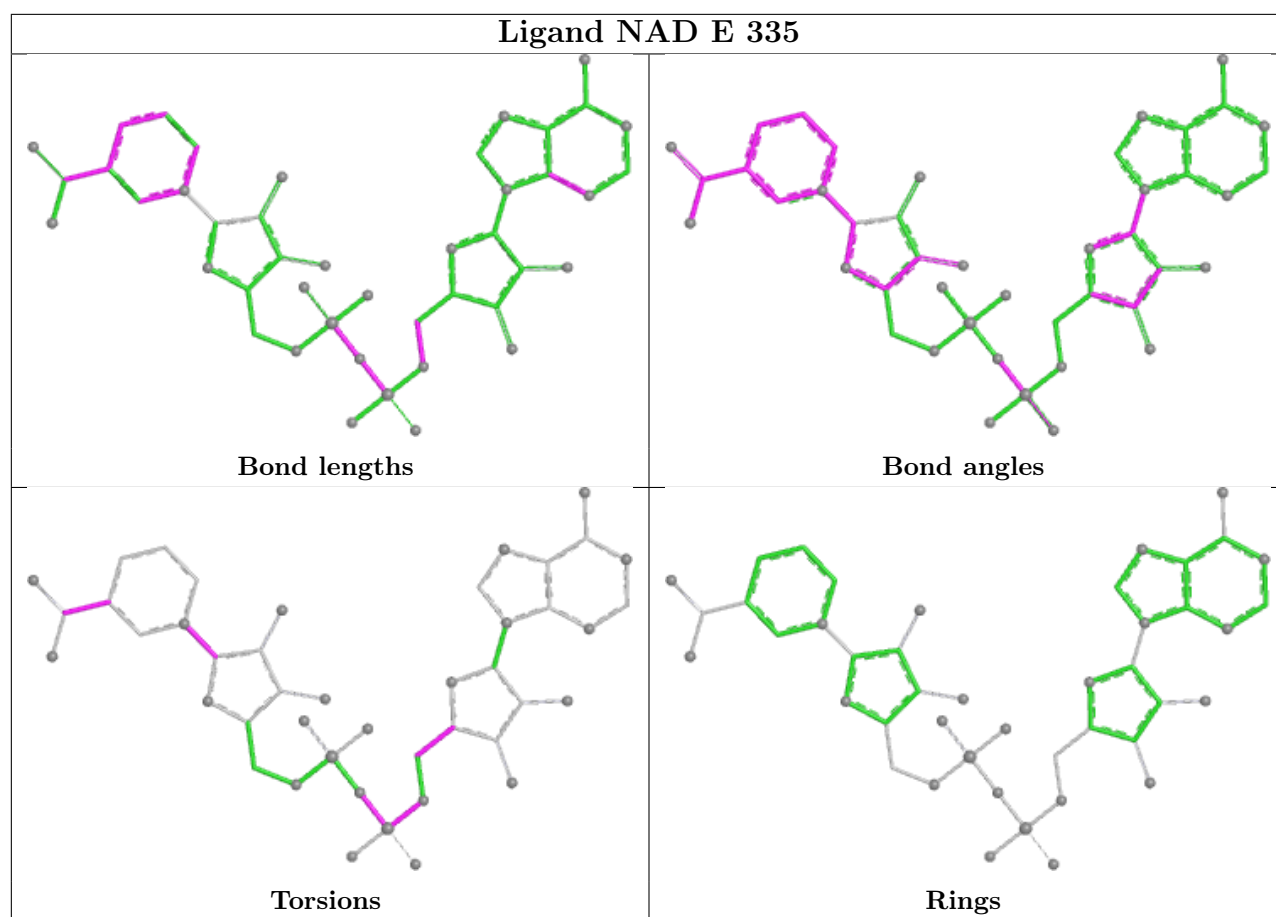
11 monomers are involved in 19 short contacts:

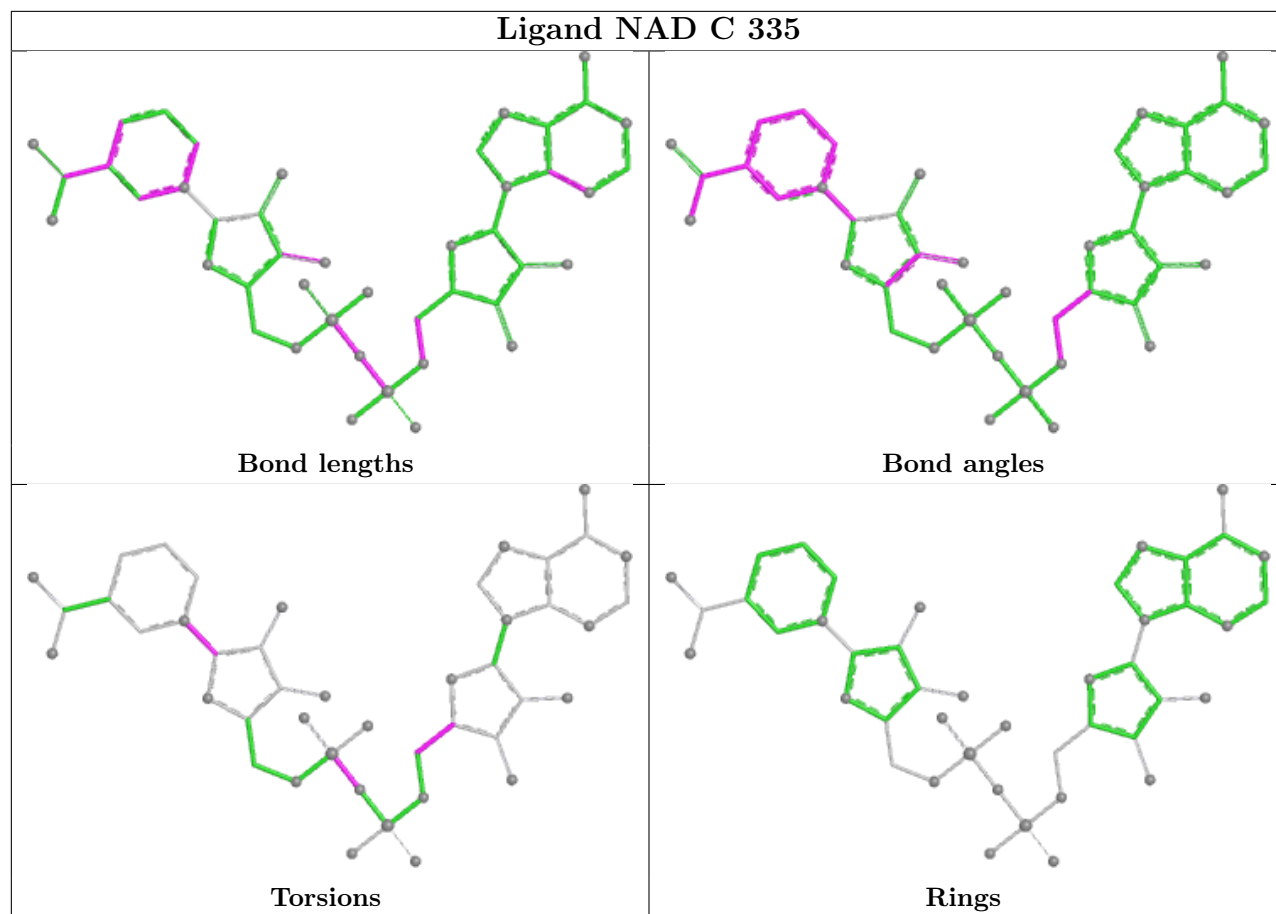
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	338	SO4	1	0
2	D	335	NAD	3	0
2	O	335	NAD	1	0
2	E	335	NAD	5	0
2	G	335	NAD	1	0
3	E	334	SO4	1	0
2	B	335	NAD	1	0
2	A	335	NAD	1	0
3	E	337	SO4	1	0
2	F	335	NAD	2	0
2	H	335	NAD	2	0

