



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:08 PM UTC

PDB ID : 2C9G / pdb_00002c9g
EMDB ID : EMD-1178
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON
BASE DODECAHEDRON
Authors : Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.;
Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.
Deposited on : 2005-12-12
Resolution : 9.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

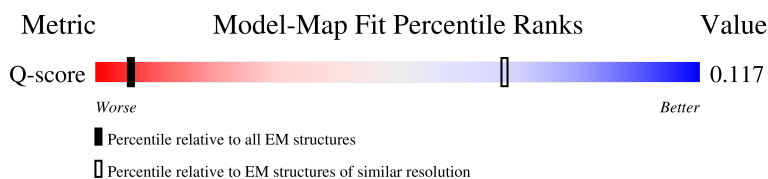
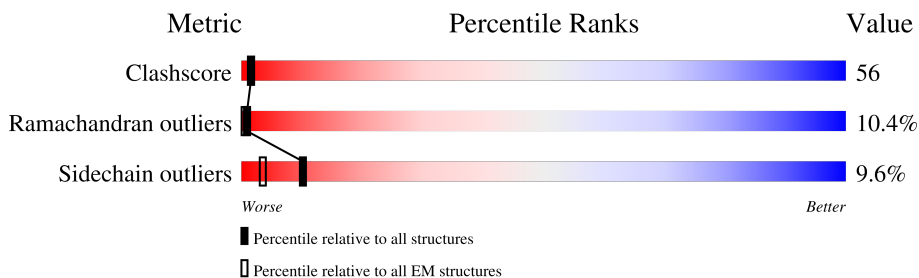
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	228 (8.80 - 9.80)

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

Mol	Chain	Length	Quality of chain
1	A	523	17% 26% 44% 14% • 14%
1	B	523	18% 26% 44% 15% • 14%
1	C	523	18% 26% 44% 15% • 14%
1	D	523	17% 26% 43% 15% • 14%

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Mol	Chain	Length	Quality of chain
1	E	523	18% 25% 44% 15% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

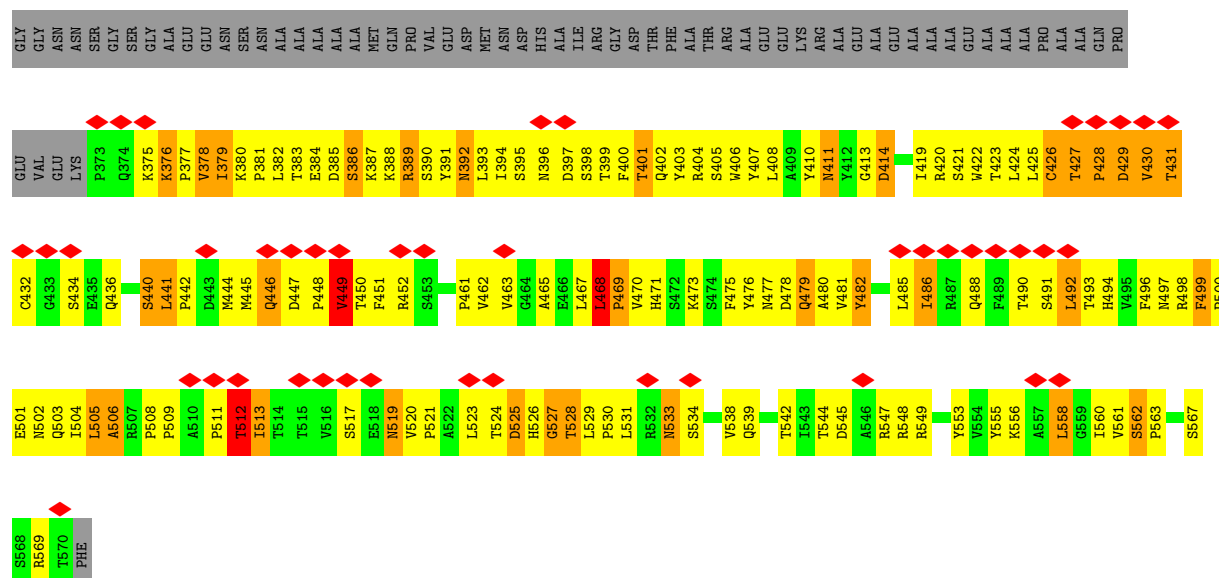
- Molecule 1 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	B	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	C	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	D	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	E	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		

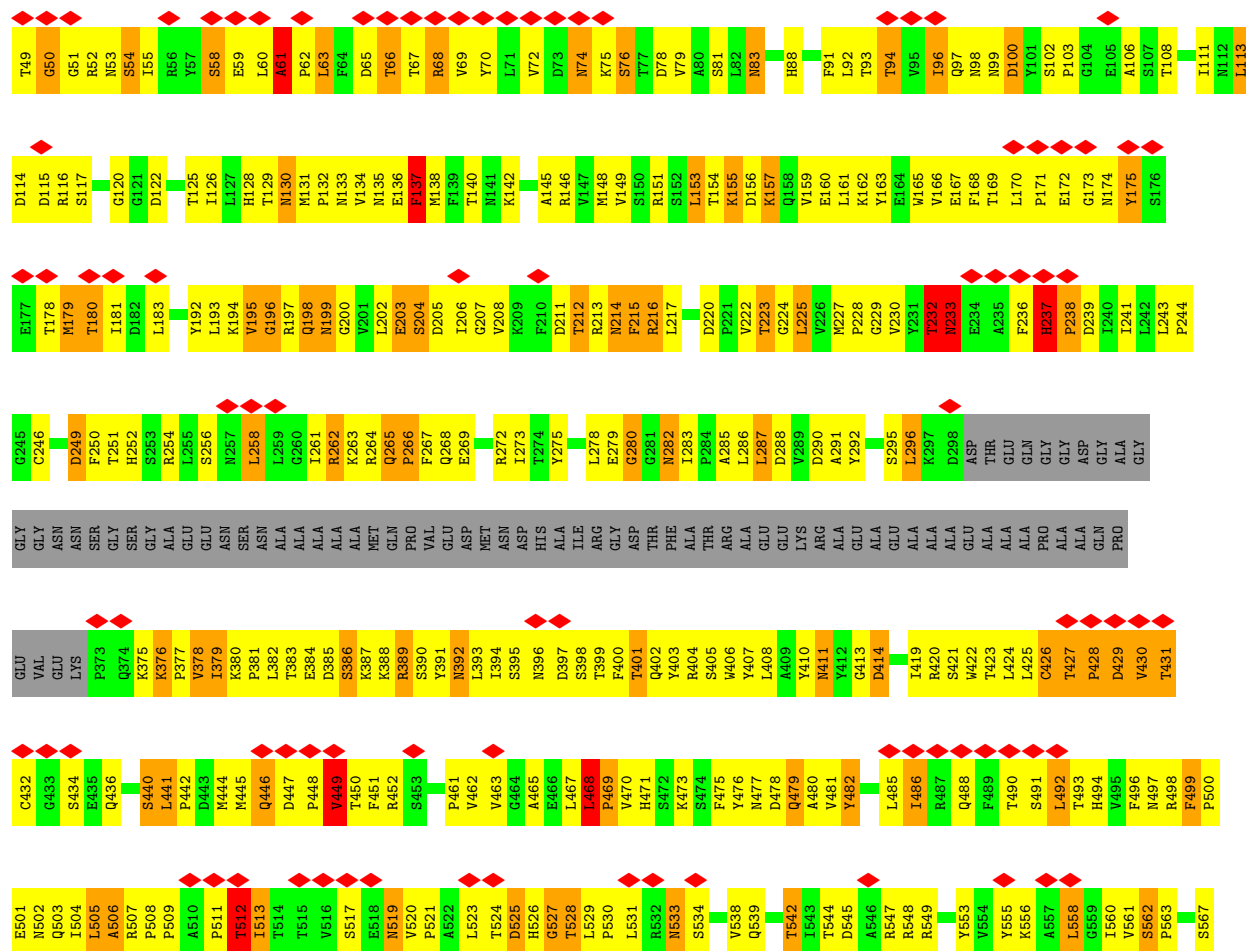


Government	Percentage
Current government	18%
Previous government	26%
Current government	44%
Previous government	15%
Current government	14%



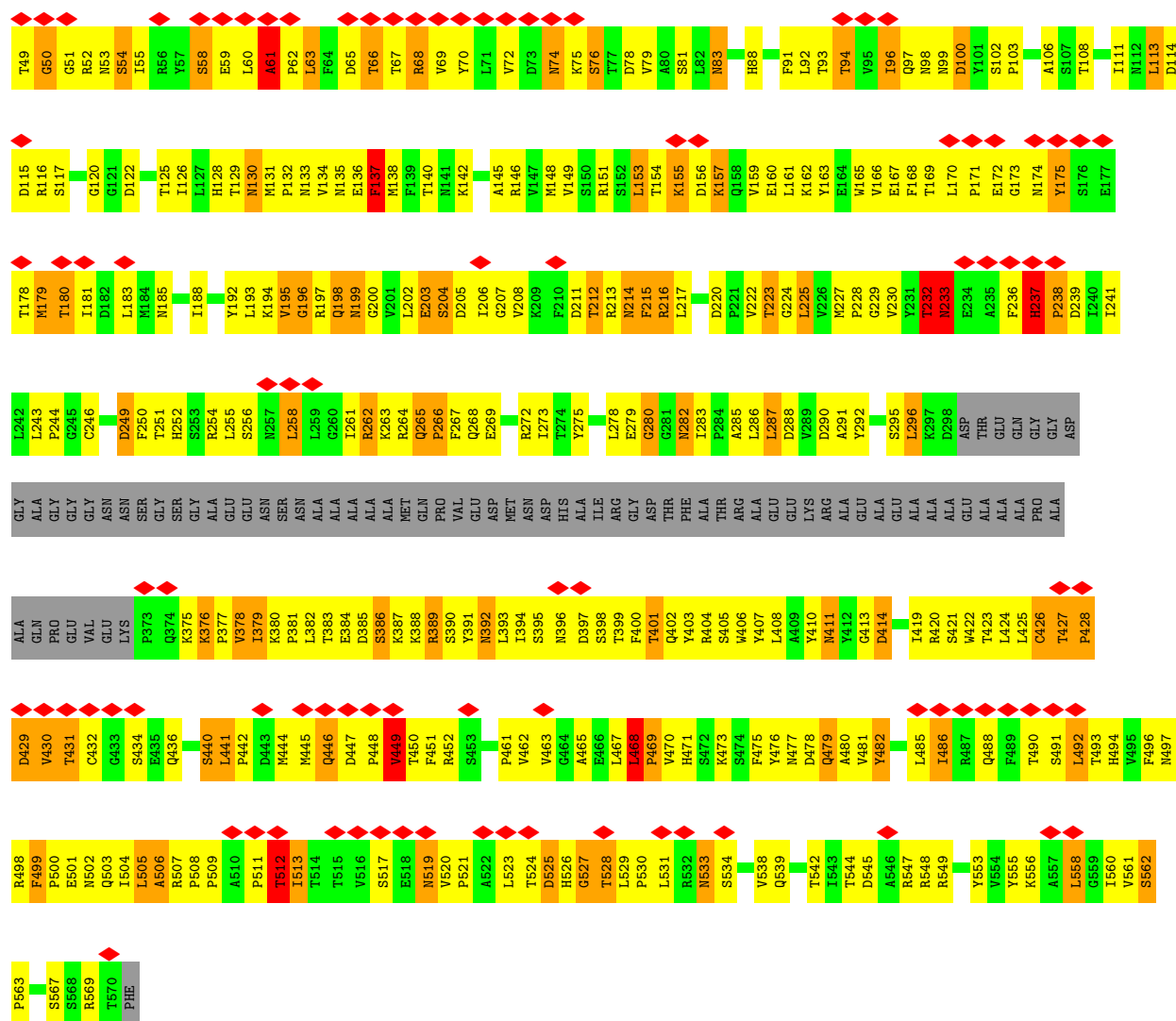


• Molecule 1: PENTON PROTEIN





• Molecule 1: PENTON PROTEIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1849	Depositor
Resolution determination method	Not provided	
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51020	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	509.000	Depositor
Minimum map value	-335.000	Depositor
Average map value	3.055	Depositor
Map value standard deviation	52.415	Depositor
Recommended contour level	91.9	Depositor
Map size ($\text{\AA}$)	382.23, 382.23, 382.23	wwPDB
Map dimensions	279, 279, 279	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.74	1/3652 (0.0%)	1.26	44/4971 (0.9%)
1	B	0.74	1/3652 (0.0%)	1.26	44/4971 (0.9%)
1	C	0.74	1/3652 (0.0%)	1.26	44/4971 (0.9%)
1	D	0.74	1/3652 (0.0%)	1.26	44/4971 (0.9%)
1	E	0.74	1/3652 (0.0%)	1.27	44/4971 (0.9%)
All	All	0.74	5/18260 (0.0%)	1.26	220/24855 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	ARG	C-N	-5.73	1.25	1.33
1	E	569	ARG	C-N	-5.73	1.25	1.33
1	C	569	ARG	C-N	-5.68	1.25	1.33
1	D	569	ARG	C-N	-5.68	1.25	1.33
1	B	569	ARG	C-N	-5.65	1.25	1.33

