



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:36 PM UTC

PDB ID : 6CRJ / pdb_00006crj
EMDB ID : EMD-7564
Title : Mouse norovirus model using the crystal structure of MNV P domain and the Norwalkvirus shell domain
Authors : Smith, T.J.
Deposited on : 2018-03-19
Resolution : 8.00 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

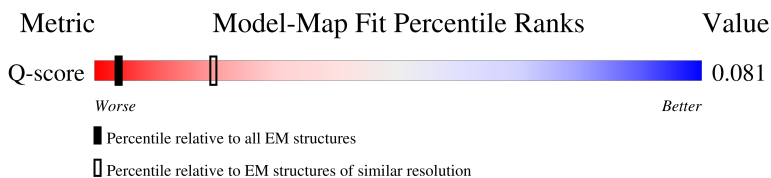
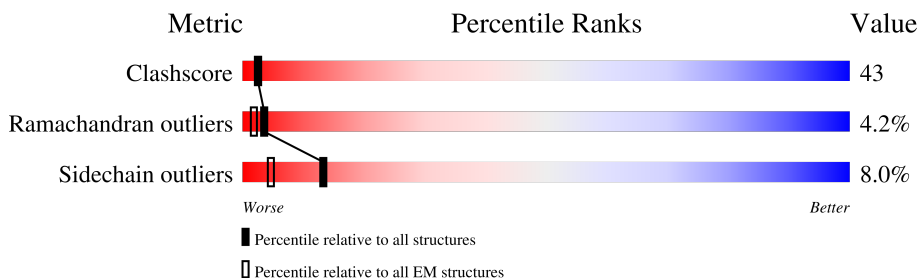
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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

Mol	Chain	Length	Quality of chain
1	A	531	
1	B	531	
1	C	531	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11749 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 Norwalk virus, MNV-1 capsid protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	527	Total	C	N	O	S	0	0
			3997	2555	672	752	18		
1	A	508	Total	C	N	O	S	0	0
			3876	2484	651	723	18		
1	C	508	Total	C	N	O	S	0	0
			3876	2484	651	723	18		

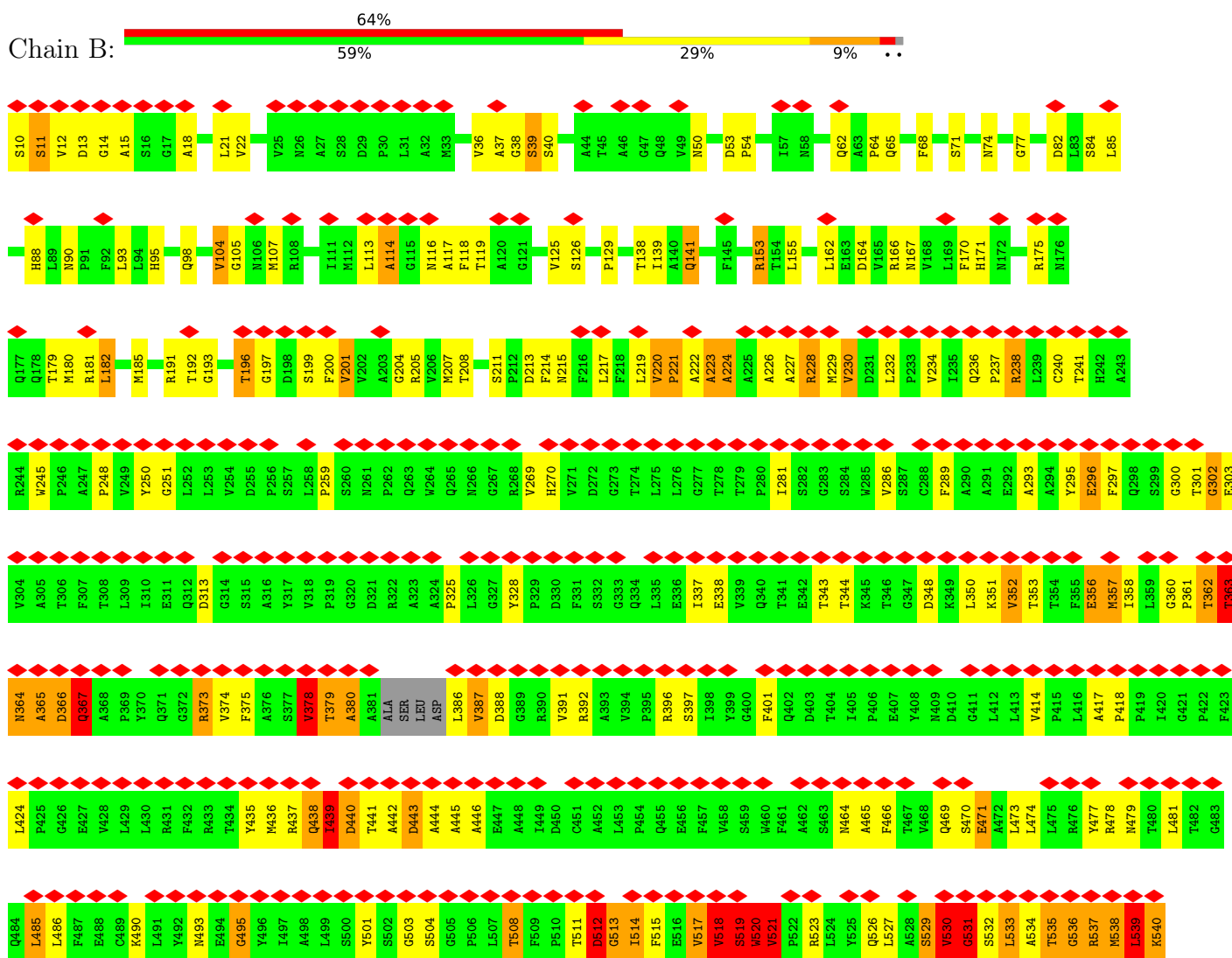
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ALA	-	linker	UNP Q83884
B	223	ALA	-	linker	UNP Q83884
B	224	ALA	-	linker	UNP Q83884
B	225	ALA	-	linker	UNP Q83884
B	226	ALA	-	linker	UNP Q83884
B	227	ALA	-	linker	UNP Q83884
A	222	ALA	-	linker	UNP Q83884
A	223	ALA	-	linker	UNP Q83884
A	224	ALA	-	linker	UNP Q83884
A	225	ALA	-	linker	UNP Q83884
A	226	ALA	-	linker	UNP Q83884
A	227	ALA	-	linker	UNP Q83884
C	222	ALA	-	linker	UNP Q83884
C	223	ALA	-	linker	UNP Q83884
C	224	ALA	-	linker	UNP Q83884
C	225	ALA	-	linker	UNP Q83884
C	226	ALA	-	linker	UNP Q83884
C	227	ALA	-	linker	UNP Q83884

3 Residue-property plots

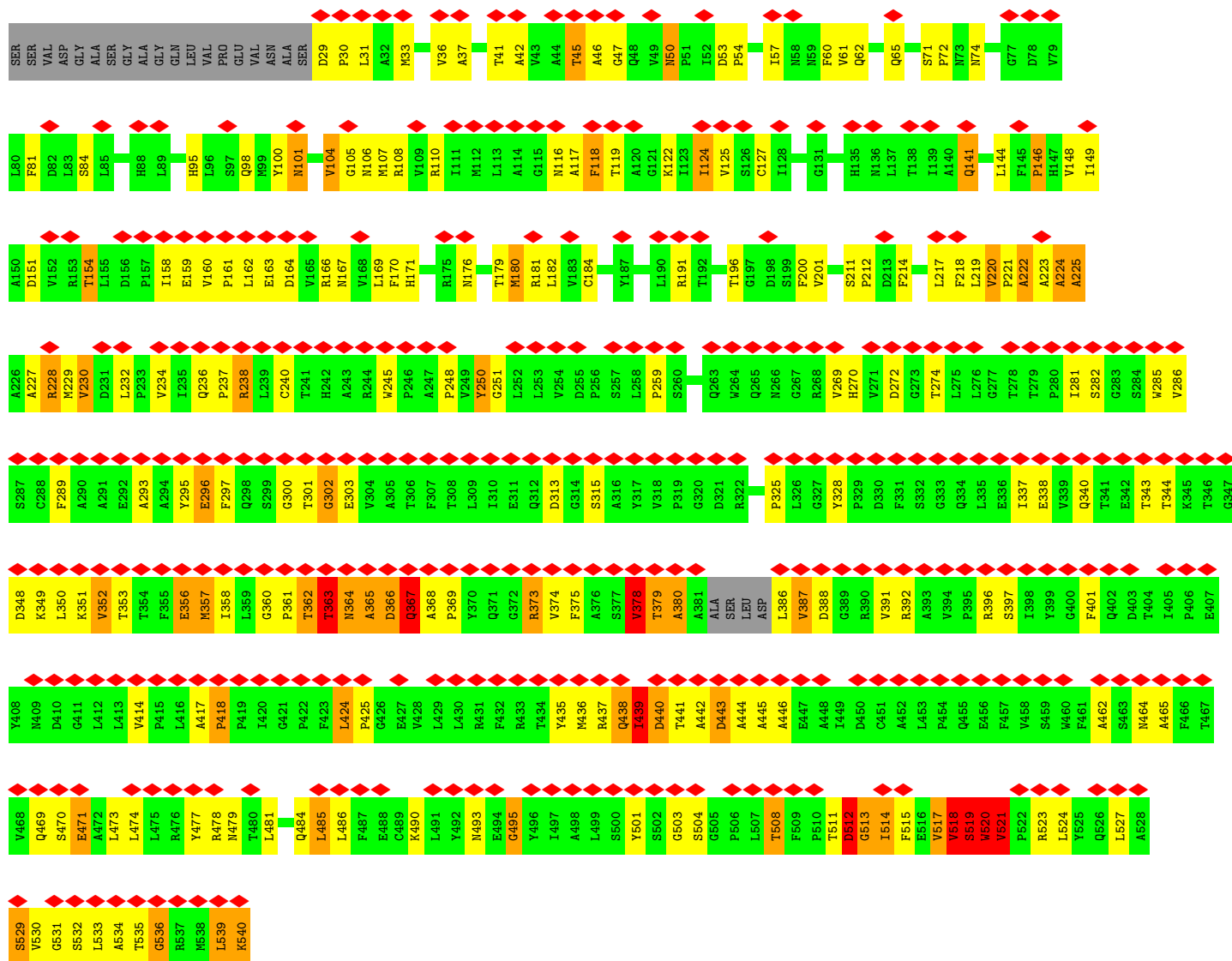
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Norwalk virus, MNV-1 capsid protein chimera