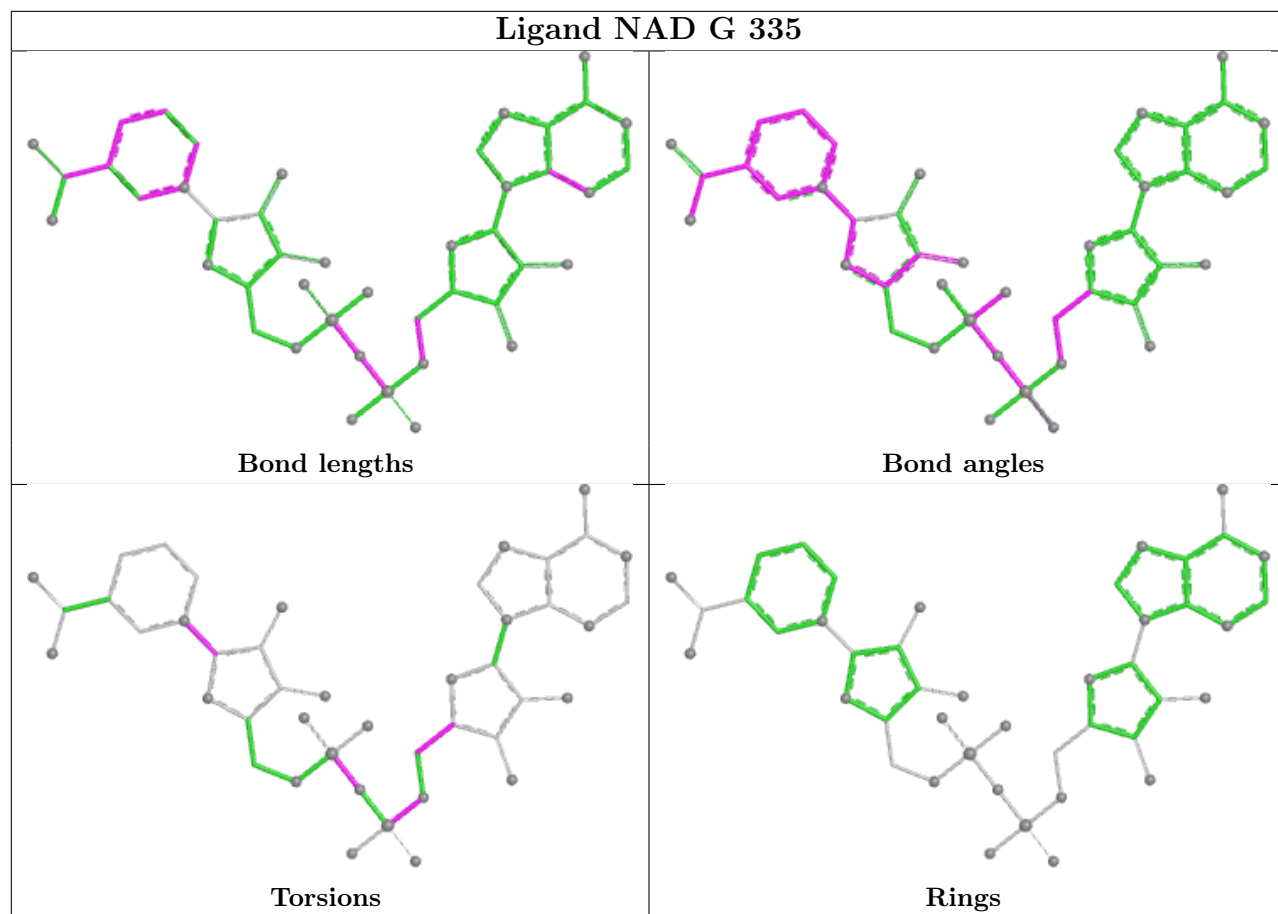
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