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	GLY	N-CA-C	12.01	127.14	112.73
1	D	207	GLY	N-CA-C	11.97	127.10	112.73
1	A	207	GLY	N-CA-C	11.94	127.06	112.73
1	C	207	GLY	N-CA-C	11.94	127.06	112.73
1	B	207	GLY	N-CA-C	11.94	127.06	112.73
1	B	265	GLN	CA-C-N	10.99	133.58	119.84
1	B	265	GLN	C-N-CA	10.99	133.58	119.84
1	C	265	GLN	CA-C-N	10.96	133.54	119.84
1	C	265	GLN	C-N-CA	10.96	133.54	119.84
1	E	265	GLN	CA-C-N	10.95	133.53	119.84
1	E	265	GLN	C-N-CA	10.95	133.53	119.84
1	A	265	GLN	CA-C-N	10.94	133.51	119.84
1	A	265	GLN	C-N-CA	10.94	133.51	119.84
1	D	265	GLN	CA-C-N	10.90	133.46	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	GLN	C-N-CA	10.90	133.46	119.84
1	D	468	LEU	CA-C-N	9.91	132.22	119.84
1	D	468	LEU	C-N-CA	9.91	132.22	119.84
1	E	468	LEU	CA-C-N	9.89	132.21	119.84
1	E	468	LEU	C-N-CA	9.89	132.21	119.84
1	A	468	LEU	CA-C-N	9.86	132.16	119.84
1	A	468	LEU	C-N-CA	9.86	132.16	119.84
1	C	468	LEU	CA-C-N	9.86	132.16	119.84
1	C	468	LEU	C-N-CA	9.86	132.16	119.84
1	B	468	LEU	CA-C-N	9.80	132.09	119.84
1	B	468	LEU	C-N-CA	9.80	132.09	119.84
1	B	441	LEU	CA-C-N	8.82	130.87	119.84
1	B	441	LEU	C-N-CA	8.82	130.87	119.84
1	A	441	LEU	CA-C-N	8.76	130.79	119.84
1	A	441	LEU	C-N-CA	8.76	130.79	119.84
1	C	441	LEU	CA-C-N	8.74	130.77	119.84
1	C	441	LEU	C-N-CA	8.74	130.77	119.84
1	E	441	LEU	CA-C-N	8.72	130.74	119.84
1	E	441	LEU	C-N-CA	8.72	130.74	119.84
1	D	441	LEU	CA-C-N	8.71	130.73	119.84
1	D	441	LEU	C-N-CA	8.71	130.73	119.84
1	A	396	ASN	N-CA-C	-8.56	103.00	113.19
1	D	396	ASN	N-CA-C	-8.54	103.03	113.19
1	E	396	ASN	N-CA-C	-8.53	103.04	113.19
1	B	396	ASN	N-CA-C	-8.52	103.06	113.19
1	C	396	ASN	N-CA-C	-8.50	103.08	113.19
1	D	61	ALA	CA-C-N	8.39	128.71	119.90
1	D	61	ALA	C-N-CA	8.39	128.71	119.90
1	A	61	ALA	CA-C-N	8.36	128.68	119.90
1	A	61	ALA	C-N-CA	8.36	128.68	119.90
1	B	61	ALA	CA-C-N	8.35	128.67	119.90
1	B	61	ALA	C-N-CA	8.35	128.67	119.90
1	C	61	ALA	CA-C-N	8.33	128.65	119.90
1	C	61	ALA	C-N-CA	8.33	128.65	119.90
1	E	61	ALA	CA-C-N	8.33	128.64	119.90
1	E	61	ALA	C-N-CA	8.33	128.64	119.90
1	A	76	SER	N-CA-C	8.05	120.77	111.11
1	D	76	SER	N-CA-C	8.04	120.76	111.11
1	E	76	SER	N-CA-C	8.04	120.76	111.11
1	C	76	SER	N-CA-C	8.03	120.74	111.11
1	B	76	SER	N-CA-C	7.98	120.69	111.11
1	A	376	LYS	CA-C-N	7.70	128.66	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	LYS	C-N-CA	7.70	128.66	120.12
1	B	376	LYS	CA-C-N	7.69	128.66	120.12
1	B	376	LYS	C-N-CA	7.69	128.66	120.12
1	E	376	LYS	CA-C-N	7.68	128.65	120.12
1	E	376	LYS	C-N-CA	7.68	128.65	120.12
1	D	376	LYS	CA-C-N	7.68	128.64	120.12
1	D	376	LYS	C-N-CA	7.68	128.64	120.12
1	C	376	LYS	CA-C-N	7.66	128.62	120.12
1	C	376	LYS	C-N-CA	7.66	128.62	120.12
1	D	103	PRO	N-CA-C	-7.55	103.28	113.40
1	A	103	PRO	N-CA-C	-7.53	103.31	113.40
1	B	103	PRO	N-CA-C	-7.52	103.33	113.40
1	C	103	PRO	N-CA-C	-7.52	103.32	113.40
1	E	103	PRO	N-CA-C	-7.51	103.34	113.40
1	D	488	GLN	N-CA-C	-7.40	104.06	113.23
1	A	488	GLN	N-CA-C	-7.38	104.08	113.23
1	A	427	THR	CA-C-N	7.37	129.05	119.84
1	A	427	THR	C-N-CA	7.37	129.05	119.84
1	B	488	GLN	N-CA-C	-7.37	104.09	113.23
1	E	488	GLN	N-CA-C	-7.36	104.10	113.23
1	B	427	THR	CA-C-N	7.36	129.03	119.84
1	B	427	THR	C-N-CA	7.36	129.03	119.84
1	E	427	THR	CA-C-N	7.35	129.02	119.84
1	E	427	THR	C-N-CA	7.35	129.02	119.84
1	D	427	THR	CA-C-N	7.34	129.02	119.84
1	D	427	THR	C-N-CA	7.34	129.02	119.84
1	C	488	GLN	N-CA-C	-7.34	104.13	113.23
1	C	427	THR	CA-C-N	7.34	129.01	119.84
1	C	427	THR	C-N-CA	7.34	129.01	119.84
1	C	447	ASP	CA-C-N	7.15	128.78	119.84
1	C	447	ASP	C-N-CA	7.15	128.78	119.84
1	B	447	ASP	CA-C-N	7.13	128.75	119.84
1	B	447	ASP	C-N-CA	7.13	128.75	119.84
1	D	447	ASP	CA-C-N	7.12	128.74	119.84
1	D	447	ASP	C-N-CA	7.12	128.74	119.84
1	A	447	ASP	CA-C-N	7.10	128.72	119.84
1	A	447	ASP	C-N-CA	7.10	128.72	119.84
1	E	447	ASP	CA-C-N	7.10	128.72	119.84
1	E	447	ASP	C-N-CA	7.10	128.72	119.84
1	D	512	THR	N-CA-C	-6.71	100.35	110.28
1	B	512	THR	N-CA-C	-6.68	100.39	110.28
1	A	512	THR	N-CA-C	-6.67	100.41	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	512	THR	N-CA-C	-6.66	100.42	110.28
1	C	512	THR	N-CA-C	-6.65	100.44	110.28
1	C	100	ASP	N-CA-C	6.52	121.25	113.16
1	A	100	ASP	N-CA-C	6.50	121.22	113.16
1	D	100	ASP	N-CA-C	6.47	121.18	113.16
1	B	100	ASP	N-CA-C	6.46	121.17	113.16
1	E	100	ASP	N-CA-C	6.45	121.16	113.16
1	A	81	SER	N-CA-C	6.38	121.25	112.90
1	E	81	SER	N-CA-C	6.38	121.25	112.90
1	C	81	SER	N-CA-C	6.37	121.25	112.90
1	B	81	SER	N-CA-C	6.36	121.23	112.90
1	D	81	SER	N-CA-C	6.34	121.21	112.90
1	B	63	LEU	N-CA-C	-6.17	99.34	109.40
1	A	63	LEU	N-CA-C	-6.16	99.36	109.40
1	D	63	LEU	N-CA-C	-6.12	99.42	109.40
1	C	63	LEU	N-CA-C	-6.11	99.44	109.40
1	E	63	LEU	N-CA-C	-6.09	99.47	109.40
1	B	113	LEU	N-CA-C	-6.00	101.39	110.28
1	A	113	LEU	N-CA-C	-6.00	101.41	110.28
1	E	113	LEU	N-CA-C	-6.00	101.41	110.28
1	D	113	LEU	N-CA-C	-5.98	101.43	110.28
1	C	558	LEU	CA-C-N	-5.93	117.61	121.65
1	C	558	LEU	C-N-CA	-5.93	117.61	121.65
1	E	558	LEU	CA-C-N	-5.91	117.63	121.65
1	E	558	LEU	C-N-CA	-5.91	117.63	121.65
1	B	558	LEU	CA-C-N	-5.88	117.65	121.65
1	B	558	LEU	C-N-CA	-5.88	117.65	121.65
1	C	94	THR	N-CA-C	-5.85	99.66	108.96
1	D	175	TYR	N-CA-C	5.85	118.77	109.65
1	B	175	TYR	N-CA-C	5.84	118.76	109.65
1	A	175	TYR	N-CA-C	5.83	118.75	109.65
1	B	94	THR	N-CA-C	-5.83	99.70	108.96
1	A	94	THR	N-CA-C	-5.82	99.71	108.96
1	B	505	LEU	N-CA-C	-5.82	106.22	113.15
1	E	505	LEU	N-CA-C	-5.82	106.22	113.15
1	D	558	LEU	CA-C-N	-5.81	117.70	121.65
1	D	558	LEU	C-N-CA	-5.81	117.70	121.65
1	D	94	THR	N-CA-C	-5.80	99.73	108.96
1	E	94	THR	N-CA-C	-5.80	99.73	108.96
1	D	505	LEU	N-CA-C	-5.80	106.25	113.15
1	E	175	TYR	N-CA-C	5.79	118.69	109.65
1	D	477	ASN	N-CA-C	5.79	117.73	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	TYR	N-CA-C	5.78	118.66	109.65
1	A	558	LEU	CA-C-N	-5.77	117.72	121.65
1	A	558	LEU	C-N-CA	-5.77	117.72	121.65
1	B	70	TYR	N-CA-C	5.77	118.31	108.90
1	B	477	ASN	N-CA-C	5.77	117.70	108.41
1	C	477	ASN	N-CA-C	5.75	117.67	108.41
1	A	505	LEU	N-CA-C	-5.75	106.31	113.15
1	C	505	LEU	N-CA-C	-5.75	106.31	113.15
1	D	70	TYR	N-CA-C	5.74	118.26	108.90
1	C	70	TYR	N-CA-C	5.74	118.26	108.90
1	E	477	ASN	N-CA-C	5.74	117.65	108.41
1	A	70	TYR	N-CA-C	5.73	118.24	108.90
1	A	477	ASN	N-CA-C	5.72	117.63	108.41
1	E	70	TYR	N-CA-C	5.72	118.22	108.90
1	D	282	ASN	N-CA-C	-5.59	100.56	109.96
1	E	282	ASN	N-CA-C	-5.59	100.57	109.96
1	C	113	LEU	N-CA-C	-5.59	101.37	110.20
1	B	282	ASN	N-CA-C	-5.57	100.61	109.96
1	C	282	ASN	N-CA-C	-5.56	100.61	109.96
1	A	282	ASN	N-CA-C	-5.54	100.65	109.96
1	B	55	ILE	N-CA-C	-5.51	99.21	107.37
1	D	55	ILE	N-CA-C	-5.50	99.23	107.37
1	E	55	ILE	N-CA-C	-5.48	99.25	107.37
1	C	55	ILE	N-CA-C	-5.48	99.26	107.37
1	A	55	ILE	N-CA-C	-5.45	99.30	107.37
1	C	237	HIS	CA-C-N	5.43	125.43	119.89
1	C	237	HIS	C-N-CA	5.43	125.43	119.89
1	E	426	CYS	N-CA-C	5.41	116.50	108.60
1	C	411	ASN	N-CA-C	5.41	119.04	112.23
1	A	237	HIS	CA-C-N	5.40	125.39	119.89
1	A	237	HIS	C-N-CA	5.40	125.39	119.89
1	C	137	PHE	N-CA-C	-5.38	99.35	110.80
1	E	137	PHE	N-CA-C	-5.38	99.35	110.80
1	B	137	PHE	N-CA-C	-5.37	99.36	110.80
1	C	426	CYS	N-CA-C	5.37	116.44	108.60
1	B	426	CYS	N-CA-C	5.37	116.44	108.60
1	A	426	CYS	N-CA-C	5.37	116.44	108.60
1	B	411	ASN	N-CA-C	5.37	118.99	112.23
1	B	237	HIS	CA-C-N	5.37	125.36	119.89
1	B	237	HIS	C-N-CA	5.37	125.36	119.89
1	A	137	PHE	N-CA-C	-5.35	99.40	110.80
1	D	411	ASN	N-CA-C	5.35	118.97	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ASN	N-CA-C	5.34	118.96	112.23
1	D	426	CYS	N-CA-C	5.33	116.39	108.60
1	D	137	PHE	N-CA-C	-5.32	99.46	110.80
1	E	411	ASN	N-CA-C	5.32	118.93	112.23
1	E	237	HIS	CA-C-N	5.32	125.31	119.89
1	E	237	HIS	C-N-CA	5.32	125.31	119.89
1	D	237	HIS	CA-C-N	5.28	125.28	119.89
1	D	237	HIS	C-N-CA	5.28	125.28	119.89
1	B	180	THR	N-CA-C	-5.21	105.24	111.03
1	E	180	THR	N-CA-C	-5.20	105.26	111.03
1	C	180	THR	N-CA-C	-5.20	105.26	111.03
1	E	225	LEU	N-CA-C	5.20	117.08	109.24
1	A	180	THR	N-CA-C	-5.19	105.27	111.03
1	E	96	ILE	CB-CA-C	-5.18	105.64	111.23
1	B	225	LEU	N-CA-C	5.18	117.06	109.24
1	C	96	ILE	CB-CA-C	-5.17	105.64	111.23
1	B	499	PHE	CA-C-N	5.14	126.27	119.84
1	B	499	PHE	C-N-CA	5.14	126.27	119.84
1	D	180	THR	N-CA-C	-5.14	105.32	111.03
1	D	225	LEU	N-CA-C	5.14	117.00	109.24
1	C	449	VAL	N-CA-C	5.14	120.03	109.34
1	A	225	LEU	N-CA-C	5.14	117.00	109.24
1	D	449	VAL	N-CA-C	5.13	120.02	109.34
1	A	449	VAL	N-CA-C	5.13	120.02	109.34
1	A	96	ILE	CB-CA-C	-5.13	105.69	111.23
1	C	225	LEU	N-CA-C	5.12	116.98	109.24
1	B	449	VAL	N-CA-C	5.12	119.99	109.34
1	E	449	VAL	N-CA-C	5.12	119.98	109.34
1	E	499	PHE	CA-C-N	5.10	126.21	119.84
1	E	499	PHE	C-N-CA	5.10	126.21	119.84
1	C	499	PHE	CA-C-N	5.09	126.21	119.84
1	C	499	PHE	C-N-CA	5.09	126.21	119.84
1	D	96	ILE	CB-CA-C	-5.09	105.73	111.23
1	A	499	PHE	CA-C-N	5.08	126.19	119.84
1	A	499	PHE	C-N-CA	5.08	126.19	119.84
1	B	96	ILE	CB-CA-C	-5.05	105.78	111.23
1	D	499	PHE	CA-C-N	5.03	126.13	119.84
1	D	499	PHE	C-N-CA	5.03	126.13	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	3568	0	3498	426	0
1	B	3568	0	3498	434	0
1	C	3568	0	3498	436	0
1	D	3568	0	3498	441	0
1	E	3568	0	3498	443	0
All	All	17840	0	17490	1980	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (1980) 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:B:452:ARG:HH21	1:C:99:ASN:HB3	1.14	1.13
1:C:452:ARG:HH21	1:D:99:ASN:HB3	1.14	1.11
1:D:452:ARG:HH21	1:E:99:ASN:HB3	1.14	1.10
1:A:99:ASN:HB3	1:E:452:ARG:HH21	1.14	1.07
1:A:452:ARG:HH21	1:B:99:ASN:HB3	1.14	1.06
1:D:68:ARG:HG2	1:D:68:ARG:HH11	1.25	1.02
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.25	1.01
1:E:68:ARG:HH11	1:E:68:ARG:HG2	1.25	0.99
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.25	0.98
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.25	0.97
1:D:444:MET:HE1	1:D:561:VAL:HG21	1.47	0.96
1:A:444:MET:HE1	1:A:561:VAL:HG21	1.47	0.96
1:E:444:MET:HE1	1:E:561:VAL:HG21	1.47	0.94
1:C:444:MET:HE1	1:C:561:VAL:HG21	1.47	0.94
1:B:444:MET:HE1	1:B:561:VAL:HG21	1.47	0.93
1:C:452:ARG:NH2	1:D:99:ASN:HB3	1.86	0.91
1:B:278:LEU:HD23	1:B:419:ILE:HD12	1.53	0.91
1:A:99:ASN:HB3	1:E:452:ARG:NH2	1.86	0.91
1:A:278:LEU:HD23	1:A:419:ILE:HD12	1.53	0.91
1:B:292:TYR:HA	1:B:377:PRO:CG	2.01	0.90
1:C:292:TYR:HA	1:C:377:PRO:CG	2.01	0.90
1:A:452:ARG:NH2	1:B:99:ASN:HB3	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LEU:HD23	1:E:419:ILE:HD12	1.53	0.90
1:D:292:TYR:HA	1:D:377:PRO:CG	2.02	0.90
1:E:292:TYR:HA	1:E:377:PRO:CG	2.01	0.90
1:B:452:ARG:NH2	1:C:99:ASN:HB3	1.86	0.90
1:B:295:SER:HB3	1:B:377:PRO:HG3	1.51	0.90
1:C:376:LYS:HB3	1:C:377:PRO:HD2	1.55	0.89
1:D:451:PHE:HD2	1:D:461:PRO:HA	1.38	0.89
1:B:68:ARG:HH12	1:B:562:SER:HB3	1.38	0.89
1:C:295:SER:HB3	1:C:377:PRO:HG3	1.51	0.89
1:D:452:ARG:NH2	1:E:99:ASN:HB3	1.86	0.89
1:B:376:LYS:HB3	1:B:377:PRO:HD2	1.55	0.89
1:D:68:ARG:HH12	1:D:562:SER:HB3	1.38	0.89
1:D:295:SER:HB3	1:D:377:PRO:HG3	1.51	0.89
1:D:376:LYS:HB3	1:D:377:PRO:HD2	1.54	0.89
1:C:451:PHE:HD2	1:C:461:PRO:HA	1.38	0.89
1:D:278:LEU:HD23	1:D:419:ILE:HD12	1.53	0.89
1:A:295:SER:HB3	1:A:377:PRO:HG3	1.51	0.89
1:E:295:SER:HB3	1:E:377:PRO:HG3	1.50	0.88
1:A:451:PHE:HD2	1:A:461:PRO:HA	1.38	0.88
1:C:278:LEU:HD23	1:C:419:ILE:HD12	1.53	0.88
1:A:292:TYR:HA	1:A:377:PRO:CG	2.02	0.88
1:A:68:ARG:HH12	1:A:562:SER:HB3	1.38	0.88
1:E:376:LYS:HB3	1:E:377:PRO:HD2	1.55	0.88
1:E:451:PHE:HD2	1:E:461:PRO:HA	1.38	0.88
1:A:376:LYS:HB3	1:A:377:PRO:HD2	1.54	0.87
1:C:68:ARG:HH12	1:C:562:SER:HB3	1.38	0.87
1:E:68:ARG:HH12	1:E:562:SER:HB3	1.38	0.87
1:B:211:ASP:HA	1:B:508:PRO:CG	2.05	0.87
1:B:262:ARG:NH1	1:C:130:ASN:HD22	1.73	0.87
1:A:52:ARG:HB3	1:A:117:SER:OG	1.75	0.86
1:A:130:ASN:HD22	1:E:262:ARG:NH1	1.73	0.86
1:D:83:ASN:HD22	1:D:91:PHE:HB2	1.40	0.86
1:D:504:ILE:HG22	1:D:505:LEU:HD23	1.57	0.86
1:E:52:ARG:HB3	1:E:117:SER:OG	1.75	0.86
1:B:504:ILE:HG22	1:B:505:LEU:HD23	1.57	0.86
1:C:211:ASP:HA	1:C:508:PRO:CG	2.05	0.86
1:E:211:ASP:HA	1:E:508:PRO:CG	2.05	0.86
1:E:504:ILE:HG22	1:E:505:LEU:HD23	1.57	0.86
1:D:262:ARG:NH1	1:E:130:ASN:HD22	1.73	0.86
1:B:451:PHE:HD2	1:B:461:PRO:HA	1.38	0.85
1:A:83:ASN:HD22	1:A:91:PHE:HB2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:HA	1:A:508:PRO:CG	2.05	0.85
1:A:262:ARG:NH1	1:B:130:ASN:HD22	1.74	0.85
1:C:52:ARG:HB3	1:C:117:SER:OG	1.75	0.85
1:D:211:ASP:HA	1:D:508:PRO:CG	2.05	0.85
1:B:193:LEU:HD11	1:B:498:ARG:HH12	1.41	0.85
1:C:58:SER:O	1:C:60:LEU:N	2.09	0.85
1:B:52:ARG:HB3	1:B:117:SER:OG	1.75	0.85
1:C:262:ARG:NH1	1:D:130:ASN:HD22	1.73	0.85
1:B:58:SER:O	1:B:60:LEU:N	2.09	0.85
1:B:83:ASN:HD22	1:B:91:PHE:HB2	1.40	0.85
1:C:504:ILE:HG22	1:C:505:LEU:HD23	1.57	0.85
1:E:83:ASN:HD22	1:E:91:PHE:HB2	1.40	0.85
1:A:504:ILE:HG22	1:A:505:LEU:HD23	1.58	0.84
1:C:83:ASN:HD22	1:C:91:PHE:HB2	1.40	0.84
1:D:52:ARG:HB3	1:D:117:SER:OG	1.75	0.84
1:E:58:SER:O	1:E:60:LEU:N	2.09	0.84
1:D:178:THR:HG21	1:D:511:PRO:HD2	1.60	0.84
1:D:58:SER:O	1:D:60:LEU:N	2.09	0.84
1:E:156:ASP:O	1:E:157:LYS:HG3	1.78	0.84
1:A:214:ASN:C	1:A:214:ASN:HD22	1.86	0.84
1:D:193:LEU:HD11	1:D:498:ARG:HH12	1.41	0.84
1:C:178:THR:HG21	1:C:511:PRO:HD2	1.60	0.84
1:A:58:SER:O	1:A:60:LEU:N	2.09	0.84
1:A:193:LEU:HD11	1:A:498:ARG:HH12	1.41	0.83
1:C:193:LEU:HD11	1:C:498:ARG:HH12	1.41	0.83
1:D:214:ASN:C	1:D:214:ASN:HD22	1.86	0.83
1:A:156:ASP:O	1:A:157:LYS:HG3	1.78	0.83
1:C:156:ASP:O	1:C:157:LYS:HG3	1.78	0.83
1:D:468:LEU:HD12	1:D:469:PRO:HD2	1.59	0.83
1:C:49:THR:HG23	1:C:53:ASN:OD1	1.79	0.83
1:B:178:THR:HG21	1:B:511:PRO:HD2	1.59	0.83
1:B:214:ASN:C	1:B:214:ASN:HD22	1.86	0.83
1:D:156:ASP:O	1:D:157:LYS:HG3	1.78	0.83
1:E:193:LEU:HD11	1:E:498:ARG:HH12	1.41	0.83
1:E:49:THR:HG23	1:E:53:ASN:OD1	1.79	0.83
1:E:214:ASN:C	1:E:214:ASN:HD22	1.86	0.83
1:E:178:THR:HG21	1:E:511:PRO:HD2	1.60	0.82
1:B:156:ASP:O	1:B:157:LYS:HG3	1.78	0.82
1:E:468:LEU:HD12	1:E:469:PRO:HD2	1.59	0.82
1:D:49:THR:HG23	1:D:53:ASN:OD1	1.79	0.82
1:B:49:THR:HG23	1:B:53:ASN:OD1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:HG23	1:A:53:ASN:OD1	1.79	0.82
1:C:468:LEU:HD12	1:C:469:PRO:HD2	1.60	0.82
1:D:544:THR:CG2	1:D:548:ARG:HA	2.10	0.82
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.60	0.82
1:C:214:ASN:HD22	1:C:214:ASN:C	1.86	0.82
1:A:178:THR:HG21	1:A:511:PRO:HD2	1.60	0.81
1:A:384:GLU:HG2	1:A:390:SER:HA	1.62	0.81
1:A:468:LEU:HD12	1:A:469:PRO:HD2	1.59	0.81
1:B:544:THR:CG2	1:B:548:ARG:HA	2.10	0.81
1:C:544:THR:CG2	1:C:548:ARG:HA	2.10	0.81
1:C:68:ARG:HG2	1:C:68:ARG:NH1	1.92	0.81
1:A:544:THR:CG2	1:A:548:ARG:HA	2.10	0.81
1:B:384:GLU:HG2	1:B:390:SER:HA	1.62	0.80
1:E:544:THR:CG2	1:E:548:ARG:HA	2.10	0.80
1:C:384:GLU:HG2	1:C:390:SER:HA	1.62	0.80
1:B:68:ARG:HG2	1:B:68:ARG:NH1	1.92	0.80
1:E:384:GLU:HG2	1:E:390:SER:HA	1.62	0.80
1:B:74:ASN:ND2	1:B:556:LYS:HZ1	1.79	0.79
1:C:237:HIS:CD2	1:C:425:LEU:HD11	2.18	0.79
1:D:389:ARG:HD3	1:D:502:ASN:HD22	1.47	0.79
1:A:68:ARG:HG2	1:A:68:ARG:NH1	1.92	0.79
1:D:237:HIS:CD2	1:D:425:LEU:HD11	2.18	0.79
1:E:237:HIS:CD2	1:E:425:LEU:HD11	2.18	0.79
1:B:237:HIS:CD2	1:B:425:LEU:HD11	2.17	0.79
1:D:384:GLU:HG2	1:D:390:SER:HA	1.62	0.79
1:C:74:ASN:ND2	1:C:556:LYS:HZ1	1.81	0.78
1:A:237:HIS:CD2	1:A:425:LEU:HD11	2.18	0.78
1:C:249:ASP:C	1:C:249:ASP:OD1	2.26	0.78
1:D:249:ASP:C	1:D:249:ASP:OD1	2.26	0.78
1:A:249:ASP:C	1:A:249:ASP:OD1	2.26	0.78
1:B:389:ARG:HD3	1:B:502:ASN:HD22	1.47	0.78
1:A:154:THR:OG1	1:A:160:GLU:HB2	1.84	0.77
1:B:249:ASP:C	1:B:249:ASP:OD1	2.27	0.77
1:E:154:THR:OG1	1:E:160:GLU:HB2	1.84	0.77
1:B:154:THR:OG1	1:B:160:GLU:HB2	1.84	0.77
1:C:379:ILE:O	1:C:381:PRO:HD3	1.85	0.77
1:E:389:ARG:HD3	1:E:502:ASN:HD22	1.47	0.77
1:A:379:ILE:O	1:A:381:PRO:HD3	1.85	0.77
1:D:154:THR:OG1	1:D:160:GLU:HB2	1.84	0.77
1:E:249:ASP:C	1:E:249:ASP:OD1	2.26	0.77
1:A:389:ARG:HD3	1:A:502:ASN:HD22	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ARG:HD3	1:C:502:ASN:HD22	1.47	0.77
1:B:211:ASP:HA	1:B:508:PRO:HG3	1.67	0.77
1:C:154:THR:OG1	1:C:160:GLU:HB2	1.84	0.77
1:C:211:ASP:HA	1:C:508:PRO:HG3	1.67	0.77
1:A:403:TYR:CE1	1:A:504:ILE:HG21	2.21	0.76
1:C:403:TYR:CE1	1:C:504:ILE:HG21	2.21	0.76
1:D:292:TYR:HA	1:D:377:PRO:HG2	1.67	0.76
1:D:403:TYR:CE1	1:D:504:ILE:HG21	2.21	0.76
1:E:379:ILE:O	1:E:381:PRO:HD3	1.85	0.76
1:A:211:ASP:HA	1:A:508:PRO:HG3	1.67	0.76
1:B:403:TYR:CE1	1:B:504:ILE:HG21	2.21	0.76
1:B:379:ILE:O	1:B:381:PRO:HD3	1.85	0.76
1:C:292:TYR:HA	1:C:377:PRO:HG2	1.67	0.76
1:D:74:ASN:ND2	1:D:556:LYS:HZ1	1.84	0.76
1:E:292:TYR:HA	1:E:377:PRO:HG2	1.67	0.76
1:C:475:PHE:O	1:C:513:ILE:HA	1.87	0.76
1:B:292:TYR:HA	1:B:377:PRO:HG2	1.67	0.75
1:D:379:ILE:O	1:D:381:PRO:HD3	1.85	0.75
1:E:403:TYR:CE1	1:E:504:ILE:HG21	2.21	0.75
1:A:74:ASN:ND2	1:A:556:LYS:HZ1	1.84	0.75
1:C:68:ARG:NH1	1:C:562:SER:HB3	2.01	0.75
1:B:475:PHE:O	1:B:513:ILE:HA	1.87	0.75
1:D:452:ARG:HE	1:E:98:ASN:HD21	1.34	0.75
1:B:451:PHE:CD2	1:B:461:PRO:HA	2.22	0.75
1:D:211:ASP:HA	1:D:508:PRO:HG3	1.67	0.75
1:E:475:PHE:O	1:E:513:ILE:HA	1.87	0.75
1:A:68:ARG:NH1	1:A:562:SER:HB3	2.01	0.75
1:E:211:ASP:HA	1:E:508:PRO:HG3	1.67	0.75
1:D:68:ARG:NH1	1:D:562:SER:HB3	2.01	0.74
1:D:451:PHE:CD2	1:D:461:PRO:HA	2.22	0.74
1:E:68:ARG:NH1	1:E:562:SER:HB3	2.01	0.74
1:A:292:TYR:HA	1:A:377:PRO:HG2	1.67	0.74
1:B:68:ARG:NH1	1:B:562:SER:HB3	2.01	0.74
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.53	0.74
1:C:295:SER:O	1:C:296:LEU:HB2	1.88	0.74
1:C:451:PHE:CD2	1:C:461:PRO:HA	2.22	0.74
1:E:68:ARG:HG2	1:E:68:ARG:NH1	1.92	0.74
1:E:403:TYR:HD1	1:E:504:ILE:HD13	1.52	0.74
1:A:403:TYR:HD1	1:A:504:ILE:HD13	1.52	0.74
1:A:475:PHE:O	1:A:513:ILE:HA	1.87	0.74
1:C:142:LYS:HG2	1:C:169:THR:HG22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:PHE:O	1:D:513:ILE:HA	1.86	0.74
1:B:295:SER:O	1:B:296:LEU:HB2	1.88	0.74
1:E:295:SER:O	1:E:296:LEU:HB2	1.88	0.74
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.53	0.74
1:D:142:LYS:HG2	1:D:169:THR:HG22	1.70	0.74
1:B:452:ARG:HE	1:C:98:ASN:HD21	1.34	0.73
1:B:243:LEU:HD21	1:B:403:TYR:CE2	2.23	0.73
1:D:68:ARG:HG2	1:D:68:ARG:NH1	1.92	0.73
1:E:451:PHE:CD2	1:E:461:PRO:HA	2.22	0.73
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.53	0.73
1:B:403:TYR:HD1	1:B:504:ILE:HD13	1.52	0.73
1:D:243:LEU:HD21	1:D:403:TYR:CE2	2.24	0.73
1:A:452:ARG:HE	1:B:98:ASN:HD21	1.34	0.73
1:B:441:LEU:HD12	1:B:445:MET:HE2	1.71	0.73
1:C:403:TYR:HD1	1:C:504:ILE:HD13	1.52	0.73
1:C:452:ARG:HE	1:D:98:ASN:HD21	1.34	0.73
1:D:468:LEU:CD1	1:D:469:PRO:HD2	2.19	0.73
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.70	0.73
1:A:295:SER:O	1:A:296:LEU:HB2	1.88	0.73
1:C:243:LEU:HD21	1:C:403:TYR:CE2	2.23	0.73
1:E:441:LEU:HD12	1:E:445:MET:HE2	1.71	0.73
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.24	0.73
1:D:295:SER:O	1:D:296:LEU:HB2	1.88	0.73
1:D:403:TYR:HD1	1:D:504:ILE:HD13	1.52	0.73
1:E:148:MET:HA	1:E:163:TYR:HD2	1.54	0.73
1:A:98:ASN:HD21	1:E:452:ARG:HE	1.34	0.72
1:D:244:PRO:HA	1:D:275:TYR:CD2	2.24	0.72
1:D:544:THR:HG22	1:D:548:ARG:HA	1.71	0.72
1:D:441:LEU:HD12	1:D:445:MET:HE2	1.71	0.72
1:A:468:LEU:CD1	1:A:469:PRO:HD2	2.19	0.72
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.53	0.72
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.23	0.72
1:B:142:LYS:HG2	1:B:169:THR:HG22	1.70	0.72
1:B:148:MET:HA	1:B:163:TYR:HD2	1.54	0.72
1:B:544:THR:HG22	1:B:548:ARG:HA	1.71	0.72
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.53	0.72
1:E:142:LYS:HG2	1:E:169:THR:HG22	1.70	0.72
1:A:451:PHE:CD2	1:A:461:PRO:HA	2.22	0.72
1:E:197:ARG:HG3	1:E:198:GLN:N	2.05	0.72
1:A:197:ARG:HG3	1:A:198:GLN:N	2.05	0.72
1:B:244:PRO:HA	1:B:275:TYR:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:LEU:HD21	1:E:403:TYR:CE2	2.23	0.72
1:E:244:PRO:HA	1:E:275:TYR:CD2	2.24	0.72
1:B:468:LEU:CD1	1:B:469:PRO:HD2	2.19	0.72
1:D:148:MET:HA	1:D:163:TYR:HD2	1.54	0.72
1:E:468:LEU:CD1	1:E:469:PRO:HD2	2.19	0.72
1:A:441:LEU:HD12	1:A:445:MET:HE2	1.71	0.72
1:C:148:MET:HA	1:C:163:TYR:HD2	1.54	0.71
1:C:244:PRO:HA	1:C:275:TYR:CD2	2.24	0.71
1:A:544:THR:HG22	1:A:548:ARG:HA	1.70	0.71
1:C:544:THR:HG22	1:C:548:ARG:HA	1.70	0.71
1:E:544:THR:HG22	1:E:548:ARG:HA	1.71	0.71
1:A:436:GLN:HE22	1:B:74:ASN:ND2	1.88	0.71
1:C:441:LEU:HD12	1:C:445:MET:HE2	1.71	0.71
1:C:468:LEU:CD1	1:C:469:PRO:HD2	2.19	0.71
1:D:197:ARG:HG3	1:D:198:GLN:N	2.05	0.71
1:A:419:ILE:HG22	1:A:423:THR:CG2	2.21	0.71
1:B:419:ILE:HG22	1:B:423:THR:CG2	2.21	0.71
1:C:197:ARG:HG3	1:C:198:GLN:N	2.05	0.71
1:D:436:GLN:HE22	1:E:74:ASN:ND2	1.88	0.71
1:A:74:ASN:ND2	1:E:436:GLN:HE22	1.89	0.71
1:A:243:LEU:HD21	1:A:403:TYR:CD2	2.26	0.71
1:A:148:MET:HA	1:A:163:TYR:HD2	1.54	0.71
1:B:197:ARG:HG3	1:B:198:GLN:N	2.05	0.71
1:C:419:ILE:HG22	1:C:423:THR:CG2	2.21	0.71
1:E:419:ILE:HG22	1:E:423:THR:CG2	2.21	0.71
1:C:436:GLN:HE22	1:D:74:ASN:ND2	1.89	0.71
1:C:243:LEU:HD21	1:C:403:TYR:CD2	2.26	0.70
1:E:249:ASP:HB2	1:E:272:ARG:HG2	1.73	0.70
1:D:419:ILE:HG22	1:D:423:THR:CG2	2.21	0.70
1:B:436:GLN:HE22	1:C:74:ASN:ND2	1.89	0.70
1:C:122:ASP:OD1	1:C:528:THR:HB	1.91	0.70
1:C:217:LEU:HB2	1:C:232:THR:HG21	1.73	0.70
1:E:243:LEU:HD21	1:E:403:TYR:CD2	2.26	0.70
1:A:122:ASP:OD1	1:A:528:THR:HB	1.91	0.70
1:B:160:GLU:OE2	1:B:162:LYS:HE3	1.91	0.70
1:D:249:ASP:HB2	1:D:272:ARG:HG2	1.73	0.70
1:B:122:ASP:OD1	1:B:528:THR:HB	1.91	0.70
1:A:160:GLU:OE2	1:A:162:LYS:HE3	1.91	0.70
1:B:215:PHE:CE1	1:B:241:ILE:HD11	2.27	0.70
1:D:217:LEU:HB2	1:D:232:THR:HG21	1.73	0.70
1:D:243:LEU:HD21	1:D:403:TYR:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLU:OE2	1:E:162:LYS:HE3	1.91	0.70
1:C:160:GLU:OE2	1:C:162:LYS:HE3	1.91	0.70
1:D:122:ASP:OD1	1:D:528:THR:HB	1.91	0.70
1:E:217:LEU:HB2	1:E:232:THR:HG21	1.73	0.70
1:A:419:ILE:HG22	1:A:423:THR:HG21	1.75	0.69
1:B:243:LEU:HD21	1:B:403:TYR:CD2	2.26	0.69
1:B:249:ASP:HB2	1:B:272:ARG:HG2	1.73	0.69
1:A:249:ASP:HB2	1:A:272:ARG:HG2	1.73	0.69
1:C:444:MET:HG2	1:C:444:MET:O	1.92	0.69
1:D:215:PHE:CE1	1:D:241:ILE:HD11	2.27	0.69
1:C:215:PHE:CE1	1:C:241:ILE:HD11	2.27	0.69
1:C:249:ASP:HB2	1:C:272:ARG:HG2	1.73	0.69
1:E:122:ASP:OD1	1:E:528:THR:HB	1.91	0.69
1:B:419:ILE:HG22	1:B:423:THR:HG21	1.75	0.69
1:B:444:MET:O	1:B:444:MET:HG2	1.92	0.69
1:D:419:ILE:HG22	1:D:423:THR:HG21	1.75	0.69
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.27	0.69
1:D:160:GLU:OE2	1:D:162:LYS:HE3	1.91	0.69
1:E:512:THR:O	1:E:513:ILE:HB	1.93	0.69
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.73	0.68
1:B:217:LEU:HB2	1:B:232:THR:HG21	1.73	0.68
1:D:444:MET:O	1:D:444:MET:HG2	1.92	0.68
1:A:142:LYS:HD3	1:A:167:GLU:OE2	1.93	0.68
1:E:215:PHE:CE1	1:E:241:ILE:HD11	2.27	0.68
1:E:444:MET:HG2	1:E:444:MET:O	1.92	0.68
1:D:142:LYS:HD3	1:D:167:GLU:OE2	1.93	0.68
1:D:512:THR:O	1:D:513:ILE:HB	1.93	0.68
1:E:142:LYS:HD3	1:E:167:GLU:OE2	1.93	0.68
1:A:512:THR:O	1:A:513:ILE:HB	1.93	0.68
1:E:278:LEU:HD22	1:E:406:TRP:HA	1.76	0.68
1:C:419:ILE:HG22	1:C:423:THR:HG21	1.75	0.68
1:A:444:MET:O	1:A:444:MET:HG2	1.92	0.68
1:B:142:LYS:HD3	1:B:167:GLU:OE2	1.94	0.68
1:E:419:ILE:HG22	1:E:423:THR:HG21	1.75	0.68
1:A:146:ARG:O	1:A:246:CYS:HB2	1.94	0.68
1:B:149:VAL:HG23	1:B:195:VAL:HG11	1.76	0.68
1:B:512:THR:O	1:B:513:ILE:HB	1.93	0.68
1:A:386:SER:O	1:A:387:LYS:HB2	1.94	0.67
1:D:217:LEU:HB2	1:D:232:THR:CG2	2.25	0.67
1:E:149:VAL:HG23	1:E:195:VAL:HG11	1.76	0.67
1:C:217:LEU:HB2	1:C:232:THR:CG2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:HG23	1:D:195:VAL:HG11	1.76	0.67
1:E:217:LEU:HB2	1:E:232:THR:CG2	2.25	0.67
1:A:278:LEU:HD22	1:A:406:TRP:HA	1.76	0.67
1:D:278:LEU:HD22	1:D:406:TRP:HA	1.76	0.67
1:A:149:VAL:HG23	1:A:195:VAL:HG11	1.76	0.67
1:C:83:ASN:OD1	1:C:83:ASN:N	2.27	0.67
1:C:142:LYS:HD3	1:C:167:GLU:OE2	1.94	0.67
1:C:227:MET:HB2	1:C:228:PRO:HD3	1.76	0.67
1:C:512:THR:O	1:C:513:ILE:HB	1.93	0.67
1:D:386:SER:O	1:D:387:LYS:HB2	1.94	0.67
1:E:386:SER:O	1:E:387:LYS:HB2	1.94	0.67
1:B:217:LEU:HB2	1:B:232:THR:CG2	2.25	0.67
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.76	0.67
1:B:227:MET:HB2	1:B:228:PRO:HD3	1.76	0.67
1:D:227:MET:HB2	1:D:228:PRO:HD3	1.76	0.67
1:C:452:ARG:HH22	1:D:99:ASN:HD22	1.43	0.67
1:D:146:ARG:O	1:D:246:CYS:HB2	1.94	0.67
1:C:146:ARG:O	1:C:246:CYS:HB2	1.94	0.66
1:D:468:LEU:HD12	1:D:469:PRO:CD	2.25	0.66
1:E:146:ARG:O	1:E:246:CYS:HB2	1.94	0.66
1:A:426:CYS:HA	1:B:132:PRO:HG3	1.77	0.66
1:B:468:LEU:HD12	1:B:469:PRO:CD	2.26	0.66
1:C:426:CYS:HA	1:D:132:PRO:HG3	1.77	0.66
1:C:430:VAL:HG21	1:C:517:SER:N	2.10	0.66
1:D:452:ARG:HH22	1:E:99:ASN:HD22	1.43	0.66
1:B:278:LEU:HD22	1:B:406:TRP:HA	1.76	0.66
1:C:149:VAL:HG23	1:C:195:VAL:HG11	1.76	0.66
1:B:146:ARG:O	1:B:246:CYS:HB2	1.94	0.66
1:B:386:SER:O	1:B:387:LYS:HB2	1.94	0.66
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.25	0.66
1:A:468:LEU:HD12	1:A:469:PRO:CD	2.26	0.66
1:C:278:LEU:HD22	1:C:406:TRP:HA	1.76	0.66
1:C:386:SER:O	1:C:387:LYS:HB2	1.94	0.66
1:D:430:VAL:HG21	1:D:517:SER:N	2.11	0.66
1:A:452:ARG:HH22	1:B:99:ASN:HD22	1.43	0.66
1:B:426:CYS:HA	1:C:132:PRO:HG3	1.77	0.66
1:C:468:LEU:HD12	1:C:469:PRO:CD	2.26	0.66
1:E:227:MET:HB2	1:E:228:PRO:HD3	1.76	0.66
1:A:99:ASN:HD22	1:E:452:ARG:HH22	1.43	0.65
1:A:132:PRO:HG3	1:E:426:CYS:HA	1.77	0.65
1:B:430:VAL:HG21	1:B:517:SER:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:N	1:B:393:LEU:HD12	2.12	0.65
1:D:60:LEU:O	1:D:61:ALA:HB3	1.97	0.65
1:E:430:VAL:HG21	1:E:517:SER:N	2.11	0.65
1:D:193:LEU:HD11	1:D:498:ARG:NH1	2.12	0.65
1:D:426:CYS:HA	1:E:132:PRO:HG3	1.77	0.65
1:A:393:LEU:HD12	1:A:393:LEU:N	2.12	0.65
1:A:430:VAL:HG21	1:A:517:SER:N	2.10	0.65
1:B:60:LEU:O	1:B:61:ALA:HB3	1.97	0.65
1:C:60:LEU:O	1:C:61:ALA:HB3	1.97	0.65
1:A:436:GLN:HE22	1:B:74:ASN:HD21	1.45	0.65
1:B:452:ARG:HH22	1:C:99:ASN:HD22	1.43	0.65
1:D:393:LEU:HD12	1:D:393:LEU:N	2.12	0.65
1:D:436:GLN:NE2	1:E:74:ASN:HD21	1.95	0.65
1:E:133:ASN:HB2	1:E:174:ASN:OD1	1.97	0.65
1:A:211:ASP:O	1:A:212:THR:HG22	1.97	0.64
1:C:193:LEU:HD11	1:C:498:ARG:NH1	2.12	0.64
1:C:211:ASP:O	1:C:212:THR:HG22	1.97	0.64
1:D:436:GLN:HE22	1:E:74:ASN:HD21	1.45	0.64
1:C:513:ILE:O	1:C:513:ILE:HG22	1.97	0.64
1:E:468:LEU:HD12	1:E:469:PRO:CD	2.26	0.64
1:C:393:LEU:HD12	1:C:393:LEU:N	2.12	0.64
1:E:60:LEU:O	1:E:61:ALA:HB3	1.97	0.64
1:B:436:GLN:NE2	1:C:74:ASN:HD21	1.95	0.64
1:E:393:LEU:N	1:E:393:LEU:HD12	2.12	0.64
1:B:278:LEU:O	1:B:404:ARG:HD3	1.98	0.64
1:B:436:GLN:HE22	1:C:74:ASN:HD21	1.46	0.64
1:E:513:ILE:HG22	1:E:513:ILE:O	1.97	0.64
1:C:436:GLN:NE2	1:D:74:ASN:HD21	1.96	0.64
1:D:513:ILE:O	1:D:513:ILE:HG22	1.97	0.64
1:A:133:ASN:HB2	1:A:174:ASN:OD1	1.97	0.64
1:E:278:LEU:O	1:E:404:ARG:HD3	1.98	0.64
1:E:493:THR:HG21	1:E:497:ASN:O	1.99	0.64
1:E:499:PHE:N	1:E:500:PRO:HD3	2.13	0.64
1:A:74:ASN:HD21	1:E:436:GLN:NE2	1.95	0.63
1:B:133:ASN:HB2	1:B:174:ASN:OD1	1.97	0.63
1:C:133:ASN:HB2	1:C:174:ASN:OD1	1.97	0.63
1:A:436:GLN:NE2	1:B:74:ASN:HD21	1.95	0.63
1:B:493:THR:HG21	1:B:497:ASN:O	1.99	0.63
1:B:513:ILE:HG22	1:B:513:ILE:O	1.97	0.63
1:C:436:GLN:HE22	1:D:74:ASN:HD21	1.45	0.63
1:C:499:PHE:N	1:C:500:PRO:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LEU:HD23	1:D:287:LEU:C	2.24	0.63
1:B:211:ASP:O	1:B:212:THR:HG22	1.97	0.63
1:B:499:PHE:N	1:B:500:PRO:HD3	2.13	0.63
1:D:211:ASP:O	1:D:212:THR:HG22	1.97	0.63
1:D:278:LEU:O	1:D:404:ARG:HD3	1.98	0.63
1:D:499:PHE:N	1:D:500:PRO:HD3	2.13	0.63
1:A:60:LEU:O	1:A:61:ALA:HB3	1.97	0.63
1:E:211:ASP:O	1:E:212:THR:HG22	1.97	0.63
1:C:493:THR:HG21	1:C:497:ASN:O	1.98	0.63
1:A:493:THR:HG21	1:A:497:ASN:O	1.98	0.63
1:C:278:LEU:O	1:C:404:ARG:HD3	1.98	0.63
1:D:133:ASN:HB2	1:D:174:ASN:OD1	1.97	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.63
1:A:287:LEU:HD23	1:A:287:LEU:C	2.24	0.63
1:C:287:LEU:HD23	1:C:287:LEU:C	2.24	0.63
1:E:134:VAL:HA	1:E:140:THR:OG1	1.99	0.63
1:E:83:ASN:OD1	1:E:83:ASN:N	2.26	0.63
1:E:148:MET:HA	1:E:163:TYR:CD2	2.34	0.63
1:A:499:PHE:N	1:A:500:PRO:HD3	2.13	0.62
1:B:193:LEU:HD11	1:B:498:ARG:NH1	2.12	0.62
1:D:134:VAL:HA	1:D:140:THR:OG1	1.99	0.62
1:A:513:ILE:O	1:A:513:ILE:HG22	1.97	0.62
1:B:134:VAL:HA	1:B:140:THR:OG1	1.99	0.62
1:D:148:MET:HA	1:D:163:TYR:CD2	2.34	0.62
1:D:544:THR:HG21	1:D:548:ARG:HD2	1.81	0.62
1:A:278:LEU:O	1:A:404:ARG:HD3	1.98	0.62
1:C:378:VAL:HG12	1:C:379:ILE:N	2.14	0.62
1:D:125:THR:HG23	1:D:524:THR:CG2	2.29	0.62
1:B:287:LEU:C	1:B:287:LEU:HD23	2.24	0.62
1:E:214:ASN:C	1:E:214:ASN:ND2	2.55	0.62
1:A:378:VAL:HG12	1:A:379:ILE:N	2.15	0.62
1:B:125:THR:HG23	1:B:524:THR:CG2	2.29	0.62
1:E:287:LEU:HD23	1:E:287:LEU:C	2.24	0.62
1:A:544:THR:HG21	1:A:548:ARG:HD2	1.81	0.62
1:D:258:LEU:HD12	1:D:258:LEU:O	2.00	0.62
1:E:544:THR:HG21	1:E:548:ARG:HD2	1.81	0.62
1:A:125:THR:HG23	1:A:524:THR:CG2	2.29	0.62
1:A:258:LEU:HD12	1:A:258:LEU:O	2.00	0.62
1:B:178:THR:CG2	1:B:511:PRO:HD2	2.29	0.62
1:B:544:THR:HG21	1:B:548:ARG:HD2	1.81	0.62
1:A:148:MET:HA	1:A:163:TYR:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:MET:HA	1:B:163:TYR:CD2	2.34	0.62
1:D:493:THR:HG21	1:D:497:ASN:O	1.99	0.62
1:B:125:THR:CG2	1:B:526:HIS:NE2	2.63	0.62
1:C:125:THR:HG23	1:C:524:THR:CG2	2.29	0.62
1:C:134:VAL:HA	1:C:140:THR:OG1	1.99	0.62
1:C:148:MET:HA	1:C:163:TYR:CD2	2.34	0.62
1:E:125:THR:HG23	1:E:524:THR:CG2	2.29	0.62
1:A:125:THR:CG2	1:A:526:HIS:NE2	2.63	0.62
1:A:233:ASN:CG	1:A:233:ASN:O	2.43	0.62
1:B:60:LEU:O	1:B:60:LEU:HG	2.00	0.62
1:C:494:HIS:C	1:C:496:PHE:H	2.07	0.62
1:D:125:THR:CG2	1:D:526:HIS:NE2	2.63	0.61
1:E:378:VAL:HG12	1:E:379:ILE:N	2.15	0.61
1:B:394:ILE:HG23	1:B:398:SER:HB2	1.82	0.61
1:D:60:LEU:O	1:D:60:LEU:HG	2.00	0.61
1:E:125:THR:CG2	1:E:526:HIS:NE2	2.63	0.61
1:A:193:LEU:HD11	1:A:498:ARG:NH1	2.12	0.61
1:A:394:ILE:HG23	1:A:398:SER:HB2	1.82	0.61
1:E:220:ASP:OD1	1:E:222:VAL:HG12	2.00	0.61
1:E:233:ASN:CG	1:E:233:ASN:O	2.43	0.61
1:B:220:ASP:OD1	1:B:222:VAL:HG12	2.00	0.61
1:D:394:ILE:HG23	1:D:398:SER:HB2	1.82	0.61
1:B:233:ASN:CG	1:B:233:ASN:O	2.43	0.61
1:B:378:VAL:HG12	1:B:379:ILE:N	2.15	0.61
1:C:220:ASP:OD1	1:C:222:VAL:HG12	2.00	0.61
1:E:60:LEU:O	1:E:60:LEU:HG	2.00	0.61
1:E:444:MET:HB2	1:E:539:GLN:OE1	2.01	0.61
1:A:74:ASN:HD21	1:E:436:GLN:HE22	1.46	0.61
1:D:220:ASP:OD1	1:D:222:VAL:HG12	2.00	0.61
1:A:494:HIS:C	1:A:496:PHE:H	2.08	0.61
1:B:258:LEU:HD12	1:B:258:LEU:O	2.00	0.61
1:C:258:LEU:HD12	1:C:258:LEU:O	2.00	0.61
1:C:444:MET:HB2	1:C:539:GLN:OE1	2.00	0.61
1:C:394:ILE:HG23	1:C:398:SER:HB2	1.82	0.61
1:D:178:THR:CG2	1:D:511:PRO:HD2	2.30	0.61
1:E:193:LEU:HD11	1:E:498:ARG:NH1	2.12	0.61
1:A:220:ASP:OD1	1:A:222:VAL:HG12	2.00	0.61
1:B:444:MET:HB2	1:B:539:GLN:OE1	2.01	0.61
1:B:494:HIS:C	1:B:496:PHE:H	2.08	0.61
1:C:125:THR:CG2	1:C:526:HIS:NE2	2.63	0.61
1:C:233:ASN:O	1:C:233:ASN:CG	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:THR:HG21	1:C:548:ARG:HD2	1.81	0.61
1:D:378:VAL:HG12	1:D:379:ILE:N	2.15	0.61
1:C:178:THR:CG2	1:C:511:PRO:HD2	2.30	0.60
1:D:444:MET:HB2	1:D:539:GLN:OE1	2.01	0.60
1:E:258:LEU:HD12	1:E:258:LEU:O	2.00	0.60
1:A:214:ASN:C	1:A:214:ASN:ND2	2.55	0.60
1:C:440:SER:HB3	1:C:461:PRO:O	2.02	0.60
1:D:440:SER:HB3	1:D:461:PRO:O	2.01	0.60
1:A:263:LYS:NZ	1:A:268:GLN:HB2	2.16	0.60
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.84	0.60
1:B:125:THR:HG21	1:B:526:HIS:NE2	2.17	0.60
1:B:394:ILE:HG23	1:B:395:SER:H	1.67	0.60
1:C:60:LEU:O	1:C:60:LEU:HG	2.00	0.60
1:D:494:HIS:C	1:D:496:PHE:H	2.07	0.60
1:E:263:LYS:NZ	1:E:268:GLN:HB2	2.16	0.60
1:B:425:LEU:HD23	1:C:172:GLU:HB3	1.83	0.60
1:D:75:LYS:HZ2	1:D:94:THR:HG23	1.67	0.60
1:D:125:THR:HG21	1:D:526:HIS:NE2	2.16	0.60
1:E:383:THR:HG22	1:E:384:GLU:HG3	1.83	0.60
1:A:125:THR:HG21	1:A:526:HIS:NE2	2.17	0.60
1:A:394:ILE:HG23	1:A:395:SER:H	1.67	0.60
1:B:220:ASP:HB2	1:B:227:MET:HG2	1.84	0.60
1:C:383:THR:HG22	1:C:384:GLU:HG3	1.84	0.60
1:D:440:SER:C	1:D:442:PRO:HD3	2.27	0.60
1:E:394:ILE:HG23	1:E:395:SER:H	1.66	0.60
1:A:60:LEU:O	1:A:60:LEU:HG	2.00	0.60
1:A:440:SER:HB3	1:A:461:PRO:O	2.02	0.60
1:D:233:ASN:CG	1:D:233:ASN:O	2.42	0.60
1:D:383:THR:HG22	1:D:384:GLU:HG3	1.84	0.60
1:A:440:SER:C	1:A:442:PRO:HD3	2.27	0.60
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.01	0.60
1:B:278:LEU:CD2	1:B:406:TRP:HA	2.32	0.60
1:C:440:SER:C	1:C:442:PRO:HD3	2.27	0.60
1:D:449:VAL:CG2	1:E:67:THR:HG21	2.32	0.60
1:E:125:THR:HG21	1:E:526:HIS:NE2	2.17	0.60
1:A:172:GLU:HB3	1:E:425:LEU:HD23	1.83	0.60