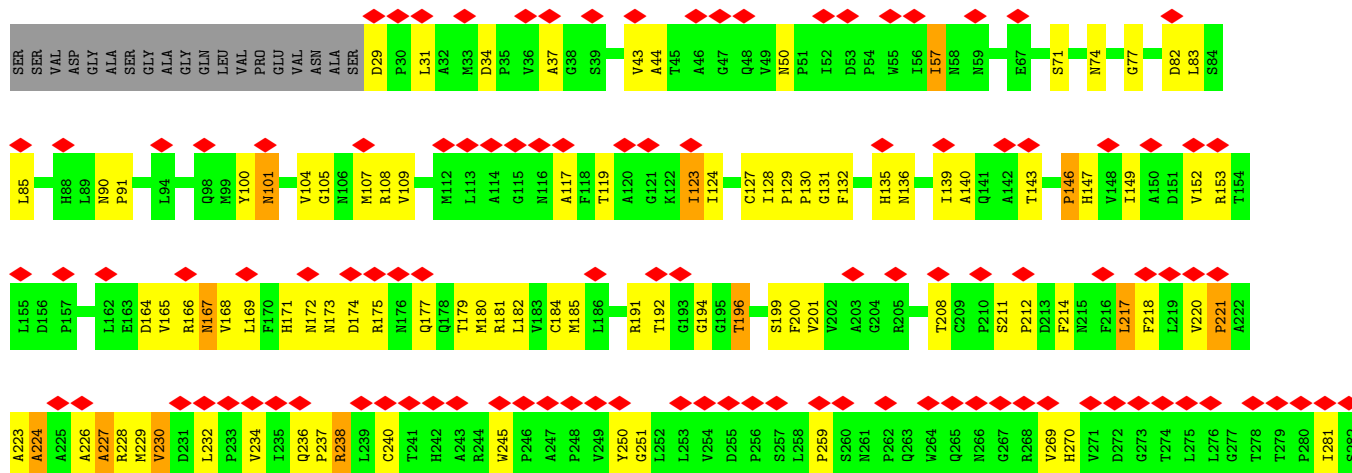


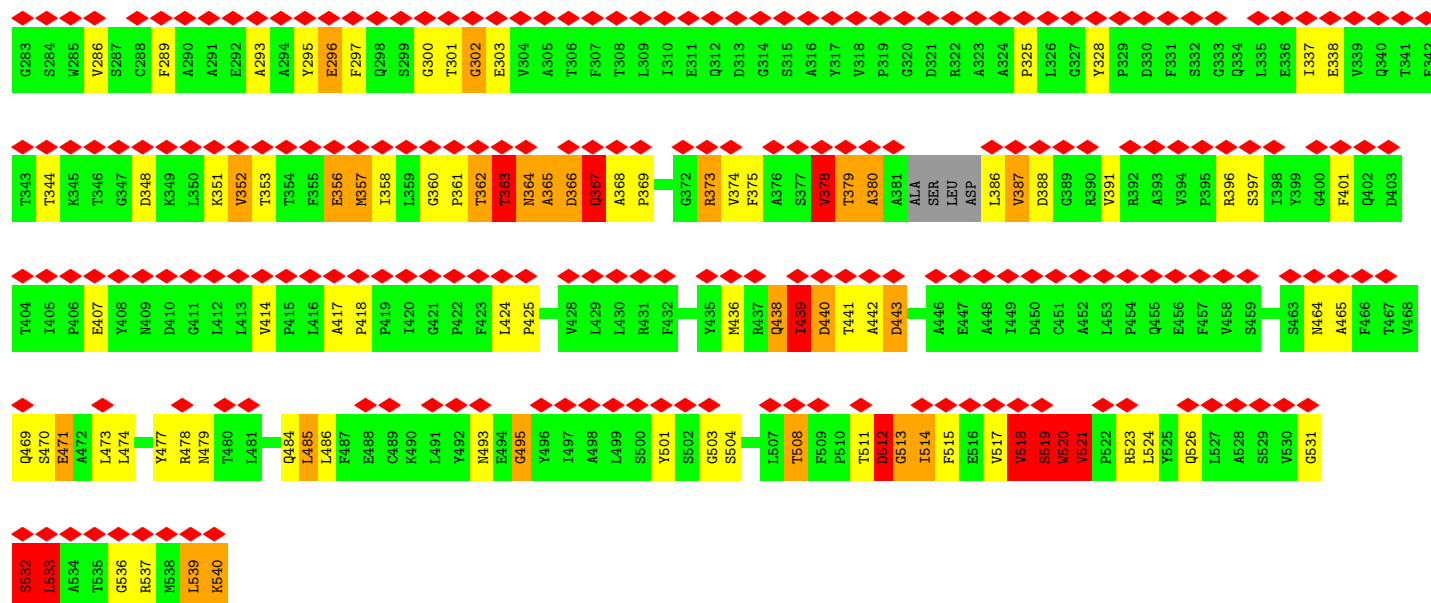
- Molecule 1: Norwalk virus, MNV-1 capsid protein chimera





• Molecule 1: Norwalk virus, MNV-1 capsid protein chimera





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20425	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI EAGLE (2k x 2k)	Depositor
Maximum map value	14.876	Depositor
Minimum map value	-11.954	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.934	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	599.0016, 599.0016, 599.0016	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5598999, 1.5598999, 1.5598999	Depositor

5 Model quality

5.1 Standard geometry

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	1.22	15/3979 (0.4%)	1.43	54/5449 (1.0%)
1	B	1.23	17/4101 (0.4%)	1.51	67/5616 (1.2%)
1	C	1.24	17/3979 (0.4%)	1.57	58/5449 (1.1%)
All	All	1.23	49/12059 (0.4%)	1.50	179/16514 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	4
1	B	2	4
1	C	2	4
All	All	6	12

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	532	SER	C-N	-8.49	1.23	1.34
1	C	536	GLY	C-N	-7.42	1.24	1.33
1	B	533	LEU	CA-C	-7.35	1.43	1.53
1	A	251	GLY	N-CA	6.58	1.52	1.45
1	B	251	GLY	N-CA	6.55	1.52	1.45
1	C	532	SER	CA-C	-6.51	1.44	1.52
1	C	251	GLY	N-CA	6.47	1.52	1.45
1	C	512	ASP	C-O	-6.29	1.15	1.24
1	B	512	ASP	C-O	-6.27	1.15	1.24
1	A	512	ASP	C-O	-6.27	1.15	1.24
1	A	238	ARG	N-CA	6.16	1.54	1.46
1	C	238	ARG	N-CA	6.14	1.54	1.46
1	C	514	ILE	N-CA	6.14	1.53	1.46
1	B	238	ARG	N-CA	6.12	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	ILE	N-CA	6.09	1.53	1.46
1	B	514	ILE	N-CA	6.08	1.53	1.46
1	C	378	VAL	CA-C	-5.78	1.46	1.53
1	B	529	SER	C-N	-5.77	1.25	1.33
1	A	378	VAL	CA-C	-5.75	1.46	1.53
1	B	378	VAL	CA-C	-5.73	1.46	1.53
1	B	495	GLY	N-CA	5.71	1.52	1.45
1	A	495	GLY	N-CA	5.69	1.52	1.45
1	C	495	GLY	N-CA	5.69	1.52	1.45
1	C	513	GLY	N-CA	-5.65	1.36	1.45
1	B	513	GLY	N-CA	-5.63	1.36	1.45
1	A	513	GLY	N-CA	-5.63	1.36	1.45
1	A	418	PRO	C-O	-5.51	1.18	1.24
1	C	418	PRO	C-O	-5.50	1.18	1.24
1	B	418	PRO	C-O	-5.49	1.18	1.24
1	B	539	LEU	CA-C	-5.44	1.45	1.52
1	B	286	VAL	N-CA	-5.32	1.40	1.46
1	C	286	VAL	N-CA	-5.32	1.40	1.46
1	A	286	VAL	N-CA	-5.29	1.40	1.46
1	C	387	VAL	CA-CB	5.29	1.60	1.54
1	A	515	PHE	N-CA	5.28	1.52	1.46
1	B	387	VAL	CA-CB	5.28	1.60	1.54
1	B	517	VAL	N-CA	5.26	1.52	1.46
1	C	360	GLY	N-CA	5.25	1.50	1.43
1	A	517	VAL	N-CA	5.24	1.52	1.46
1	C	517	VAL	N-CA	5.23	1.52	1.46
1	A	387	VAL	CA-CB	5.22	1.60	1.54
1	B	515	PHE	N-CA	5.20	1.52	1.46
1	C	515	PHE	N-CA	5.20	1.52	1.46
1	C	325	PRO	CA-C	5.19	1.58	1.52
1	B	360	GLY	N-CA	5.18	1.50	1.43
1	B	325	PRO	CA-C	5.16	1.58	1.52
1	A	325	PRO	CA-C	5.15	1.58	1.52
1	A	360	GLY	N-CA	5.14	1.50	1.43
1	A	531	GLY	CA-C	5.07	1.57	1.51