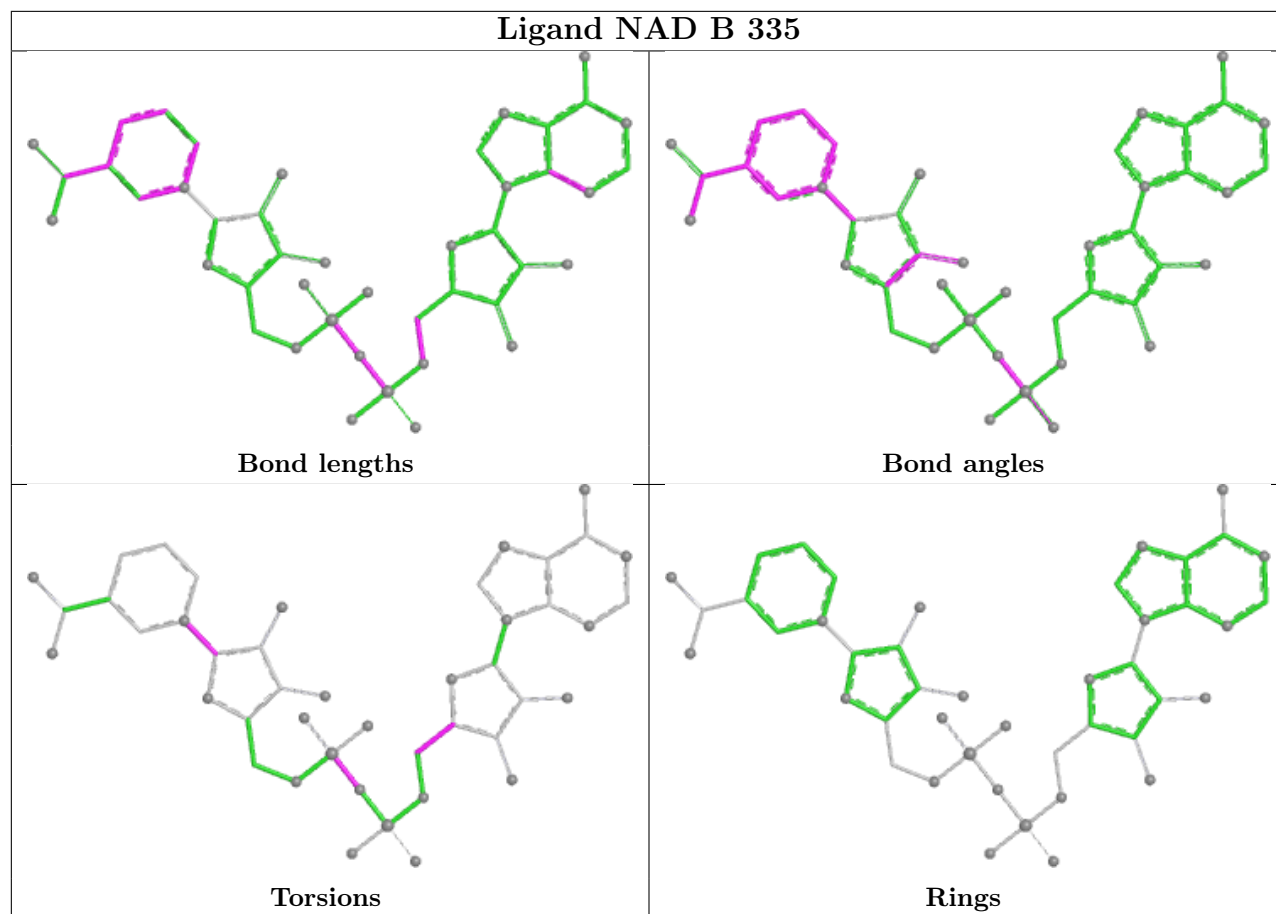


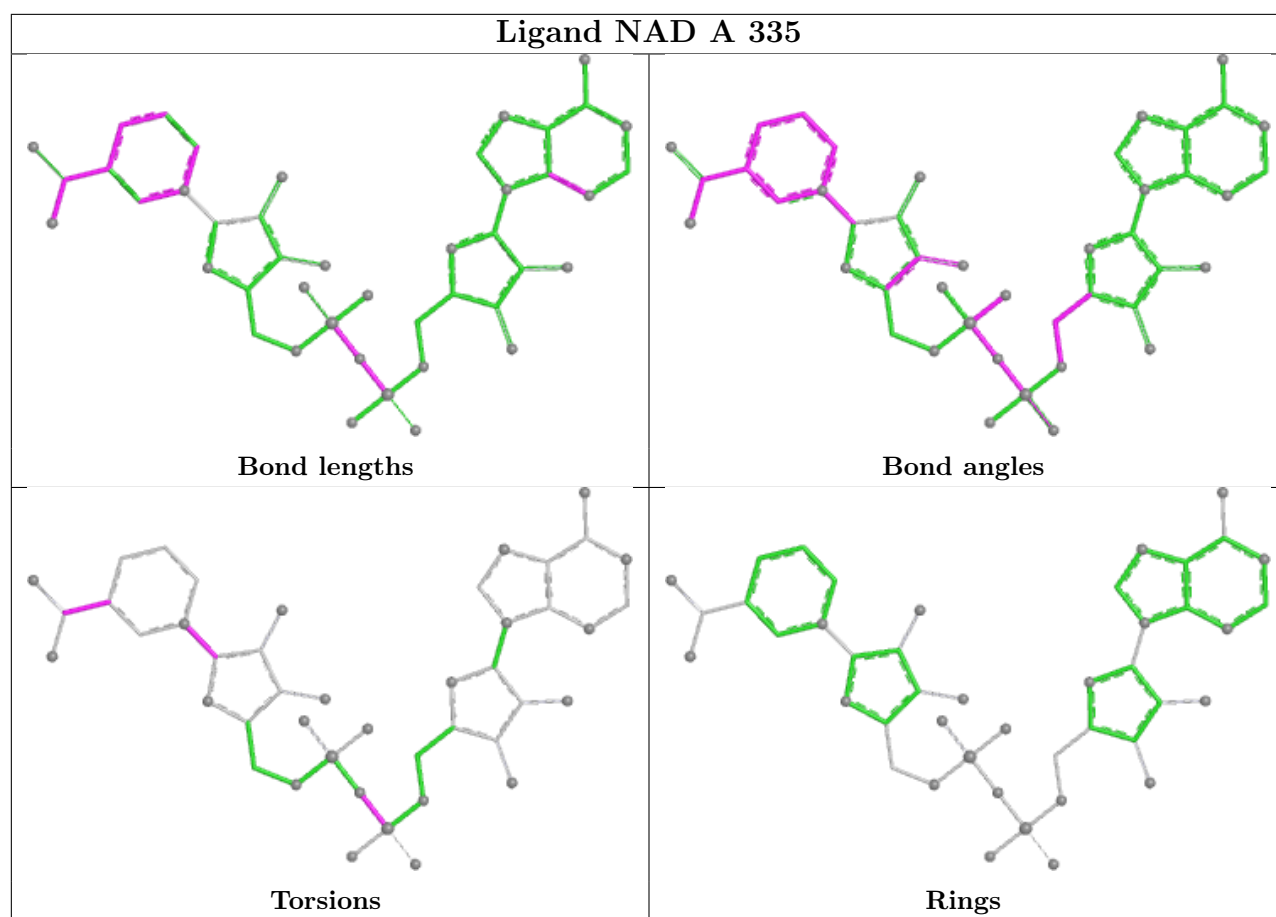


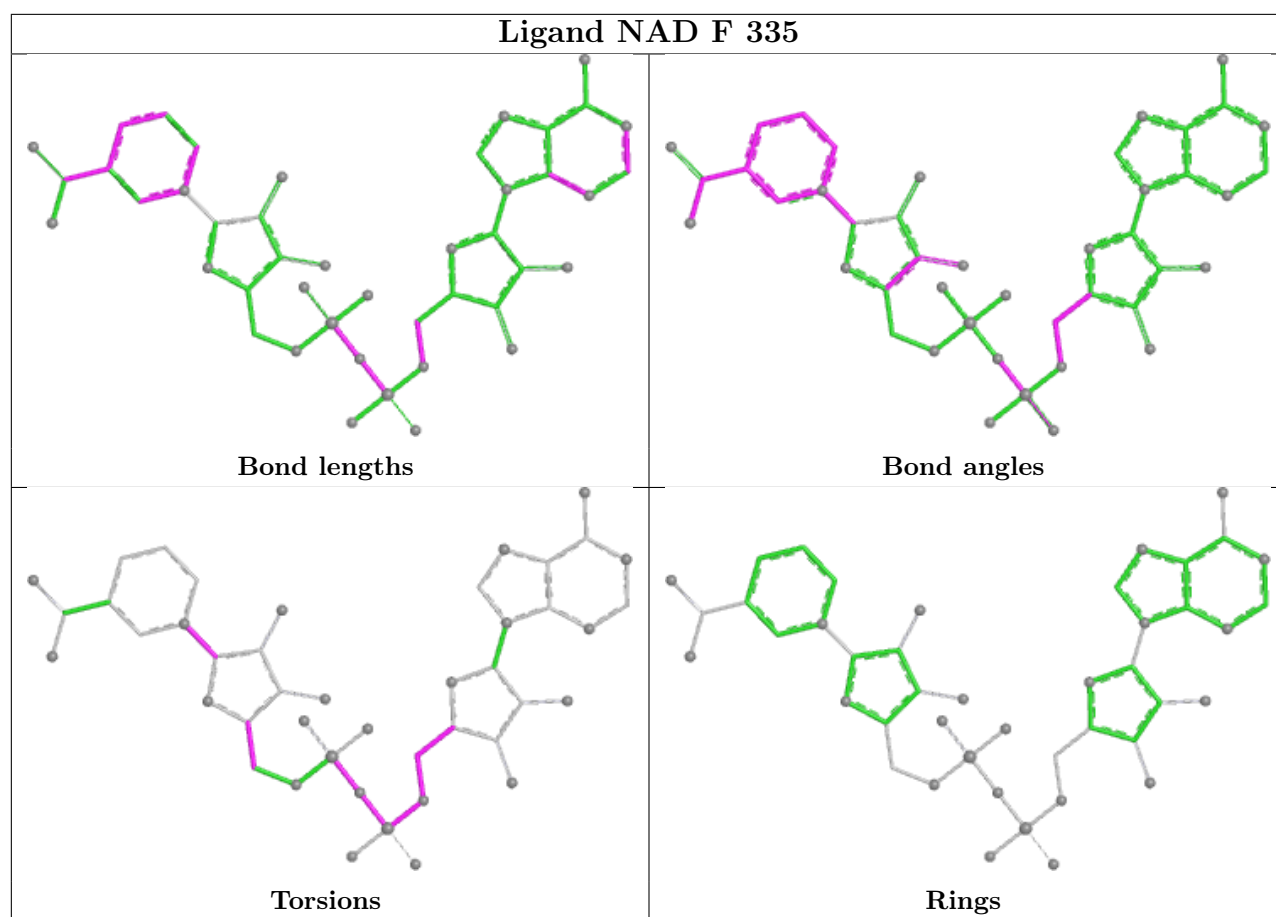


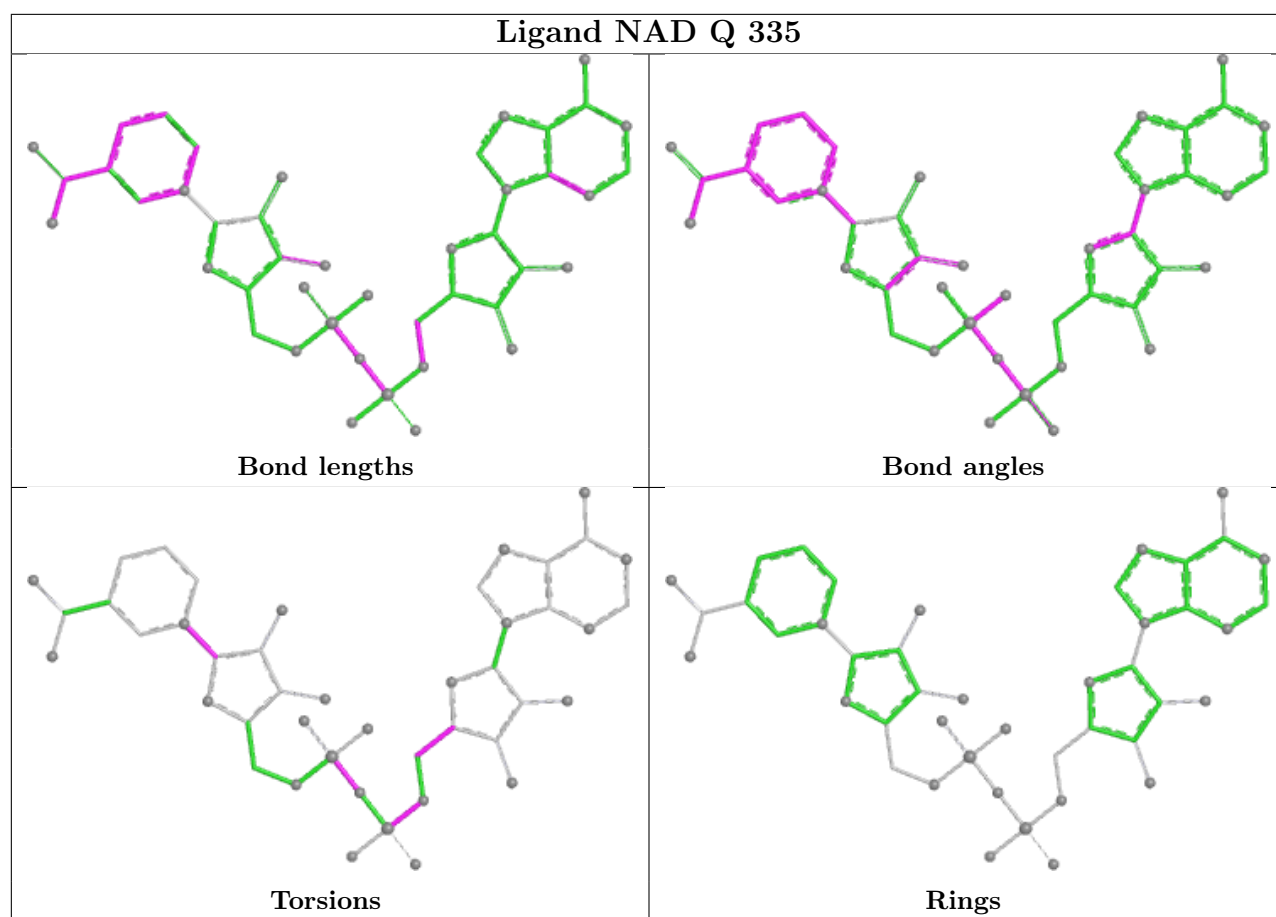


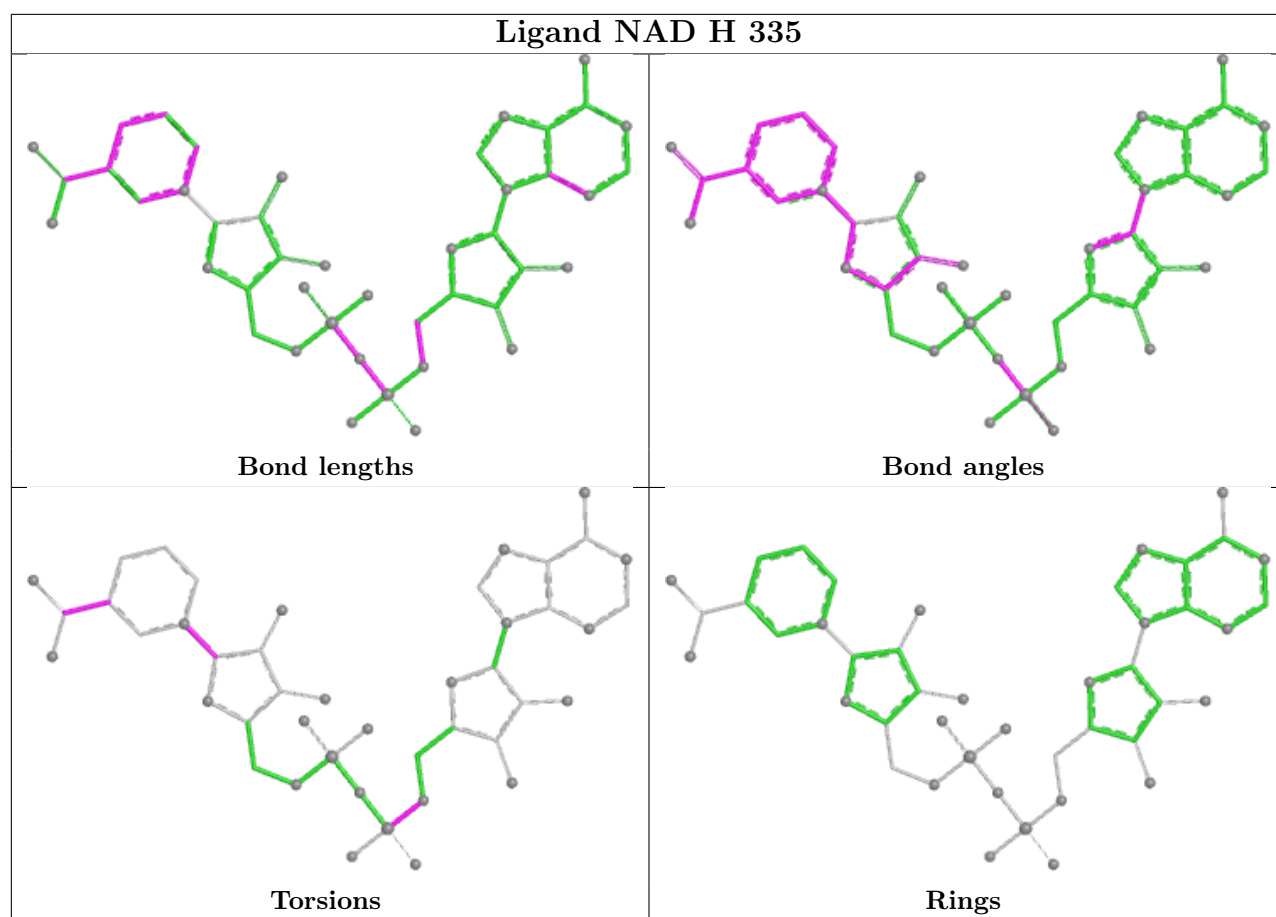












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	337/337 (100%)	-0.16	0 100 100	29, 42, 59, 80	0
1	B	337/337 (100%)	-0.04	1 (0%) 90 88	31, 46, 63, 71	0
1	C	337/337 (100%)	0.04	1 (0%) 90 88	31, 48, 69, 81	0
1	D	336/337 (99%)	0.49	7 (2%) 63 58	35, 62, 79, 96	0
1	E	336/337 (99%)	2.20	174 (51%) 0 0	55, 87, 108, 114	0
1	F	336/337 (99%)	1.56	99 (29%) 1 1	43, 88, 105, 113	0
1	G	336/337 (99%)	1.06	60 (17%) 3 3	34, 69, 91, 101	0
1	H	335/337 (99%)	1.14	48 (14%) 6 5	48, 83, 103, 114	0
1	O	337/337 (100%)	-0.39	0 100 100	19, 31, 45, 56	0
1	Q	336/337 (99%)	-0.12	0 100 100	21, 39, 58, 81	0
All	All	3363/3370 (99%)	0.58	390 (11%) 9 7	19, 56, 99, 114	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	116	VAL	6.4
1	E	228	ILE	6.2
1	E	187	ALA	5.8
1	E	271	LEU	5.8
1	E	270	ILE	5.6
1	E	117	ILE	5.3
1	E	267	LEU	5.1
1	E	324	LEU	4.7
1	E	244	VAL	4.7
1	E	29	ALA	4.7
1	E	255	VAL	4.7
1	F	130	VAL	4.6
1	E	44	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	93	ILE	4.5
1	E	193	LEU	4.5
1	E	118	ILE	4.4
1	F	329	ALA	4.4
1	E	87	LEU	4.4
1	E	225	LEU	4.4
1	E	92	VAL	4.3
1	E	143	ILE	4.3
1	F	214	VAL	4.3
1	E	308	ILE	4.3
1	F	119	THR	4.2
1	E	129	VAL	4.2
1	E	15	PHE	4.2
1	E	273	VAL	4.2
1	E	115	LYS	4.1
1	E	180	GLY	4.1
1	E	328	VAL	4.1
1	E	153	CYS	4.0
1	E	215	ALA	4.0
1	H	87	LEU	4.0
1	F	137	TYR	4.0
1	E	105	ALA	4.0
1	E	305	VAL	4.0
1	E	291	THR	3.9
1	E	155	ALA	3.9
1	E	325	ALA	3.9
1	E	246	VAL	3.9
1	E	292	ILE	3.9
1	F	146	ASN	3.8
1	E	91	ILE	3.8
1	G	308	ILE	3.8
1	F	27	ILE	3.8
1	F	155	ALA	3.8
1	F	25	LEU	3.8
1	E	30	ILE	3.7
1	E	160	VAL	3.7
1	E	216	LEU	3.7
1	E	52	ILE	3.7
1	E	24	PRO	3.7
1	E	310	TRP	3.7
1	E	263	ALA	3.7
1	E	321	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	258	ALA	3.6
1	E	258	ALA	3.6
1	E	48	SER	3.6
1	E	252	ALA	3.6
1	F	1	LEU	3.6
1	H	63	ALA	3.5
1	E	130	VAL	3.5
1	F	217	VAL	3.5
1	E	203	ILE	3.5
1	E	119	THR	3.5
1	E	309	ALA	3.5
1	F	131	GLY	3.4
1	F	216	LEU	3.4
1	G	296	LEU	3.4
1	E	144	ILE	3.4
1	E	154	LEU	3.4
1	E	158	VAL	3.4
1	F	324	LEU	3.4
1	G	273	VAL	3.4
1	F	225	LEU	3.3
1	E	18(A)	TRP	3.3
1	F	128	TYR	3.3
1	E	28	ILE	3.3
1	F	40	ALA	3.2
1	F	46	TYR	3.2
1	F	14	ASN	3.2
1	G	269	GLY	3.2
1	F	29	ALA	3.2
1	D	322	VAL	3.2
1	G	244	VAL	3.2
1	G	169	LYS	3.2
1	E	205	PRO	3.2
1	F	322	VAL	3.2
1	F	24	PRO	3.1
1	E	208	THR	3.1
1	G	292	ILE	3.1
1	E	3	VAL	3.1
1	E	217	VAL	3.1
1	E	259	PHE	3.1
1	F	8	PHE	3.1
1	F	48	SER	3.1
1	F	100	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	175	THR	3.1
1	G	171	THR	3.1
1	G	307	VAL	3.1
1	B	0(A)	ALA	3.1
1	G	167	ILE	3.1
1	E	142	PRO	3.0
1	E	27	ILE	3.0
1	F	74	VAL	3.0
1	G	251	PHE	3.0
1	F	52	ILE	3.0
1	E	204	VAL	3.0
1	F	328	VAL	3.0
1	G	130	VAL	3.0
1	H	332	TRP	3.0
1	F	87	LEU	3.0
1	H	62	THR	3.0
1	F	84	TRP	3.0
1	H	193	LEU	2.9