1:A:220:ASP:HB2	1:A:227:MET:HG2	1.84	0.60
1:A:449:VAL:CG2	1:B:67:THR:HG21	2.32	0.60
1:A:501:GLU:CD	1:A:501:GLU:H	2.10	0.60
1:C:410:TYR:CD1	1:C:420:ARG:HA	2.37	0.60
1:E:494:HIS:C	1:E:496:PHE:H	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:HD11	1:C:403:TYR:HE2	1.67	0.60
1:C:394:ILE:HG23	1:C:395:SER:H	1.67	0.60
1:C:449:VAL:CG2	1:D:67:THR:HG21	2.32	0.60
1:E:278:LEU:CD2	1:E:406:TRP:HA	2.32	0.60
1:A:425:LEU:HD23	1:B:172:GLU:HB3	1.84	0.59
1:B:75:LYS:HZ2	1:B:94:THR:HG23	1.67	0.59
1:C:389:ARG:NH1	1:C:389:ARG:HG2	2.17	0.59
1:D:278:LEU:CD2	1:D:406:TRP:HA	2.32	0.59
1:D:389:ARG:HG2	1:D:389:ARG:NH1	2.17	0.59
1:D:410:TYR:CD1	1:D:420:ARG:HA	2.37	0.59
1:D:425:LEU:HD23	1:E:172:GLU:HB3	1.84	0.59
1:E:501:GLU:H	1:E:501:GLU:CD	2.10	0.59
1:A:67:THR:HG21	1:E:449:VAL:CG2	2.32	0.59
1:C:220:ASP:HB2	1:C:227:MET:HG2	1.84	0.59
1:E:282:ASN:HD21	1:E:404:ARG:HE	1.51	0.59
1:E:389:ARG:HG2	1:E:389:ARG:NH1	2.17	0.59
1:A:389:ARG:NH1	1:A:389:ARG:HG2	2.17	0.59
1:B:263:LYS:NZ	1:B:268:GLN:HB2	2.16	0.59
1:B:410:TYR:CD1	1:B:420:ARG:HA	2.37	0.59
1:D:220:ASP:HB2	1:D:227:MET:HG2	1.84	0.59
1:E:278:LEU:HD23	1:E:419:ILE:CD1	2.30	0.59
1:E:394:ILE:HG23	1:E:398:SER:HB2	1.82	0.59
1:E:440:SER:HB3	1:E:461:PRO:O	2.01	0.59
1:A:410:TYR:CD1	1:A:420:ARG:HA	2.37	0.59
1:B:449:VAL:CG2	1:C:67:THR:HG21	2.32	0.59
1:D:243:LEU:HD11	1:D:403:TYR:HE2	1.67	0.59
1:E:243:LEU:HD11	1:E:403:TYR:HE2	1.67	0.59
1:A:378:VAL:O	1:A:380:LYS:N	2.35	0.59
1:B:383:THR:HG22	1:B:384:GLU:HG3	1.83	0.59
1:B:440:SER:C	1:B:442:PRO:HD3	2.27	0.59
1:B:525:ASP:C	1:B:525:ASP:OD1	2.45	0.59
1:E:378:VAL:O	1:E:380:LYS:N	2.36	0.59
1:E:410:TYR:CD1	1:E:420:ARG:HA	2.37	0.59
1:B:282:ASN:HD21	1:B:404:ARG:HE	1.50	0.59
1:B:501:GLU:H	1:B:501:GLU:CD	2.10	0.59
1:C:378:VAL:O	1:C:380:LYS:N	2.36	0.59
1:D:243:LEU:CD2	1:D:403:TYR:CD2	2.86	0.59
1:B:243:LEU:CD2	1:B:403:TYR:CD2	2.86	0.59
1:C:263:LYS:NZ	1:C:268:GLN:HB2	2.16	0.59
1:C:425:LEU:HD23	1:D:172:GLU:HB3	1.83	0.59
1:B:224:GLY:O	1:B:399:THR:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:HG21	1:C:526:HIS:NE2	2.17	0.59
1:C:501:GLU:CD	1:C:501:GLU:H	2.10	0.59
1:C:520:VAL:CG2	1:C:521:PRO:HD2	2.33	0.59
1:D:385:ASP:O	1:D:386:SER:C	2.45	0.59
1:A:178:THR:CG2	1:A:511:PRO:HD2	2.30	0.59
1:A:278:LEU:CD2	1:A:406:TRP:HA	2.32	0.59
1:C:211:ASP:CG	1:C:212:THR:H	2.10	0.59
1:C:214:ASN:C	1:C:214:ASN:ND2	2.55	0.59
1:C:525:ASP:C	1:C:525:ASP:OD1	2.45	0.59
1:D:74:ASN:HD22	1:D:556:LYS:HZ1	1.51	0.59
1:D:501:GLU:CD	1:D:501:GLU:H	2.10	0.59
1:D:525:ASP:C	1:D:525:ASP:OD1	2.45	0.59
1:E:211:ASP:CG	1:E:212:THR:H	2.10	0.59
1:E:440:SER:C	1:E:442:PRO:HD3	2.27	0.59
1:E:520:VAL:CG2	1:E:521:PRO:HD2	2.33	0.59
1:C:278:LEU:CD2	1:C:406:TRP:HA	2.32	0.59
1:A:197:ARG:HG3	1:A:198:GLN:CG	2.33	0.58
1:A:211:ASP:CG	1:A:212:THR:H	2.10	0.58
1:B:197:ARG:HG3	1:B:198:GLN:CG	2.33	0.58
1:B:243:LEU:HD11	1:B:403:TYR:HE2	1.67	0.58
1:C:243:LEU:CD2	1:C:403:TYR:CD2	2.86	0.58
1:C:282:ASN:HD21	1:C:404:ARG:HE	1.50	0.58
1:E:525:ASP:C	1:E:525:ASP:OD1	2.45	0.58
1:A:525:ASP:C	1:A:525:ASP:OD1	2.45	0.58
1:B:378:VAL:O	1:B:380:LYS:N	2.35	0.58
1:B:389:ARG:HG2	1:B:389:ARG:NH1	2.17	0.58
1:C:224:GLY:O	1:C:399:THR:HB	2.03	0.58
1:E:220:ASP:HB2	1:E:227:MET:HG2	1.84	0.58
1:E:224:GLY:O	1:E:399:THR:HB	2.03	0.58
1:B:278:LEU:HD23	1:B:419:ILE:CD1	2.30	0.58
1:B:385:ASP:O	1:B:386:SER:C	2.45	0.58
1:C:197:ARG:HG3	1:C:198:GLN:CG	2.33	0.58
1:C:385:ASP:O	1:C:386:SER:C	2.45	0.58
1:D:154:THR:HG22	1:D:155:LYS:N	2.19	0.58
1:D:263:LYS:NZ	1:D:268:GLN:HB2	2.16	0.58
1:D:394:ILE:HG23	1:D:395:SER:H	1.67	0.58
1:E:243:LEU:CD2	1:E:403:TYR:CD2	2.86	0.58
1:A:203:GLU:C	1:A:205:ASP:H	2.11	0.58
1:A:224:GLY:O	1:A:399:THR:HB	2.03	0.58
1:A:282:ASN:HD21	1:A:404:ARG:HE	1.50	0.58
1:B:154:THR:HG22	1:B:155:LYS:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:C	1:C:239:ASP:OD1	2.45	0.58
1:D:282:ASN:HD21	1:D:404:ARG:HE	1.50	0.58
1:E:154:THR:HG22	1:E:155:LYS:N	2.18	0.58
1:A:243:LEU:CD2	1:A:403:TYR:CD2	2.86	0.58
1:A:385:ASP:O	1:A:386:SER:C	2.45	0.58
1:B:440:SER:HB3	1:B:461:PRO:O	2.02	0.58
1:C:278:LEU:HD23	1:C:419:ILE:CD1	2.30	0.58
1:D:211:ASP:CG	1:D:212:THR:H	2.10	0.58
1:E:178:THR:CG2	1:E:511:PRO:HD2	2.30	0.58
1:E:239:ASP:OD1	1:E:239:ASP:C	2.46	0.58
1:E:385:ASP:O	1:E:386:SER:C	2.46	0.58
1:A:478:ASP:C	1:A:480:ALA:H	2.12	0.58
1:A:520:VAL:CG2	1:A:521:PRO:HD2	2.33	0.58
1:B:211:ASP:O	1:B:212:THR:CG2	2.52	0.58
1:C:410:TYR:HE2	1:D:172:GLU:OE1	1.87	0.58
1:D:211:ASP:O	1:D:212:THR:CG2	2.52	0.58
1:B:478:ASP:C	1:B:480:ALA:H	2.12	0.58
1:D:478:ASP:C	1:D:480:ALA:H	2.12	0.58
1:A:172:GLU:OE1	1:E:410:TYR:HE2	1.87	0.58
1:C:211:ASP:O	1:C:212:THR:CG2	2.52	0.58
1:C:478:ASP:C	1:C:480:ALA:H	2.12	0.58
1:A:278:LEU:HD23	1:A:419:ILE:CD1	2.30	0.58
1:C:203:GLU:C	1:C:205:ASP:H	2.11	0.58
1:E:211:ASP:O	1:E:212:THR:CG2	2.52	0.58
1:A:154:THR:HG22	1:A:155:LYS:N	2.19	0.58
1:A:211:ASP:O	1:A:212:THR:CG2	2.52	0.58
1:D:378:VAL:O	1:D:380:LYS:N	2.35	0.58
1:A:239:ASP:C	1:A:239:ASP:OD1	2.46	0.57
1:C:154:THR:HG22	1:C:155:LYS:N	2.18	0.57
1:A:243:LEU:HD11	1:A:403:TYR:HE2	1.67	0.57
1:A:282:ASN:ND2	1:A:404:ARG:HE	2.03	0.57
1:A:410:TYR:HE2	1:B:172:GLU:OE1	1.87	0.57
1:B:211:ASP:CG	1:B:212:THR:H	2.10	0.57
1:B:410:TYR:HE2	1:C:172:GLU:OE1	1.87	0.57
1:E:203:GLU:C	1:E:205:ASP:H	2.11	0.57
1:B:282:ASN:ND2	1:B:404:ARG:HE	2.03	0.57
1:D:197:ARG:HG3	1:D:198:GLN:CG	2.33	0.57
1:D:224:GLY:O	1:D:399:THR:HB	2.03	0.57
1:D:410:TYR:HE2	1:E:172:GLU:OE1	1.87	0.57
1:E:197:ARG:HG3	1:E:198:GLN:CG	2.33	0.57
1:B:520:VAL:CG2	1:B:521:PRO:HD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:C	1:B:205:ASP:H	2.11	0.57
1:D:403:TYR:CD1	1:D:504:ILE:HD13	2.39	0.57
1:B:214:ASN:C	1:B:214:ASN:ND2	2.55	0.57
1:D:53:ASN:O	1:D:54:SER:C	2.48	0.57
1:D:282:ASN:ND2	1:D:404:ARG:HE	2.03	0.57
1:D:482:TYR:CE1	1:D:486:ILE:HD12	2.40	0.57
1:D:520:VAL:CG2	1:D:521:PRO:HD2	2.33	0.57
1:B:239:ASP:C	1:B:239:ASP:OD1	2.45	0.57
1:C:567:SER:HB2	1:D:49:THR:HG21	1.87	0.57
1:B:482:TYR:CE1	1:B:486:ILE:HD12	2.40	0.57
1:A:134:VAL:HG22	1:A:173:GLY:O	2.05	0.56
1:E:134:VAL:HG22	1:E:173:GLY:O	2.05	0.56
1:E:282:ASN:ND2	1:E:404:ARG:HE	2.03	0.56
1:A:482:TYR:CE1	1:A:486:ILE:HD12	2.40	0.56
1:E:478:ASP:C	1:E:480:ALA:H	2.12	0.56
1:A:567:SER:HB2	1:B:49:THR:HG21	1.87	0.56
1:B:134:VAL:HG22	1:B:173:GLY:O	2.05	0.56
1:B:392:ASN:HB3	1:B:402:GLN:NE2	2.21	0.56
1:B:434:SER:N	1:C:555:TYR:HE2	2.04	0.56
1:B:479:GLN:O	1:B:479:GLN:HG2	2.05	0.56
1:C:74:ASN:HD22	1:C:556:LYS:HZ1	1.51	0.56
1:C:282:ASN:ND2	1:C:404:ARG:HE	2.02	0.56
1:D:479:GLN:O	1:D:479:GLN:HG2	2.05	0.56
1:E:273:ILE:O	1:E:273:ILE:HG23	2.05	0.56
1:E:479:GLN:O	1:E:479:GLN:HG2	2.05	0.56
1:C:125:THR:CG2	1:C:524:THR:HG23	2.36	0.56
1:A:434:SER:N	1:B:555:TYR:HE2	2.04	0.56
1:C:392:ASN:HB3	1:C:402:GLN:NE2	2.21	0.56
1:D:392:ASN:HB3	1:D:402:GLN:NE2	2.21	0.56
1:D:567:SER:HB2	1:E:49:THR:HG21	1.87	0.56
1:E:392:ASN:HB3	1:E:402:GLN:NE2	2.21	0.56
1:A:125:THR:CG2	1:A:524:THR:HG23	2.35	0.56
1:B:53:ASN:O	1:B:54:SER:C	2.48	0.56
1:B:403:TYR:CD1	1:B:504:ILE:HD13	2.39	0.56
1:C:482:TYR:CE1	1:C:486:ILE:HD12	2.40	0.56
1:D:239:ASP:C	1:D:239:ASP:OD1	2.45	0.56
1:D:273:ILE:HG23	1:D:273:ILE:O	2.05	0.56
1:E:74:ASN:ND2	1:E:556:LYS:HZ1	2.04	0.56
1:A:53:ASN:O	1:A:54:SER:C	2.48	0.56
1:A:392:ASN:HB3	1:A:402:GLN:NE2	2.21	0.56
1:D:203:GLU:C	1:D:205:ASP:H	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ASN:O	1:E:54:SER:C	2.48	0.56
1:A:67:THR:O	1:A:68:ARG:HG2	2.06	0.56
1:B:273:ILE:O	1:B:273:ILE:HG23	2.05	0.56
1:B:419:ILE:O	1:B:423:THR:HG22	2.06	0.56
1:B:567:SER:HB2	1:C:49:THR:HG21	1.87	0.56
1:D:134:VAL:HG22	1:D:173:GLY:O	2.05	0.56
1:E:482:TYR:CE1	1:E:486:ILE:HD12	2.40	0.56
1:A:273:ILE:HG23	1:A:273:ILE:O	2.05	0.56
1:E:125:THR:CG2	1:E:524:THR:HG23	2.35	0.56
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.66	0.56
1:A:493:THR:HG22	1:A:494:HIS:N	2.21	0.56
1:C:53:ASN:O	1:C:54:SER:C	2.48	0.56
1:C:403:TYR:CD1	1:C:504:ILE:HD13	2.39	0.56
1:A:555:TYR:HE2	1:E:434:SER:N	2.04	0.55
1:C:283:ILE:O	1:C:401:THR:HG23	2.07	0.55
1:C:434:SER:N	1:D:555:TYR:HE2	2.04	0.55
1:D:67:THR:O	1:D:68:ARG:HG2	2.06	0.55
1:A:49:THR:HG21	1:E:567:SER:HB2	1.87	0.55
1:A:479:GLN:O	1:A:479:GLN:HG2	2.05	0.55
1:B:125:THR:CG2	1:B:524:THR:HG23	2.36	0.55
1:B:403:TYR:HD1	1:B:504:ILE:CD1	2.20	0.55
1:A:283:ILE:O	1:A:401:THR:HG23	2.07	0.55
1:A:494:HIS:C	1:A:496:PHE:N	2.64	0.55
1:B:283:ILE:O	1:B:401:THR:HG23	2.07	0.55
1:C:197:ARG:HG3	1:C:198:GLN:H	1.71	0.55
1:D:68:ARG:HH11	1:D:68:ARG:CG	2.07	0.55
1:D:403:TYR:HD1	1:D:504:ILE:CD1	2.19	0.55
1:D:419:ILE:O	1:D:423:THR:HG22	2.06	0.55
1:E:283:ILE:O	1:E:401:THR:HG23	2.06	0.55
1:A:428:PRO:O	1:A:429:ASP:HB3	2.06	0.55
1:C:266:PRO:C	1:C:268:GLN:H	2.15	0.55
1:C:395:SER:C	1:C:397:ASP:H	2.14	0.55
1:A:419:ILE:O	1:A:423:THR:HG22	2.06	0.55
1:C:449:VAL:HG22	1:D:67:THR:HG21	1.89	0.55
1:C:479:GLN:HG2	1:C:479:GLN:O	2.05	0.55
1:C:67:THR:O	1:C:68:ARG:HG2	2.06	0.55
1:D:125:THR:CG2	1:D:524:THR:HG23	2.35	0.55
1:E:67:THR:O	1:E:68:ARG:HG2	2.06	0.55
1:E:493:THR:HG22	1:E:494:HIS:N	2.21	0.55
1:A:74:ASN:HD22	1:A:556:LYS:HZ1	1.51	0.55
1:B:449:VAL:HG22	1:C:67:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:VAL:HG22	1:C:173:GLY:O	2.05	0.55
1:D:436:GLN:CD	1:E:556:LYS:HZ3	2.14	0.55
1:D:449:VAL:HG22	1:E:67:THR:HG21	1.89	0.55
1:A:449:VAL:HG22	1:B:67:THR:HG21	1.89	0.55
1:B:67:THR:O	1:B:68:ARG:HG2	2.06	0.55
1:C:136:GLU:O	1:C:137:PHE:HB2	2.07	0.55
1:D:266:PRO:C	1:D:268:GLN:H	2.15	0.55
1:D:493:THR:HG22	1:D:494:HIS:N	2.21	0.55
1:E:197:ARG:HG3	1:E:198:GLN:H	1.71	0.55
1:A:197:ARG:HG3	1:A:198:GLN:H	1.71	0.55
1:A:266:PRO:C	1:A:268:GLN:H	2.15	0.55
1:C:273:ILE:HG23	1:C:273:ILE:O	2.05	0.55
1:D:215:PHE:HE1	1:D:241:ILE:HD11	1.71	0.55
1:A:529:LEU:HD21	1:B:68:ARG:NE	2.22	0.55
1:B:136:GLU:O	1:B:137:PHE:HB2	2.07	0.55
1:D:434:SER:N	1:E:555:TYR:HE2	2.04	0.55
1:E:419:ILE:O	1:E:423:THR:HG22	2.06	0.55
1:A:403:TYR:CD1	1:A:504:ILE:HD13	2.39	0.54
1:B:266:PRO:C	1:B:268:GLN:H	2.15	0.54
1:C:419:ILE:O	1:C:423:THR:HG22	2.06	0.54
1:D:83:ASN:OD1	1:D:83:ASN:N	2.26	0.54
1:C:544:THR:HG21	1:C:548:ARG:HA	1.89	0.54
1:D:278:LEU:HD23	1:D:419:ILE:CD1	2.30	0.54
1:D:283:ILE:O	1:D:401:THR:HG23	2.07	0.54
1:E:266:PRO:C	1:E:268:GLN:H	2.14	0.54
1:A:505:LEU:O	1:A:506:ALA:O	2.26	0.54
1:B:263:LYS:HZ3	1:B:268:GLN:HB2	1.73	0.54
1:B:395:SER:C	1:B:397:ASP:H	2.14	0.54
1:D:136:GLU:O	1:D:137:PHE:HB2	2.07	0.54
1:E:428:PRO:O	1:E:429:ASP:HB3	2.07	0.54
1:B:529:LEU:HD21	1:C:68:ARG:NE	2.23	0.54
1:D:395:SER:C	1:D:397:ASP:H	2.14	0.54
1:D:428:PRO:O	1:D:429:ASP:HB3	2.06	0.54
1:B:493:THR:HG22	1:B:494:HIS:N	2.21	0.54
1:D:463:VAL:HB	1:D:529:LEU:CD1	2.38	0.54
1:B:494:HIS:C	1:B:496:PHE:N	2.64	0.54
1:E:215:PHE:HE1	1:E:241:ILE:HD11	1.71	0.54
1:E:192:TYR:CZ	1:E:197:ARG:HB3	2.43	0.54
1:E:208:VAL:HG23	1:E:208:VAL:O	2.08	0.54
1:E:389:ARG:HG2	1:E:389:ARG:HH11	1.73	0.54
1:E:505:LEU:O	1:E:506:ALA:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NE	1:E:529:LEU:HD21	2.23	0.54
1:A:136:GLU:O	1:A:137:PHE:HB2	2.07	0.54
1:A:395:SER:C	1:A:397:ASP:H	2.14	0.54
1:B:192:TYR:CZ	1:B:197:ARG:HB3	2.43	0.54
1:C:428:PRO:O	1:C:429:ASP:HB3	2.06	0.54
1:C:505:LEU:O	1:C:506:ALA:O	2.26	0.54
1:D:197:ARG:HG3	1:D:198:GLN:H	1.71	0.54
1:D:505:LEU:O	1:D:506:ALA:O	2.26	0.54
1:E:463:VAL:HB	1:E:529:LEU:CD1	2.38	0.54
1:A:192:TYR:CZ	1:A:197:ARG:HB3	2.43	0.54
1:B:208:VAL:HG23	1:B:208:VAL:O	2.08	0.54
1:B:428:PRO:O	1:B:429:ASP:HB3	2.06	0.54
1:C:192:TYR:CZ	1:C:197:ARG:HB3	2.43	0.54
1:C:493:THR:HG22	1:C:494:HIS:N	2.21	0.54
1:D:192:TYR:CZ	1:D:197:ARG:HB3	2.43	0.54
1:A:67:THR:HG21	1:E:449:VAL:HG22	1.89	0.54
1:B:197:ARG:HG3	1:B:198:GLN:H	1.71	0.53
1:E:544:THR:HG21	1:E:548:ARG:HA	1.89	0.53
1:B:544:THR:HG21	1:B:548:ARG:HA	1.89	0.53
1:D:449:VAL:HG12	1:D:450:THR:N	2.23	0.53
1:E:403:TYR:HD1	1:E:504:ILE:CD1	2.19	0.53
1:B:215:PHE:HE1	1:B:241:ILE:HD11	1.71	0.53
1:B:74:ASN:HD22	1:B:556:LYS:HZ1	1.51	0.53
1:B:154:THR:CG2	1:B:155:LYS:N	2.72	0.53
1:B:389:ARG:HG2	1:B:389:ARG:HH11	1.73	0.53
1:D:151:ARG:HG3	1:D:161:LEU:CD2	2.39	0.53
1:A:93:THR:HG22	1:A:94:THR:N	2.23	0.53
1:A:295:SER:HB3	1:A:377:PRO:CG	2.33	0.53
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.73	0.53
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.38	0.53
1:B:452:ARG:NH2	1:C:99:ASN:HD22	2.07	0.53
1:C:93:THR:HG22	1:C:94:THR:N	2.23	0.53
1:D:208:VAL:HG23	1:D:208:VAL:O	2.08	0.53
1:D:529:LEU:HD21	1:E:68:ARG:NE	2.23	0.53
1:C:69:VAL:CG2	1:C:561:VAL:HB	2.39	0.53
1:C:403:TYR:HD1	1:C:504:ILE:CD1	2.19	0.53
1:C:529:LEU:HD21	1:D:68:ARG:NE	2.23	0.53
1:D:154:THR:CG2	1:D:155:LYS:N	2.72	0.53
1:E:136:GLU:O	1:E:137:PHE:HB2	2.07	0.53
1:A:263:LYS:HZ3	1:A:268:GLN:HB2	1.74	0.53
1:C:386:SER:O	1:C:387:LYS:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:CG2	1:D:561:VAL:HB	2.39	0.53
1:D:93:THR:HG22	1:D:94:THR:N	2.23	0.53
1:D:151:ARG:HG3	1:D:161:LEU:HD21	1.91	0.53
1:D:389:ARG:HG2	1:D:389:ARG:HH11	1.73	0.53
1:B:197:ARG:C	1:B:199:ASN:H	2.17	0.53
1:B:449:VAL:HG12	1:B:450:THR:N	2.23	0.53
1:B:505:LEU:O	1:B:506:ALA:O	2.26	0.53
1:C:151:ARG:HG3	1:C:161:LEU:HD21	1.91	0.53
1:C:154:THR:CG2	1:C:155:LYS:N	2.72	0.53
1:C:236:PHE:O	1:C:237:HIS:HB3	2.09	0.53
1:E:69:VAL:CG2	1:E:561:VAL:HB	2.39	0.53
1:E:292:TYR:HA	1:E:377:PRO:HG3	1.91	0.53
1:B:222:VAL:HG13	1:B:223:THR:N	2.24	0.53
1:E:151:ARG:HG3	1:E:161:LEU:HD21	1.91	0.53
1:A:544:THR:HG21	1:A:548:ARG:HA	1.89	0.52
1:C:197:ARG:CG	1:C:198:GLN:N	2.72	0.52
1:C:208:VAL:O	1:C:208:VAL:HG23	2.08	0.52
1:C:222:VAL:HG13	1:C:223:THR:N	2.24	0.52
1:C:295:SER:HB3	1:C:377:PRO:CG	2.33	0.52
1:E:120:GLY:O	1:E:563:PRO:HA	2.10	0.52
1:E:151:ARG:HG3	1:E:161:LEU:CD2	2.39	0.52
1:A:215:PHE:HE1	1:A:241:ILE:HD11	1.71	0.52
1:A:449:VAL:HG12	1:A:450:THR:N	2.23	0.52
1:B:69:VAL:CG2	1:B:561:VAL:HB	2.39	0.52
1:C:180:THR:HG21	1:C:258:LEU:CD2	2.40	0.52
1:D:236:PHE:O	1:D:237:HIS:HB3	2.09	0.52
1:D:266:PRO:O	1:D:268:GLN:N	2.43	0.52
1:E:93:THR:HG22	1:E:94:THR:N	2.23	0.52
1:E:494:HIS:C	1:E:496:PHE:N	2.64	0.52
1:A:69:VAL:CG2	1:A:561:VAL:HB	2.39	0.52
1:A:151:ARG:HG3	1:A:161:LEU:CD2	2.39	0.52
1:A:154:THR:CG2	1:A:155:LYS:N	2.72	0.52
1:A:197:ARG:C	1:A:199:ASN:H	2.17	0.52
1:A:386:SER:O	1:A:387:LYS:CB	2.57	0.52
1:B:120:GLY:O	1:B:563:PRO:HA	2.10	0.52
1:B:151:ARG:HG3	1:B:161:LEU:HD21	1.91	0.52
1:D:180:THR:HG21	1:D:258:LEU:CD2	2.40	0.52
1:D:494:HIS:C	1:D:496:PHE:N	2.64	0.52
1:E:263:LYS:HZ3	1:E:268:GLN:HB2	1.74	0.52
1:A:452:ARG:NH2	1:B:99:ASN:HD22	2.06	0.52
1:B:180:THR:HG21	1:B:258:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:O	1:B:268:GLN:N	2.43	0.52
1:B:463:VAL:HB	1:B:529:LEU:CD1	2.38	0.52
1:C:151:ARG:HG3	1:C:161:LEU:CD2	2.39	0.52
1:C:389:ARG:HG2	1:C:389:ARG:HH11	1.73	0.52
1:C:449:VAL:HG12	1:C:450:THR:N	2.23	0.52
1:E:171:PRO:O	1:E:175:TYR:OH	2.25	0.52
1:E:180:THR:HG21	1:E:258:LEU:CD2	2.40	0.52
1:E:236:PHE:O	1:E:237:HIS:HB3	2.09	0.52
1:B:197:ARG:CG	1:B:198:GLN:N	2.72	0.52
1:D:197:ARG:CG	1:D:198:GLN:N	2.72	0.52
1:D:441:LEU:N	1:D:442:PRO:HD3	2.24	0.52
1:E:154:THR:CG2	1:E:155:LYS:N	2.71	0.52
1:E:395:SER:C	1:E:397:ASP:H	2.14	0.52
1:E:449:VAL:HG12	1:E:450:THR:N	2.23	0.52
1:A:208:VAL:HG23	1:A:208:VAL:O	2.08	0.52
1:A:211:ASP:HA	1:A:508:PRO:HG2	1.89	0.52
1:C:403:TYR:CD1	1:C:504:ILE:HG21	2.45	0.52
1:C:520:VAL:HG23	1:C:521:PRO:HD2	1.92	0.52
1:D:386:SER:O	1:D:387:LYS:CB	2.57	0.52
1:E:197:ARG:CG	1:E:198:GLN:N	2.72	0.52
1:E:520:VAL:HG23	1:E:521:PRO:HD2	1.92	0.52
1:A:171:PRO:O	1:A:175:TYR:OH	2.25	0.52
1:A:266:PRO:O	1:A:268:GLN:N	2.43	0.52
1:A:403:TYR:HD1	1:A:504:ILE:CD1	2.20	0.52
1:C:211:ASP:HA	1:C:508:PRO:HG2	1.89	0.52
1:C:262:ARG:HH11	1:D:130:ASN:HD22	1.55	0.52
1:C:413:GLY:O	1:C:414:ASP:C	2.53	0.52
1:C:463:VAL:HB	1:C:529:LEU:CD1	2.38	0.52
1:E:222:VAL:HG13	1:E:223:THR:N	2.24	0.52
1:E:386:SER:O	1:E:387:LYS:CB	2.57	0.52
1:A:99:ASN:HD22	1:E:452:ARG:NH2	2.07	0.52
1:A:197:ARG:CG	1:A:198:GLN:N	2.72	0.52
1:A:222:VAL:HG13	1:A:223:THR:N	2.24	0.52
1:B:125:THR:HG22	1:B:524:THR:HG23	1.92	0.52
1:B:151:ARG:HG3	1:B:161:LEU:CD2	2.39	0.52
1:B:403:TYR:CD1	1:B:504:ILE:HG21	2.45	0.52
1:D:120:GLY:O	1:D:563:PRO:HA	2.10	0.52
1:D:222:VAL:HG13	1:D:223:THR:N	2.24	0.52
1:D:413:GLY:O	1:D:414:ASP:C	2.53	0.52
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.40	0.52
1:B:93:THR:HG22	1:B:94:THR:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:THR:CG2	1:D:524:THR:CG2	2.88	0.52
1:D:151:ARG:HB3	1:D:200:GLY:O	2.10	0.52
1:D:197:ARG:C	1:D:199:ASN:H	2.17	0.52
1:B:413:GLY:O	1:B:414:ASP:C	2.53	0.52
1:C:263:LYS:HZ3	1:C:268:GLN:HB2	1.74	0.52
1:E:197:ARG:C	1:E:199:ASN:H	2.17	0.52
1:E:295:SER:HB3	1:E:377:PRO:CG	2.33	0.52
1:E:403:TYR:CD1	1:E:504:ILE:HG21	2.45	0.52
1:A:441:LEU:N	1:A:442:PRO:HD3	2.24	0.51
1:C:125:THR:CG2	1:C:524:THR:CG2	2.88	0.51
1:C:197:ARG:C	1:C:199:ASN:H	2.17	0.51
1:C:494:HIS:C	1:C:496:PHE:N	2.64	0.51
1:D:452:ARG:NH2	1:E:99:ASN:HD22	2.06	0.51
1:C:151:ARG:HB3	1:C:200:GLY:O	2.10	0.51
1:C:215:PHE:HE1	1:C:241:ILE:HD11	1.71	0.51
1:C:295:SER:OG	1:C:377:PRO:HD3	2.10	0.51
1:E:151:ARG:HB3	1:E:200:GLY:O	2.10	0.51
1:A:125:THR:CG2	1:A:524:THR:CG2	2.88	0.51
1:B:233:ASN:C	1:B:233:ASN:OD1	2.54	0.51
1:B:441:LEU:N	1:B:442:PRO:HD3	2.24	0.51
1:D:138:MET:HB3	1:D:254:ARG:NH1	2.26	0.51
1:D:295:SER:OG	1:D:377:PRO:HD3	2.10	0.51
1:E:125:THR:CG2	1:E:524:THR:CG2	2.88	0.51
1:A:151:ARG:HG3	1:A:161:LEU:HD21	1.91	0.51
1:A:151:ARG:HB3	1:A:200:GLY:O	2.10	0.51
1:A:236:PHE:O	1:A:237:HIS:HB3	2.09	0.51
1:B:130:ASN:HA	1:B:519:ASN:CG	2.36	0.51
1:C:125:THR:HG22	1:C:524:THR:HG23	1.92	0.51
1:C:132:PRO:HD3	1:C:553:TYR:CE2	2.46	0.51
1:C:171:PRO:O	1:C:175:TYR:OH	2.25	0.51
1:D:425:LEU:HD12	1:D:426:CYS:N	2.26	0.51
1:E:132:PRO:HD3	1:E:553:TYR:CE2	2.46	0.51
1:A:120:GLY:O	1:A:563:PRO:HA	2.10	0.51
1:A:130:ASN:HA	1:A:519:ASN:CG	2.36	0.51
1:A:295:SER:OG	1:A:377:PRO:HD3	2.10	0.51
1:A:413:GLY:O	1:A:414:ASP:C	2.53	0.51
1:B:125:THR:CG2	1:B:524:THR:CG2	2.88	0.51
1:B:211:ASP:HA	1:B:508:PRO:HG2	1.89	0.51
1:B:422:TRP:H	1:B:422:TRP:CD1	2.29	0.51
1:C:75:LYS:HZ2	1:C:94:THR:HG23	1.75	0.51
1:D:125:THR:HG22	1:D:524:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:NH1	1:E:424:LEU:HD13	2.26	0.51
1:A:520:VAL:HG23	1:A:521:PRO:HD2	1.92	0.51
1:B:132:PRO:HD3	1:B:553:TYR:CE2	2.46	0.51
1:B:138:MET:HB3	1:B:254:ARG:NH1	2.26	0.51
1:B:151:ARG:HB3	1:B:200:GLY:O	2.10	0.51
1:B:264:ARG:NH1	1:B:424:LEU:HD13	2.26	0.51
1:B:295:SER:OG	1:B:377:PRO:HD3	2.10	0.51
1:C:120:GLY:O	1:C:563:PRO:HA	2.10	0.51
1:C:451:PHE:CE1	1:D:97:GLN:HB2	2.46	0.51
1:D:132:PRO:HD3	1:D:553:TYR:CE2	2.46	0.51
1:D:211:ASP:C	1:D:212:THR:CG2	2.84	0.51
1:D:547:ARG:O	1:D:548:ARG:HB2	2.11	0.51
1:E:425:LEU:HD12	1:E:426:CYS:N	2.25	0.51
1:A:60:LEU:O	1:A:61:ALA:CB	2.59	0.51
1:B:295:SER:HB3	1:B:377:PRO:CG	2.33	0.51
1:C:60:LEU:O	1:C:61:ALA:CB	2.59	0.51
1:C:130:ASN:HA	1:C:519:ASN:CG	2.36	0.51
1:C:138:MET:HB3	1:C:254:ARG:NH1	2.26	0.51
1:C:441:LEU:N	1:C:442:PRO:HD3	2.24	0.51
1:D:295:SER:HB3	1:D:377:PRO:CG	2.33	0.51
1:D:544:THR:HG21	1:D:548:ARG:HA	1.89	0.51
1:E:125:THR:HG22	1:E:524:THR:HG23	1.92	0.51
1:E:403:TYR:CD1	1:E:504:ILE:HD13	2.39	0.51
1:A:97:GLN:HB2	1:E:451:PHE:CE1	2.46	0.51
1:A:264:ARG:NH1	1:A:424:LEU:HD13	2.26	0.51
1:A:403:TYR:CD1	1:A:504:ILE:HG21	2.45	0.51
1:B:211:ASP:C	1:B:212:THR:CG2	2.84	0.51
1:B:451:PHE:CE1	1:C:97:GLN:HB2	2.46	0.51
1:B:520:VAL:HG23	1:B:521:PRO:HD2	1.92	0.51
1:C:491:SER:O	1:C:492:LEU:O	2.29	0.51
1:D:403:TYR:CD1	1:D:504:ILE:HG21	2.45	0.51
1:D:430:VAL:HG23	1:D:517:SER:HB2	1.93	0.51
1:E:197:ARG:HG3	1:E:198:GLN:HG2	1.93	0.51
1:E:211:ASP:C	1:E:212:THR:CG2	2.84	0.51
1:E:413:GLY:O	1:E:414:ASP:C	2.53	0.51
1:A:422:TRP:CD1	1:A:422:TRP:H	2.29	0.51
1:C:425:LEU:HD12	1:C:426:CYS:N	2.25	0.51
1:D:264:ARG:NH1	1:D:424:LEU:HD13	2.26	0.51
1:E:295:SER:OG	1:E:377:PRO:HD3	2.10	0.51
1:E:441:LEU:N	1:E:442:PRO:HD3	2.24	0.51
1:A:132:PRO:HD3	1:A:553:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HB3	1:A:254:ARG:NH1	2.26	0.51
1:A:451:PHE:CE1	1:B:97:GLN:HB2	2.46	0.51
1:B:236:PHE:O	1:B:237:HIS:HB3	2.09	0.51
1:C:264:ARG:NH1	1:C:424:LEU:HD13	2.26	0.51
1:C:452:ARG:NH2	1:D:99:ASN:HD22	2.07	0.51
1:D:130:ASN:HA	1:D:519:ASN:CG	2.36	0.51
1:D:451:PHE:CE1	1:E:97:GLN:HB2	2.46	0.51
1:A:125:THR:HG22	1:A:524:THR:HG23	1.92	0.50
1:A:233:ASN:C	1:A:233:ASN:OD1	2.54	0.50
1:B:135:ASN:HA	1:B:172:GLU:HG2	1.93	0.50
1:C:422:TRP:CD1	1:C:422:TRP:H	2.29	0.50
1:D:214:ASN:C	1:D:214:ASN:ND2	2.55	0.50
1:A:98:ASN:ND2	1:E:452:ARG:HE	2.08	0.50
1:A:211:ASP:C	1:A:212:THR:CG2	2.84	0.50
1:B:427:THR:HG23	1:B:428:PRO:HD2	1.94	0.50
1:B:451:PHE:CE1	1:C:97:GLN:HG3	2.47	0.50
1:C:211:ASP:C	1:C:212:THR:CG2	2.84	0.50
1:C:567:SER:CB	1:D:49:THR:HG21	2.41	0.50
1:D:233:ASN:O	1:D:233:ASN:OD1	2.30	0.50
1:D:451:PHE:HE1	1:E:97:GLN:HG3	1.76	0.50
1:D:520:VAL:HG23	1:D:521:PRO:HD2	1.92	0.50
1:E:430:VAL:HG23	1:E:517:SER:HB2	1.93	0.50
1:A:547:ARG:O	1:A:548:ARG:HB2	2.11	0.50
1:C:233:ASN:C	1:C:233:ASN:OD1	2.54	0.50
1:D:197:ARG:HG3	1:D:198:GLN:HG2	1.93	0.50
1:D:243:LEU:CD2	1:D:403:TYR:HD2	2.24	0.50
1:E:130:ASN:HA	1:E:519:ASN:CG	2.36	0.50
1:E:138:MET:HB3	1:E:254:ARG:NH1	2.26	0.50
1:A:233:ASN:O	1:A:233:ASN:OD1	2.30	0.50
1:A:451:PHE:HE1	1:B:97:GLN:HG3	1.76	0.50
1:B:60:LEU:O	1:B:61:ALA:CB	2.59	0.50
1:D:60:LEU:O	1:D:61:ALA:CB	2.59	0.50
1:E:192:TYR:CD2	1:E:193:LEU:HD23	2.47	0.50
1:E:233:ASN:C	1:E:233:ASN:OD1	2.54	0.50
1:A:197:ARG:HG3	1:A:198:GLN:HG2	1.93	0.50
1:A:451:PHE:CE1	1:B:97:GLN:HG3	2.47	0.50
1:C:135:ASN:HA	1:C:172:GLU:HG2	1.94	0.50
1:C:266:PRO:O	1:C:268:GLN:N	2.43	0.50
1:C:451:PHE:CE1	1:D:97:GLN:HG3	2.47	0.50
1:C:544:THR:HG22	1:C:545:ASP:N	2.27	0.50
1:D:263:LYS:HZ3	1:D:268:GLN:HB2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:SER:CB	1:E:49:THR:HG21	2.41	0.50
1:E:211:ASP:HA	1:E:508:PRO:HG2	1.89	0.50
1:E:243:LEU:CD2	1:E:403:TYR:HD2	2.24	0.50
1:A:97:GLN:HG3	1:E:451:PHE:CE1	2.47	0.50
1:A:243:LEU:CD2	1:A:403:TYR:HD2	2.24	0.50
1:A:491:SER:O	1:A:492:LEU:O	2.29	0.50
1:C:178:THR:O	1:C:181:ILE:N	2.45	0.50
1:C:192:TYR:CD2	1:C:193:LEU:HD23	2.47	0.50
1:D:192:TYR:CD2	1:D:193:LEU:HD23	2.47	0.50
1:D:422:TRP:CD1	1:D:422:TRP:H	2.29	0.50
1:D:427:THR:HG23	1:D:428:PRO:HD2	1.94	0.50
1:E:243:LEU:CD2	1:E:244:PRO:HD3	2.42	0.50
1:E:427:THR:HG23	1:E:428:PRO:HD2	1.94	0.50
1:A:178:THR:O	1:A:181:ILE:N	2.45	0.50
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.50
1:A:567:SER:CB	1:B:49:THR:HG21	2.41	0.50
1:B:61:ALA:HB1	1:B:62:PRO:CD	2.42	0.50
1:B:491:SER:O	1:B:492:LEU:O	2.29	0.50
1:B:544:THR:HG22	1:B:545:ASP:N	2.26	0.50
1:B:547:ARG:O	1:B:548:ARG:HB2	2.11	0.50
1:B:567:SER:CB	1:C:49:THR:HG21	2.41	0.50
1:C:451:PHE:HE1	1:D:97:GLN:HG3	1.77	0.50
1:D:237:HIS:ND1	1:D:238:PRO:O	2.45	0.50
1:E:422:TRP:H	1:E:422:TRP:CD1	2.29	0.50
1:A:61:ALA:HB1	1:A:62:PRO:CD	2.42	0.50
1:B:243:LEU:CD2	1:B:244:PRO:HD3	2.42	0.50
1:B:425:LEU:HD12	1:B:426:CYS:N	2.26	0.50
1:C:61:ALA:HB1	1:C:62:PRO:CD	2.42	0.50
1:C:233:ASN:O	1:C:233:ASN:OD1	2.30	0.50
1:C:547:ARG:O	1:C:548:ARG:HB2	2.11	0.50
1:D:114:ASP:OD1	1:D:115:ASP:N	2.45	0.50
1:D:135:ASN:HA	1:D:172:GLU:HG2	1.94	0.50
1:D:451:PHE:CE1	1:E:97:GLN:HG3	2.47	0.50
1:D:491:SER:O	1:D:492:LEU:O	2.29	0.50
1:E:61:ALA:HB1	1:E:62:PRO:CD	2.42	0.50
1:A:192:TYR:CD2	1:A:193:LEU:HD23	2.47	0.50
1:B:233:ASN:O	1:B:233:ASN:OD1	2.30	0.50
1:B:386:SER:O	1:B:387:LYS:CB	2.57	0.50
1:C:114:ASP:OD1	1:C:115:ASP:N	2.45	0.50
1:C:243:LEU:CD2	1:C:244:PRO:HD3	2.42	0.50
1:E:178:THR:O	1:E:181:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:PRO:O	1:E:268:GLN:N	2.43	0.50
1:E:547:ARG:O	1:E:548:ARG:HB2	2.11	0.50
1:A:49:THR:HG21	1:E:567:SER:CB	2.42	0.49
1:A:425:LEU:HD12	1:A:426:CYS:N	2.26	0.49
1:B:178:THR:O	1:B:181:ILE:N	2.45	0.49
1:D:178:THR:O	1:D:181:ILE:N	2.45	0.49
1:D:197:ARG:HG3	1:D:198:GLN:HG3	1.94	0.49
1:E:202:LEU:O	1:E:203:GLU:C	2.55	0.49
1:E:544:THR:HG22	1:E:545:ASP:N	2.26	0.49
1:A:126:ILE:HG23	1:A:523:LEU:HD23	1.94	0.49
1:A:394:ILE:HG22	1:A:400:PHE:O	2.12	0.49
1:A:486:ILE:HD11	1:E:485:LEU:HD11	1.94	0.49
1:B:481:VAL:HG21	1:C:482:TYR:OH	2.12	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG2	1.93	0.49
1:D:243:LEU:HD22	1:D:244:PRO:CD	2.43	0.49
1:D:436:GLN:NE2	1:E:556:LYS:HZ3	2.09	0.49
1:E:258:LEU:HD12	1:E:258:LEU:C	2.37	0.49
1:B:171:PRO:O	1:B:175:TYR:OH	2.25	0.49
1:B:203:GLU:C	1:B:205:ASP:N	2.71	0.49
1:B:212:THR:HG23	1:B:508:PRO:HB3	1.94	0.49
1:D:126:ILE:HG23	1:D:523:LEU:HD23	1.94	0.49
1:D:212:THR:HG23	1:D:508:PRO:HB3	1.94	0.49
1:D:233:ASN:OD1	1:D:233:ASN:C	2.54	0.49
1:D:243:LEU:CD2	1:D:244:PRO:HD3	2.42	0.49
1:D:544:THR:HG22	1:D:545:ASP:N	2.26	0.49
1:E:114:ASP:OD1	1:E:115:ASP:N	2.45	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:430:VAL:HG23	1:A:517:SER:HB2	1.93	0.49
1:B:129:THR:HG22	1:B:553:TYR:O	2.13	0.49
1:D:61:ALA:HB1	1:D:62:PRO:CD	2.42	0.49
1:D:395:SER:C	1:D:397:ASP:N	2.71	0.49
1:E:491:SER:O	1:E:492:LEU:O	2.29	0.49
1:A:129:THR:HG22	1:A:553:TYR:O	2.13	0.49
1:A:481:VAL:HG21	1:B:482:TYR:OH	2.13	0.49
1:A:485:LEU:HD11	1:B:486:ILE:HD11	1.95	0.49
1:C:91:PHE:CD2	1:C:91:PHE:N	2.81	0.49
1:C:237:HIS:ND1	1:C:238:PRO:O	2.45	0.49
1:C:243:LEU:HD22	1:C:244:PRO:CD	2.43	0.49
1:E:67:THR:OG1	1:E:68:ARG:N	2.45	0.49
1:B:114:ASP:OD1	1:B:115:ASP:N	2.45	0.49
1:B:243:LEU:CD2	1:B:403:TYR:HD2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:HH11	1:C:130:ASN:HD22	1.55	0.49
1:C:212:THR:HG23	1:C:508:PRO:HB3	1.94	0.49
1:D:258:LEU:HD12	1:D:258:LEU:C	2.37	0.49
1:E:60:LEU:O	1:E:61:ALA:CB	2.59	0.49
1:E:125:THR:HG22	1:E:526:HIS:NE2	2.28	0.49
1:E:135:ASN:HA	1:E:172:GLU:HG2	1.94	0.49
1:E:394:ILE:HG22	1:E:400:PHE:O	2.12	0.49
1:A:114:ASP:OD1	1:A:115:ASP:N	2.45	0.49
1:A:262:ARG:HH11	1:B:130:ASN:HD22	1.56	0.49
1:B:197:ARG:HG3	1:B:198:GLN:HG2	1.93	0.49
1:B:394:ILE:HG22	1:B:400:PHE:O	2.12	0.49
1:C:394:ILE:HG22	1:C:400:PHE:O	2.13	0.49
1:E:129:THR:HG22	1:E:553:TYR:O	2.13	0.49
1:E:243:LEU:HD22	1:E:244:PRO:CD	2.43	0.49
1:A:97:GLN:HG3	1:E:451:PHE:HE1	1.77	0.49
1:A:452:ARG:HE	1:B:98:ASN:ND2	2.08	0.49
1:B:451:PHE:HE1	1:C:97:GLN:HG3	1.76	0.49
1:E:75:LYS:HZ2	1:E:94:THR:HG23	1.78	0.49
1:E:126:ILE:HG23	1:E:523:LEU:HD23	1.94	0.49
1:E:211:ASP:OD1	1:E:213:ARG:HG2	2.13	0.49
1:E:233:ASN:O	1:E:233:ASN:OD1	2.30	0.49
1:A:203:GLU:C	1:A:205:ASP:N	2.70	0.49
1:B:243:LEU:HD22	1:B:244:PRO:CD	2.43	0.49
1:B:430:VAL:HG23	1:B:517:SER:HB2	1.93	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG3	1.94	0.49
1:C:430:VAL:HG23	1:C:517:SER:HB2	1.93	0.49
1:C:468:LEU:HD12	1:C:468:LEU:C	2.38	0.49
1:D:203:GLU:C	1:D:205:ASP:N	2.70	0.49
1:E:449:VAL:HG12	1:E:450:THR:HG23	1.95	0.49
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.94	0.49
1:A:451:PHE:HE2	1:A:462:VAL:HG23	1.78	0.49
1:B:192:TYR:CD2	1:B:193:LEU:HD23	2.47	0.49
1:B:452:ARG:HE	1:C:98:ASN:ND2	2.08	0.49
1:C:427:THR:HG23	1:C:428:PRO:HD2	1.94	0.49
1:D:125:THR:HG22	1:D:526:HIS:NE2	2.28	0.49
1:D:129:THR:HG22	1:D:553:TYR:O	2.13	0.49
1:D:481:VAL:HG21	1:E:482:TYR:OH	2.13	0.49
1:A:212:THR:HG23	1:A:508:PRO:HB3	1.94	0.48
1:A:427:THR:HG23	1:A:428:PRO:HD2	1.94	0.48
1:C:243:LEU:CD2	1:C:403:TYR:HD2	2.24	0.48
1:C:258:LEU:HD12	1:C:258:LEU:C	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG22	1:D:561:VAL:HB	1.95	0.48
1:D:203:GLU:O	1:D:205:ASP:N	2.46	0.48
1:D:214:ASN:HD21	1:D:216:ARG:HG2	1.78	0.48
1:A:391:TYR:O	1:A:392:ASN:C	2.57	0.48
1:A:482:TYR:OH	1:E:481:VAL:HG21	2.12	0.48
1:B:98:ASN:HD22	1:B:99:ASN:N	2.11	0.48
1:B:545:ASP:OD1	1:B:549:ARG:HG2	2.13	0.48
1:C:69:VAL:HG22	1:C:561:VAL:HB	1.95	0.48
1:C:203:GLU:O	1:C:205:ASP:N	2.46	0.48
1:C:449:VAL:HG12	1:C:450:THR:HG23	1.95	0.48
1:D:66:THR:HA	1:D:563:PRO:O	2.13	0.48
1:D:211:ASP:HA	1:D:508:PRO:HG2	1.89	0.48
1:E:203:GLU:O	1:E:205:ASP:N	2.46	0.48
1:E:468:LEU:HD12	1:E:468:LEU:C	2.38	0.48
1:A:125:THR:HG22	1:A:526:HIS:NE2	2.28	0.48
1:A:243:LEU:HD22	1:A:244:PRO:CD	2.43	0.48
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.95	0.48
1:B:237:HIS:ND1	1:B:238:PRO:O	2.45	0.48
1:C:202:LEU:O	1:C:203:GLU:C	2.55	0.48
1:C:211:ASP:OD1	1:C:213:ARG:HG2	2.13	0.48
1:C:292:TYR:HA	1:C:377:PRO:HG3	1.90	0.48
1:C:389:ARG:CD	1:C:502:ASN:HD22	2.23	0.48
1:D:91:PHE:N	1:D:91:PHE:CD2	2.81	0.48
1:A:91:PHE:N	1:A:91:PHE:CD2	2.81	0.48
1:A:154:THR:HG1	1:A:160:GLU:HB2	1.78	0.48
1:A:214:ASN:HD21	1:A:216:ARG:HG2	1.78	0.48
1:C:451:PHE:HE2	1:C:462:VAL:HG23	1.78	0.48
1:C:481:VAL:HG21	1:D:482:TYR:OH	2.12	0.48
1:D:106:ALA:C	1:D:108:THR:N	2.71	0.48
1:D:476:TYR:HD1	1:D:513:ILE:HD12	1.79	0.48
1:D:545:ASP:OD1	1:D:549:ARG:HG2	2.13	0.48
1:A:66:THR:HA	1:A:563:PRO:O	2.14	0.48
1:A:202:LEU:O	1:A:203:GLU:C	2.55	0.48
1:A:258:LEU:HD12	1:A:258:LEU:C	2.37	0.48
1:A:468:LEU:HD12	1:A:468:LEU:C	2.38	0.48
1:A:545:ASP:OD1	1:A:549:ARG:HG2	2.13	0.48
1:B:258:LEU:HD12	1:B:258:LEU:C	2.38	0.48
1:B:444:MET:HB2	1:B:539:GLN:CD	2.39	0.48
1:B:485:LEU:HD11	1:C:486:ILE:HD11	1.94	0.48
1:C:66:THR:HA	1:C:563:PRO:O	2.13	0.48
1:C:126:ILE:HG23	1:C:523:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ARG:HE	1:D:98:ASN:ND2	2.08	0.48
1:D:394:ILE:HG22	1:D:400:PHE:O	2.13	0.48
1:D:444:MET:HB2	1:D:539:GLN:CD	2.39	0.48
1:D:452:ARG:HE	1:E:98:ASN:ND2	2.08	0.48
1:D:468:LEU:HD12	1:D:468:LEU:C	2.38	0.48
1:E:69:VAL:HG22	1:E:561:VAL:HB	1.95	0.48
1:E:212:THR:HG23	1:E:508:PRO:HB3	1.94	0.48
1:E:451:PHE:HE2	1:E:462:VAL:HG23	1.78	0.48
1:A:67:THR:OG1	1:A:68:ARG:N	2.45	0.48
1:A:106:ALA:C	1:A:108:THR:H	2.22	0.48
1:A:444:MET:HB2	1:A:539:GLN:CD	2.39	0.48
1:B:197:ARG:HG3	1:B:198:GLN:HG3	1.94	0.48
1:B:211:ASP:OD1	1:B:213:ARG:HG2	2.13	0.48
1:B:292:TYR:HA	1:B:377:PRO:HG3	1.90	0.48
1:C:129:THR:HG22	1:C:553:TYR:O	2.13	0.48
1:D:485:LEU:HD11	1:E:486:ILE:HD11	1.95	0.48
1:A:111:ILE:HD13	1:E:449:VAL:HG11	1.96	0.48
1:A:243:LEU:CD2	1:A:403:TYR:CE2	2.96	0.48
1:B:66:THR:HA	1:B:563:PRO:O	2.13	0.48
1:B:202:LEU:O	1:B:203:GLU:C	2.55	0.48
1:C:98:ASN:HD22	1:C:99:ASN:N	2.11	0.48
1:C:125:THR:HG22	1:C:526:HIS:NE2	2.28	0.48
1:C:391:TYR:O	1:C:392:ASN:C	2.57	0.48
1:C:545:ASP:OD1	1:C:549:ARG:HG2	2.13	0.48
1:D:243:LEU:HD22	1:D:244:PRO:HD2	1.96	0.48
1:D:538:VAL:HG23	1:D:538:VAL:O	2.14	0.48
1:E:214:ASN:HD21	1:E:216:ARG:HG2	1.78	0.48
1:E:237:HIS:ND1	1:E:238:PRO:O	2.45	0.48
1:E:444:MET:HB2	1:E:539:GLN:CD	2.39	0.48
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.94	0.48
1:A:243:LEU:HD22	1:A:244:PRO:HD2	1.96	0.48
1:B:126:ILE:HG23	1:B:523:LEU:HD23	1.94	0.48
1:E:98:ASN:HD22	1:E:99:ASN:N	2.11	0.48
1:E:243:LEU:HD22	1:E:244:PRO:HD2	1.96	0.48
1:A:389:ARG:CD	1:A:502:ASN:HD22	2.23	0.48
1:A:481:VAL:O	1:A:482:TYR:C	2.57	0.48
1:B:476:TYR:HD1	1:B:513:ILE:HD12	1.79	0.48
1:B:538:VAL:O	1:B:538:VAL:HG23	2.14	0.48
1:D:171:PRO:O	1:D:175:TYR:OH	2.25	0.48
1:E:391:TYR:O	1:E:392:ASN:C	2.57	0.48
1:B:125:THR:HG22	1:B:526:HIS:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HA	1:B:206:ILE:HG13	1.96	0.48
1:B:203:GLU:O	1:B:205:ASP:N	2.46	0.48
1:B:214:ASN:HD21	1:B:216:ARG:HG2	1.79	0.48
1:C:243:LEU:CD2	1:C:403:TYR:CE2	2.96	0.48
1:C:444:MET:HB2	1:C:539:GLN:CD	2.39	0.48
1:D:211:ASP:OD1	1:D:213:ARG:HG2	2.13	0.48
1:E:91:PHE:CD2	1:E:91:PHE:N	2.81	0.48
1:A:130:ASN:HD22	1:E:262:ARG:HH11	1.55	0.47
1:A:203:GLU:O	1:A:205:ASP:N	2.46	0.47
1:A:538:VAL:HG23	1:A:538:VAL:O	2.14	0.47
1:D:106:ALA:C	1:D:108:THR:H	2.22	0.47
1:E:197:ARG:HG3	1:E:198:GLN:HG3	1.94	0.47
1:E:410:TYR:O	1:E:420:ARG:HD3	2.14	0.47
1:E:538:VAL:HG23	1:E:538:VAL:O	2.14	0.47
1:A:83:ASN:OD1	1:A:83:ASN:N	2.26	0.47
1:A:436:GLN:OE1	1:A:436:GLN:N	2.38	0.47
1:A:449:VAL:HG11	1:B:111:ILE:HD13	1.96	0.47
1:B:499:PHE:N	1:B:500:PRO:CD	2.77	0.47
1:C:214:ASN:HD21	1:C:216:ARG:HG2	1.78	0.47
1:C:395:SER:C	1:C:397:ASP:N	2.71	0.47
1:C:410:TYR:O	1:C:420:ARG:HD3	2.14	0.47
1:C:481:VAL:O	1:C:482:TYR:C	2.57	0.47
1:D:430:VAL:CG2	1:D:431:THR:N	2.77	0.47
1:D:449:VAL:HG12	1:D:450:THR:HG23	1.95	0.47
1:D:499:PHE:N	1:D:500:PRO:CD	2.78	0.47
1:D:508:PRO:HA	1:D:509:PRO:HD3	1.73	0.47
1:E:106:ALA:C	1:E:108:THR:H	2.22	0.47
1:E:545:ASP:OD1	1:E:549:ARG:HG2	2.13	0.47
1:A:211:ASP:OD1	1:A:213:ARG:HG2	2.13	0.47
1:A:410:TYR:O	1:A:420:ARG:HD3	2.14	0.47
1:A:431:THR:O	1:A:432:CYS:HB2	2.14	0.47
1:B:243:LEU:HD22	1:B:244:PRO:HD2	1.96	0.47
1:B:431:THR:O	1:B:432:CYS:HB2	2.14	0.47
1:B:451:PHE:HE2	1:B:462:VAL:HG23	1.78	0.47
1:C:243:LEU:HD22	1:C:244:PRO:HD2	1.96	0.47