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	532	SER	CA-C-N	-32.04	83.19	121.64
1	C	532	SER	C-N-CA	-32.04	83.19	121.64
1	B	530	VAL	CB-CA-C	-17.42	82.72	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	LEU	CA-C-N	-13.68	97.08	121.70
1	B	539	LEU	C-N-CA	-13.68	97.08	121.70
1	A	517	VAL	CA-C-N	11.99	143.29	121.70
1	A	517	VAL	C-N-CA	11.99	143.29	121.70
1	C	517	VAL	CA-C-N	11.99	143.29	121.70
1	C	517	VAL	C-N-CA	11.99	143.29	121.70
1	B	517	VAL	CA-C-N	11.99	143.28	121.70
1	B	517	VAL	C-N-CA	11.99	143.28	121.70
1	B	531	GLY	CA-C-N	-10.90	100.71	121.54
1	B	531	GLY	C-N-CA	-10.90	100.71	121.54
1	A	520	TRP	CA-C-N	10.47	140.54	121.70
1	A	520	TRP	C-N-CA	10.47	140.54	121.70
1	C	520	TRP	CA-C-N	10.45	140.52	121.70
1	C	520	TRP	C-N-CA	10.45	140.52	121.70
1	B	520	TRP	CA-C-N	10.44	140.49	121.70
1	B	520	TRP	C-N-CA	10.44	140.49	121.70
1	B	529	SER	CA-C-N	-9.94	104.09	121.97
1	B	529	SER	C-N-CA	-9.94	104.09	121.97
1	B	526	GLN	OE1-CD-NE2	-9.42	113.18	122.60
1	C	518	VAL	CA-C-N	9.26	138.36	121.70
1	C	518	VAL	C-N-CA	9.26	138.36	121.70
1	B	518	VAL	CA-C-N	9.25	138.35	121.70
1	B	518	VAL	C-N-CA	9.25	138.35	121.70
1	A	518	VAL	CA-C-N	9.23	138.32	121.70
1	A	518	VAL	C-N-CA	9.23	138.32	121.70
1	A	504	SER	N-CA-C	8.98	125.18	114.04
1	C	504	SER	N-CA-C	8.96	125.14	114.04
1	B	504	SER	N-CA-C	8.95	125.14	114.04
1	B	387	VAL	N-CA-C	8.59	121.22	109.80
1	C	387	VAL	N-CA-C	8.56	121.19	109.80
1	C	532	SER	O-C-N	-8.56	111.20	122.59
1	A	387	VAL	N-CA-C	8.56	121.18	109.80
1	C	532	SER	CB-CA-C	-7.95	94.61	110.42
1	B	538	MET	CB-CA-C	-7.92	94.66	110.42
1	B	539	LEU	CB-CA-C	-7.80	94.90	110.42
1	A	414	VAL	CA-C-N	-7.68	111.84	119.90
1	A	414	VAL	C-N-CA	-7.68	111.84	119.90
1	C	414	VAL	CA-C-N	-7.63	111.88	119.90
1	C	414	VAL	C-N-CA	-7.63	111.88	119.90
1	B	414	VAL	CA-C-N	-7.62	111.89	119.90
1	B	414	VAL	C-N-CA	-7.62	111.89	119.90
1	B	514	ILE	N-CA-C	7.53	118.71	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ILE	N-CA-C	7.52	118.70	108.17
1	C	514	ILE	N-CA-C	7.50	118.67	108.17
1	B	414	VAL	N-CA-C	7.50	115.34	109.19
1	C	414	VAL	N-CA-C	7.45	115.30	109.19
1	A	414	VAL	N-CA-C	7.43	115.28	109.19
1	B	538	MET	CA-C-N	-7.36	107.47	121.54
1	B	538	MET	C-N-CA	-7.36	107.47	121.54
1	B	380	ALA	N-CA-C	-7.34	103.22	111.14
1	A	380	ALA	N-CA-C	-7.34	103.22	111.14
1	C	380	ALA	N-CA-C	-7.33	103.22	111.14
1	A	167	ASN	N-CA-C	-7.25	104.69	113.97
1	A	217	LEU	N-CA-C	7.03	120.07	108.48
1	C	373	ARG	N-CA-C	7.01	119.89	108.26
1	B	373	ARG	N-CA-C	6.97	119.83	108.26
1	A	373	ARG	N-CA-C	6.96	119.81	108.26
1	C	521	VAL	N-CA-C	6.91	130.34	111.00
1	A	521	VAL	N-CA-C	6.90	130.32	111.00
1	B	521	VAL	N-CA-C	6.90	130.32	111.00
1	C	360	GLY	CA-C-N	6.89	128.46	119.84
1	C	360	GLY	C-N-CA	6.89	128.46	119.84
1	A	360	GLY	CA-C-N	6.88	128.44	119.84
1	A	360	GLY	C-N-CA	6.88	128.44	119.84
1	B	360	GLY	CA-C-N	6.87	128.43	119.84
1	B	360	GLY	C-N-CA	6.87	128.43	119.84
1	A	529	SER	CA-C-N	-6.84	109.65	121.97
1	A	529	SER	C-N-CA	-6.84	109.65	121.97
1	B	199	SER	N-CA-C	-6.82	104.83	113.01
1	C	515	PHE	N-CA-C	6.81	120.59	109.76
1	A	515	PHE	N-CA-C	6.80	120.57	109.76
1	A	517	VAL	CA-C-O	-6.80	113.02	121.11
1	C	175	ARG	N-CA-C	-6.80	105.02	113.38
1	B	515	PHE	N-CA-C	6.79	120.56	109.76
1	B	517	VAL	CA-C-O	-6.75	113.07	121.11
1	A	358	ILE	CB-CA-C	-6.75	102.80	110.96
1	C	517	VAL	CA-C-O	-6.75	113.08	121.11
1	B	358	ILE	CB-CA-C	-6.74	102.80	110.96
1	B	526	GLN	CG-CD-NE2	6.73	126.50	116.40
1	C	358	ILE	CB-CA-C	-6.73	102.82	110.96
1	B	439	ILE	CA-C-N	6.63	133.63	121.70
1	B	439	ILE	C-N-CA	6.63	133.63	121.70
1	C	439	ILE	CA-C-N	6.63	133.63	121.70
1	C	439	ILE	C-N-CA	6.63	133.63	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ILE	CA-C-N	6.63	133.63	121.70
1	A	439	ILE	C-N-CA	6.63	133.63	121.70
1	B	65	GLN	N-CA-C	-6.56	102.56	111.55
1	A	508	THR	N-CA-CB	-6.54	99.74	110.52
1	B	535	THR	CA-C-N	6.51	134.18	121.41
1	B	535	THR	C-N-CA	6.51	134.18	121.41
1	C	508	THR	N-CA-CB	-6.51	99.78	110.52
1	B	508	THR	N-CA-CB	-6.48	99.83	110.52
1	C	117	ALA	N-CA-C	-6.41	105.46	113.28
1	C	533	LEU	N-CA-C	6.33	118.92	108.48
1	C	34	ASP	N-CA-C	-6.33	102.10	110.07
1	A	250	TYR	N-CA-C	-6.29	106.24	114.04
1	C	250	TYR	N-CA-C	-6.29	106.25	114.04
1	C	531	GLY	N-CA-C	-6.29	98.28	113.18
1	C	532	SER	CA-C-O	-6.27	111.55	120.51
1	B	250	TYR	N-CA-C	-6.25	106.28	114.04
1	A	117	ALA	N-CA-C	-6.24	105.67	113.28
1	C	217	LEU	N-CA-C	6.16	123.91	110.80
1	C	146	PRO	N-CA-C	-6.14	101.58	111.03
1	A	519	SER	CA-C-N	6.10	133.19	121.54
1	A	519	SER	C-N-CA	6.10	133.19	121.54
1	C	519	SER	CA-C-N	6.09	133.18	121.54
1	C	519	SER	C-N-CA	6.09	133.18	121.54
1	B	519	SER	CA-C-N	6.09	133.18	121.54
1	B	519	SER	C-N-CA	6.09	133.18	121.54
1	A	539	LEU	N-CA-C	-6.08	104.65	111.28
1	B	378	VAL	CB-CA-C	-6.00	104.81	111.35
1	B	530	VAL	CA-C-N	5.99	133.15	121.41
1	B	530	VAL	C-N-CA	5.99	133.15	121.41
1	C	378	VAL	CB-CA-C	-5.98	104.83	111.35
1	B	417	ALA	N-CA-C	-5.98	101.83	110.08
1	C	417	ALA	N-CA-C	-5.97	101.84	110.08
1	A	417	ALA	N-CA-C	-5.95	101.87	110.08
1	A	378	VAL	CB-CA-C	-5.95	104.87	111.35
1	C	232	LEU	CA-C-N	5.92	125.68	119.76
1	C	232	LEU	C-N-CA	5.92	125.68	119.76
1	B	232	LEU	CA-C-N	5.92	125.68	119.76
1	B	232	LEU	C-N-CA	5.92	125.68	119.76
1	A	232	LEU	CA-C-N	5.87	125.63	119.76
1	A	232	LEU	C-N-CA	5.87	125.63	119.76
1	B	193	GLY	N-CA-C	-5.85	104.24	112.60
1	C	167	ASN	N-CA-C	-5.83	106.33	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	GLN	N-CA-C	-5.78	103.37	110.65
1	B	167	ASN	N-CA-C	-5.71	106.45	113.41
1	C	44	ALA	N-CA-C	5.70	117.49	111.28
1	A	176	ASN	N-CA-C	-5.68	106.39	113.38
1	B	512	ASP	O-C-N	-5.67	114.85	122.22
1	B	197	GLY	N-CA-C	-5.62	99.86	113.18
1	C	512	ASP	O-C-N	-5.62	114.91	122.22
1	A	512	ASP	O-C-N	-5.62	114.91	122.22
1	A	146	PRO	N-CA-C	-5.52	102.53	111.03
1	C	517	VAL	N-CA-C	-5.41	101.85	109.21
1	B	517	VAL	N-CA-C	-5.39	101.88	109.21
1	B	201	VAL	N-CA-C	-5.36	100.12	108.81
1	A	517	VAL	N-CA-C	-5.36	101.92	109.21
1	C	128	ILE	CA-C-N	5.33	123.50	119.66
1	C	128	ILE	C-N-CA	5.33	123.50	119.66
1	C	199	SER	N-CA-C	-5.30	106.32	112.89
1	B	50	ASN	CA-C-N	5.26	125.16	119.85
1	B	50	ASN	C-N-CA	5.26	125.16	119.85
1	A	245	TRP	CA-C-N	-5.23	113.30	119.84
1	A	245	TRP	C-N-CA	-5.23	113.30	119.84
1	A	50	ASN	CA-C-N	5.22	125.43	120.31
1	A	50	ASN	C-N-CA	5.22	125.43	120.31
1	C	240	CYS	N-CA-C	5.22	118.24	110.52
1	A	504	SER	CA-C-N	5.21	131.08	121.70
1	A	504	SER	C-N-CA	5.21	131.08	121.70
1	C	504	SER	CA-C-N	5.21	131.07	121.70
1	C	504	SER	C-N-CA	5.21	131.07	121.70
1	B	245	TRP	CA-C-N	-5.20	113.34	119.84
1	B	245	TRP	C-N-CA	-5.20	113.34	119.84
1	B	504	SER	CA-C-N	5.20	131.06	121.70
1	B	504	SER	C-N-CA	5.20	131.06	121.70
1	C	245	TRP	CA-C-N	-5.20	113.34	119.84
1	C	245	TRP	C-N-CA	-5.20	113.34	119.84
1	B	538	MET	N-CA-C	5.19	121.86	110.80
1	A	240	CYS	N-CA-C	5.19	118.20	110.52
1	B	211	SER	N-CA-C	-5.19	102.66	110.24
1	B	240	CYS	N-CA-C	5.19	118.20	110.52
1	B	39	SER	N-CA-C	5.18	117.60	111.33
1	B	217	LEU	N-CA-C	5.17	121.81	110.80
1	A	211	SER	N-CA-C	-5.11	103.03	110.08
1	C	172	ASN	N-CA-C	-5.09	101.39	109.59
1	A	104	VAL	CB-CA-C	-5.09	103.96	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	GLU	N-CA-C	5.05	119.44	113.28
1	A	471	GLU	N-CA-C	5.04	119.43	113.28
1	A	154	THR	N-CA-C	5.04	117.78	110.42
1	C	358	ILE	N-CA-CB	5.03	116.73	111.00
1	C	471	GLU	N-CA-C	5.03	119.42	113.28
1	A	238	ARG	N-CA-C	-5.02	107.11	113.18
1	A	358	ILE	N-CA-CB	5.01	116.71	111.00
1	C	539	LEU	N-CA-C	-5.00	105.96	111.71

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	518	VAL	CA
1	B	521	VAL	CA
1	A	518	VAL	CA
1	A	521	VAL	CA
1	C	518	VAL	CA
1	C	521	VAL	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	GLN	Peptide
1	A	512	ASP	Peptide
1	A	518	VAL	Peptide
1	A	519	SER	Peptide
1	B	438	GLN	Peptide
1	B	512	ASP	Peptide
1	B	518	VAL	Peptide
1	B	519	SER	Peptide
1	C	438	GLN	Peptide
1	C	512	ASP	Peptide
1	C	518	VAL	Peptide
1	C	519	SER	Peptide

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	3876	0	3810	513	0
1	B	3997	0	3923	438	0
1	C	3876	0	3814	388	0
All	All	11749	0	11547	998	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 43.