1	E	128	TYR	2.9
1	G	241	ASP	2.9
1	E	229	ALA	2.9
1	F	129	VAL	2.9
1	F	160	VAL	2.9
1	G	305	VAL	2.9
1	E	64	ILE	2.9
1	E	221	LEU	2.9
1	G	242	LEU	2.9
1	E	22	ASP	2.9
1	F	32	ASP	2.9
1	E	0(A)	ALA	2.9
1	E	213	ALA	2.9
1	F	15	PHE	2.9
1	E	161	LEU	2.8
1	G	309	ALA	2.8
1	E	157	PHE	2.8
1	E	218	LEU	2.8
1	F	242	LEU	2.8
1	E	251	PHE	2.8
1	H	139	HIS	2.8
1	H	52	ILE	2.8
1	F	31	ASN	2.8
1	E	25	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	104	GLY	2.8
1	E	53	PHE	2.8
1	G	246	VAL	2.8
1	E	327	ILE	2.8
1	E	262	SER	2.8
1	E	242	LEU	2.8
1	F	218	LEU	2.8
1	G	152	ASN	2.7
1	G	298	MET	2.7
1	E	283	PHE	2.7
1	E	307	VAL	2.7
1	E	145	SER	2.7
1	D	59	PRO	2.7
1	F	164	LYS	2.7
1	E	16	LEU	2.7
1	E	206	THR	2.7
1	E	156	PRO	2.7
1	G	245	GLN	2.7
1	F	274	CYS	2.7
1	G	271	LEU	2.7
1	E	316	GLY	2.7
1	F	223	GLY	2.7
1	E	84	TRP	2.7
1	E	240	VAL	2.7
1	E	250	THR	2.7
1	H	27	ILE	2.6
1	G	187	ALA	2.6
1	H	29	ALA	2.6
1	F	168	ILE	2.6
1	F	267	LEU	2.6
1	H	44	LEU	2.6
1	F	270	ILE	2.6
1	G	228	ILE	2.6
1	E	137	TYR	2.6
1	E	194	ARG	2.6
1	F	108	HIS	2.6
1	E	274	CYS	2.6
1	F	259	PHE	2.6
1	G	252	ALA	2.6
1	E	11	ILE	2.6
1	E	230	LEU	2.6
1	G	156	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	31	ASN	2.6
1	H	165	PHE	2.6
1	G	188	SER	2.5
1	H	84	TRP	2.5
1	H	186	ASP	2.5
1	E	139	HIS	2.5
1	E	60(A)	GLY	2.5
1	G	37	VAL	2.5
1	H	113	ALA	2.5
1	G	202	ASN	2.5
1	G	278	LEU	2.5
1	E	12	GLY	2.5
1	F	73	VAL	2.5
1	F	44	LEU	2.5
1	H	185	LEU	2.5
1	E	214	VAL	2.5
1	E	165	PHE	2.5
1	E	127	THR	2.5
1	E	151	THR	2.5
1	E	285	CYS	2.5
1	F	122(A)	LYS	2.5
1	E	284	ARG	2.5
1	G	293	ASP	2.5
1	E	131	GLY	2.5
1	E	299	VAL	2.5
1	G	160	VAL	2.5
1	H	57	VAL	2.5
1	H	130	VAL	2.5
1	E	40	ALA	2.5
1	G	165	PHE	2.5
1	H	105	ALA	2.5
1	E	306	LYS	2.4
1	E	1	LEU	2.4
1	F	5	ILE	2.4
1	E	170	GLY	2.4
1	G	229	ALA	2.4
1	H	134	ALA	2.4
1	E	102	ARG	2.4
1	H	1	LEU	2.4
1	H	110	GLU	2.4
1	E	21	LYS	2.4
1	E	74	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	37	VAL	2.4
1	H	92	VAL	2.4
1	E	49	THR	2.4
1	E	179	THR	2.4
1	F	28	ILE	2.4
1	G	230	LEU	2.4
1	H	184	LEU	2.4
1	G	247	SER	2.4
1	E	269	GLY	2.4
1	F	134	ALA	2.4
1	H	99	PHE	2.4
1	E	109	ILE	2.4
1	F	109	ILE	2.4
1	H	64	ILE	2.4
1	E	169	LYS	2.4
1	H	0	LYS	2.4
1	E	57	VAL	2.4
1	E	100	VAL	2.4
1	E	257	ALA	2.4
1	F	43	LEU	2.3
1	E	167	ILE	2.3
1	F	330	ASN	2.3
1	E	149	CYS	2.3
1	E	112	GLY	2.3
1	E	17	ARG	2.3
1	F	116	VAL	2.3
1	G	193	LEU	2.3
1	H	70	ILE	2.3
1	E	33	THR	2.3
1	E	264	GLU	2.3
1	F	107	LYS	2.3
1	E	239	VAL	2.3
1	H	37	VAL	2.3
1	H	187	ALA	2.3
1	H	28	ILE	2.3
1	F	42	HIS	2.3
1	G	175	THR	2.3
1	E	268	LYS	2.3
1	E	13	ARG	2.3
1	H	24	PRO	2.3
1	F	104	GLY	2.3
1	F	273	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	240	VAL	2.3
1	H	73	VAL	2.3
1	F	161	LEU	2.3
1	E	196	ALA	2.3
1	E	211	ALA	2.3
1	G	200	ALA	2.3
1	E	38	LYS	2.3
1	E	69	LYS	2.3
1	E	146	ASN	2.3
1	G	331	ASN	2.3
1	E	39	GLN	2.3
1	E	132	VAL	2.3
1	E	184	LEU	2.3
1	G	158	VAL	2.3
1	G	217	VAL	2.3
1	E	329	ALA	2.2
1	F	325	ALA	2.2
1	H	143	ILE	2.2
1	F	18(B)	HIS	2.2
1	G	306	LYS	2.2
1	G	174	THR	2.2