1:E:65:ASP:O	1:E:66:THR:C	2.58	0.47
1:E:481:VAL:O	1:E:482:TYR:C	2.57	0.47
1:A:203:GLU:HA	1:A:206:ILE:HG13	1.96	0.47
1:A:405:SER:HB3	1:A:408:LEU:HB2	1.97	0.47
1:B:391:TYR:O	1:B:392:ASN:C	2.57	0.47
1:B:430:VAL:CG2	1:B:431:THR:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:MET:HE3	1:B:463:VAL:HG11	1.97	0.47
1:C:154:THR:HG1	1:C:160:GLU:HB2	1.79	0.47
1:C:203:GLU:C	1:C:205:ASP:N	2.70	0.47
1:D:98:ASN:HD22	1:D:99:ASN:N	2.12	0.47
1:E:66:THR:HA	1:E:563:PRO:O	2.14	0.47
1:E:203:GLU:C	1:E:205:ASP:N	2.71	0.47
1:E:476:TYR:HD1	1:E:513:ILE:HD12	1.79	0.47
1:A:430:VAL:CG2	1:A:431:THR:N	2.77	0.47
1:A:499:PHE:N	1:A:500:PRO:CD	2.78	0.47
1:B:468:LEU:HD12	1:B:468:LEU:C	2.38	0.47
1:C:149:VAL:CG2	1:C:195:VAL:HG11	2.45	0.47
1:C:485:LEU:HD11	1:D:486:ILE:HD11	1.94	0.47
1:D:202:LEU:O	1:D:203:GLU:C	2.55	0.47
1:D:216:ARG:HG3	1:D:216:ARG:O	2.15	0.47
1:E:216:ARG:HG3	1:E:216:ARG:O	2.15	0.47
1:E:243:LEU:CD2	1:E:403:TYR:CE2	2.96	0.47
1:A:69:VAL:HG22	1:A:561:VAL:HB	1.95	0.47
1:A:78:ASP:OD1	1:A:94:THR:HG22	2.15	0.47
1:A:98:ASN:HD22	1:A:99:ASN:N	2.11	0.47
1:A:216:ARG:HG3	1:A:216:ARG:O	2.15	0.47
1:A:419:ILE:C	1:A:421:SER:N	2.72	0.47
1:A:476:TYR:HD1	1:A:513:ILE:HD12	1.79	0.47
1:C:65:ASP:O	1:C:66:THR:C	2.58	0.47
1:C:558:LEU:HD23	1:C:558:LEU:HA	1.62	0.47
1:D:405:SER:HB3	1:D:408:LEU:HB2	1.97	0.47
1:D:502:ASN:C	1:D:504:ILE:H	2.23	0.47
1:E:106:ALA:C	1:E:108:THR:N	2.71	0.47
1:B:69:VAL:HG22	1:B:561:VAL:HB	1.95	0.47
1:B:216:ARG:O	1:B:216:ARG:HG3	2.15	0.47
1:B:410:TYR:O	1:B:420:ARG:HD3	2.14	0.47
1:B:449:VAL:HG12	1:B:450:THR:HG23	1.95	0.47
1:B:449:VAL:HG11	1:C:111:ILE:HD13	1.95	0.47
1:B:481:VAL:O	1:B:482:TYR:C	2.57	0.47
1:C:106:ALA:C	1:C:108:THR:H	2.22	0.47
1:C:131:MET:HA	1:C:553:TYR:CD2	2.50	0.47
1:C:449:VAL:HG11	1:D:111:ILE:HD13	1.96	0.47
1:D:67:THR:OG1	1:D:68:ARG:N	2.45	0.47
1:D:131:MET:HA	1:D:553:TYR:CD2	2.50	0.47
1:D:410:TYR:O	1:D:420:ARG:HD3	2.14	0.47
1:E:74:ASN:HD22	1:E:556:LYS:HZ1	1.61	0.47
1:E:180:THR:HG21	1:E:258:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:THR:O	1:E:432:CYS:HB2	2.14	0.47
1:A:445:MET:HE3	1:A:463:VAL:HG11	1.97	0.47
1:C:478:ASP:C	1:C:480:ALA:N	2.73	0.47
1:D:449:VAL:HG11	1:E:111:ILE:HD13	1.96	0.47
1:E:131:MET:HA	1:E:553:TYR:CD2	2.50	0.47
1:E:261:ILE:HD12	1:E:406:TRP:CE3	2.50	0.47
1:A:60:LEU:HD21	1:E:451:PHE:O	2.15	0.47
1:A:106:ALA:C	1:A:108:THR:N	2.71	0.47
1:A:261:ILE:HD12	1:A:406:TRP:CE3	2.50	0.47
1:C:389:ARG:HH11	1:C:389:ARG:CG	2.28	0.47
1:D:451:PHE:HE2	1:D:462:VAL:HG23	1.78	0.47
1:E:389:ARG:HH11	1:E:389:ARG:CG	2.28	0.47
1:E:430:VAL:CG2	1:E:431:THR:N	2.77	0.47
1:A:395:SER:C	1:A:397:ASP:N	2.71	0.47
1:A:502:ASN:C	1:A:504:ILE:H	2.23	0.47
1:B:91:PHE:CD2	1:B:91:PHE:N	2.81	0.47
1:C:78:ASP:OD1	1:C:94:THR:HG22	2.14	0.47
1:C:265:GLN:HA	1:C:266:PRO:HD2	1.57	0.47
1:C:430:VAL:CG2	1:C:431:THR:N	2.78	0.47
1:D:203:GLU:HA	1:D:206:ILE:HG13	1.96	0.47
1:D:389:ARG:HH11	1:D:389:ARG:CG	2.28	0.47
1:E:405:SER:HB3	1:E:408:LEU:HB2	1.97	0.47
1:B:65:ASP:O	1:B:66:THR:C	2.57	0.46
1:B:106:ALA:C	1:B:108:THR:H	2.22	0.46
1:B:131:MET:HA	1:B:553:TYR:CD2	2.50	0.46
1:B:261:ILE:HD12	1:B:406:TRP:CE3	2.50	0.46
1:B:405:SER:HB3	1:B:408:LEU:HB2	1.97	0.46
1:C:203:GLU:HA	1:C:206:ILE:HG13	1.96	0.46
1:D:391:TYR:O	1:D:392:ASN:C	2.57	0.46
1:D:478:ASP:C	1:D:480:ALA:N	2.73	0.46
1:E:178:THR:C	1:E:180:THR:N	2.73	0.46
1:A:131:MET:HA	1:A:553:TYR:CD2	2.50	0.46
1:A:180:THR:O	1:A:181:ILE:C	2.58	0.46
1:A:237:HIS:ND1	1:A:238:PRO:O	2.45	0.46
1:A:450:THR:HG21	1:B:96:ILE:CD1	2.46	0.46
1:A:451:PHE:O	1:B:60:LEU:HD21	2.16	0.46
1:C:106:ALA:C	1:C:108:THR:N	2.71	0.46
1:C:476:TYR:HD1	1:C:513:ILE:HD12	1.79	0.46
1:D:138:MET:HB3	1:D:254:ARG:HH11	1.80	0.46
1:D:197:ARG:O	1:D:199:ASN:N	2.43	0.46
1:D:292:TYR:HA	1:D:377:PRO:HG3	1.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:MET:HE3	1:E:254:ARG:NH1	2.31	0.46
1:A:180:THR:HG21	1:A:258:LEU:HD23	1.97	0.46
1:A:389:ARG:HH11	1:A:389:ARG:CG	2.29	0.46
1:B:83:ASN:OD1	1:B:83:ASN:N	2.26	0.46
1:B:508:PRO:HA	1:B:509:PRO:HD3	1.73	0.46
1:C:180:THR:HG21	1:C:258:LEU:HD23	1.97	0.46
1:D:261:ILE:HD12	1:D:406:TRP:CE3	2.50	0.46
1:E:138:MET:HB3	1:E:254:ARG:HH11	1.80	0.46
1:A:65:ASP:O	1:A:66:THR:C	2.58	0.46
1:A:75:LYS:HZ2	1:A:94:THR:HG23	1.80	0.46
1:A:96:ILE:CD1	1:E:450:THR:HG21	2.46	0.46
1:B:211:ASP:C	1:B:212:THR:HG23	2.41	0.46
1:B:395:SER:C	1:B:397:ASP:N	2.71	0.46
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.71	0.46
1:C:180:THR:O	1:C:181:ILE:C	2.58	0.46
1:C:215:PHE:O	1:C:216:ARG:HB3	2.15	0.46
1:C:431:THR:O	1:C:432:CYS:HB2	2.14	0.46
1:D:78:ASP:OD1	1:D:94:THR:HG22	2.14	0.46
1:E:203:GLU:HA	1:E:206:ILE:HG13	1.96	0.46
1:E:419:ILE:C	1:E:421:SER:N	2.72	0.46
1:A:51:GLY:HA3	1:A:116:ARG:HH12	1.81	0.46
1:A:138:MET:HE3	1:A:254:ARG:NH1	2.31	0.46
1:A:178:THR:C	1:A:180:THR:N	2.73	0.46
1:A:513:ILE:HD12	1:A:513:ILE:N	2.31	0.46
1:B:68:ARG:NH1	1:B:68:ARG:CG	2.66	0.46
1:B:180:THR:O	1:B:181:ILE:C	2.58	0.46
1:B:376:LYS:CB	1:B:377:PRO:HD2	2.32	0.46
1:C:451:PHE:O	1:D:60:LEU:HD21	2.16	0.46
1:D:146:ARG:HE	1:D:246:CYS:HA	1.80	0.46
1:D:383:THR:C	1:D:384:GLU:HG3	2.41	0.46
1:D:410:TYR:CE2	1:E:172:GLU:OE1	2.69	0.46
1:D:450:THR:HG21	1:E:96:ILE:CD1	2.46	0.46
1:D:451:PHE:O	1:E:60:LEU:HD21	2.16	0.46
1:D:481:VAL:O	1:D:482:TYR:C	2.57	0.46
1:E:146:ARG:HE	1:E:246:CYS:HA	1.79	0.46
1:A:427:THR:HA	1:A:428:PRO:HD3	1.75	0.46
1:B:51:GLY:HA3	1:B:116:ARG:HH12	1.81	0.46
1:B:78:ASP:OD1	1:B:94:THR:HG22	2.15	0.46
1:B:180:THR:HG21	1:B:258:LEU:HD23	1.97	0.46
1:B:202:LEU:O	1:B:205:ASP:OD1	2.34	0.46
1:C:51:GLY:HA3	1:C:116:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASP:C	1:C:212:THR:HG23	2.41	0.46
1:C:244:PRO:HA	1:C:275:TYR:CE2	2.51	0.46
1:C:538:VAL:HG23	1:C:538:VAL:O	2.14	0.46
1:E:78:ASP:OD1	1:E:94:THR:HG22	2.14	0.46
1:A:146:ARG:HE	1:A:246:CYS:HA	1.80	0.46
1:A:178:THR:O	1:A:180:THR:N	2.49	0.46
1:A:544:THR:HG23	1:A:549:ARG:N	2.31	0.46
1:B:450:THR:HG21	1:C:96:ILE:CD1	2.45	0.46
1:C:138:MET:HB3	1:C:254:ARG:HH11	1.80	0.46
1:C:146:ARG:HE	1:C:246:CYS:HA	1.80	0.46
1:C:178:THR:O	1:C:180:THR:N	2.49	0.46
1:D:178:THR:O	1:D:180:THR:N	2.49	0.46
1:A:73:ASP:OD1	1:A:73:ASP:N	2.42	0.46
1:A:132:PRO:HD3	1:A:553:TYR:CD2	2.51	0.46
1:B:135:ASN:HB2	1:B:172:GLU:OE2	2.16	0.46
1:B:151:ARG:NH1	1:B:205:ASP:OD2	2.49	0.46
1:B:215:PHE:O	1:B:216:ARG:HB3	2.15	0.46
1:B:287:LEU:HD23	1:B:288:ASP:C	2.41	0.46
1:B:419:ILE:C	1:B:421:SER:N	2.72	0.46
1:C:261:ILE:HD12	1:C:406:TRP:CE3	2.50	0.46
1:C:544:THR:HG23	1:C:549:ARG:N	2.31	0.46
1:E:295:SER:CB	1:E:377:PRO:HG3	2.36	0.46
1:A:135:ASN:HB2	1:A:172:GLU:OE2	2.16	0.46
1:A:138:MET:HB3	1:A:254:ARG:HH11	1.80	0.46
1:A:211:ASP:C	1:A:212:THR:HG23	2.41	0.46
1:A:215:PHE:O	1:A:216:ARG:HB3	2.15	0.46
1:A:287:LEU:HD23	1:A:288:ASP:C	2.41	0.46
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.76	0.46
1:B:146:ARG:HE	1:B:246:CYS:HA	1.80	0.46
1:B:244:PRO:HA	1:B:275:TYR:CE2	2.51	0.46
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.75	0.46
1:C:502:ASN:C	1:C:504:ILE:H	2.23	0.46
1:C:513:ILE:HD12	1:C:513:ILE:N	2.31	0.46
1:D:51:GLY:HA3	1:D:116:ARG:HH12	1.81	0.46
1:D:132:PRO:HD3	1:D:553:TYR:CD2	2.51	0.46
1:D:295:SER:CB	1:D:377:PRO:HG3	2.36	0.46
1:E:202:LEU:O	1:E:205:ASP:OD1	2.34	0.46
1:E:215:PHE:O	1:E:216:ARG:HB3	2.15	0.46
1:E:478:ASP:C	1:E:480:ALA:N	2.73	0.46
1:E:502:ASN:C	1:E:504:ILE:H	2.23	0.46
1:B:106:ALA:C	1:B:108:THR:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:MET:HE3	1:B:254:ARG:NH1	2.31	0.46
1:B:178:THR:O	1:B:180:THR:N	2.49	0.46
1:B:225:LEU:HD22	1:B:285:ALA:O	2.16	0.46
1:B:237:HIS:CD2	1:B:425:LEU:CD1	2.97	0.46
1:B:383:THR:C	1:B:384:GLU:HG3	2.41	0.46
1:B:389:ARG:HH11	1:B:389:ARG:CG	2.28	0.46
1:C:178:THR:C	1:C:180:THR:N	2.73	0.46
1:C:405:SER:HB3	1:C:408:LEU:HB2	1.97	0.46
1:C:499:PHE:N	1:C:500:PRO:CD	2.77	0.46
1:D:135:ASN:HB2	1:D:172:GLU:OE2	2.16	0.46
1:D:202:LEU:O	1:D:205:ASP:OD1	2.34	0.46
1:E:178:THR:O	1:E:180:THR:N	2.49	0.46
1:E:211:ASP:C	1:E:212:THR:HG23	2.41	0.46
1:E:395:SER:C	1:E:397:ASP:N	2.71	0.46
1:E:445:MET:HE3	1:E:463:VAL:HG11	1.97	0.46
1:A:225:LEU:HD22	1:A:285:ALA:O	2.16	0.45
1:B:132:PRO:HD3	1:B:553:TYR:CD2	2.51	0.45
1:B:493:THR:CG2	1:B:494:HIS:N	2.79	0.45
1:B:513:ILE:HD12	1:B:513:ILE:N	2.31	0.45
1:C:151:ARG:NH1	1:C:205:ASP:OD2	2.49	0.45
1:C:216:ARG:HG3	1:C:216:ARG:O	2.15	0.45
1:C:295:SER:CB	1:C:377:PRO:HG3	2.36	0.45
1:C:450:THR:HG21	1:D:96:ILE:CD1	2.46	0.45
1:D:180:THR:O	1:D:181:ILE:C	2.58	0.45
1:D:197:ARG:CG	1:D:198:GLN:H	2.29	0.45
1:D:215:PHE:O	1:D:216:ARG:HB3	2.15	0.45
1:D:244:PRO:HA	1:D:275:TYR:CE2	2.51	0.45
1:E:180:THR:O	1:E:181:ILE:C	2.58	0.45
1:A:93:THR:HG22	1:A:94:THR:O	2.16	0.45
1:A:151:ARG:NH1	1:A:205:ASP:OD2	2.49	0.45
1:A:493:THR:HG22	1:A:494:HIS:O	2.16	0.45
1:B:451:PHE:O	1:C:60:LEU:HD21	2.16	0.45
1:C:135:ASN:HA	1:C:172:GLU:CG	2.46	0.45
1:C:504:ILE:C	1:C:506:ALA:H	2.25	0.45
1:D:138:MET:HE3	1:D:254:ARG:NH1	2.31	0.45
1:D:211:ASP:C	1:D:212:THR:HG23	2.41	0.45
1:D:287:LEU:HD23	1:D:288:ASP:C	2.41	0.45
1:D:431:THR:O	1:D:432:CYS:HB2	2.14	0.45
1:D:544:THR:HG23	1:D:549:ARG:N	2.31	0.45
1:E:244:PRO:HA	1:E:275:TYR:CE2	2.51	0.45
1:E:493:THR:HG22	1:E:494:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:THR:HG23	1:E:549:ARG:N	2.31	0.45
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.75	0.45
1:A:410:TYR:CE2	1:B:172:GLU:OE1	2.69	0.45
1:B:135:ASN:HA	1:B:172:GLU:CG	2.47	0.45
1:B:178:THR:C	1:B:180:THR:N	2.73	0.45
1:C:138:MET:HE3	1:C:254:ARG:NH1	2.31	0.45
1:C:436:GLN:HE21	1:D:558:LEU:HD11	1.81	0.45
1:C:493:THR:HG22	1:C:494:HIS:O	2.16	0.45
1:C:493:THR:CG2	1:C:494:HIS:N	2.80	0.45
1:D:195:VAL:HG12	1:D:196:GLY:N	2.32	0.45
1:D:290:ASP:O	1:D:291:ALA:C	2.60	0.45
1:D:436:GLN:HE21	1:E:558:LEU:HD11	1.81	0.45
1:D:445:MET:HE3	1:D:463:VAL:HG11	1.97	0.45
1:D:493:THR:CG2	1:D:494:HIS:N	2.80	0.45
1:E:135:ASN:HA	1:E:172:GLU:CG	2.46	0.45
1:E:287:LEU:HD23	1:E:288:ASP:C	2.41	0.45
1:A:558:LEU:HD11	1:E:436:GLN:HE21	1.81	0.45
1:B:504:ILE:C	1:B:506:ALA:H	2.24	0.45
1:C:146:ARG:HB2	1:C:165:TRP:CD2	2.52	0.45
1:C:197:ARG:CG	1:C:198:GLN:H	2.29	0.45
1:C:445:MET:HE3	1:C:463:VAL:HG11	1.97	0.45
1:D:178:THR:C	1:D:180:THR:N	2.73	0.45
1:E:51:GLY:HA3	1:E:116:ARG:HH12	1.81	0.45
1:E:93:THR:HG22	1:E:94:THR:O	2.16	0.45
1:A:135:ASN:HA	1:A:172:GLU:CG	2.47	0.45
1:A:295:SER:CB	1:A:377:PRO:HG3	2.36	0.45
1:A:383:THR:C	1:A:384:GLU:HG3	2.41	0.45
1:B:135:ASN:N	1:B:140:THR:OG1	2.47	0.45
1:B:265:GLN:HA	1:B:266:PRO:HD2	1.57	0.45
1:B:436:GLN:HE21	1:C:558:LEU:HD11	1.81	0.45
1:B:502:ASN:C	1:B:504:ILE:H	2.23	0.45
1:C:68:ARG:NH1	1:C:68:ARG:CG	2.66	0.45
1:C:202:LEU:O	1:C:205:ASP:OD1	2.34	0.45
1:C:225:LEU:HD22	1:C:285:ALA:O	2.16	0.45
1:C:237:HIS:CD2	1:C:425:LEU:CD1	2.97	0.45
1:C:383:THR:C	1:C:384:GLU:HG3	2.41	0.45
1:D:135:ASN:HA	1:D:172:GLU:CG	2.47	0.45
1:D:146:ARG:HB2	1:D:165:TRP:CD2	2.52	0.45
1:D:170:LEU:HB3	1:D:171:PRO:HD2	1.99	0.45
1:D:225:LEU:HD22	1:D:285:ALA:O	2.16	0.45
1:D:446:GLN:O	1:D:448:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:LEU:HB3	1:E:171:PRO:HD2	1.99	0.45
1:E:195:VAL:HG12	1:E:196:GLY:N	2.32	0.45
1:E:225:LEU:HD22	1:E:285:ALA:O	2.16	0.45
1:A:146:ARG:HB2	1:A:165:TRP:CD2	2.52	0.45
1:A:202:LEU:O	1:A:205:ASP:OD1	2.34	0.45
1:B:93:THR:HG22	1:B:94:THR:O	2.16	0.45
1:B:243:LEU:CD2	1:B:403:TYR:CE2	2.96	0.45
1:B:529:LEU:HD21	1:C:68:ARG:HE	1.82	0.45
1:D:151:ARG:NH1	1:D:205:ASP:OD2	2.49	0.45
1:E:135:ASN:HB2	1:E:172:GLU:OE2	2.16	0.45
1:E:383:THR:C	1:E:384:GLU:HG3	2.41	0.45
1:A:436:GLN:HE21	1:B:558:LEU:HD11	1.81	0.45
1:B:527:GLY:HA3	1:C:68:ARG:NH2	2.32	0.45
1:C:132:PRO:HD3	1:C:553:TYR:CD2	2.51	0.45
1:C:463:VAL:HB	1:C:529:LEU:HD13	1.99	0.45
1:D:180:THR:HG21	1:D:258:LEU:HD23	1.97	0.45
1:D:243:LEU:HD23	1:D:244:PRO:HD3	1.99	0.45
1:D:419:ILE:C	1:D:421:SER:N	2.72	0.45
1:D:513:ILE:HD12	1:D:513:ILE:N	2.31	0.45
1:E:132:PRO:HD3	1:E:553:TYR:CD2	2.51	0.45
1:E:446:GLN:O	1:E:448:PRO:HD3	2.17	0.45
1:E:499:PHE:N	1:E:500:PRO:CD	2.77	0.45
1:A:446:GLN:O	1:A:448:PRO:HD3	2.17	0.45
1:B:197:ARG:CG	1:B:198:GLN:H	2.30	0.45
1:B:544:THR:HG23	1:B:549:ARG:N	2.31	0.45
1:C:135:ASN:HB2	1:C:172:GLU:OE2	2.16	0.45
1:C:436:GLN:OE1	1:C:436:GLN:N	2.38	0.45
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.82	0.45
1:D:250:PHE:O	1:D:252:HIS:N	2.50	0.45
1:E:513:ILE:HD12	1:E:513:ILE:N	2.31	0.45
1:E:525:ASP:OD1	1:E:525:ASP:O	2.35	0.45
1:A:243:LEU:HD23	1:A:244:PRO:HD3	1.99	0.45
1:A:292:TYR:HA	1:A:377:PRO:HG3	1.91	0.45
1:B:195:VAL:HG12	1:B:196:GLY:N	2.32	0.45
1:B:290:ASP:O	1:B:291:ALA:C	2.60	0.45
1:C:287:LEU:HD23	1:C:288:ASP:C	2.41	0.45
1:D:525:ASP:OD1	1:D:525:ASP:O	2.35	0.45
1:E:493:THR:CG2	1:E:494:HIS:N	2.80	0.45
1:B:49:THR:O	1:B:50:GLY:C	2.60	0.45
1:B:129:THR:HB	1:B:130:ASN:H	1.65	0.45
1:B:138:MET:HB3	1:B:254:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:CG2	1:B:195:VAL:HG11	2.45	0.45
1:C:195:VAL:HG12	1:C:196:GLY:N	2.32	0.45
1:C:225:LEU:HD13	1:C:287:LEU:HA	1.99	0.45
1:C:419:ILE:C	1:C:421:SER:N	2.72	0.45
1:C:533:ASN:OD1	1:C:533:ASN:N	2.50	0.45
1:D:65:ASP:O	1:D:66:THR:C	2.57	0.45
1:D:529:LEU:HD21	1:E:68:ARG:HE	1.82	0.45
1:E:290:ASP:O	1:E:291:ALA:C	2.60	0.45
1:E:476:TYR:HD1	1:E:513:ILE:CD1	2.30	0.45
1:A:75:LYS:NZ	1:A:94:THR:HG23	2.33	0.44
1:A:197:ARG:O	1:A:199:ASN:N	2.43	0.44
1:A:250:PHE:O	1:A:252:HIS:N	2.50	0.44
1:A:525:ASP:OD1	1:A:525:ASP:O	2.35	0.44
1:B:146:ARG:HB2	1:B:165:TRP:CD2	2.52	0.44
1:B:170:LEU:HB3	1:B:171:PRO:HD2	1.99	0.44
1:B:295:SER:CB	1:B:377:PRO:HG3	2.36	0.44
1:B:493:THR:HG22	1:B:494:HIS:O	2.16	0.44
1:C:49:THR:O	1:C:50:GLY:C	2.60	0.44
1:C:217:LEU:CB	1:C:232:THR:HG21	2.46	0.44
1:C:525:ASP:OD1	1:C:525:ASP:O	2.35	0.44
1:D:504:ILE:C	1:D:506:ALA:H	2.25	0.44
1:E:151:ARG:NH1	1:E:205:ASP:OD2	2.49	0.44
1:A:172:GLU:OE1	1:E:410:TYR:CE2	2.68	0.44
1:C:229:GLY:O	1:C:286:LEU:HD13	2.18	0.44
1:D:493:THR:HG22	1:D:494:HIS:O	2.16	0.44
1:E:250:PHE:O	1:E:252:HIS:N	2.50	0.44
1:E:389:ARG:CD	1:E:502:ASN:HD22	2.23	0.44
1:E:420:ARG:HG3	1:E:420:ARG:O	2.17	0.44
1:E:533:ASN:OD1	1:E:533:ASN:N	2.50	0.44
1:A:476:TYR:HD1	1:A:513:ILE:CD1	2.30	0.44
1:A:529:LEU:HD21	1:B:68:ARG:HE	1.82	0.44
1:B:225:LEU:HD13	1:B:287:LEU:HA	2.00	0.44
1:B:229:GLY:O	1:B:286:LEU:HD13	2.18	0.44
1:C:230:VAL:HG13	1:C:503:GLN:CD	2.43	0.44
1:D:217:LEU:CB	1:D:232:THR:HG21	2.46	0.44
1:D:389:ARG:CD	1:D:502:ASN:HD22	2.23	0.44
1:E:68:ARG:NH1	1:E:68:ARG:CG	2.66	0.44
1:E:75:LYS:NZ	1:E:94:THR:HG23	2.32	0.44
1:E:243:LEU:HD23	1:E:244:PRO:HD3	1.99	0.44
1:E:504:ILE:C	1:E:506:ALA:H	2.25	0.44
1:A:229:GLY:O	1:A:286:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HH21	1:A:432:CYS:C	2.26	0.44
1:A:533:ASN:OD1	1:A:533:ASN:N	2.50	0.44
1:B:243:LEU:HD23	1:B:244:PRO:HD3	1.99	0.44
1:B:476:TYR:HD1	1:B:513:ILE:CD1	2.30	0.44
1:C:75:LYS:NZ	1:C:94:THR:HG23	2.32	0.44
1:C:93:THR:HG22	1:C:94:THR:O	2.17	0.44
1:C:254:ARG:HH21	1:C:432:CYS:C	2.26	0.44
1:C:262:ARG:NH1	1:D:130:ASN:ND2	2.55	0.44
1:C:410:TYR:CE2	1:D:172:GLU:OE1	2.68	0.44
1:C:527:GLY:HA3	1:D:68:ARG:NH2	2.32	0.44
1:D:265:GLN:HA	1:D:266:PRO:HD2	1.57	0.44
1:E:63:LEU:HA	1:E:63:LEU:HD12	1.82	0.44
1:A:195:VAL:HG12	1:A:196:GLY:N	2.32	0.44
1:A:429:ASP:OD1	1:A:432:CYS:N	2.51	0.44
1:B:250:PHE:O	1:B:252:HIS:N	2.50	0.44
1:B:446:GLN:O	1:B:448:PRO:HD3	2.17	0.44
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.82	0.44
1:C:250:PHE:O	1:C:252:HIS:N	2.50	0.44
1:C:290:ASP:O	1:C:291:ALA:C	2.60	0.44
1:D:93:THR:HG22	1:D:94:THR:O	2.17	0.44
1:D:230:VAL:HG13	1:D:503:GLN:CD	2.43	0.44
1:D:295:SER:O	1:D:296:LEU:CB	2.64	0.44
1:D:429:ASP:OD1	1:D:432:CYS:N	2.51	0.44
1:E:146:ARG:HB2	1:E:165:TRP:CD2	2.52	0.44
1:E:229:GLY:O	1:E:286:LEU:HD13	2.18	0.44
1:B:558:LEU:HA	1:B:558:LEU:HD23	1.62	0.44
1:C:243:LEU:HD23	1:C:244:PRO:HD3	1.99	0.44
1:D:75:LYS:NZ	1:D:94:THR:HG23	2.32	0.44
1:A:560:ILE:HD11	1:E:465:ALA:HB3	2.00	0.44
1:B:261:ILE:HD12	1:B:406:TRP:CZ3	2.53	0.44
1:B:436:GLN:OE1	1:B:436:GLN:N	2.39	0.44
1:B:463:VAL:HB	1:B:529:LEU:HD13	1.99	0.44
1:B:478:ASP:C	1:B:480:ALA:N	2.73	0.44
1:C:264:ARG:HG3	1:C:264:ARG:O	2.18	0.44
1:E:128:HIS:HD2	1:E:555:TYR:HD2	1.66	0.44
1:A:68:ARG:HE	1:E:529:LEU:HD21	1.82	0.44
1:A:83:ASN:ND2	1:A:92:LEU:O	2.51	0.44
1:A:197:ARG:CG	1:A:198:GLN:H	2.30	0.44
1:B:420:ARG:HG3	1:B:420:ARG:O	2.17	0.44
1:C:83:ASN:ND2	1:C:92:LEU:O	2.51	0.44
1:C:128:HIS:HD2	1:C:555:TYR:HD2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:O	1:C:420:ARG:HG3	2.17	0.44
1:D:533:ASN:OD1	1:D:533:ASN:N	2.50	0.44
1:E:225:LEU:HD13	1:E:287:LEU:HA	1.99	0.44
1:E:261:ILE:HD12	1:E:406:TRP:CZ3	2.53	0.44
1:A:68:ARG:NH2	1:E:527:GLY:HA3	2.32	0.44
1:A:170:LEU:HB3	1:A:171:PRO:HD2	1.99	0.44
1:A:478:ASP:C	1:A:480:ALA:N	2.73	0.44
1:C:170:LEU:HB3	1:C:171:PRO:HD2	1.99	0.44
1:C:446:GLN:O	1:C:448:PRO:HD3	2.17	0.44
1:D:154:THR:HG1	1:D:160:GLU:HB2	1.79	0.44
1:E:83:ASN:ND2	1:E:92:LEU:O	2.51	0.44
1:A:130:ASN:ND2	1:E:262:ARG:NH1	2.55	0.43
1:A:230:VAL:HG13	1:A:503:GLN:CD	2.43	0.43
1:A:493:THR:CG2	1:A:494:HIS:N	2.79	0.43
1:A:527:GLY:HA3	1:B:68:ARG:NH2	2.32	0.43
1:B:467:LEU:HD12	1:B:467:LEU:HA	1.83	0.43
1:B:525:ASP:OD1	1:B:525:ASP:O	2.35	0.43
1:C:261:ILE:HD12	1:C:406:TRP:CZ3	2.53	0.43
1:D:83:ASN:ND2	1:D:92:LEU:O	2.51	0.43
1:D:135:ASN:N	1:D:140:THR:OG1	2.47	0.43
1:D:420:ARG:HG3	1:D:420:ARG:O	2.17	0.43
1:E:436:GLN:OE1	1:E:436:GLN:N	2.39	0.43
1:A:225:LEU:HD13	1:A:287:LEU:HA	1.99	0.43
1:A:264:ARG:HG3	1:A:264:ARG:O	2.18	0.43
1:B:533:ASN:OD1	1:B:533:ASN:N	2.50	0.43
1:C:202:LEU:C	1:C:204:SER:N	2.75	0.43
1:D:49:THR:O	1:D:50:GLY:C	2.60	0.43
1:D:261:ILE:HD12	1:D:406:TRP:CZ3	2.53	0.43
1:D:527:GLY:HA3	1:E:68:ARG:NH2	2.33	0.43
1:E:74:ASN:ND2	1:E:556:LYS:NZ	2.66	0.43
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.51	0.43
1:A:290:ASP:O	1:A:291:ALA:C	2.60	0.43
1:A:393:LEU:N	1:A:393:LEU:CD1	2.81	0.43
1:A:467:LEU:HD13	1:B:126:ILE:HG21	2.01	0.43
1:B:83:ASN:ND2	1:B:92:LEU:O	2.51	0.43
1:C:429:ASP:OD1	1:C:432:CYS:N	2.51	0.43
1:C:524:THR:OG1	1:C:525:ASP:N	2.52	0.43
1:D:211:ASP:CG	1:D:212:THR:N	2.77	0.43
1:D:254:ARG:HH21	1:D:432:CYS:C	2.26	0.43
1:A:49:THR:O	1:A:50:GLY:C	2.60	0.43
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:VAL:C	1:B:471:HIS:HD2	2.27	0.43
1:D:225:LEU:HD13	1:D:287:LEU:HA	1.99	0.43
1:D:262:ARG:HH11	1:E:130:ASN:HD22	1.55	0.43
1:E:49:THR:O	1:E:50:GLY:C	2.60	0.43
1:E:197:ARG:CG	1:E:198:GLN:H	2.29	0.43
1:A:237:HIS:CD2	1:A:425:LEU:CD1	2.97	0.43
1:A:504:ILE:C	1:A:506:ALA:H	2.25	0.43
1:B:411:ASN:OD1	1:C:172:GLU:N	2.52	0.43
1:B:467:LEU:HD13	1:C:126:ILE:HG21	2.00	0.43
1:B:497:ASN:O	1:B:500:PRO:HD3	2.19	0.43
1:C:436:GLN:CD	1:D:556:LYS:HZ3	2.27	0.43
1:D:229:GLY:O	1:D:286:LEU:HD13	2.18	0.43
1:E:211:ASP:CG	1:E:212:THR:N	2.77	0.43
1:E:230:VAL:HG13	1:E:503:GLN:CD	2.43	0.43
1:E:268:GLN:O	1:E:269:GLU:C	2.61	0.43
1:A:497:ASN:O	1:A:500:PRO:HD3	2.19	0.43
1:A:524:THR:OG1	1:A:525:ASP:N	2.52	0.43
1:A:527:GLY:HA3	1:B:68:ARG:HH21	1.84	0.43
1:B:227:MET:C	1:B:229:GLY:H	2.27	0.43
1:B:393:LEU:N	1:B:393:LEU:CD1	2.81	0.43
1:B:465:ALA:HB3	1:C:560:ILE:HD11	2.00	0.43
1:C:476:TYR:HD1	1:C:513:ILE:CD1	2.30	0.43
1:C:527:GLY:HA3	1:D:68:ARG:HH21	1.84	0.43
1:E:149:VAL:CG2	1:E:195:VAL:HG11	2.45	0.43
1:A:68:ARG:NH1	1:A:562:SER:CB	2.79	0.43
1:A:419:ILE:O	1:A:421:SER:N	2.52	0.43
1:A:429:ASP:OD1	1:A:429:ASP:C	2.62	0.43
1:A:508:PRO:HA	1:A:509:PRO:HD3	1.73	0.43
1:B:254:ARG:HH21	1:B:432:CYS:C	2.26	0.43
1:B:262:ARG:NH1	1:C:130:ASN:ND2	2.55	0.43
1:B:429:ASP:OD1	1:B:432:CYS:N	2.51	0.43
1:D:463:VAL:HB	1:D:529:LEU:HD13	1.99	0.43
1:E:254:ARG:HH21	1:E:432:CYS:C	2.26	0.43
1:E:427:THR:HA	1:E:428:PRO:HD3	1.75	0.43
1:A:126:ILE:HG21	1:E:467:LEU:HD13	2.00	0.43
1:A:406:TRP:O	1:A:407:TYR:C	2.62	0.43
1:B:230:VAL:HG13	1:B:503:GLN:CD	2.43	0.43
1:C:195:VAL:O	1:C:196:GLY:C	2.62	0.43
1:C:429:ASP:OD1	1:C:429:ASP:C	2.62	0.43
1:C:465:ALA:HB3	1:D:560:ILE:HD11	2.00	0.43
1:C:529:LEU:HD21	1:D:68:ARG:HE	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LEU:CD2	1:D:403:TYR:CE2	2.96	0.43
1:D:436:GLN:OE1	1:D:436:GLN:N	2.38	0.43
1:E:264:ARG:HG3	1:E:264:ARG:O	2.18	0.43
1:A:202:LEU:C	1:A:204:SER:N	2.75	0.43
1:A:420:ARG:O	1:A:420:ARG:HG3	2.17	0.43
1:D:227:MET:C	1:D:229:GLY:H	2.27	0.43
1:D:393:LEU:N	1:D:393:LEU:CD1	2.81	0.43
1:D:406:TRP:O	1:D:407:TYR:C	2.62	0.43
1:E:154:THR:HG1	1:E:160:GLU:HB2	1.79	0.43
1:E:217:LEU:CB	1:E:232:THR:HG21	2.46	0.43
1:E:463:VAL:HB	1:E:529:LEU:HD13	1.99	0.43
1:A:128:HIS:HD2	1:A:555:TYR:HD2	1.66	0.43
1:A:214:ASN:O	1:A:216:ARG:N	2.50	0.43
1:A:261:ILE:HD12	1:A:406:TRP:CZ3	2.53	0.43
1:B:264:ARG:HG3	1:B:264:ARG:O	2.18	0.43
1:B:524:THR:OG1	1:B:525:ASP:N	2.52	0.43
1:C:197:ARG:O	1:C:199:ASN:N	2.43	0.43
1:C:227:MET:C	1:C:229:GLY:H	2.27	0.43
1:C:406:TRP:O	1:C:407:TYR:C	2.61	0.43
1:D:195:VAL:O	1:D:196:GLY:C	2.62	0.43
1:D:264:ARG:HG3	1:D:264:ARG:O	2.18	0.43
1:D:429:ASP:OD1	1:D:429:ASP:C	2.62	0.43
1:E:68:ARG:NH1	1:E:562:SER:CB	2.79	0.43
1:E:275:TYR:CE1	1:E:404:ARG:HD2	2.54	0.43
1:E:419:ILE:O	1:E:421:SER:N	2.52	0.43
1:A:227:MET:C	1:A:229:GLY:H	2.27	0.42
1:A:279:GLU:O	1:A:280:GLY:O	2.38	0.42
1:A:556:LYS:HZ3	1:E:436:GLN:CD	2.27	0.42
1:B:527:GLY:HA3	1:C:68:ARG:HH21	1.84	0.42
1:C:194:LYS:O	1:C:194:LYS:HG2	2.19	0.42
1:C:419:ILE:O	1:C:421:SER:N	2.52	0.42
1:D:394:ILE:HG23	1:D:395:SER:N	2.34	0.42
1:E:265:GLN:HA	1:E:266:PRO:HD2	1.57	0.42
1:E:497:ASN:O	1:E:500:PRO:HD3	2.19	0.42
1:A:451:PHE:CE1	1:B:97:GLN:CB	3.03	0.42
1:A:470:VAL:C	1:A:471:HIS:HD2	2.27	0.42
1:B:419:ILE:O	1:B:421:SER:N	2.52	0.42
1:D:68:ARG:NH1	1:D:562:SER:CB	2.79	0.42
1:D:275:TYR:CE1	1:D:404:ARG:HD2	2.54	0.42
1:D:470:VAL:C	1:D:471:HIS:HD2	2.27	0.42
1:D:476:TYR:HD1	1:D:513:ILE:CD1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ASP:OD1	1:E:429:ASP:C	2.62	0.42
1:C:268:GLN:O	1:C:269:GLU:C	2.61	0.42
1:C:411:ASN:OD1	1:D:172:GLU:N	2.51	0.42
1:C:430:VAL:O	1:C:432:CYS:N	2.53	0.42
1:C:467:LEU:HD12	1:C:467:LEU:HA	1.83	0.42
1:D:128:HIS:HD2	1:D:555:TYR:HD2	1.66	0.42
1:D:278:LEU:CD2	1:D:419:ILE:HD12	2.38	0.42
1:A:53:ASN:O	1:A:54:SER:O	2.38	0.42
1:B:75:LYS:NZ	1:B:94:THR:HG23	2.32	0.42
1:B:128:HIS:HD2	1:B:555:TYR:HD2	1.66	0.42
1:B:389:ARG:CD	1:B:502:ASN:HD22	2.23	0.42
1:B:410:TYR:CE2	1:C:172:GLU:OE1	2.68	0.42
1:C:497:ASN:O	1:C:500:PRO:HD3	2.19	0.42
1:D:149:VAL:CG2	1:D:195:VAL:HG11	2.45	0.42
1:D:411:ASN:OD1	1:E:172:GLU:N	2.52	0.42
1:E:203:GLU:H	1:E:203:GLU:HG2	1.69	0.42
1:A:172:GLU:N	1:E:411:ASN:OD1	2.52	0.42
1:B:178:THR:O	1:B:179:MET:C	2.63	0.42
1:B:451:PHE:CE1	1:C:97:GLN:CB	3.03	0.42
1:C:393:LEU:N	1:C:393:LEU:CD1	2.81	0.42
1:C:470:VAL:C	1:C:471:HIS:HD2	2.27	0.42
1:D:419:ILE:O	1:D:421:SER:N	2.52	0.42
1:E:237:HIS:CD2	1:E:425:LEU:CD1	2.97	0.42
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.62	0.42
1:B:194:LYS:O	1:B:194:LYS:HG2	2.19	0.42
1:B:211:ASP:CG	1:B:212:THR:N	2.77	0.42
1:B:230:VAL:HG13	1:B:503:GLN:NE2	2.35	0.42
1:B:275:TYR:CE1	1:B:404:ARG:HD2	2.54	0.42
1:B:295:SER:O	1:B:296:LEU:CB	2.64	0.42
1:B:406:TRP:O	1:B:407:TYR:C	2.62	0.42
1:C:230:VAL:HG13	1:C:503:GLN:NE2	2.35	0.42
1:C:275:TYR:CE1	1:C:404:ARG:HD2	2.54	0.42
1:D:93:THR:CG2	1:D:94:THR:N	2.83	0.42
1:D:230:VAL:HG13	1:D:503:GLN:NE2	2.35	0.42
1:E:53:ASN:O	1:E:54:SER:O	2.38	0.42
1:E:93:THR:CG2	1:E:94:THR:N	2.83	0.42
1:E:135:ASN:N	1:E:140:THR:OG1	2.47	0.42
1:E:230:VAL:HG13	1:E:503:GLN:NE2	2.35	0.42
1:E:406:TRP:O	1:E:407:TYR:C	2.62	0.42
1:A:98:ASN:ND2	1:A:98:ASN:C	2.78	0.42
1:A:230:VAL:HG13	1:A:503:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:HB3	1:B:560:ILE:HD11	2.00	0.42
1:B:237:HIS:NE2	1:B:425:LEU:CD1	2.83	0.42
1:C:211:ASP:CG	1:C:212:THR:N	2.77	0.42
1:D:279:GLU:O	1:D:280:GLY:O	2.37	0.42
1:D:467:LEU:HD13	1:E:126:ILE:HG21	2.01	0.42
1:D:524:THR:OG1	1:D:525:ASP:N	2.52	0.42
1:D:527:GLY:HA3	1:E:68:ARG:HH21	1.84	0.42
1:E:145:ALA:HB3	1:E:168:PHE:CE1	2.44	0.42
1:E:178:THR:O	1:E:179:MET:C	2.63	0.42
1:E:470:VAL:C	1:E:471:HIS:HD2	2.27	0.42
1:A:153:LEU:O	1:A:154:THR:C	2.62	0.42
1:A:411:ASN:OD1	1:B:172:GLU:N	2.52	0.42
1:A:430:VAL:O	1:A:432:CYS:N	2.53	0.42
1:B:202:LEU:C	1:B:204:SER:N	2.75	0.42
1:C:279:GLU:O	1:C:280:GLY:O	2.38	0.42
1:D:406:TRP:HE1	1:D:419:ILE:HG21	1.85	0.42
1:D:451:PHE:CE1	1:E:97:GLN:CB	3.03	0.42
1:D:465:ALA:HB3	1:E:560:ILE:HD11	2.00	0.42
1:D:497:ASN:O	1:D:500:PRO:HD3	2.19	0.42
1:E:475:PHE:CD1	1:E:475:PHE:N	2.88	0.42
1:A:68:ARG:HH21	1:E:527:GLY:HA3	1.84	0.42
1:B:195:VAL:O	1:B:196:GLY:C	2.62	0.42
1:B:197:ARG:O	1:B:199:ASN:N	2.43	0.42
1:B:279:GLU:O	1:B:280:GLY:O	2.38	0.42
1:C:178:THR:O	1:C:179:MET:C	2.63	0.42
1:D:53:ASN:O	1:D:54:SER:O	2.38	0.42
1:E:153:LEU:O	1:E:154:THR:C	2.62	0.42
1:E:194:LYS:O	1:E:194:LYS:HG2	2.19	0.42
1:E:202:LEU:C	1:E:204:SER:N	2.75	0.42
1:E:227:MET:C	1:E:229:GLY:H	2.27	0.42
1:A:237:HIS:NE2	1:A:425:LEU:CD1	2.83	0.42
1:B:68:ARG:NH1	1:B:562:SER:CB	2.79	0.42
1:B:475:PHE:N	1:B:475:PHE:CD1	2.88	0.42
1:C:406:TRP:HE1	1:C:419:ILE:HG21	1.85	0.42
1:C:467:LEU:HD13	1:D:126:ILE:HG21	2.01	0.42
1:D:194:LYS:O	1:D:194:LYS:HG2	2.19	0.42
1:D:237:HIS:NE2	1:D:425:LEU:CD1	2.83	0.42
1:E:430:VAL:O	1:E:432:CYS:N	2.53	0.42
1:E:501:GLU:O	1:E:501:GLU:HG2	2.20	0.42
1:E:524:THR:OG1	1:E:525:ASP:N	2.52	0.42
1:A:149:VAL:CG2	1:A:195:VAL:HG11	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:O	1:A:382:LEU:C	2.63	0.41
1:B:507:ARG:O	1:B:508:PRO:C	2.63	0.41
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.66	0.41
1:D:129:THR:HB	1:D:130:ASN:H	1.65	0.41
1:D:202:LEU:C	1:D:204:SER:N	2.75	0.41
1:E:131:MET:HA	1:E:132:PRO:HD3	1.87	0.41
1:E:381:PRO:O	1:E:382:LEU:C	2.63	0.41
1:E:507:ARG:O	1:E:508:PRO:C	2.63	0.41
1:A:194:LYS:HG2	1:A:194:LYS:O	2.19	0.41
1:A:195:VAL:O	1:A:196:GLY:C	2.62	0.41
1:B:53:ASN:O	1:B:54:SER:O	2.38	0.41
1:B:154:THR:HG1	1:B:160:GLU:HB2	1.83	0.41
1:B:394:ILE:HG23	1:B:395:SER:N	2.34	0.41
1:B:406:TRP:HE1	1:B:419:ILE:HG21	1.85	0.41
1:B:429:ASP:OD1	1:B:429:ASP:C	2.62	0.41
1:B:430:VAL:O	1:B:432:CYS:N	2.53	0.41
1:B:468:LEU:HA	1:B:469:PRO:HD3	1.76	0.41
1:C:266:PRO:C	1:C:268:GLN:N	2.78	0.41
1:D:430:VAL:O	1:D:432:CYS:N	2.53	0.41
1:E:195:VAL:O	1:E:196:GLY:C	2.62	0.41
1:E:279:GLU:O	1:E:280:GLY:O	2.38	0.41
1:E:376:LYS:CB	1:E:377:PRO:HD2	2.32	0.41
1:A:275:TYR:CE1	1:A:404:ARG:HD2	2.54	0.41
1:B:93:THR:CG2	1:B:94:THR:N	2.83	0.41
1:B:266:PRO:C	1:B:268:GLN:N	2.79	0.41
1:B:450:THR:HG21	1:C:96:ILE:HD13	2.03	0.41
1:C:153:LEU:O	1:C:154:THR:C	2.62	0.41
1:C:214:ASN:O	1:C:216:ARG:N	2.50	0.41
1:C:419:ILE:HG22	1:C:423:THR:HG22	2.02	0.41
1:C:451:PHE:CE1	1:D:97:GLN:CB	3.03	0.41
1:E:149:VAL:O	1:E:149:VAL:HG22	2.21	0.41
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.92	0.41
1:E:406:TRP:HE1	1:E:419:ILE:HG21	1.85	0.41
1:B:88:HIS:CD2	1:B:555:TYR:O	2.74	0.41
1:B:268:GLN:O	1:B:269:GLU:C	2.61	0.41
1:C:135:ASN:N	1:C:140:THR:OG1	2.47	0.41
1:C:237:HIS:NE2	1:C:425:LEU:CD1	2.83	0.41
1:C:501:GLU:O	1:C:501:GLU:HG2	2.20	0.41
1:D:268:GLN:O	1:D:269:GLU:C	2.61	0.41
1:D:501:GLU:HG2	1:D:501:GLU:O	2.20	0.41
1:D:530:PRO:HG3	1:E:66:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:HIS:NE2	1:E:425:LEU:CD1	2.83	0.41
1:A:135:ASN:N	1:A:140:THR:OG1	2.47	0.41
1:B:67:THR:OG1	1:B:68:ARG:N	2.45	0.41
1:C:88:HIS:CD2	1:C:555:TYR:O	2.74	0.41
1:C:381:PRO:O	1:C:382:LEU:C	2.63	0.41
1:C:382:LEU:HA	1:C:382:LEU:HD12	1.75	0.41
1:D:214:ASN:O	1:D:216:ARG:N	2.50	0.41
1:D:265:GLN:NE2	1:D:268:GLN:NE2	2.68	0.41
1:D:382:LEU:HD12	1:D:382:LEU:HA	1.75	0.41
1:B:530:PRO:HG3	1:C:66:THR:O	2.21	0.41
1:C:211:ASP:OD1	1:C:212:THR:N	2.35	0.41
1:C:475:PHE:CD1	1:C:475:PHE:N	2.88	0.41
1:E:197:ARG:O	1:E:199:ASN:N	2.43	0.41
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.91	0.41
1:E:266:PRO:C	1:E:268:GLN:N	2.78	0.41
1:E:508:PRO:HA	1:E:509:PRO:HD3	1.73	0.41
1:A:153:LEU:HD23	1:A:159:VAL:HG12	2.03	0.41
1:A:203:GLU:H	1:A:203:GLU:HG2	1.69	0.41
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.85	0.41
1:A:419:ILE:HG22	1:A:423:THR:HG22	2.02	0.41
1:A:430:VAL:HG23	1:A:431:THR:N	2.36	0.41
1:A:530:PRO:HG3	1:B:66:THR:O	2.21	0.41
1:C:149:VAL:HG22	1:C:149:VAL:O	2.21	0.41
1:C:265:GLN:NE2	1:C:268:GLN:NE2	2.68	0.41
1:E:214:ASN:O	1:E:216:ARG:N	2.50	0.41
1:E:265:GLN:NE2	1:E:268:GLN:NE2	2.68	0.41
1:E:393:LEU:N	1:E:393:LEU:CD1	2.81	0.41
1:E:429:ASP:OD1	1:E:432:CYS:N	2.51	0.41
1:E:441:LEU:HD12	1:E:445:MET:CE	2.48	0.41
1:A:97:GLN:CB	1:E:451:PHE:CE1	3.03	0.41
1:A:475:PHE:CD1	1:A:475:PHE:N	2.88	0.41
1:B:214:ASN:O	1:B:216:ARG:N	2.50	0.41
1:C:180:THR:HG21	1:C:258:LEU:HD21	2.03	0.41
1:C:430:VAL:HG23	1:C:431:THR:N	2.36	0.41
1:C:450:THR:HG21	1:D:96:ILE:HD13	2.03	0.41
1:D:507:ARG:O	1:D:508:PRO:C	2.63	0.41
1:E:113:LEU:HD23	1:E:113:LEU:HA	1.71	0.41
1:A:93:THR:CG2	1:A:94:THR:N	2.83	0.41
1:A:96:ILE:HD13	1:E:450:THR:HG21	2.03	0.41
1:A:265:GLN:NE2	1:A:268:GLN:NE2	2.68	0.41
1:A:501:GLU:HG2	1:A:501:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.71	0.41
1:B:185:ASN:O	1:B:188:ILE:HB	2.21	0.41
1:B:243:LEU:CD1	1:B:403:TYR:HE2	2.33	0.41
1:B:381:PRO:HG2	1:B:381:PRO:O	2.21	0.41
1:C:68:ARG:NH1	1:C:562:SER:CB	2.79	0.41
1:C:98:ASN:ND2	1:C:98:ASN:C	2.78	0.41
1:D:134:VAL:HG21	1:D:175:TYR:CE2	2.56	0.41
1:D:153:LEU:HD23	1:D:159:VAL:HG12	2.03	0.41
1:D:394:ILE:CG2	1:D:398:SER:HB2	2.51	0.41
1:D:475:PHE:CD1	1:D:475:PHE:N	2.88	0.41
1:E:88:HIS:CD2	1:E:555:TYR:O	2.74	0.41
1:E:129:THR:HB	1:E:130:ASN:H	1.65	0.41
1:E:153:LEU:HD23	1:E:159:VAL:HG12	2.03	0.41
1:A:66:THR:O	1:E:530:PRO:HG3	2.21	0.41
1:A:217:LEU:CB	1:A:232:THR:HG21	2.46	0.41
1:B:98:ASN:HD22	1:B:98:ASN:C	2.29	0.41
1:B:414:ASP:C	1:B:414:ASP:OD1	2.64	0.41
1:B:430:VAL:HG23	1:B:431:THR:N	2.36	0.41
1:C:53:ASN:O	1:C:54:SER:O	2.38	0.41
1:C:131:MET:HA	1:C:132:PRO:HD3	1.87	0.41
1:C:414:ASP:C	1:C:414:ASP:OD1	2.64	0.41
1:D:96:ILE:HD13	1:D:96:ILE:HA	1.87	0.41
1:D:131:MET:HA	1:D:132:PRO:HD3	1.87	0.41
1:D:149:VAL:HG22	1:D:149:VAL:O	2.21	0.41
1:D:178:THR:O	1:D:179:MET:C	2.63	0.41
1:D:266:PRO:C	1:D:268:GLN:N	2.78	0.41
1:E:295:SER:O	1:E:296:LEU:CB	2.64	0.41
1:A:178:THR:O	1:A:179:MET:C	2.63	0.40
1:B:63:LEU:HA	1:B:63:LEU:HD12	1.82	0.40
1:B:153:LEU:HD23	1:B:159:VAL:HG12	2.03	0.40
1:B:501:GLU:HG2	1:B:501:GLU:O	2.20	0.40
1:C:93:THR:CG2	1:C:94:THR:N	2.83	0.40
1:C:96:ILE:HG22	1:C:98:ASN:H	1.86	0.40
1:D:96:ILE:HG22	1:D:98:ASN:H	1.86	0.40
1:D:98:ASN:HD22	1:D:98:ASN:C	2.30	0.40
1:D:430:VAL:HG23	1:D:431:THR:N	2.36	0.40
1:D:542:THR:O	1:D:542:THR:HG22	2.21	0.40
1:E:468:LEU:HA	1:E:469:PRO:HD3	1.76	0.40
1:A:220:ASP:HA	1:A:221:PRO:HD2	1.89	0.40
1:C:129:THR:HB	1:C:130:ASN:H	1.65	0.40
1:C:153:LEU:HD23	1:C:159:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:O	1:D:154:THR:C	2.62	0.40
1:D:180:THR:HG21	1:D:258:LEU:HD21	2.03	0.40
1:D:198:GLN:H	1:D:198:GLN:HG3	1.63	0.40
1:D:381:PRO:O	1:D:382:LEU:C	2.63	0.40
1:E:414:ASP:C	1:E:414:ASP:OD1	2.64	0.40
1:A:180:THR:HG21	1:A:258:LEU:HD21	2.03	0.40
1:B:132:PRO:HD2	1:B:135:ASN:HD22	1.86	0.40
1:C:508:PRO:HA	1:C:509:PRO:HD3	1.73	0.40
1:C:530:PRO:HG3	1:D:66:THR:O	2.21	0.40
1:D:75:LYS:HB3	1:D:78:ASP:OD2	2.22	0.40
1:E:185:ASN:O	1:E:188:ILE:HB	2.21	0.40
1:B:75:LYS:HB3	1:B:78:ASP:OD2	2.22	0.40
1:B:96:ILE:HG22	1:B:98:ASN:H	1.86	0.40
1:B:265:GLN:NE2	1:B:268:GLN:NE2	2.68	0.40
1:C:73:ASP:OD1	1:C:73:ASP:N	2.42	0.40
1:C:134:VAL:HG21	1:C:175:TYR:CE2	2.56	0.40
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.44	0.40
1:D:441:LEU:HD12	1:D:445:MET:CE	2.47	0.40
1:E:98:ASN:HD22	1:E:98:ASN:C	2.29	0.40
1:E:243:LEU:CG	1:E:403:TYR:CE2	3.05	0.40
1:E:419:ILE:HA	1:E:422:TRP:NE1	2.37	0.40
1:A:134:VAL:HG21	1:A:175:TYR:CE2	2.56	0.40
1:A:149:VAL:HG22	1:A:149:VAL:O	2.21	0.40
1:A:211:ASP:OD1	1:A:212:THR:N	2.35	0.40
1:B:278:LEU:CD2	1:B:419:ILE:HD12	2.38	0.40
1:C:381:PRO:O	1:C:381:PRO:HG2	2.21	0.40
1:D:88:HIS:CD2	1:D:555:TYR:O	2.74	0.40
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.71	0.40
1:E:197:ARG:C	1:E:199:ASN:N	2.80	0.40
1:E:394:ILE:HG23	1:E:395:SER:N	2.34	0.40
1:E:468:LEU:HD12	1:E:469:PRO:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	6
1	B	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	6
1	C	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	6
1	D	444/523 (85%)	323 (73%)	75 (17%)	46 (10%)	0	6
1	E	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	6
All	All	2220/2615 (85%)	1619 (73%)	371 (17%)	230 (10%)	1	6