All (998) 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:445:ALA:CA	1:A:350:LEU:HB2	1.24	1.67
1:A:169:LEU:HD12	1:C:168:VAL:CA	1.30	1.62
1:A:425:PRO:HD3	1:C:425:PRO:CG	1.25	1.61
1:B:445:ALA:HA	1:A:350:LEU:CB	1.28	1.57
1:B:446:ALA:CB	1:A:350:LEU:HD21	1.29	1.53
1:A:274:THR:CG2	1:C:537:ARG:CB	1.85	1.52
1:A:274:THR:CG2	1:C:537:ARG:HB2	1.05	1.51
1:A:169:LEU:CD1	1:C:168:VAL:CA	1.85	1.50
1:B:373:ARG:NH1	1:B:375:PHE:HZ	1.00	1.50
1:B:62:GLN:CD	1:C:140:ALA:HB2	1.37	1.50
1:C:373:ARG:NH1	1:C:375:PHE:HZ	1.00	1.47
1:B:343:THR:HG21	1:A:435:TYR:CB	1.43	1.46
1:C:356:GLU:CG	1:C:379:THR:HG22	1.46	1.46
1:B:539:LEU:HG	1:B:540:LYS:CD	1.42	1.45
1:B:539:LEU:CG	1:B:540:LYS:HD2	1.47	1.45
1:B:364:ASN:N	1:B:365:ALA:HB2	1.27	1.45
1:A:169:LEU:HD11	1:C:168:VAL:C	1.38	1.45
1:A:45:THR:HG22	1:C:166:ARG:CB	1.47	1.44
1:A:169:LEU:CG	1:C:168:VAL:HA	1.45	1.44
1:A:356:GLU:CG	1:A:379:THR:HG22	1.46	1.44
1:A:169:LEU:CD1	1:C:168:VAL:C	1.89	1.44
1:B:446:ALA:CB	1:A:343:THR:HG22	1.48	1.44
1:C:364:ASN:N	1:C:365:ALA:HB2	1.27	1.44
1:A:274:THR:HG23	1:C:537:ARG:CB	1.44	1.43
1:B:343:THR:HB	1:A:435:TYR:CG	1.49	1.43
1:B:343:THR:CB	1:A:435:TYR:CD2	2.01	1.43
1:B:343:THR:HB	1:A:435:TYR:CD2	1.54	1.42
1:B:356:GLU:CG	1:B:379:THR:HG22	1.46	1.42
1:A:101:ASN:HD22	1:C:131:GLY:C	1.27	1.42
1:A:373:ARG:NH1	1:A:375:PHE:HZ	1.00	1.42
1:A:373:ARG:NH1	1:A:375:PHE:CZ	1.87	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ARG:NH1	1:C:526:GLN:HE22	1.17	1.41
1:A:364:ASN:N	1:A:365:ALA:HB2	1.27	1.41
1:B:62:GLN:CD	1:C:140:ALA:CB	1.94	1.40
1:B:373:ARG:NH1	1:B:375:PHE:CZ	1.87	1.40
1:A:425:PRO:CD	1:C:425:PRO:CG	2.01	1.39
1:C:373:ARG:NH1	1:C:375:PHE:CZ	1.87	1.39
1:B:62:GLN:NE2	1:C:140:ALA:CB	1.87	1.37
1:C:363:THR:C	1:C:365:ALA:HB2	1.49	1.35
1:B:445:ALA:HA	1:A:350:LEU:CA	1.55	1.35
1:C:220:VAL:CG1	1:C:221:PRO:HD2	1.56	1.35
1:B:363:THR:C	1:B:365:ALA:HB2	1.49	1.35
1:A:363:THR:C	1:A:365:ALA:HB2	1.49	1.34
1:A:169:LEU:CD1	1:C:168:VAL:HA	1.50	1.33
1:A:227:ALA:HB1	1:A:228:ARG:NH1	1.44	1.33
1:A:425:PRO:CD	1:C:425:PRO:HG3	1.56	1.33
1:A:425:PRO:HD3	1:C:425:PRO:CB	1.56	1.32
1:A:523:ARG:HD3	1:C:526:GLN:NE2	1.43	1.32
1:C:227:ALA:CB	1:C:228:ARG:HA	1.43	1.32
1:B:445:ALA:CA	1:A:350:LEU:CB	1.91	1.31
1:A:101:ASN:ND2	1:C:131:GLY:C	1.88	1.31
1:B:343:THR:CB	1:A:435:TYR:CG	2.10	1.29
1:B:207:MET:CE	1:C:143:THR:HG21	1.61	1.29
1:C:532:SER:C	1:C:533:LEU:HD22	1.53	1.29
1:B:446:ALA:HB1	1:A:343:THR:CG2	1.59	1.29
1:C:227:ALA:HB1	1:C:228:ARG:CA	1.57	1.29
1:B:392:ARG:CD	1:A:250:TYR:OH	1.78	1.28
1:A:378:VAL:O	1:A:380:ALA:N	1.66	1.28
1:A:462:ALA:HB1	1:C:540:LYS:NZ	1.47	1.28
1:B:226:ALA:HB1	1:B:228:ARG:CZ	1.63	1.27
1:A:523:ARG:NH1	1:C:526:GLN:NE2	1.78	1.27
1:B:62:GLN:NE2	1:C:140:ALA:HB2	0.94	1.26
1:B:378:VAL:O	1:B:380:ALA:N	1.66	1.26
1:A:169:LEU:HD12	1:C:168:VAL:N	1.48	1.26
1:B:446:ALA:HB2	1:A:350:LEU:CD2	1.59	1.25
1:B:446:ALA:CB	1:A:350:LEU:CD2	2.03	1.25
1:A:45:THR:O	1:C:166:ARG:N	1.68	1.25
1:A:220:VAL:CG1	1:C:132:PHE:CE1	2.19	1.25
1:C:378:VAL:O	1:C:380:ALA:N	1.66	1.24
1:B:343:THR:HG22	1:A:446:ALA:CB	1.67	1.24
1:B:437:ARG:HH21	1:A:352:VAL:CG1	1.48	1.24
1:A:535:THR:O	1:A:536:GLY:O	1.54	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ARG:NE	1:A:352:VAL:HG21	1.50	1.23
1:A:98:GLN:O	1:A:222:ALA:O	1.56	1.22
1:B:350:LEU:HB2	1:A:445:ALA:CA	1.65	1.22
1:A:227:ALA:HB1	1:A:228:ARG:CZ	1.70	1.21
1:A:220:VAL:HG13	1:C:132:PHE:CE1	1.74	1.21
1:B:350:LEU:CB	1:A:445:ALA:HA	1.63	1.20
1:A:523:ARG:CZ	1:C:526:GLN:HE22	1.54	1.20
1:A:523:ARG:CD	1:C:526:GLN:NE2	2.01	1.20
1:B:350:LEU:HD21	1:A:446:ALA:CB	1.72	1.20
1:A:45:THR:HB	1:C:166:ARG:O	1.32	1.20
1:B:11:SER:OG	1:C:29:ASP:OD2	1.59	1.19
1:A:274:THR:HG21	1:C:537:ARG:CB	1.60	1.18
1:A:362:THR:HA	1:A:363:THR:CG2	1.72	1.18
1:B:343:THR:OG1	1:A:435:TYR:CD2	1.88	1.18
1:C:362:THR:HA	1:C:363:THR:CG2	1.72	1.18
1:B:362:THR:HA	1:B:363:THR:CG2	1.72	1.18
1:C:364:ASN:N	1:C:365:ALA:CB	2.07	1.17
1:A:485:LEU:HD12	1:A:485:LEU:N	1.39	1.17
1:A:220:VAL:CG1	1:C:132:PHE:HE1	1.57	1.16
1:B:485:LEU:N	1:B:485:LEU:HD12	1.39	1.16
1:B:350:LEU:HD21	1:A:446:ALA:HB2	1.26	1.16
1:B:364:ASN:N	1:B:365:ALA:CB	2.07	1.16
1:A:169:LEU:HD11	1:C:169:LEU:N	1.58	1.16
1:A:364:ASN:N	1:A:365:ALA:CB	2.07	1.16
1:B:343:THR:CG2	1:A:435:TYR:CB	2.24	1.16
1:C:485:LEU:N	1:C:485:LEU:HD12	1.39	1.16
1:B:352:VAL:CG1	1:A:437:ARG:HH21	1.59	1.15
1:B:343:THR:HG22	1:A:446:ALA:HB1	1.15	1.15
1:B:530:VAL:CG2	1:B:531:GLY:N	1.89	1.15
1:A:45:THR:CG2	1:C:166:ARG:HB2	1.77	1.15
1:A:532:SER:O	1:A:534:ALA:N	1.78	1.14
1:C:366:ASP:O	1:C:367:GLN:HB2	1.44	1.14
1:A:523:ARG:HH11	1:C:526:GLN:NE2	1.36	1.13
1:B:366:ASP:O	1:B:367:GLN:HB2	1.44	1.13
1:A:45:THR:CG2	1:C:166:ARG:CB	2.28	1.12
1:A:356:GLU:HG2	1:A:379:THR:HG22	1.14	1.12
1:C:356:GLU:HG2	1:C:379:THR:CG2	1.80	1.12
1:A:45:THR:C	1:C:166:ARG:O	1.92	1.12
1:A:462:ALA:CB	1:C:540:LYS:NZ	2.13	1.12
1:B:356:GLU:HG2	1:B:379:THR:CG2	1.80	1.11
1:C:220:VAL:O	1:C:221:PRO:O	1.68	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HG	1:C:168:VAL:HA	1.15	1.11
1:B:200:PHE:CE1	1:C:191:ARG:HD2	1.87	1.10
1:B:226:ALA:CB	1:B:228:ARG:CZ	2.30	1.10
1:B:350:LEU:CD2	1:A:446:ALA:HB2	1.78	1.09
1:A:356:GLU:HG2	1:A:379:THR:CG2	1.80	1.09
1:B:446:ALA:HB3	1:A:350:LEU:HD21	1.10	1.09
1:B:362:THR:CA	1:B:363:THR:HG23	1.82	1.09
1:A:45:THR:HG21	1:C:168:VAL:O	1.48	1.09
1:B:435:TYR:CE2	1:A:343:THR:O	2.05	1.08
1:C:220:VAL:HG13	1:C:221:PRO:HD2	1.17	1.08
1:B:392:ARG:HD2	1:A:250:TYR:HH	0.98	1.08
1:A:220:VAL:HG11	1:C:132:PHE:CD1	1.87	1.08
1:B:392:ARG:HD2	1:A:250:TYR:OH	1.41	1.08
1:A:45:THR:HB	1:C:166:ARG:C	1.76	1.08
1:B:220:VAL:HG13	1:B:221:PRO:HD2	1.12	1.08
1:A:362:THR:CA	1:A:363:THR:HG23	1.82	1.08
1:C:362:THR:CA	1:C:363:THR:HG23	1.82	1.08
1:B:530:VAL:HG23	1:B:531:GLY:N	1.48	1.08
1:B:356:GLU:HG2	1:B:379:THR:HG22	1.14	1.07
1:B:445:ALA:CB	1:A:350:LEU:H	1.67	1.07
1:A:366:ASP:O	1:A:367:GLN:HB2	1.44	1.07
1:B:226:ALA:HA	1:B:228:ARG:HH12	1.16	1.07
1:C:356:GLU:HG2	1:C:379:THR:HG22	1.14	1.07
1:C:356:GLU:HG3	1:C:379:THR:HG22	1.34	1.07
1:B:356:GLU:HG3	1:B:379:THR:HG22	1.34	1.06
1:B:350:LEU:HB2	1:A:445:ALA:HA	1.08	1.06
1:B:485:LEU:N	1:B:485:LEU:CD1	2.18	1.06
1:B:485:LEU:H	1:B:485:LEU:CD1	1.68	1.06
1:A:485:LEU:H	1:A:485:LEU:CD1	1.68	1.06
1:C:485:LEU:H	1:C:485:LEU:CD1	1.68	1.06
1:C:532:SER:CA	1:C:533:LEU:HD22	1.84	1.06
1:B:445:ALA:C	1:A:350:LEU:HB2	1.75	1.06