1	G	290	THR	2.2
1	F	19	GLY	2.2
1	E	70	ILE	2.2
1	F	169	LYS	2.2
1	G	259	PHE	2.2
1	H	263	ALA	2.2
1	E	171	THR	2.2
1	F	127	THR	2.2
1	D	128	TYR	2.2
1	E	231	ARG	2.2
1	E	323	ASP	2.2
1	F	7	GLY	2.2
1	G	287	ASP	2.2
1	G	267	LEU	2.2
1	H	25	LEU	2.2
1	E	37	VAL	2.2
1	E	66	VAL	2.2
1	F	89	ILE	2.2
1	F	139	HIS	2.2
1	E	297	THR	2.2
1	F	142	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	50	LEU	2.2
1	F	51	GLY	2.2
1	F	92	VAL	2.2
1	G	132	VAL	2.2
1	E	89	ILE	2.2
1	E	332	TRP	2.2
1	F	11	ILE	2.2
1	F	10	ARG	2.2
1	H	137	TYR	2.2
1	E	58	LYS	2.2
1	F	0	LYS	2.2
1	G	164	LYS	2.2
1	F	227	GLY	2.2
1	H	43	LEU	2.2
1	F	312	ASP	2.2
1	G	275	ASP	2.2
1	E	286	SER	2.2
1	F	30	ILE	2.2
1	G	270	ILE	2.2
1	G	157	PHE	2.2
1	F	315	TRP	2.1
1	E	36	GLY	2.1
1	E	188	SER	2.1
1	E	243	VAL	2.1
1	G	168	ILE	2.1
1	G	279	VAL	2.1
1	G	283	PHE	2.1
1	H	157	PHE	2.1
1	F	18(A)	TRP	2.1
1	H	59	PRO	2.1
1	F	288	PHE	2.1
1	F	211	ALA	2.1
1	G	257	ALA	2.1
1	E	20	ARG	2.1
1	E	121	PRO	2.1
1	H	201	LEU	2.1
1	E	152	ASN	2.1
1	G	330	ASN	2.1
1	F	36	GLY	2.1
1	H	180	GLY	2.1
1	F	321	VAL	2.1
1	H	109	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	116	VAL	2.1
1	E	134	ALA	2.1
1	H	60	SER	2.1
1	E	159	LYS	2.1
1	F	85	LYS	2.1
1	E	59	PRO	2.1
1	F	219	PRO	2.1
1	E	245	GLN	2.1
1	H	81	LEU	2.1
1	F	313	ASN	2.1
1	F	88	GLY	2.1
1	F	125	ILE	2.1
1	F	143	ILE	2.1
1	F	311	TYR	2.1
1	G	27	ILE	2.1
1	H	30	ILE	2.1
1	D	37	VAL	2.1
1	E	279	VAL	2.1
1	F	57	VAL	2.1
1	E	77	ARG	2.0
1	E	191	ARG	2.0
1	E	289	SER	2.0
1	F	39	GLN	2.0
1	E	76	ASN	2.0
1	F	226	ASN	2.0
1	E	209	GLY	2.0
1	H	7	GLY	2.0
1	C	0(A)	ALA	2.0
1	F	136	ALA	2.0
1	F	215	ALA	2.0
1	D	188	SER	2.0
1	E	177	SER	2.0
1	D	332	TRP	2.0
1	F	151	THR	2.0
1	G	304	MET	2.0
1	E	296	LEU	2.0
1	F	64	ILE	2.0
1	D	214	VAL	2.0
1	E	320	ARG	2.0
1	H	102	ARG	2.0
1	E	178	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	E	337	5/5	0.62	0.18	116,117,117,117	5
3	SO4	D	336	5/5	0.65	0.22	84,84,85,86	5
3	SO4	A	341	5/5	0.66	0.14	108,108,109,109	5
3	SO4	G	334	5/5	0.71	0.20	87,87,88,89	5
3	SO4	F	334	5/5	0.72	0.13	111,111,111,112	0
3	SO4	B	334	5/5	0.72	0.14	91,91,92,92	5
3	SO4	G	339	5/5	0.72	0.12	114,114,114,114	5
3	SO4	G	338	5/5	0.74	0.11	96,96,97,97	5
3	SO4	O	339	5/5	0.77	0.18	87,87,88,88	5
3	SO4	H	337	5/5	0.78	0.11	80,81,82,82	5
3	SO4	D	337	5/5	0.78	0.17	89,90,90,90	5
3	SO4	O	337	5/5	0.79	0.20	72,74,75,75	5
3	SO4	G	337	5/5	0.79	0.15	101,102,102,102	5
3	SO4	E	336	5/5	0.80	0.12	78,79,79,80	5
3	SO4	O	334	5/5	0.81	0.12	74,74,75,77	5
3	SO4	H	334	5/5	0.81	0.15	79,80,80,81	5
2	NAD	E	335	44/44	0.83	0.16	87,97,102,104	0
3	SO4	F	337	5/5	0.83	0.13	85,86,86,87	5
3	SO4	E	338	5/5	0.84	0.16	87,87,88,88	5
3	SO4	A	334	5/5	0.84	0.12	79,79,80,81	5
3	SO4	D	334	5/5	0.84	0.11	75,76,76,76	5
3	SO4	O	338	5/5	0.85	0.13	88,89,90,90	5
2	NAD	F	335	44/44	0.85	0.15	67,73,81,81	0
2	NAD	H	335	44/44	0.86	0.13	83,87,95,96	0
3	SO4	A	339	5/5	0.87	0.16	104,104,105,106	5
3	SO4	Q	334	5/5	0.88	0.15	73,75,75,75	5
3	SO4	Q	339	5/5	0.88	0.14	88,88,90,90	5