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	59	GLU
1	A	130	ASN
1	A	137	PHE
1	A	296	LEU
1	A	375	LYS
1	A	378	VAL
1	A	379	ILE
1	A	449	VAL
1	A	469	PRO
1	A	492	LEU
1	A	506	ALA
1	B	54	SER
1	B	59	GLU
1	B	130	ASN
1	B	137	PHE
1	B	296	LEU
1	B	375	LYS
1	B	378	VAL
1	B	379	ILE
1	B	449	VAL
1	B	469	PRO
1	B	492	LEU
1	B	506	ALA
1	C	54	SER
1	C	59	GLU
1	C	130	ASN
1	C	137	PHE

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Mol	Chain	Res	Type
1	C	296	LEU
1	C	375	LYS
1	C	378	VAL
1	C	379	ILE
1	C	449	VAL
1	C	469	PRO
1	C	492	LEU
1	C	506	ALA
1	D	54	SER
1	D	59	GLU
1	D	130	ASN
1	D	137	PHE
1	D	296	LEU
1	D	375	LYS
1	D	378	VAL
1	D	379	ILE
1	D	449	VAL
1	D	469	PRO
1	D	492	LEU
1	D	506	ALA
1	E	54	SER
1	E	59	GLU
1	E	130	ASN
1	E	137	PHE
1	E	296	LEU
1	E	375	LYS
1	E	378	VAL
1	E	379	ILE
1	E	449	VAL
1	E	469	PRO
1	E	492	LEU
1	E	506	ALA
1	A	50	GLY
1	A	79	VAL
1	A	157	LYS
1	A	196	GLY
1	A	204	SER
1	A	212	THR
1	A	216	ARG
1	A	251	THR
1	A	267	PHE
1	A	280	GLY