1:A:485:LEU:N	1:A:485:LEU:CD1	2.18	1.06
1:C:532:SER:C	1:C:533:LEU:CD2	2.28	1.05
1:C:485:LEU:N	1:C:485:LEU:CD1	2.18	1.05
1:B:343:THR:HG21	1:A:435:TYR:HB3	1.07	1.04
1:B:207:MET:HE3	1:C:143:THR:HG21	1.33	1.04
1:B:352:VAL:HG11	1:A:437:ARG:HH21	1.20	1.04
1:A:220:VAL:HG11	1:C:132:PHE:CE1	1.89	1.03
1:B:444:ALA:HB3	1:A:352:VAL:HG12	1.37	1.03
1:B:445:ALA:HA	1:A:350:LEU:N	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:ND2	1:C:131:GLY:O	1.88	1.03
1:A:356:GLU:HG3	1:A:379:THR:HG22	1.34	1.03
1:B:539:LEU:HA	1:B:540:LYS:HE3	1.38	1.03
1:B:248:PRO:HD3	1:A:392:ARG:NH2	1.74	1.02
1:B:446:ALA:HB2	1:A:350:LEU:HD21	1.15	1.02
1:B:228:ARG:HD3	1:B:228:ARG:N	1.72	1.02
1:A:356:GLU:CG	1:A:379:THR:CG2	2.37	1.02
1:A:523:ARG:HD3	1:C:526:GLN:HE21	0.90	1.02
1:B:343:THR:HG21	1:A:435:TYR:HB2	1.38	1.02
1:C:227:ALA:HB3	1:C:228:ARG:NE	1.72	1.02
1:B:226:ALA:HA	1:B:228:ARG:NH1	1.74	1.02
1:B:343:THR:CG2	1:A:446:ALA:HB1	1.90	1.01
1:C:296:GLU:O	1:C:297:PHE:HD2	1.43	1.01
1:A:523:ARG:CZ	1:C:526:GLN:NE2	2.18	1.01
1:C:442:ALA:O	1:C:443:ASP:HB2	1.61	1.01
1:C:229:MET:HG3	1:C:230:VAL:H	1.25	1.01
1:B:442:ALA:O	1:B:443:ASP:HB2	1.60	1.01
1:B:296:GLU:O	1:B:297:PHE:HD2	1.43	1.00
1:A:229:MET:HG3	1:A:230:VAL:N	1.73	1.00
1:B:238:ARG:HB2	1:A:313:ASP:HB2	1.40	1.00
1:C:220:VAL:HG12	1:C:221:PRO:HD2	1.40	1.00
1:B:343:THR:OG1	1:A:435:TYR:HD2	1.32	1.00
1:B:535:THR:O	1:B:537:ARG:HD3	1.61	0.99
1:A:274:THR:HG21	1:C:537:ARG:HB3	1.41	0.99
1:B:437:ARG:HH21	1:A:352:VAL:HG13	1.26	0.99
1:A:296:GLU:O	1:A:297:PHE:HD2	1.43	0.99
1:C:123:ILE:HD11	1:C:184:CYS:SG	2.02	0.99
1:B:352:VAL:HG21	1:A:437:ARG:NE	1.77	0.99
1:B:445:ALA:N	1:A:350:LEU:HB2	1.77	0.99
1:B:437:ARG:CZ	1:A:352:VAL:HG21	1.92	0.98
1:B:248:PRO:CD	1:A:392:ARG:NH2	2.26	0.98
1:B:356:GLU:CG	1:B:379:THR:CG2	2.37	0.98
1:A:462:ALA:HB1	1:C:540:LYS:HZ2	1.07	0.98
1:B:437:ARG:HH21	1:A:352:VAL:HG11	1.28	0.97
1:A:442:ALA:O	1:A:443:ASP:CB	2.13	0.97
1:C:356:GLU:CG	1:C:379:THR:CG2	2.37	0.97
1:B:437:ARG:NH2	1:A:352:VAL:HG11	1.78	0.96
1:A:45:THR:CB	1:C:166:ARG:O	2.12	0.96
1:B:437:ARG:NH2	1:A:352:VAL:CG1	2.28	0.96
1:B:442:ALA:O	1:B:443:ASP:CB	2.13	0.96
1:A:442:ALA:O	1:A:443:ASP:HB2	1.61	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG13	1:B:221:PRO:CD	1.96	0.96
1:A:535:THR:O	1:A:536:GLY:C	2.02	0.96
1:C:227:ALA:CB	1:C:228:ARG:CZ	2.43	0.96
1:A:425:PRO:HD3	1:C:425:PRO:HB3	1.43	0.96
1:A:425:PRO:HD3	1:C:425:PRO:HG3	1.19	0.96
1:C:442:ALA:O	1:C:443:ASP:CB	2.13	0.96
1:A:227:ALA:CB	1:A:228:ARG:CZ	2.44	0.96
1:C:220:VAL:CG1	1:C:221:PRO:CD	2.44	0.96
1:A:229:MET:HG3	1:A:230:VAL:H	1.27	0.95
1:B:200:PHE:CD1	1:C:191:ARG:HD2	2.02	0.95
1:A:362:THR:HA	1:A:363:THR:HG23	0.95	0.94
1:A:485:LEU:HD12	1:A:485:LEU:H	1.15	0.94
1:C:362:THR:HA	1:C:363:THR:HG23	0.95	0.94
1:A:169:LEU:HD12	1:C:168:VAL:C	1.71	0.94
1:C:477:TYR:CZ	1:C:513:GLY:HA2	2.03	0.94
1:B:531:GLY:O	1:B:533:LEU:N	2.00	0.94
1:C:303:GLU:O	1:C:378:VAL:HG23	1.68	0.94
1:B:227:ALA:H	1:B:228:ARG:NH1	1.64	0.93
1:A:477:TYR:CZ	1:A:513:GLY:HA2	2.03	0.93
1:C:363:THR:H	1:C:365:ALA:CB	1.81	0.93
1:B:62:GLN:HE22	1:C:140:ALA:HB2	1.28	0.93
1:B:226:ALA:CA	1:B:228:ARG:NH1	2.30	0.93
1:C:227:ALA:CB	1:C:228:ARG:NE	2.30	0.93
1:B:227:ALA:H	1:B:228:ARG:HH11	1.01	0.93
1:A:363:THR:H	1:A:365:ALA:CB	1.82	0.93
1:B:362:THR:HA	1:B:363:THR:HG23	0.95	0.93
1:B:226:ALA:CB	1:B:228:ARG:NH2	2.31	0.93
1:B:363:THR:H	1:B:365:ALA:CB	1.82	0.93
1:B:477:TYR:CZ	1:B:513:GLY:HA2	2.03	0.93
1:B:530:VAL:HG23	1:B:531:GLY:CA	1.99	0.92
1:A:303:GLU:O	1:A:378:VAL:HG23	1.68	0.92
1:A:425:PRO:HD3	1:C:425:PRO:HG2	1.51	0.92
1:B:352:VAL:HG11	1:A:437:ARG:NH2	1.83	0.92
1:B:18:ALA:CB	1:C:153:ARG:NH1	2.33	0.92
1:B:62:GLN:CD	1:C:140:ALA:CA	2.43	0.91
1:B:303:GLU:O	1:B:378:VAL:HG23	1.68	0.91
1:A:440:ASP:HB2	1:A:443:ASP:O	1.70	0.91
1:B:220:VAL:CG1	1:B:221:PRO:HD2	1.97	0.91
1:B:207:MET:CE	1:C:143:THR:CG2	2.48	0.91
1:A:45:THR:CG2	1:C:166:ARG:HB3	1.98	0.91
1:C:485:LEU:HD12	1:C:485:LEU:H	1.15	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ASP:HB2	1:B:443:ASP:O	1.70	0.91
1:B:435:TYR:CE2	1:A:343:THR:C	2.49	0.90
1:C:220:VAL:HG13	1:C:221:PRO:CD	1.98	0.90
1:B:226:ALA:HB2	1:B:228:ARG:NH2	1.87	0.90
1:B:529:SER:O	1:B:530:VAL:C	2.09	0.90
1:C:227:ALA:HB3	1:C:228:ARG:CZ	2.01	0.90
1:C:440:ASP:HB2	1:C:443:ASP:O	1.70	0.90
1:A:218:PHE:CE1	1:C:129:PRO:HB3	2.07	0.89
1:A:425:PRO:CD	1:C:425:PRO:HG2	2.02	0.89
1:B:446:ALA:HB2	1:A:350:LEU:HD22	1.53	0.89
1:C:473:LEU:HD23	1:C:520:TRP:H	1.38	0.89
1:A:425:PRO:CG	1:C:425:PRO:HG3	2.02	0.89
1:B:62:GLN:OE1	1:C:140:ALA:HA	1.71	0.89
1:A:170:PHE:CE1	1:C:167:ASN:CG	2.48	0.89
1:B:437:ARG:NE	1:A:352:VAL:CG2	2.34	0.88
1:A:295:TYR:OH	1:A:387:VAL:O	1.92	0.88
1:A:473:LEU:HD23	1:A:520:TRP:H	1.38	0.88
1:B:138:THR:H	1:B:141:GLN:HG3	1.39	0.88
1:A:462:ALA:CB	1:C:540:LYS:HZ1	1.78	0.87
1:A:532:SER:C	1:A:534:ALA:H	1.82	0.87
1:C:295:TYR:OH	1:C:387:VAL:O	1.92	0.87
1:C:532:SER:N	1:C:533:LEU:HD22	1.88	0.87
1:B:539:LEU:CA	1:B:540:LYS:HE3	2.04	0.87
1:B:485:LEU:HD12	1:B:485:LEU:H	1.15	0.87
1:B:350:LEU:HD21	1:A:446:ALA:HB3	1.57	0.86
1:B:392:ARG:HD3	1:A:250:TYR:OH	1.75	0.86
1:B:343:THR:CG2	1:A:435:TYR:HB3	1.97	0.86
1:B:473:LEU:HD23	1:B:520:TRP:H	1.38	0.86
1:B:531:GLY:O	1:B:532:SER:C	2.12	0.86
1:A:227:ALA:CB	1:A:228:ARG:NH1	2.37	0.86
1:B:238:ARG:HB2	1:A:313:ASP:CB	2.04	0.86
1:B:535:THR:O	1:B:537:ARG:NH1	2.07	0.86
1:A:363:THR:C	1:A:365:ALA:CB	2.45	0.86
1:B:295:TYR:OH	1:B:387:VAL:O	1.92	0.86
1:A:363:THR:CA	1:A:365:ALA:HB2	2.06	0.85
1:C:363:THR:CA	1:C:365:ALA:HB2	2.06	0.85
1:A:220:VAL:CG1	1:C:132:PHE:CD1	2.51	0.85
1:A:169:LEU:HD12	1:C:167:ASN:C	1.97	0.85
1:A:523:ARG:NE	1:C:526:GLN:NE2	2.23	0.85
1:B:343:THR:CG2	1:A:435:TYR:CG	2.56	0.85
1:B:363:THR:CA	1:B:365:ALA:HB2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:THR:C	1:B:365:ALA:CB	2.45	0.85
1:B:205:ARG:CZ	1:C:139:ILE:HD11	2.07	0.84
1:A:539:LEU:O	1:A:540:LYS:HB3	1.77	0.84
1:B:366:ASP:O	1:B:367:GLN:CB	2.24	0.84
1:B:445:ALA:CA	1:A:350:LEU:N	2.40	0.84
1:B:373:ARG:HH12	1:B:375:PHE:HZ	0.85	0.84
1:C:229:MET:HG3	1:C:230:VAL:N	1.91	0.84
1:C:373:ARG:HH12	1:C:375:PHE:HZ	0.85	0.84
1:B:437:ARG:HE	1:A:352:VAL:HG21	1.40	0.84
1:B:445:ALA:CB	1:A:350:LEU:N	2.41	0.84
1:A:274:THR:HG21	1:C:537:ARG:HB2	1.25	0.84
1:C:532:SER:O	1:C:532:SER:OG	1.69	0.84
1:B:363:THR:N	1:B:365:ALA:CB	2.41	0.83
1:B:392:ARG:NH2	1:A:248:PRO:HD3	1.94	0.83