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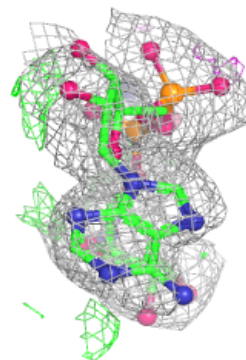
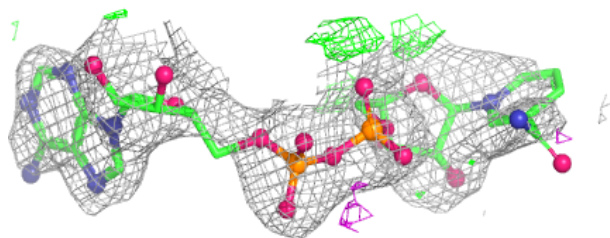
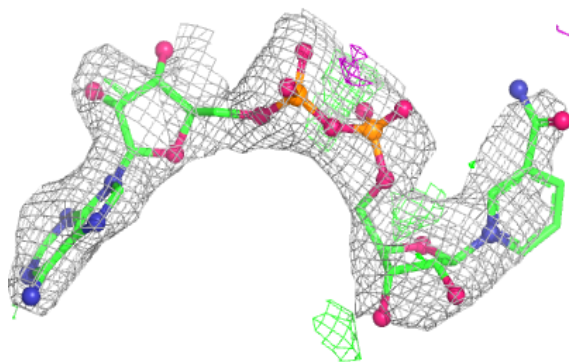
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	Q	336	5/5	0.89	0.11	69,71,72,72	0
3	SO4	B	338	5/5	0.89	0.08	75,75,76,76	5
3	SO4	O	340	5/5	0.89	0.13	68,68,69,70	5
3	SO4	E	334	5/5	0.90	0.09	60,60,61,62	5
3	SO4	G	336	5/5	0.90	0.11	67,68,68,69	5
3	SO4	B	339	5/5	0.90	0.11	69,70,71,71	5
3	SO4	B	336	5/5	0.90	0.10	52,53,53,53	5
3	SO4	C	338	5/5	0.91	0.11	62,63,64,65	5
3	SO4	H	336	5/5	0.91	0.10	77,77,78,78	5
3	SO4	C	334	5/5	0.91	0.09	79,80,80,80	5
3	SO4	F	336	5/5	0.91	0.10	56,56,59,59	5
3	SO4	C	336	5/5	0.92	0.12	67,67,68,68	0
3	SO4	Q	337	5/5	0.92	0.12	58,58,59,59	5
2	NAD	D	335	44/44	0.93	0.10	50,53,55,56	0
3	SO4	A	340	5/5	0.94	0.09	59,59,61,62	0
2	NAD	Q	335	44/44	0.94	0.08	41,48,50,51	0
3	SO4	O	336	5/5	0.94	0.08	60,62,63,63	0
2	NAD	G	335	44/44	0.94	0.09	43,47,51,52	0
3	SO4	A	338	5/5	0.94	0.07	55,56,57,58	5
2	NAD	C	335	44/44	0.94	0.09	40,45,50,51	0
3	SO4	A	337	5/5	0.95	0.07	64,65,66,68	0
3	SO4	B	337	5/5	0.95	0.07	59,60,61,61	5
2	NAD	B	335	44/44	0.95	0.08	36,44,50,51	0
3	SO4	A	336	5/5	0.96	0.10	50,50,52,52	0
3	SO4	Q	338	5/5	0.97	0.06	46,47,48,51	0
2	NAD	A	335	44/44	0.97	0.07	37,41,47,50	0
3	SO4	C	337	5/5	0.98	0.05	49,49,50,50	0
2	NAD	O	335	44/44	0.98	0.05	19,23,26,29	0