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Mol	Chain	Res	Type
1	A	386	SER
1	A	527	GLY
1	B	50	GLY
1	B	79	VAL
1	B	157	LYS
1	B	196	GLY
1	B	204	SER
1	B	212	THR
1	B	216	ARG
1	B	251	THR
1	B	267	PHE
1	B	280	GLY
1	B	386	SER
1	B	527	GLY
1	C	50	GLY
1	C	79	VAL
1	C	157	LYS
1	C	196	GLY
1	C	204	SER
1	C	212	THR
1	C	216	ARG
1	C	251	THR
1	C	267	PHE
1	C	280	GLY
1	C	386	SER
1	C	527	GLY
1	D	50	GLY
1	D	79	VAL
1	D	157	LYS
1	D	196	GLY
1	D	204	SER
1	D	212	THR
1	D	216	ARG
1	D	251	THR
1	D	267	PHE
1	D	280	GLY
1	D	386	SER
1	D	527	GLY
1	E	50	GLY
1	E	79	VAL
1	E	157	LYS
1	E	196	GLY

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Mol	Chain	Res	Type
1	E	204	SER
1	E	212	THR
1	E	216	ARG
1	E	251	THR
1	E	267	PHE
1	E	280	GLY
1	E	386	SER
1	E	527	GLY
1	A	66	THR
1	A	74	ASN
1	A	198	GLN
1	A	199	ASN
1	A	215	PHE
1	A	233	ASN
1	A	392	ASN
1	A	414	ASP
1	A	428	PRO
1	A	431	THR
1	A	479	GLN
1	B	66	THR
1	B	74	ASN
1	B	198	GLN
1	B	199	ASN
1	B	215	PHE
1	B	233	ASN
1	B	392	ASN
1	B	414	ASP
1	B	428	PRO
1	B	431	THR
1	B	479	GLN
1	C	66	THR
1	C	74	ASN
1	C	198	GLN
1	C	199	ASN
1	C	215	PHE
1	C	233	ASN
1	C	392	ASN
1	C	414	ASP
1	C	428	PRO
1	C	431	THR
1	C	479	GLN
1	D	66	THR