1:A:363:THR:N	1:A:365:ALA:CB	2.41	0.83
1:C:367:GLN:HE22	1:C:375:PHE:H	1.26	0.83
1:A:366:ASP:O	1:A:367:GLN:CB	2.24	0.83
1:B:228:ARG:HD3	1:B:228:ARG:H	1.41	0.82
1:B:228:ARG:N	1:B:228:ARG:CD	2.40	0.82
1:C:227:ALA:HB2	1:C:228:ARG:CZ	2.09	0.82
1:B:62:GLN:OE1	1:C:140:ALA:CA	2.28	0.82
1:A:373:ARG:HH12	1:A:375:PHE:HZ	0.85	0.82
1:C:363:THR:N	1:C:365:ALA:CB	2.41	0.82
1:A:274:THR:HG23	1:C:537:ARG:CG	2.10	0.82
1:B:343:THR:HB	1:A:435:TYR:CD1	2.15	0.81
1:A:45:THR:HG22	1:C:166:ARG:HB2	0.83	0.81
1:A:523:ARG:HH11	1:C:526:GLN:HE21	1.22	0.81
1:C:366:ASP:O	1:C:367:GLN:CB	2.24	0.81
1:B:437:ARG:HE	1:A:352:VAL:CB	1.92	0.81
1:A:101:ASN:ND2	1:C:131:GLY:CA	2.43	0.81
1:A:462:ALA:CB	1:C:540:LYS:HZ2	1.80	0.81
1:C:227:ALA:CB	1:C:228:ARG:CA	2.30	0.81
1:B:363:THR:N	1:B:365:ALA:HB1	1.96	0.81
1:A:220:VAL:HG11	1:C:132:PHE:HD1	1.46	0.81
1:A:524:LEU:HD13	1:C:524:LEU:HD22	1.63	0.81
1:C:229:MET:CG	1:C:230:VAL:H	1.94	0.81
1:A:363:THR:N	1:A:365:ALA:HB1	1.96	0.80
1:C:363:THR:C	1:C:365:ALA:CB	2.45	0.80
1:B:18:ALA:HB2	1:C:153:ARG:NH1	1.96	0.80
1:B:200:PHE:CD1	1:C:191:ARG:CD	2.64	0.80
1:C:363:THR:N	1:C:365:ALA:HB1	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ALA:CB	1:A:352:VAL:HG12	2.11	0.80
1:A:367:GLN:HE22	1:A:375:PHE:H	1.26	0.80
1:B:378:VAL:C	1:B:380:ALA:H	1.89	0.79
1:A:477:TYR:OH	1:A:513:GLY:HA3	1.82	0.79
1:B:445:ALA:CA	1:A:350:LEU:H	1.94	0.79
1:C:477:TYR:OH	1:C:513:GLY:HA3	1.82	0.79
1:B:437:ARG:HE	1:A:352:VAL:CG2	1.93	0.79
1:B:352:VAL:HG13	1:A:437:ARG:HH21	1.45	0.79
1:A:425:PRO:HD2	1:C:425:PRO:CG	2.13	0.79
1:B:119:THR:HG22	1:B:192:THR:HG22	1.64	0.78
1:B:238:ARG:O	1:A:285:TRP:HZ2	1.65	0.78
1:B:477:TYR:OH	1:B:513:GLY:HA3	1.82	0.78
1:B:38:GLY:HA3	1:B:213:ASP:HB3	1.64	0.78
1:B:350:LEU:CA	1:A:445:ALA:HA	2.12	0.78
1:C:227:ALA:HB1	1:C:228:ARG:HD3	1.66	0.78
1:A:223:ALA:O	1:A:224:ALA:CB	2.31	0.78
1:B:227:ALA:N	1:B:228:ARG:NH1	2.30	0.78
1:B:367:GLN:HE22	1:B:375:PHE:H	1.26	0.78
1:A:47:GLY:N	1:C:165:VAL:HG13	1.98	0.78
1:A:169:LEU:HG	1:C:168:VAL:CA	2.08	0.78
1:A:425:PRO:CD	1:C:425:PRO:CB	2.52	0.77
1:A:220:VAL:HG13	1:C:132:PHE:HE1	1.17	0.77
1:B:18:ALA:CB	1:C:153:ARG:HH12	1.95	0.77
1:B:392:ARG:NH2	1:A:248:PRO:CD	2.48	0.77
1:B:18:ALA:HA	1:C:153:ARG:HH11	1.47	0.77
1:B:238:ARG:NH2	1:A:315:SER:HB3	2.00	0.77
1:C:477:TYR:CZ	1:C:513:GLY:CA	2.68	0.77
1:B:362:THR:HG22	1:B:363:THR:HG21	1.67	0.77
1:B:364:ASN:H	1:B:365:ALA:HB2	1.46	0.77
1:B:222:ALA:O	1:B:223:ALA:CB	2.32	0.77
1:B:362:THR:HG22	1:B:363:THR:CG2	2.16	0.76
1:C:362:THR:HG22	1:C:363:THR:CG2	2.16	0.76
1:B:98:GLN:O	1:B:222:ALA:HA	1.85	0.76
1:B:343:THR:HB	1:A:435:TYR:CE2	2.20	0.76
1:B:477:TYR:CZ	1:B:513:GLY:CA	2.68	0.76
1:A:362:THR:HG22	1:A:363:THR:HG21	1.67	0.76
1:C:362:THR:HG22	1:C:363:THR:HG21	1.67	0.76
1:C:363:THR:H	1:C:365:ALA:HB1	1.50	0.76
1:A:462:ALA:HB1	1:C:540:LYS:HZ1	1.34	0.76
1:A:477:TYR:CZ	1:A:513:GLY:CA	2.68	0.76
1:B:440:ASP:HA	1:B:441:THR:HB	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:LEU:O	1:C:540:LYS:HB3	1.86	0.75
1:B:248:PRO:HD3	1:A:392:ARG:HH21	1.49	0.75
1:B:352:VAL:HG21	1:A:437:ARG:CZ	2.16	0.75
1:B:352:VAL:HG12	1:A:444:ALA:HB3	1.68	0.75
1:A:227:ALA:HA	1:A:228:ARG:NH2	2.01	0.75
1:B:62:GLN:CG	1:C:140:ALA:HB1	2.15	0.75
1:A:424:LEU:HA	1:C:425:PRO:CB	2.16	0.75
1:C:364:ASN:H	1:C:365:ALA:HB2	1.47	0.75
1:A:296:GLU:O	1:A:297:PHE:CD2	2.35	0.75
1:A:362:THR:HG22	1:A:363:THR:CG2	2.16	0.75
1:A:440:ASP:HA	1:A:441:THR:HB	1.69	0.75
1:C:174:ASP:HB2	1:C:177:GLN:HG2	1.67	0.75
1:C:378:VAL:C	1:C:380:ALA:H	1.89	0.75
1:B:62:GLN:CG	1:C:140:ALA:CB	2.63	0.75
1:B:343:THR:CG2	1:A:435:TYR:HB2	2.03	0.74
1:C:227:ALA:CB	1:C:228:ARG:CD	2.65	0.74
1:C:440:ASP:HA	1:C:441:THR:HB	1.69	0.74
1:B:343:THR:HG22	1:A:446:ALA:HB2	1.65	0.74
1:B:18:ALA:HA	1:C:153:ARG:NH1	2.03	0.74
1:B:205:ARG:NH2	1:C:139:ILE:CD1	2.50	0.74
1:C:296:GLU:O	1:C:297:PHE:CD2	2.35	0.74
1:B:363:THR:H	1:B:365:ALA:HB1	1.51	0.74
1:B:18:ALA:CA	1:C:153:ARG:HH11	2.01	0.74
1:B:445:ALA:HB2	1:A:350:LEU:H	1.50	0.74
1:B:538:MET:O	1:B:539:LEU:CB	2.25	0.73
1:B:62:GLN:CD	1:C:140:ALA:HA	2.12	0.73
1:B:343:THR:CG2	1:A:446:ALA:CB	2.54	0.73
1:B:62:GLN:CD	1:C:140:ALA:HB1	2.09	0.73
1:C:223:ALA:O	1:C:224:ALA:CB	2.36	0.73
1:C:533:LEU:CD2	1:C:533:LEU:N	2.47	0.73
1:B:207:MET:HE1	1:C:143:THR:HG21	1.67	0.72
1:B:361:PRO:O	1:B:362:THR:C	2.32	0.72
1:A:535:THR:C	1:A:536:GLY:O	2.33	0.72
1:C:223:ALA:O	1:C:224:ALA:HB3	1.88	0.72
1:B:227:ALA:N	1:B:228:ARG:HH11	1.83	0.72
1:A:524:LEU:CD1	1:C:524:LEU:HB3	2.18	0.72
1:C:344:THR:HB	1:C:348:ASP:OD2	1.90	0.72
1:A:364:ASN:H	1:A:365:ALA:HB2	1.46	0.72
1:C:361:PRO:O	1:C:362:THR:C	2.32	0.72
1:C:227:ALA:HB2	1:C:228:ARG:NH1	2.04	0.72
1:A:344:THR:HB	1:A:348:ASP:OD2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:CYS:HB2	1:C:146:PRO:HG2	1.72	0.72
1:A:229:MET:CG	1:A:230:VAL:H	2.03	0.72
1:B:129:PRO:HA	1:B:180:MET:HE2	1.71	0.71
1:B:238:ARG:CB	1:A:313:ASP:HB2	2.17	0.71
1:A:220:VAL:HG12	1:A:222:ALA:H	1.55	0.71
1:B:296:GLU:C	1:B:297:PHE:HD2	1.99	0.71
1:B:437:ARG:CZ	1:A:352:VAL:HG11	2.19	0.71
1:A:523:ARG:CD	1:C:526:GLN:CD	2.62	0.71
1:C:362:THR:HA	1:C:363:THR:CB	2.20	0.71
1:B:362:THR:HA	1:B:363:THR:CB	2.19	0.71
1:C:296:GLU:C	1:C:297:PHE:HD2	1.99	0.71
1:A:170:PHE:C	1:C:167:ASN:HD21	1.98	0.71
1:B:296:GLU:O	1:B:297:PHE:CD2	2.35	0.71
1:B:474:LEU:N	1:B:519:SER:O	2.23	0.71
1:B:344:THR:HB	1:B:348:ASP:OD2	1.90	0.70
1:A:361:PRO:O	1:A:362:THR:C	2.32	0.70
1:A:296:GLU:C	1:A:297:PHE:HD2	1.99	0.70
1:B:364:ASN:H	1:B:365:ALA:CB	2.03	0.70
1:A:45:THR:O	1:C:166:ARG:O	2.09	0.70
1:A:141:GLN:HA	1:A:144:LEU:HD12	1.74	0.70
1:A:227:ALA:CB	1:A:228:ARG:NH2	2.53	0.70
1:A:228:ARG:N	1:A:228:ARG:CD	2.55	0.69
1:A:474:LEU:N	1:A:519:SER:O	2.23	0.69
1:C:378:VAL:C	1:C:380:ALA:N	2.48	0.69
1:B:446:ALA:CB	1:A:343:THR:CG2	2.37	0.69
1:A:220:VAL:CG1	1:A:222:ALA:H	2.06	0.69
1:A:378:VAL:C	1:A:380:ALA:N	2.48	0.69
1:C:227:ALA:CB	1:C:228:ARG:HD3	2.23	0.69
1:A:462:ALA:HB2	1:C:540:LYS:HZ1	1.58	0.69
1:C:364:ASN:H	1:C:365:ALA:CB	2.03	0.69
1:B:352:VAL:CG1	1:A:437:ARG:NH2	2.42	0.69
1:A:363:THR:H	1:A:365:ALA:HB1	1.50	0.69
1:B:226:ALA:CB	1:B:228:ARG:NH1	2.54	0.69
1:A:425:PRO:CD	1:C:425:PRO:HB3	2.17	0.69
1:B:350:LEU:N	1:A:445:ALA:HA	2.07	0.68
1:B:392:ARG:NE	1:A:250:TYR:OH	2.25	0.68
1:A:418:PRO:HB3	1:C:533:LEU:H	1.58	0.68
1:A:228:ARG:N	1:A:228:ARG:HD2	2.09	0.68
1:A:362:THR:HA	1:A:363:THR:CB	2.19	0.68