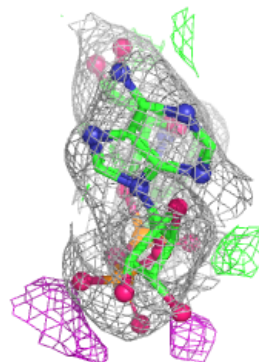
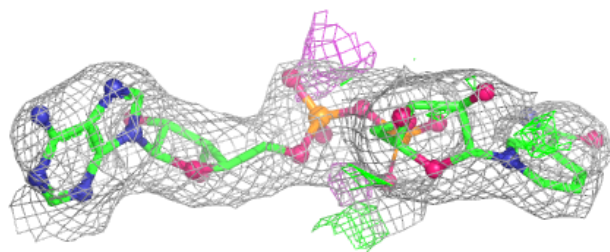
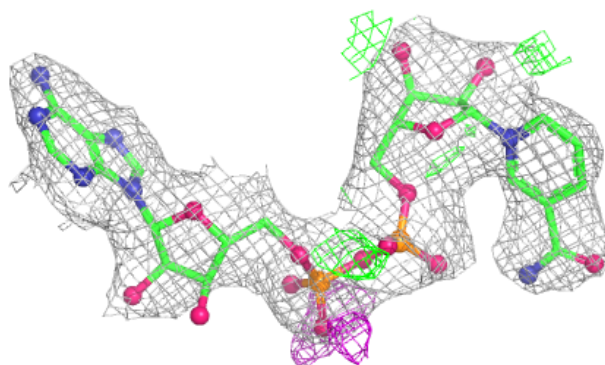
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD E 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

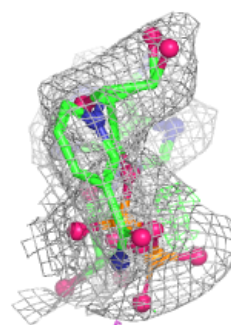
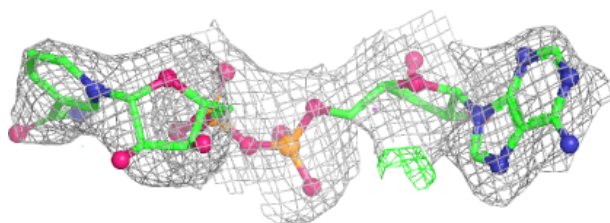
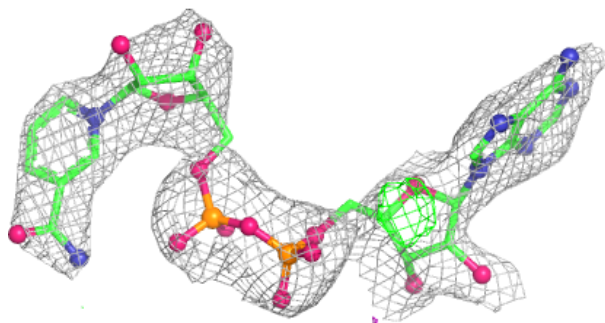
**Electron density around NAD F 335:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

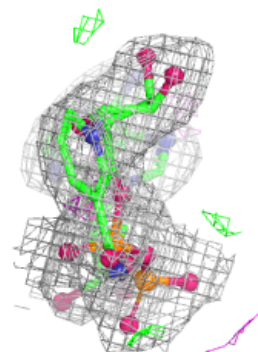
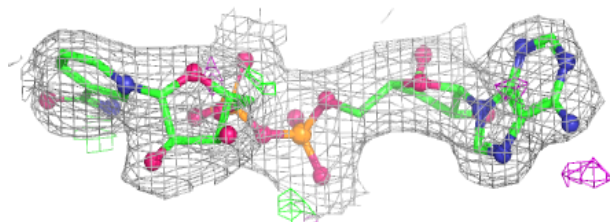
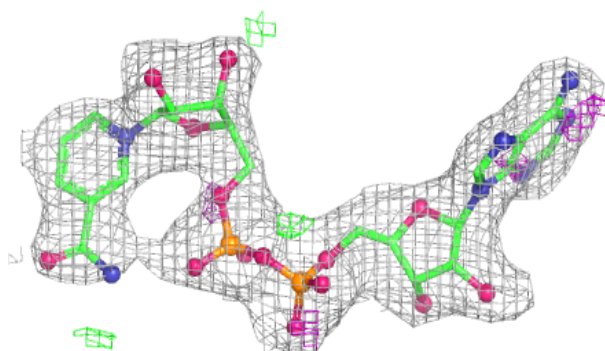


Electron density around NAD H 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

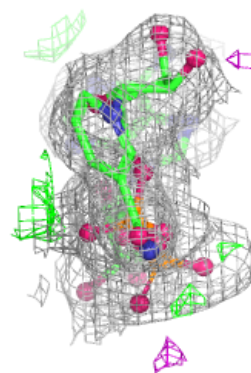
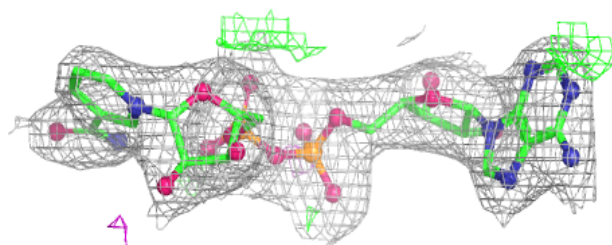
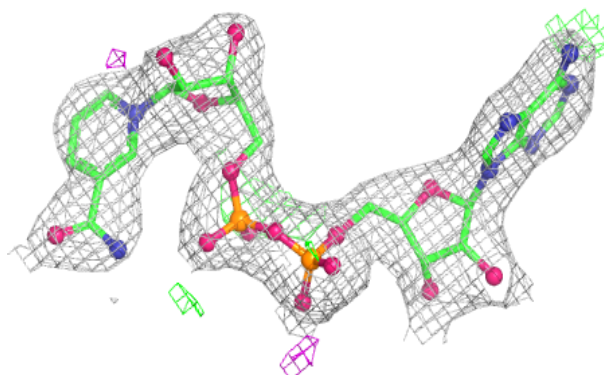
**Electron density around NAD D 335:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