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Mol	Chain	Res	Type
1	D	74	ASN
1	D	198	GLN
1	D	199	ASN
1	D	215	PHE
1	D	233	ASN
1	D	392	ASN
1	D	414	ASP
1	D	428	PRO
1	D	431	THR
1	D	479	GLN
1	E	66	THR
1	E	74	ASN
1	E	198	GLN
1	E	199	ASN
1	E	215	PHE
1	E	233	ASN
1	E	392	ASN
1	E	414	ASP
1	E	428	PRO
1	E	431	THR
1	E	479	GLN
1	A	388	LYS
1	B	388	LYS
1	C	388	LYS
1	D	388	LYS
1	E	388	LYS
1	A	155	LYS
1	A	179	MET
1	A	232	THR
1	A	490	THR
1	A	513	ILE
1	B	155	LYS
1	B	179	MET
1	B	232	THR
1	B	490	THR
1	B	513	ILE
1	C	155	LYS
1	C	179	MET
1	C	266	PRO
1	C	490	THR
1	C	513	ILE
1	D	155	LYS

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Mol	Chain	Res	Type
1	D	179	MET
1	D	490	THR
1	D	513	ILE
1	E	155	LYS
1	E	179	MET
1	E	490	THR
1	E	513	ILE
1	A	61	ALA
1	A	237	HIS
1	A	266	PRO
1	B	61	ALA
1	B	237	HIS
1	B	266	PRO
1	C	61	ALA
1	C	232	THR
1	C	237	HIS
1	D	61	ALA
1	D	232	THR
1	D	237	HIS
1	D	266	PRO
1	E	61	ALA
1	E	232	THR
1	E	237	HIS
1	E	266	PRO
1	A	486	ILE
1	B	486	ILE
1	C	486	ILE
1	D	486	ILE
1	E	486	ILE
1	B	195	VAL
1	C	195	VAL
1	D	195	VAL
1	A	195	VAL
1	E	195	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/451 (90%)	366 (91%)	38 (9%)	8	26
1	B	404/451 (90%)	365 (90%)	39 (10%)	8	24
1	C	404/451 (90%)	365 (90%)	39 (10%)	8	24
1	D	404/451 (90%)	365 (90%)	39 (10%)	8	24
1	E	404/451 (90%)	365 (90%)	39 (10%)	8	24
All	All	2020/2255 (90%)	1826 (90%)	194 (10%)	10	25

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	68	ARG
1	A	72	VAL
1	A	76	SER
1	A	83	ASN
1	A	100	ASP
1	A	102	SER
1	A	153	LEU
1	A	166	VAL
1	A	183	LEU
1	A	203	GLU
1	A	214	ASN
1	A	223	THR
1	A	232	THR
1	A	233	ASN
1	A	238	PRO
1	A	249	ASP
1	A	256	SER
1	A	258	LEU
1	A	287	LEU
1	A	389	ARG
1	A	401	THR
1	A	429	ASP
1	A	430	VAL
1	A	440	SER
1	A	446	GLN
1	A	468	LEU
1	A	473	LYS
1	A	482	TYR
1	A	512	THR
1	A	519	ASN

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Mol	Chain	Res	Type
1	A	525	ASP
1	A	528	THR
1	A	531	LEU
1	A	533	ASN
1	A	534	SER
1	A	542	THR
1	A	562	SER
1	B	58	SER
1	B	68	ARG
1	B	72	VAL
1	B	76	SER
1	B	83	ASN
1	B	100	ASP
1	B	102	SER
1	B	153	LEU
1	B	166	VAL
1	B	183	LEU
1	B	203	GLU
1	B	214	ASN
1	B	223	THR
1	B	232	THR
1	B	233	ASN
1	B	238	PRO
1	B	249	ASP
1	B	256	SER
1	B	258	LEU
1	B	262	ARG
1	B	287	LEU
1	B	389	ARG
1	B	401	THR
1	B	429	ASP
1	B	430	VAL
1	B	440	SER
1	B	446	GLN
1	B	468	LEU
1	B	473	LYS
1	B	482	TYR
1	B	512	THR
1	B	519	ASN
1	B	525	ASP
1	B	528	THR
1	B	531	LEU

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Mol	Chain	Res	Type
1	B	533	ASN
1	B	534	SER
1	B	542	THR
1	B	562	SER
1	C	58	SER
1	C	68	ARG
1	C	72	VAL
1	C	76	SER
1	C	83	ASN
1	C	100	ASP
1	C	102	SER
1	C	153	LEU
1	C	166	VAL
1	C	183	LEU
1	C	203	GLU
1	C	214	ASN
1	C	223	THR
1	C	232	THR
1	C	233	ASN
1	C	238	PRO
1	C	249	ASP
1	C	256	SER
1	C	258	LEU
1	C	262	ARG
1	C	287	LEU
1	C	389	ARG
1	C	401	THR
1	C	429	ASP
1	C	430	VAL
1	C	440	SER
1	C	446	GLN
1	C	468	LEU
1	C	473	LYS
1	C	482	TYR
1	C	512	THR
1	C	519	ASN
1	C	525	ASP
1	C	528	THR
1	C	531	LEU
1	C	533	ASN
1	C	534	SER
1	C	542	THR

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Mol	Chain	Res	Type
1	C	562	SER
1	D	58	SER
1	D	68	ARG
1	D	72	VAL
1	D	76	SER
1	D	83	ASN
1	D	100	ASP
1	D	102	SER
1	D	153	LEU
1	D	166	VAL
1	D	183	LEU
1	D	203	GLU
1	D	214	ASN
1	D	223	THR
1	D	232	THR
1	D	233	ASN
1	D	238	PRO
1	D	249	ASP
1	D	256	SER
1	D	258	LEU
1	D	262	ARG
1	D	287	LEU
1	D	389	ARG
1	D	401	THR
1	D	429	ASP
1	D	430	VAL
1	D	440	SER
1	D	446	GLN
1	D	468	LEU
1	D	473	LYS
1	D	482	TYR
1	D	512	THR
1	D	519	ASN
1	D	525	ASP
1	D	528	THR
1	D	531	LEU
1	D	533	ASN
1	D	534	SER
1	D	542	THR
1	D	562	SER
1	E	58	SER
1	E	68	ARG

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Mol	Chain	Res	Type
1	E	72	VAL
1	E	76	SER
1	E	83	ASN
1	E	100	ASP
1	E	102	SER
1	E	153	LEU
1	E	166	VAL
1	E	183	LEU
1	E	203	GLU
1	E	214	ASN
1	E	223	THR
1	E	232	THR
1	E	233	ASN
1	E	238	PRO
1	E	249	ASP
1	E	256	SER
1	E	258	LEU
1	E	262	ARG
1	E	287	LEU
1	E	389	ARG
1	E	401	THR
1	E	429	ASP
1	E	430	VAL
1	E	440	SER
1	E	446	GLN
1	E	468	LEU
1	E	473	LYS
1	E	482	TYR
1	E	512	THR
1	E	519	ASN
1	E	525	ASP
1	E	528	THR
1	E	531	LEU
1	E	533	ASN
1	E	534	SER
1	E	542	THR
1	E	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	86	ASN
1	A	98	ASN
1	A	99	ASN
1	A	128	HIS
1	A	130	ASN
1	A	199	ASN
1	A	214	ASN
1	A	265	GLN
1	A	268	GLN
1	A	282	ASN
1	A	402	GLN
1	A	459	ASN
1	A	471	HIS
1	A	503	GLN
1	B	74	ASN
1	B	86	ASN
1	B	98	ASN
1	B	99	ASN
1	B	128	HIS
1	B	130	ASN
1	B	199	ASN
1	B	214	ASN
1	B	265	GLN
1	B	268	GLN
1	B	282	ASN
1	B	402	GLN
1	B	459	ASN
1	B	471	HIS
1	B	484	GLN
1	B	503	GLN
1	C	74	ASN
1	C	86	ASN
1	C	98	ASN
1	C	99	ASN
1	C	128	HIS
1	C	130	ASN
1	C	199	ASN
1	C	214	ASN
1	C	265	GLN
1	C	268	GLN
1	C	282	ASN
1	C	402	GLN

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Mol	Chain	Res	Type
1	C	459	ASN
1	C	471	HIS
1	C	484	GLN
1	D	74	ASN
1	D	86	ASN
1	D	98	ASN
1	D	99	ASN
1	D	128	HIS
1	D	130	ASN
1	D	199	ASN
1	D	214	ASN
1	D	265	GLN
1	D	268	GLN
1	D	282	ASN
1	D	402	GLN
1	D	459	ASN
1	D	471	HIS
1	D	484	GLN
1	D	503	GLN
1	E	74	ASN
1	E	86	ASN
1	E	98	ASN
1	E	99	ASN
1	E	128	HIS
1	E	130	ASN
1	E	199	ASN
1	E	214	ASN
1	E	265	GLN
1	E	268	GLN
1	E	282	ASN
1	E	402	GLN
1	E	459	ASN
1	E	471	HIS
1	E	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

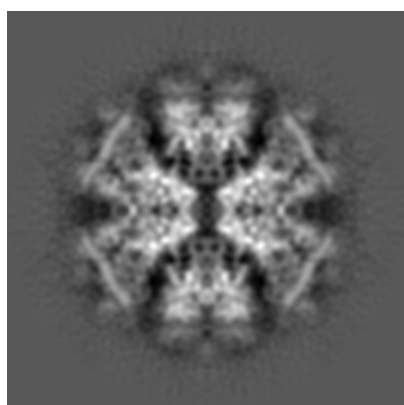
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1178. These allow visual inspection of the internal detail of the map and identification of artifacts.