1:A:230:VAL:HG11	1:A:473:LEU:HD11	1.75	0.68
1:B:18:ALA:CA	1:C:153:ARG:NH1	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:HG23	1:B:531:GLY:HA3	1.72	0.68
1:A:170:PHE:O	1:C:167:ASN:ND2	2.23	0.68
1:C:127:CYS:HB3	1:C:180:MET:HE3	1.75	0.68
1:B:343:THR:CB	1:A:435:TYR:CB	2.61	0.68
1:B:205:ARG:NE	1:C:139:ILE:HD11	2.09	0.68
1:B:444:ALA:CB	1:A:352:VAL:CG1	2.72	0.67
1:B:367:GLN:HE21	1:B:367:GLN:HA	1.59	0.67
1:B:222:ALA:O	1:B:223:ALA:HB2	1.93	0.67
1:A:272:ASP:OD2	1:C:537:ARG:CZ	2.43	0.67
1:C:474:LEU:N	1:C:519:SER:O	2.23	0.67
1:B:223:ALA:O	1:B:224:ALA:HB3	1.95	0.67
1:B:437:ARG:CZ	1:A:352:VAL:CG2	2.72	0.67
1:A:218:PHE:CZ	1:C:129:PRO:HB3	2.30	0.67
1:A:367:GLN:HA	1:A:367:GLN:HE21	1.59	0.67
1:C:477:TYR:OH	1:C:513:GLY:CA	2.43	0.67
1:B:119:THR:HG21	1:B:200:PHE:CE2	2.30	0.66
1:A:101:ASN:HD22	1:C:132:PHE:N	1.89	0.66
1:C:227:ALA:HB1	1:C:228:ARG:CD	2.24	0.66
1:C:367:GLN:HE21	1:C:367:GLN:HA	1.59	0.66
1:B:205:ARG:NH2	1:C:139:ILE:HD11	2.09	0.66
1:B:289:PHE:HE1	1:B:357:MET:HE1	1.61	0.66
1:B:530:VAL:CG2	1:B:531:GLY:CA	2.66	0.66
1:B:205:ARG:HH21	1:C:139:ILE:CD1	2.07	0.66
1:B:248:PRO:CD	1:A:392:ARG:CZ	2.74	0.66
1:B:536:GLY:O	1:B:537:ARG:HB3	1.94	0.66
1:A:289:PHE:HE1	1:A:357:MET:HE1	1.61	0.66
1:A:440:ASP:HA	1:A:441:THR:CB	2.26	0.66
1:B:62:GLN:HE21	1:C:140:ALA:HB2	1.46	0.66
1:B:230:VAL:HB	1:B:466:PHE:CG	2.30	0.66
1:B:248:PRO:CG	1:A:392:ARG:NH2	2.58	0.66
1:B:350:LEU:CB	1:A:445:ALA:CA	2.40	0.66
1:A:228:ARG:HD2	1:A:228:ARG:C	2.19	0.66
1:C:297:PHE:HB3	1:C:300:GLY:HA2	1.78	0.66
1:B:207:MET:HE1	1:C:143:THR:CG2	2.24	0.65
1:B:297:PHE:HB3	1:B:300:GLY:HA2	1.78	0.65
1:B:477:TYR:OH	1:B:513:GLY:CA	2.43	0.65
1:A:477:TYR:OH	1:A:513:GLY:CA	2.43	0.65
1:A:116:ASN:ND2	1:A:200:PHE:CE1	2.65	0.65
1:C:289:PHE:HE1	1:C:357:MET:HE1	1.61	0.65
1:A:356:GLU:HG3	1:A:379:THR:CG2	2.18	0.65
1:B:205:ARG:HE	1:C:139:ILE:HD12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ASP:HA	1:C:441:THR:CB	2.26	0.65
1:B:116:ASN:HD22	1:B:200:PHE:HE1	1.45	0.65
1:A:221:PRO:O	1:A:223:ALA:N	2.30	0.65
1:B:485:LEU:H	1:B:485:LEU:HD13	1.61	0.65
1:B:535:THR:O	1:B:537:ARG:CD	2.42	0.65
1:C:220:VAL:HG12	1:C:221:PRO:CD	2.19	0.65
1:B:440:ASP:HA	1:B:441:THR:CB	2.26	0.65
1:B:445:ALA:C	1:A:350:LEU:CB	2.15	0.65
1:C:532:SER:N	1:C:533:LEU:CD2	2.60	0.65
1:A:45:THR:O	1:C:166:ARG:CA	2.44	0.64
1:C:123:ILE:HD11	1:C:184:CYS:HG	1.58	0.64
1:B:62:GLN:HB3	1:C:140:ALA:HB1	1.78	0.64
1:B:129:PRO:HA	1:B:180:MET:CE	2.27	0.64
1:B:205:ARG:NE	1:C:139:ILE:CD1	2.60	0.64
1:B:435:TYR:OH	1:A:344:THR:C	2.40	0.64
1:B:445:ALA:HB1	1:A:349:LYS:HA	1.79	0.64
1:A:297:PHE:HB3	1:A:300:GLY:HA2	1.78	0.64
1:B:437:ARG:HA	1:A:340:GLN:OE1	1.98	0.63
1:B:539:LEU:CA	1:B:540:LYS:CE	2.77	0.63
1:A:229:MET:CG	1:A:230:VAL:N	2.54	0.63
1:C:101:ASN:HB3	1:C:220:VAL:HG21	1.81	0.63
1:B:248:PRO:HG2	1:A:392:ARG:CZ	2.29	0.63
1:B:392:ARG:HH21	1:A:248:PRO:HD3	1.64	0.63
1:A:223:ALA:O	1:A:224:ALA:HB2	1.98	0.63
1:A:227:ALA:CA	1:A:228:ARG:CZ	2.77	0.63
1:C:485:LEU:H	1:C:485:LEU:HD13	1.61	0.62
1:B:356:GLU:HG3	1:B:379:THR:CG2	2.18	0.62
1:A:228:ARG:HD2	1:A:228:ARG:H	1.64	0.62
1:A:274:THR:HG23	1:C:537:ARG:HB2	0.62	0.62
1:B:352:VAL:HG21	1:A:437:ARG:HE	1.61	0.62
1:B:439:ILE:HA	1:B:440:ASP:O	2.00	0.62
1:B:446:ALA:HB1	1:A:343:THR:HG22	0.70	0.61
1:A:45:THR:CA	1:C:166:ARG:O	2.47	0.61
1:A:478:ARG:HG2	1:A:479:ASN:N	2.15	0.61
1:A:364:ASN:H	1:A:365:ALA:CB	2.03	0.61
1:C:362:THR:HB	1:C:363:THR:OG1	2.01	0.61
1:C:478:ARG:HG2	1:C:479:ASN:N	2.15	0.61
1:B:362:THR:HB	1:B:363:THR:OG1	2.01	0.61
1:A:424:LEU:HA	1:C:425:PRO:HB2	1.81	0.61
1:C:367:GLN:NE2	1:C:375:PHE:H	1.98	0.61
1:B:248:PRO:HG2	1:A:392:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:CD	1:A:250:TYR:HH	1.75	0.61
1:A:425:PRO:HD2	1:C:425:PRO:HG2	1.79	0.61
1:B:18:ALA:CB	1:C:153:ARG:HH11	2.14	0.61
1:B:207:MET:HE2	1:C:143:THR:HG21	1.74	0.61
1:A:362:THR:HB	1:A:363:THR:OG1	2.01	0.61
1:B:478:ARG:HG2	1:B:479:ASN:N	2.15	0.61
1:C:356:GLU:HG3	1:C:379:THR:CG2	2.18	0.61
1:A:439:ILE:HA	1:A:440:ASP:O	2.00	0.61
1:A:523:ARG:HD3	1:C:526:GLN:CD	2.20	0.61
1:C:100:TYR:HA	1:C:218:PHE:O	2.01	0.61
1:B:437:ARG:NE	1:A:352:VAL:HG11	2.15	0.61
1:A:170:PHE:N	1:C:167:ASN:OD1	2.28	0.60
1:C:363:THR:CA	1:C:365:ALA:CB	2.79	0.60
1:C:439:ILE:HA	1:C:440:ASP:O	2.00	0.60
1:A:169:LEU:CD1	1:C:167:ASN:C	2.72	0.60
1:B:226:ALA:HB1	1:B:228:ARG:NE	2.14	0.60
1:B:352:VAL:HG11	1:A:437:ARG:CZ	2.31	0.60
1:B:367:GLN:NE2	1:B:375:PHE:H	1.98	0.60
1:A:101:ASN:HD21	1:C:131:GLY:CA	2.13	0.60
1:A:227:ALA:CA	1:A:228:ARG:NH2	2.64	0.60
1:C:71:SER:H	1:C:74:ASN:ND2	2.00	0.60
1:A:170:PHE:CE1	1:C:167:ASN:CB	2.60	0.60
1:B:269:VAL:HG22	1:B:270:HIS:N	2.17	0.60
1:C:289:PHE:CE1	1:C:357:MET:HE1	2.37	0.60
1:A:269:VAL:HG22	1:A:270:HIS:N	2.17	0.60
1:B:205:ARG:CZ	1:C:139:ILE:CD1	2.78	0.59
1:A:289:PHE:CE1	1:A:357:MET:HE1	2.37	0.59
1:A:119:THR:HG21	1:A:200:PHE:HE2	1.67	0.59
1:B:71:SER:H	1:B:74:ASN:HD22	1.51	0.59
1:B:192:THR:OG1	1:B:196:THR:HG23	2.02	0.59
1:A:485:LEU:H	1:A:485:LEU:HD13	1.61	0.59
1:C:220:VAL:C	1:C:221:PRO:O	2.41	0.59
1:C:477:TYR:CE1	1:C:513:GLY:HA2	2.38	0.59
1:A:101:ASN:HB2	1:C:131:GLY:O	2.01	0.59
1:A:148:VAL:HG21	1:A:160:VAL:HG22	1.84	0.59
1:B:62:GLN:CB	1:C:140:ALA:HB1	2.32	0.59
1:B:53:ASP:OD2	1:A:219:LEU:HD11	2.02	0.59
1:B:437:ARG:CB	1:A:340:GLN:OE1	2.51	0.59
1:A:220:VAL:HG21	1:C:132:PHE:CD1	2.38	0.59
1:C:269:VAL:HG22	1:C:270:HIS:N	2.17	0.58
1:B:238:ARG:HH21	1:A:315:SER:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD12	1:A:212:PRO:HA	1.85	0.58
1:A:477:TYR:CE1	1:A:513:GLY:HA2	2.38	0.58
1:C:533:LEU:N	1:C:533:LEU:HD23	2.18	0.58
1:B:289:PHE:CE1	1:B:357:MET:HE1	2.37	0.58
1:B:378:VAL:C	1:B:380:ALA:N	2.48	0.58
1:A:281:ILE:HD11	1:C:540:LYS:NZ	2.19	0.58
1:C:338:GLU:HB2	1:C:396:ARG:HD2	1.84	0.58
1:C:363:THR:N	1:C:365:ALA:HB2	2.15	0.58
1:A:220:VAL:HG12	1:A:222:ALA:CB	2.33	0.58
1:B:477:TYR:CE1	1:B:513:GLY:HA2	2.38	0.58
1:B:352:VAL:CG2	1:A:437:ARG:NE	2.62	0.58
1:B:105:GLY:HA3	1:B:214:PHE:HA	1.85	0.58
1:B:338:GLU:HB2	1:B:396:ARG:HD2	1.84	0.58
1:B:367:GLN:HE22	1:B:375:PHE:N	2.01	0.57
1:B:535:THR:C	1:B:537:ARG:HH11	2.09	0.57
1:A:71:SER:HB3	1:A:201:VAL:HG12	1.87	0.57
1:A:524:LEU:HD13	1:C:524:LEU:CD2	2.33	0.57
1:C:105:GLY:O	1:C:164:ASP:HB2	2.04	0.57
1:B:205:ARG:HE	1:C:139:ILE:CD1	2.17	0.57
1:A:218:PHE:CD2	1:C:129:PRO:HG3	2.39	0.57
1:A:338:GLU:HB2	1:A:396:ARG:HD2	1.84	0.57