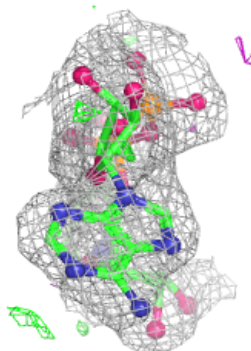
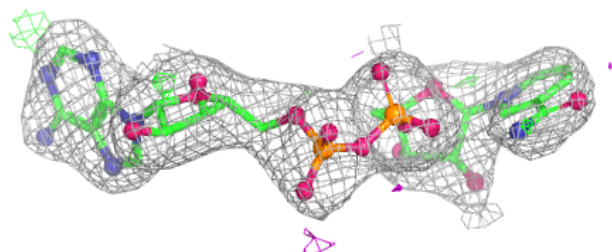
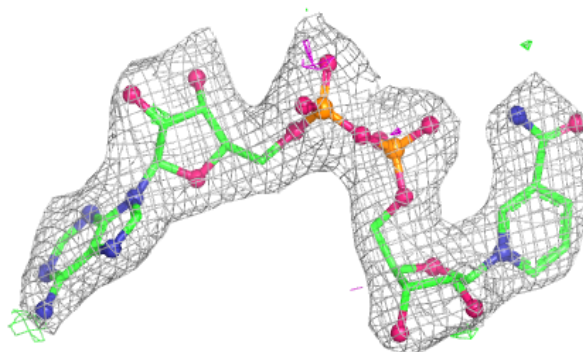


Electron density around NAD Q 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

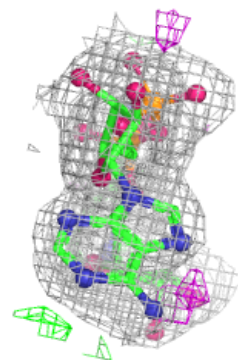
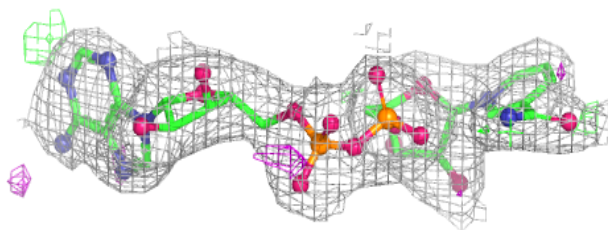
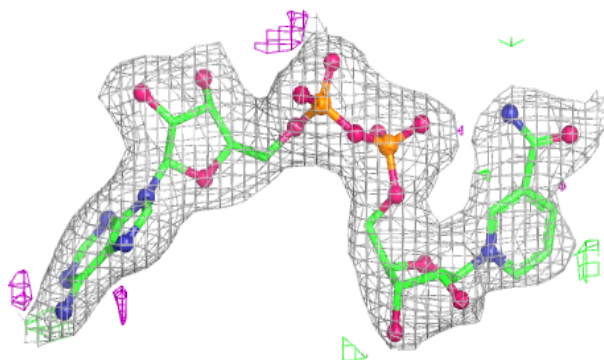
**Electron density around NAD G 335:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

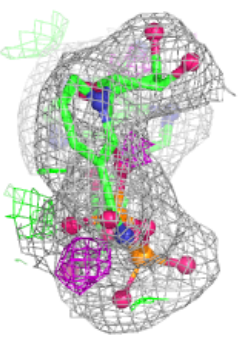
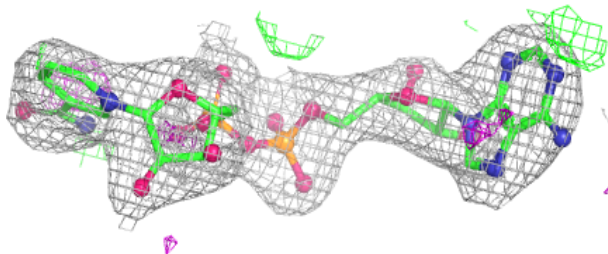
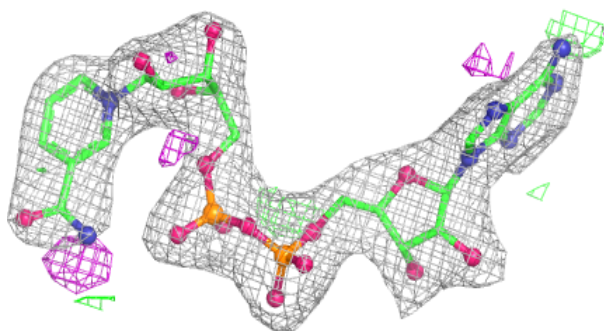


Electron density around NAD C 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

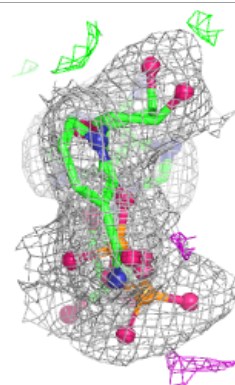
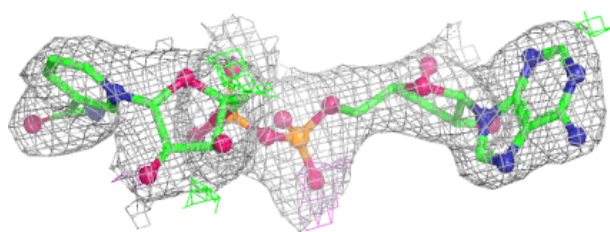
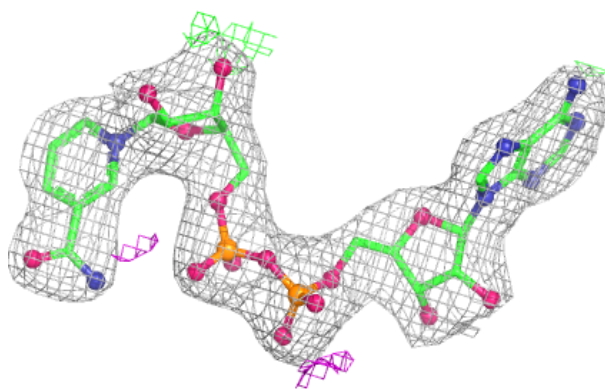
**Electron density around NAD B 335:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

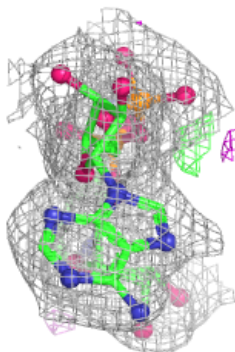
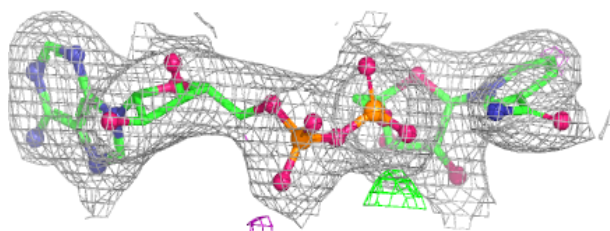
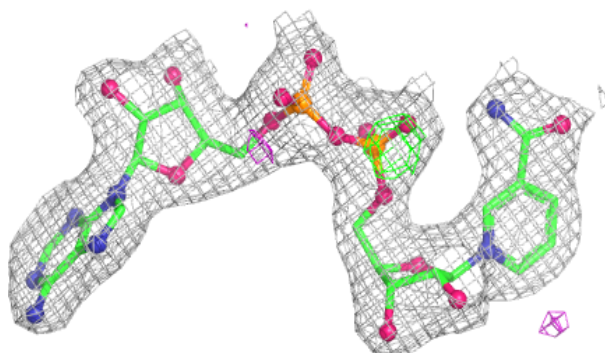


Electron density around NAD A 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD O 335:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.