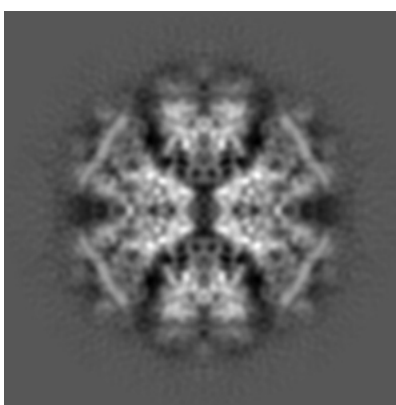
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

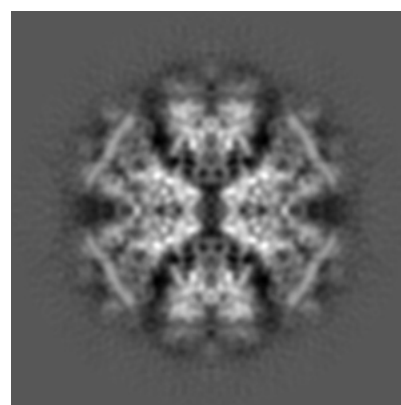
6.1.1 Primary map



X



Y

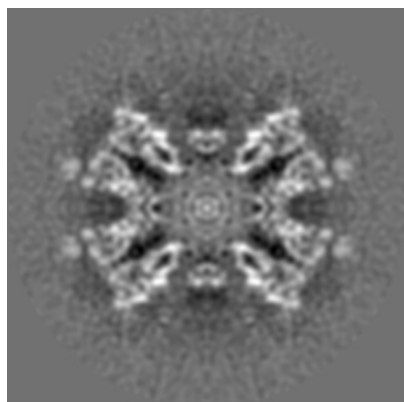


Z

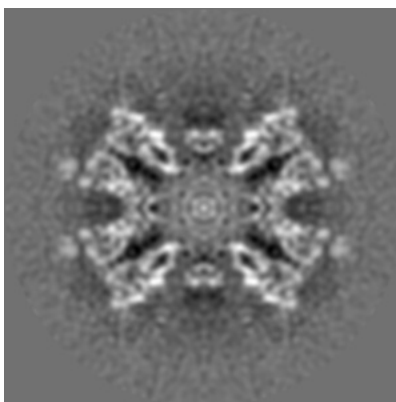
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

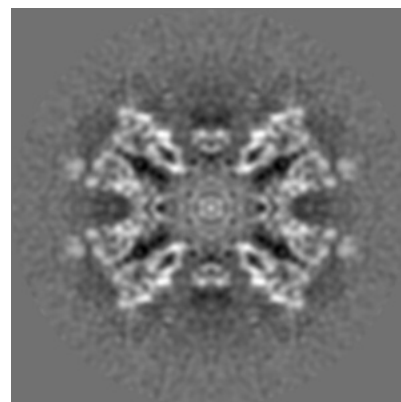
6.2.1 Primary map



X Index: 139



Y Index: 139

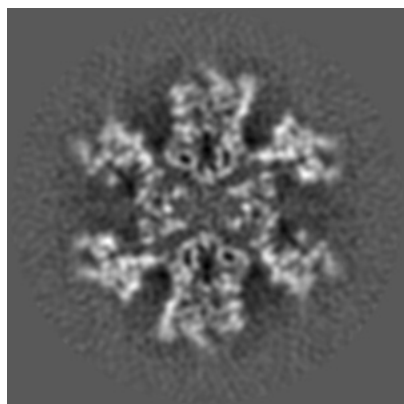


Z Index: 139

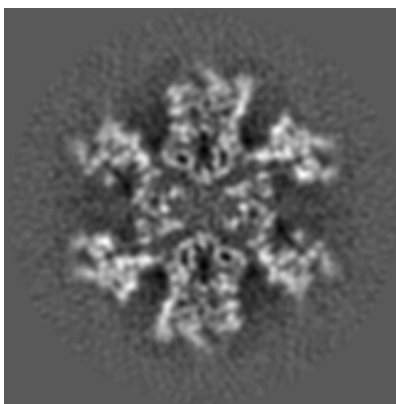
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

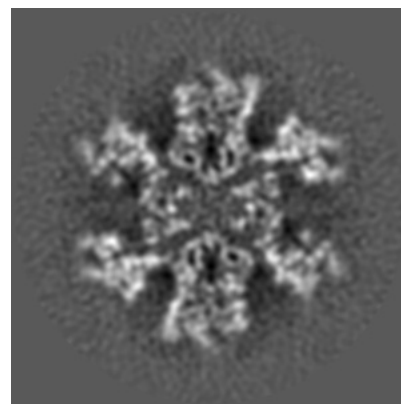
6.3.1 Primary map



X Index: 164



Y Index: 164

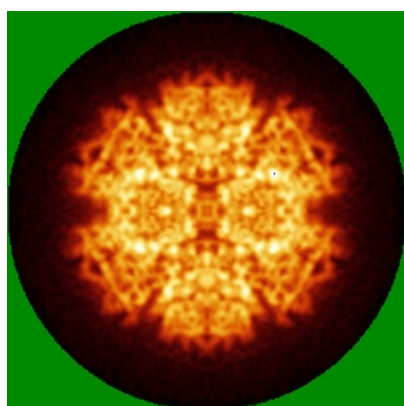


Z Index: 164

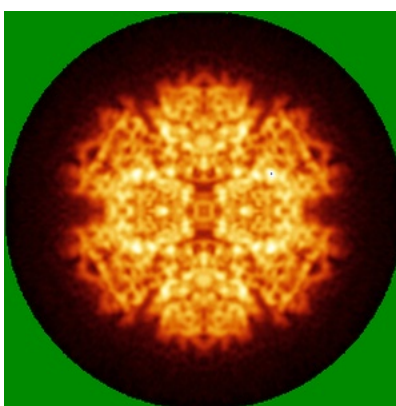
The images above show the largest variance slices of the map in three orthogonal directions.

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

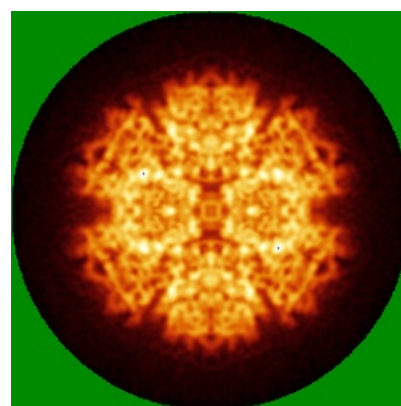
6.4.1 Primary map



X



Y

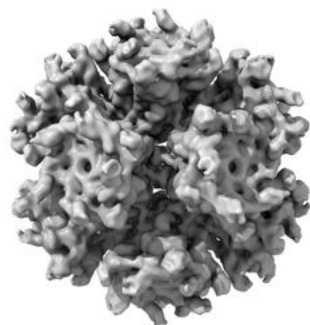


Z

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

6.5 Orthogonal surface views [i](#)

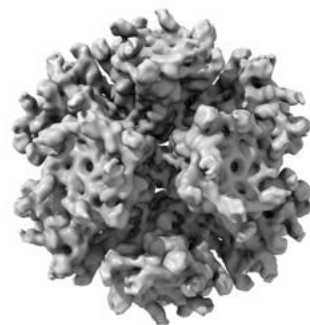
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 91.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

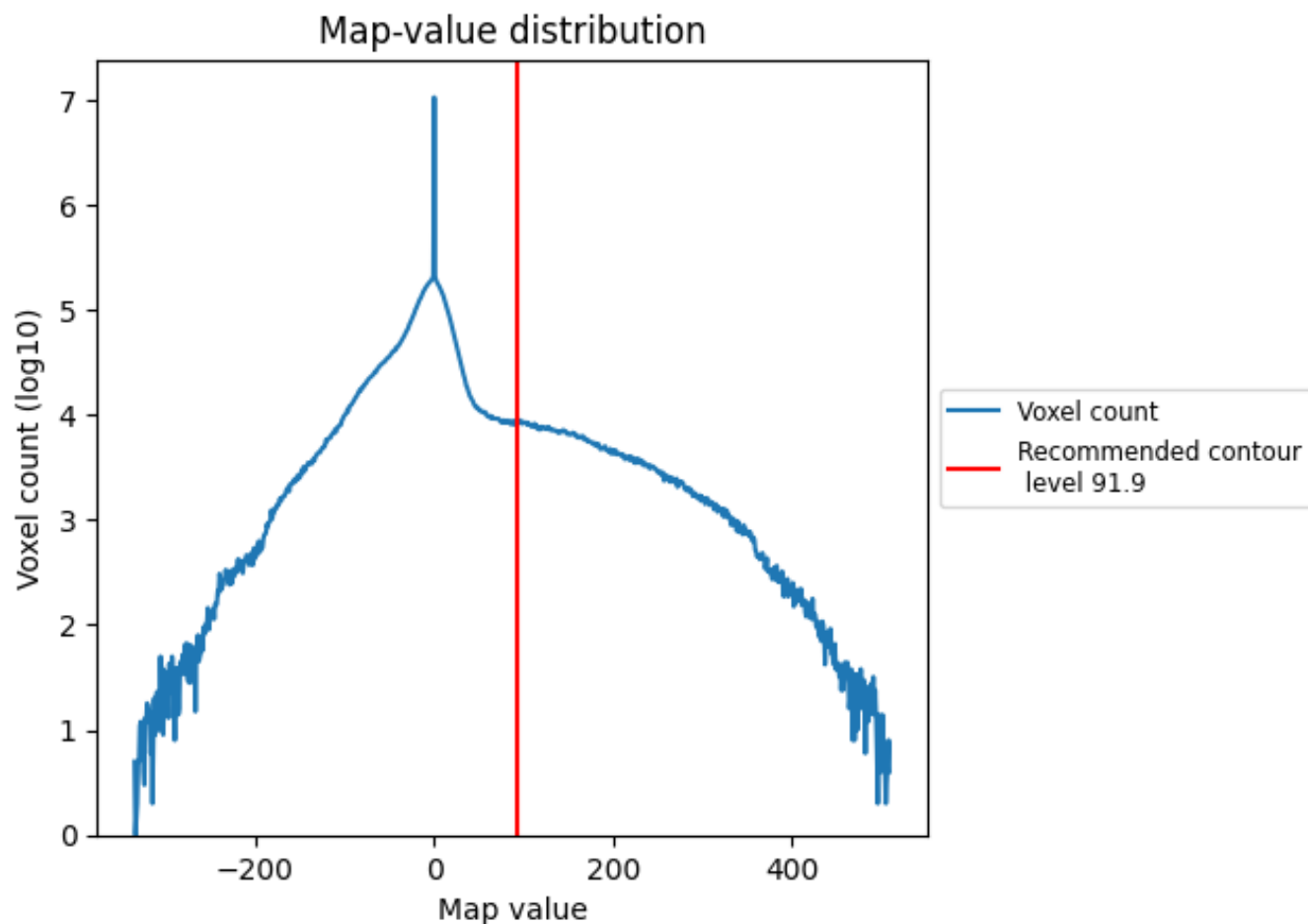
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

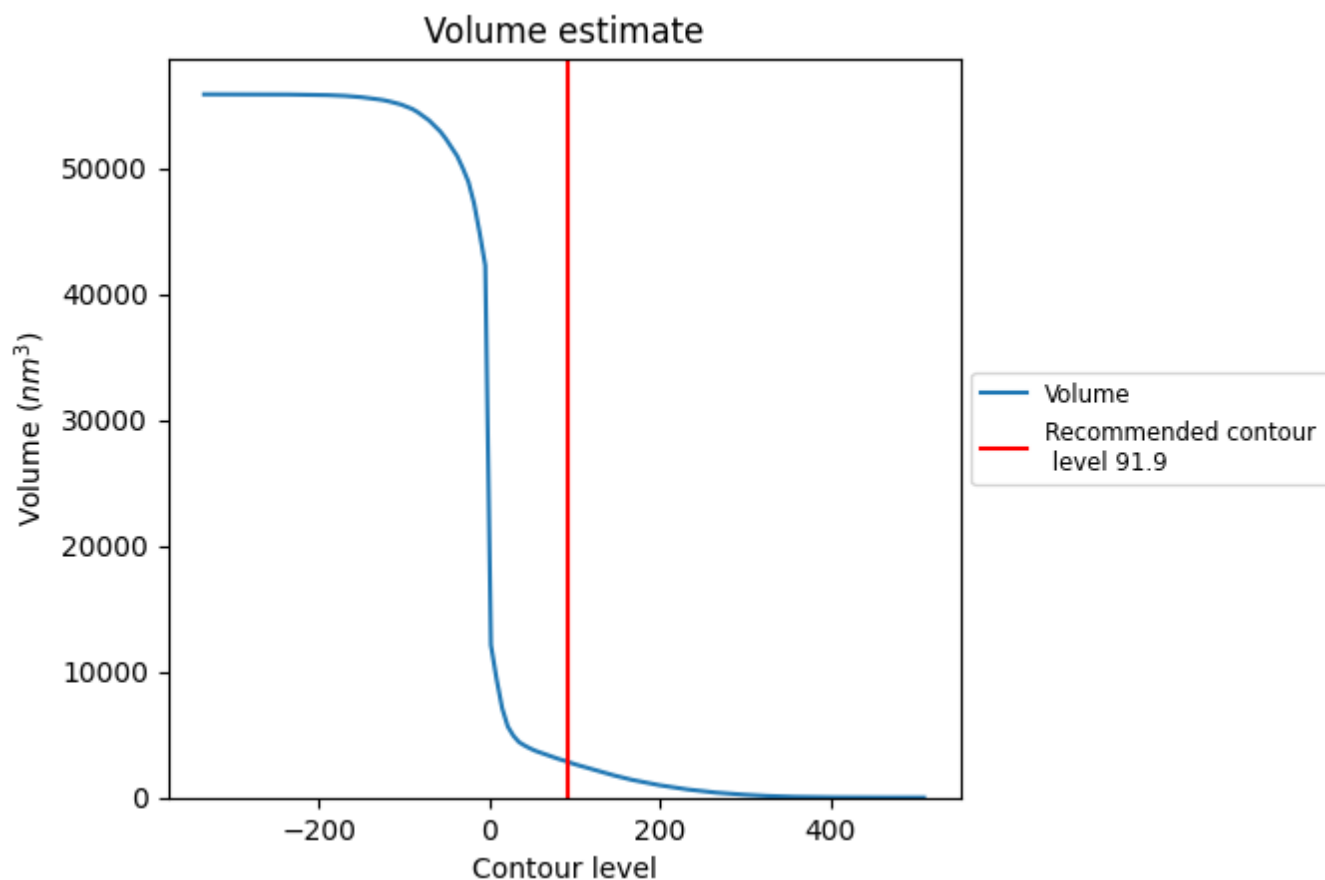
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

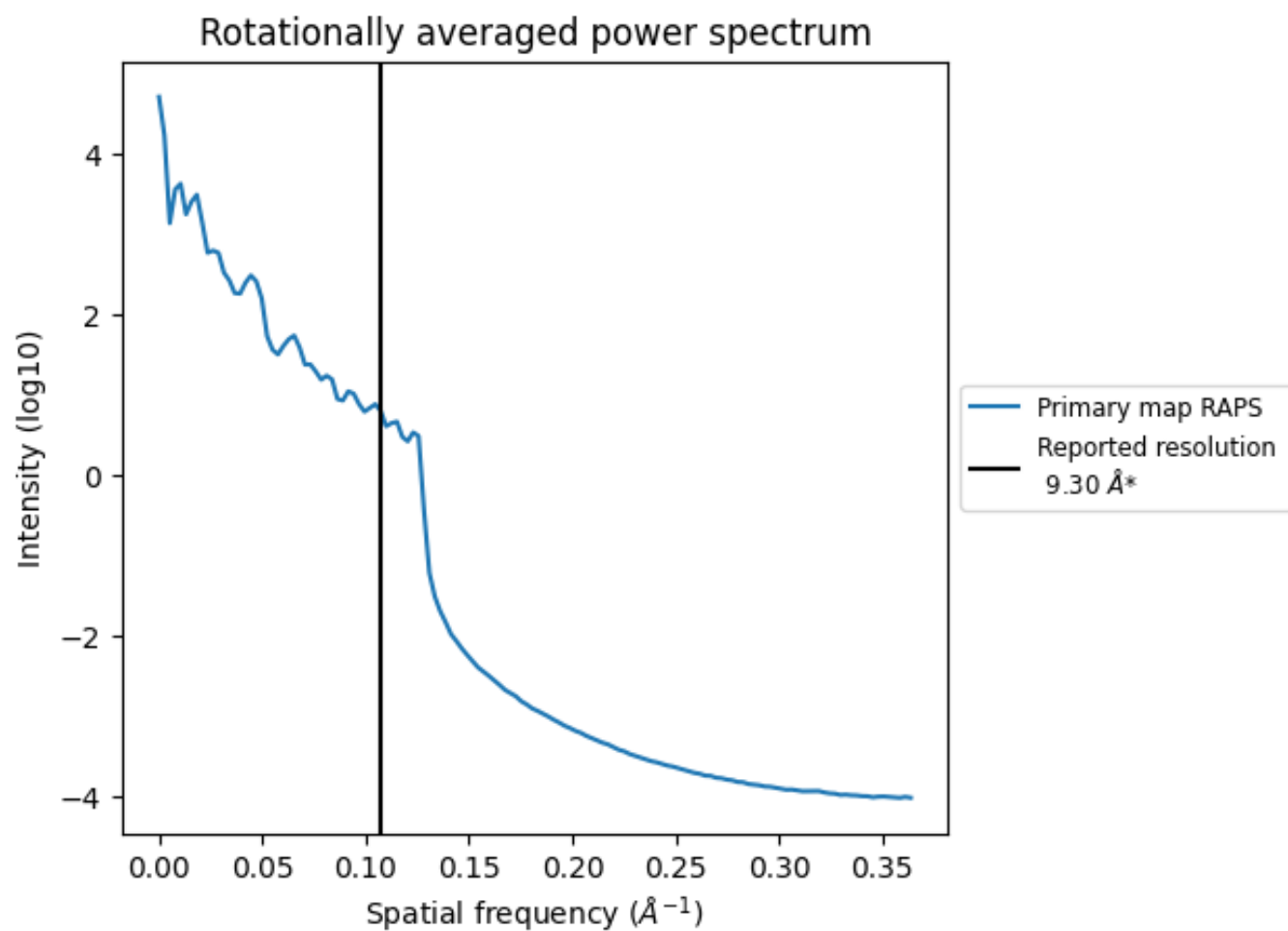
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2826 nm³; this corresponds to an approximate mass of 2552 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.108 Å⁻¹

8 Fourier-Shell correlation

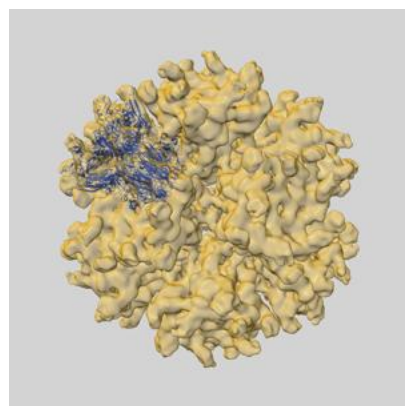
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

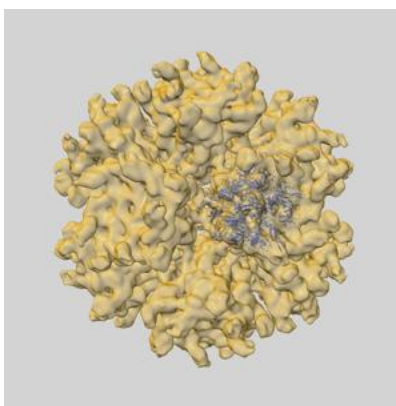
This section contains information regarding the fit between EMDB map EMD-1178 and PDB model 2C9G. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

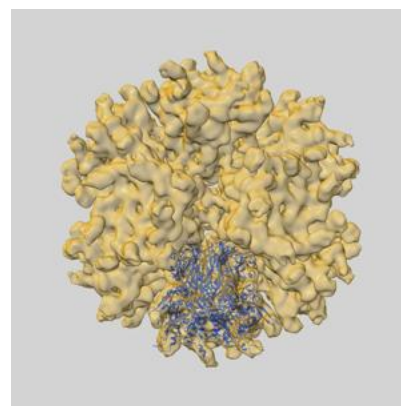
9.1.1 Map-model overlay [i](#)



X

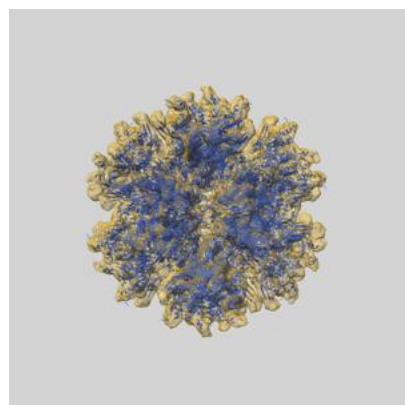


Y

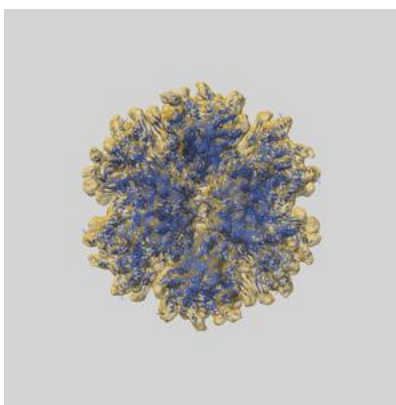


Z

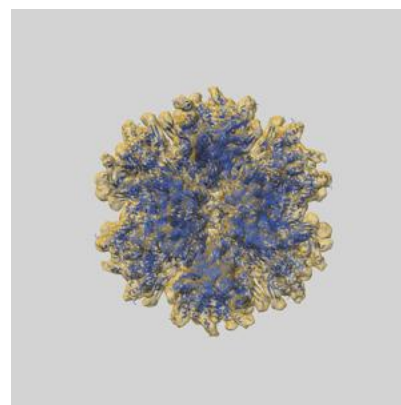
9.1.2 Map-model assembly overlay [i](#)



X



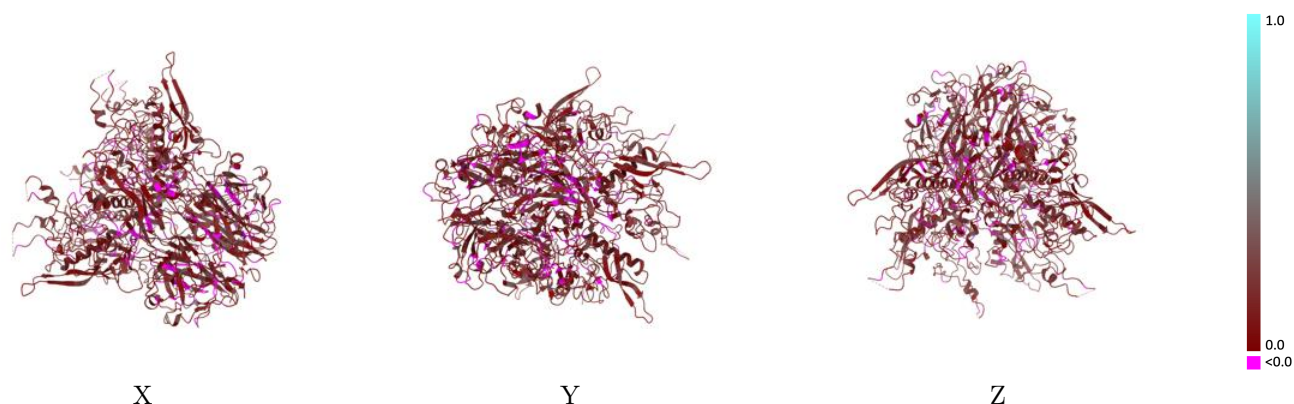
Y



Z

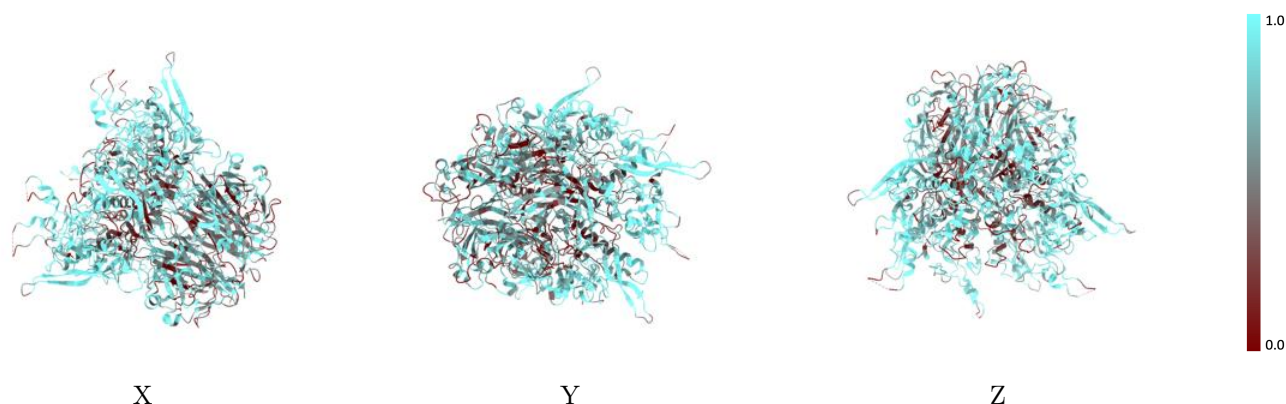
The images above show the 3D surface view of the map at the recommended contour level 91.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



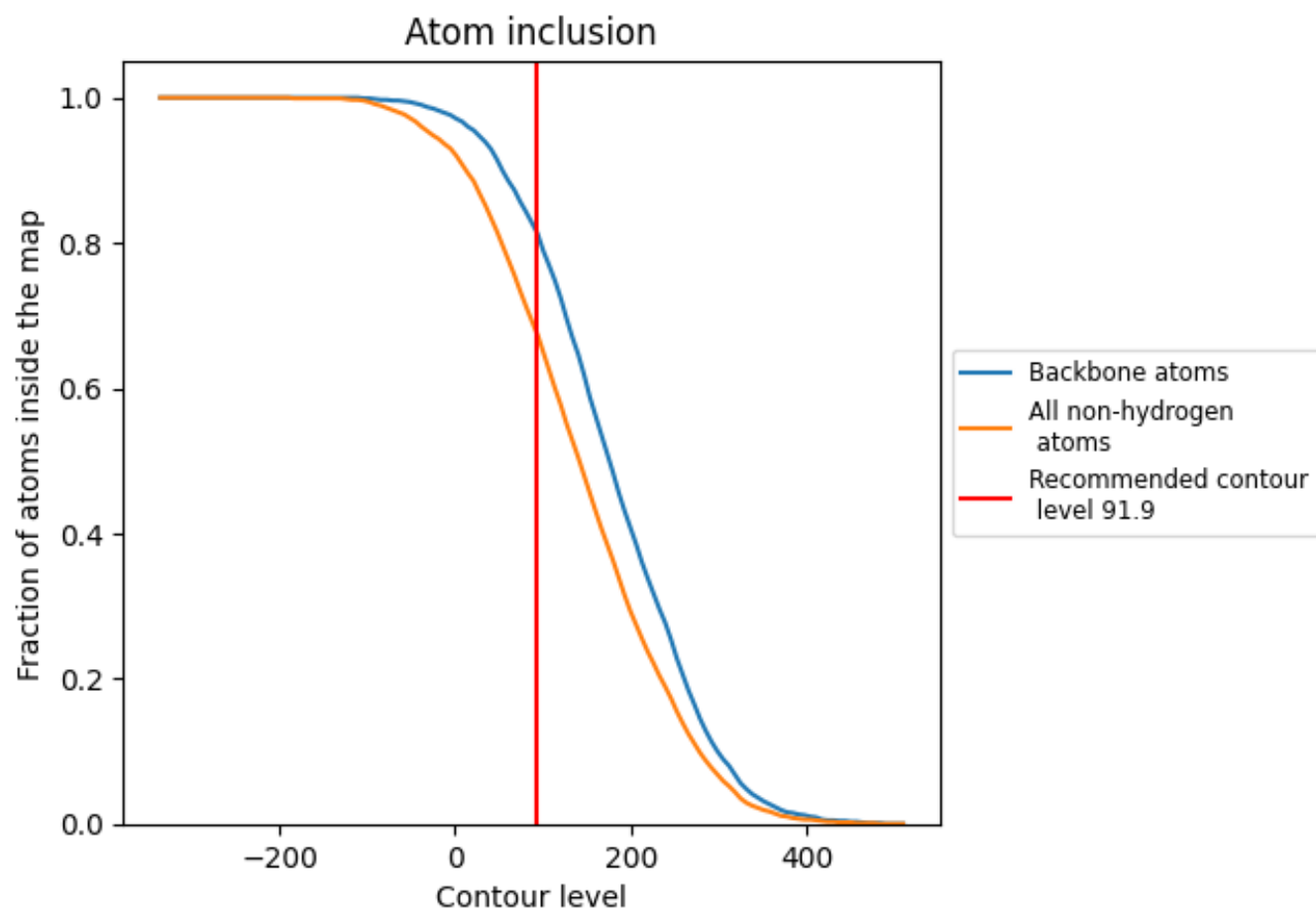
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (91.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (91.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.1170
A	0.6750	0.1170
B	0.6830	0.1170
C	0.6770	0.1170
D	0.6780	0.1170
E	0.6790	0.1180