1:C:295:TYR:N	1:C:295:TYR:CD2	2.72	0.57
1:B:18:ALA:HB1	1:C:153:ARG:HH12	1.68	0.57
1:A:125:VAL:HG12	1:A:182:LEU:HD22	1.87	0.57
1:A:295:TYR:N	1:A:295:TYR:CD2	2.72	0.57
1:A:367:GLN:HE22	1:A:375:PHE:N	2.00	0.57
1:B:200:PHE:HE1	1:C:191:ARG:HD2	1.63	0.57
1:B:295:TYR:N	1:B:295:TYR:CD2	2.72	0.57
1:B:387:VAL:HG21	1:B:391:VAL:HG12	1.86	0.57
1:B:392:ARG:CZ	1:A:248:PRO:HG2	2.35	0.57
1:C:474:LEU:HB3	1:C:518:VAL:HB	1.86	0.57
1:B:445:ALA:HB1	1:A:350:LEU:N	2.20	0.57
1:B:226:ALA:HB1	1:B:228:ARG:NH1	2.11	0.56
1:B:162:LEU:HD13	1:B:182:LEU:HG	1.86	0.56
1:B:435:TYR:HE2	1:A:343:THR:O	1.77	0.56
1:A:60:PHE:HZ	1:A:108:ARG:HD3	1.70	0.56
1:A:367:GLN:NE2	1:A:375:PHE:H	1.98	0.56
1:C:532:SER:CA	1:C:533:LEU:CD2	2.72	0.56
1:B:363:THR:CA	1:B:365:ALA:CB	2.78	0.56
1:A:387:VAL:HG21	1:A:391:VAL:HG12	1.86	0.56
1:A:474:LEU:HB3	1:A:518:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:GLN:HE22	1:C:375:PHE:N	2.00	0.56
1:C:387:VAL:HG21	1:C:391:VAL:HG12	1.86	0.56
1:C:361:PRO:O	1:C:362:THR:O	2.23	0.56
1:B:363:THR:N	1:B:365:ALA:HB2	2.15	0.56
1:C:220:VAL:O	1:C:221:PRO:C	2.44	0.56
1:C:230:VAL:HG11	1:C:473:LEU:HD11	1.87	0.56
1:B:364:ASN:CA	1:B:365:ALA:CB	2.84	0.56
1:A:37:ALA:O	1:A:166:ARG:NH2	2.38	0.56
1:A:363:THR:CA	1:A:365:ALA:CB	2.79	0.56
1:A:220:VAL:HG12	1:A:222:ALA:N	2.21	0.56
1:A:164:ASP:OD1	1:A:171:HIS:HE1	1.89	0.56
1:B:313:ASP:HB2	1:A:238:ARG:HB2	1.86	0.56
1:A:364:ASN:CA	1:A:365:ALA:CB	2.84	0.56
1:A:122:LYS:NZ	1:A:151:ASP:HB2	2.20	0.56
1:A:218:PHE:CD1	1:C:129:PRO:HB3	2.41	0.55
1:A:361:PRO:O	1:A:362:THR:O	2.23	0.55
1:A:228:ARG:N	1:A:228:ARG:NE	2.54	0.55
1:A:418:PRO:HB3	1:C:533:LEU:N	2.20	0.55
1:C:356:GLU:CD	1:C:379:THR:HG22	2.26	0.55
1:C:364:ASN:CA	1:C:365:ALA:CB	2.84	0.55
1:B:361:PRO:O	1:B:362:THR:O	2.23	0.55
1:B:539:LEU:HG	1:B:540:LYS:CE	2.29	0.55
1:B:219:LEU:HD11	1:A:53:ASP:OD2	2.06	0.55
1:B:474:LEU:HB3	1:B:518:VAL:HB	1.86	0.55
1:B:356:GLU:CD	1:B:379:THR:HG22	2.27	0.55
1:A:524:LEU:HD13	1:C:524:LEU:HB3	1.88	0.55
1:B:435:TYR:CD2	1:A:343:THR:C	2.82	0.55
1:B:538:MET:O	1:B:539:LEU:HB2	2.07	0.55
1:A:122:LYS:HD2	1:A:151:ASP:HA	1.89	0.55
1:A:462:ALA:HB2	1:C:540:LYS:NZ	2.12	0.55
1:C:234:VAL:HG23	1:C:234:VAL:O	2.07	0.55
1:B:352:VAL:CB	1:A:437:ARG:HE	2.19	0.54
1:A:229:MET:HE3	1:A:517:VAL:HG11	1.88	0.54
1:B:350:LEU:HB2	1:A:445:ALA:N	2.19	0.54
1:A:101:ASN:CG	1:C:131:GLY:O	2.48	0.54
1:A:106:ASN:HD22	1:A:163:GLU:HA	1.72	0.54
1:A:424:LEU:HA	1:C:425:PRO:HB3	1.89	0.54
1:B:392:ARG:NH2	1:A:248:PRO:CG	2.70	0.54
1:A:222:ALA:HB2	1:C:132:PHE:CE1	2.41	0.54
1:A:356:GLU:CD	1:A:379:THR:HG22	2.26	0.54
1:B:205:ARG:HH21	1:C:139:ILE:HD13	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ARG:NH2	1:A:352:VAL:CG2	2.70	0.54
1:B:437:ARG:HE	1:A:352:VAL:CG1	2.19	0.54
1:B:113:LEU:O	1:B:114:ALA:HB2	2.07	0.54
1:A:234:VAL:HG23	1:A:234:VAL:O	2.07	0.54
1:A:104:VAL:HG22	1:A:170:PHE:HB2	1.90	0.54
1:A:227:ALA:HB1	1:A:228:ARG:HH12	1.58	0.54
1:B:236:GLN:HA	1:B:513:GLY:O	2.08	0.54
1:A:45:THR:CB	1:C:166:ARG:C	2.65	0.54
1:A:236:GLN:HA	1:A:513:GLY:O	2.08	0.53
1:B:435:TYR:CD2	1:A:343:THR:O	2.59	0.53
1:C:236:GLN:HA	1:C:513:GLY:O	2.08	0.53
1:B:352:VAL:HG11	1:A:437:ARG:HE	1.72	0.53
1:A:71:SER:H	1:A:74:ASN:HD22	1.55	0.53
1:C:227:ALA:HB1	1:C:228:ARG:HA	0.61	0.53
1:B:470:SER:O	1:B:493:ASN:ND2	2.37	0.53
1:A:220:VAL:CG2	1:C:132:PHE:CD1	2.92	0.53
1:B:234:VAL:O	1:B:234:VAL:HG23	2.07	0.53
1:B:238:ARG:O	1:A:285:TRP:CZ2	2.54	0.53
1:B:350:LEU:H	1:A:445:ALA:HA	1.70	0.53
1:A:45:THR:HG21	1:C:166:ARG:HB3	1.83	0.53
1:A:105:GLY:HA3	1:A:214:PHE:HA	1.90	0.53
1:B:352:VAL:HG11	1:A:437:ARG:NE	2.23	0.53
1:B:523:ARG:O	1:B:523:ARG:HG2	2.07	0.53
1:A:523:ARG:NH2	1:C:425:PRO:O	2.36	0.53
1:A:470:SER:O	1:A:493:ASN:ND2	2.37	0.52
1:C:470:SER:O	1:C:493:ASN:ND2	2.37	0.52
1:B:437:ARG:HE	1:A:352:VAL:HG11	1.73	0.52
1:A:50:ASN:HD22	1:A:100:TYR:HE2	1.58	0.52
1:A:363:THR:N	1:A:365:ALA:HB2	2.15	0.52
1:C:37:ALA:O	1:C:166:ARG:NH2	2.42	0.52
1:C:85:LEU:HB3	1:C:179:THR:HB	1.90	0.52
1:B:164:ASP:OD2	1:B:171:HIS:HE1	1.93	0.52
1:A:45:THR:O	1:C:166:ARG:C	2.52	0.52
1:A:119:THR:HG21	1:A:200:PHE:CE2	2.45	0.52
1:C:387:VAL:CG2	1:C:391:VAL:CG1	2.88	0.52
1:B:440:ASP:CB	1:B:443:ASP:O	2.53	0.52
1:C:523:ARG:O	1:C:523:ARG:HG2	2.07	0.52
1:C:440:ASP:CB	1:C:443:ASP:O	2.53	0.52
1:B:296:GLU:C	1:B:297:PHE:CD2	2.85	0.52
1:A:387:VAL:CG2	1:A:388:ASP:N	2.73	0.52
1:C:387:VAL:HG22	1:C:391:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:HG2	1:A:379:THR:HG21	1.85	0.51
1:A:477:TYR:CE1	1:A:513:GLY:CA	2.93	0.51
1:C:211:SER:HB2	1:C:212:PRO:HD2	1.91	0.51
1:A:116:ASN:HB3	1:A:118:PHE:H	1.75	0.51
1:C:477:TYR:CE1	1:C:513:GLY:CA	2.93	0.51
1:B:229:MET:HE3	1:B:517:VAL:HG11	1.92	0.51
1:A:36:VAL:HB	1:A:106:ASN:HD21	1.75	0.51
1:B:437:ARG:CA	1:A:340:GLN:OE1	2.58	0.51
1:B:442:ALA:O	1:B:443:ASP:HB3	2.06	0.51
1:B:446:ALA:HB2	1:A:343:THR:HG22	1.75	0.51
1:C:442:ALA:O	1:C:443:ASP:HB3	2.06	0.51
1:B:437:ARG:NH2	1:A:352:VAL:HG13	2.10	0.51
1:A:387:VAL:HG22	1:A:391:VAL:CG1	2.40	0.51
1:A:524:LEU:HD12	1:C:524:LEU:HB3	1.91	0.51
1:B:343:THR:O	1:A:435:TYR:CE2	2.64	0.51
1:B:477:TYR:CE1	1:B:513:GLY:CA	2.93	0.51
1:A:387:VAL:CG2	1:A:391:VAL:CG1	2.88	0.51
1:B:387:VAL:CG2	1:B:388:ASP:N	2.73	0.51
1:A:46:ALA:N	1:C:166:ARG:O	2.42	0.51
1:B:68:PHE:CZ	1:B:204:GLY:HA3	2.46	0.51
1:B:248:PRO:CG	1:A:392:ARG:CZ	2.89	0.51
1:B:387:VAL:CG2	1:B:391:VAL:CG1	2.88	0.51
1:B:444:ALA:C	1:A:350:LEU:HB2	2.36	0.50
1:B:387:VAL:HG22	1:B:391:VAL:CG1	2.40	0.50
1:B:153:ARG:HB2	1:B:153:ARG:HH11	1.76	0.50
1:B:356:GLU:HG2	1:B:379:THR:HG21	1.85	0.50
1:C:105:GLY:HA3	1:C:214:PHE:HA	1.94	0.50
1:A:169:LEU:CG	1:C:168:VAL:CA	2.37	0.50
1:A:362:THR:CA	1:A:363:THR:CB	2.89	0.50
1:C:362:THR:CG2	1:C:363:THR:CG2	2.89	0.50
1:C:387:VAL:CG2	1:C:388:ASP:N	2.73	0.50
1:C:532:SER:O	1:C:533:LEU:HD22	2.04	0.50
1:B:486:LEU:HD12	1:B:486:LEU:N	2.26	0.50
1:A:440:ASP:HB3	1:A:441:THR:C	2.36	0.50
1:C:440:ASP:HB3	1:C:441:THR:C	2.36	0.50
1:B:129:PRO:CA	1:B:180:MET:HE2	2.41	0.50
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.77	0.50
1:B:437:ARG:HB2	1:A:340:GLN:OE1	2.12	0.50
1:A:170:PHE:CE1	1:C:167:ASN:HB2	2.07	0.50
1:A:220:VAL:CG1	1:A:222:ALA:CB	2.90	0.50
1:B:352:VAL:CG2	1:A:437:ARG:HE	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLN:HE21	1:B:367:GLN:CA	2.24	0.50
1:B:440:ASP:HB3	1:B:441:THR:C	2.36	0.50
1:A:101:ASN:HD21	1:C:130:PRO:C	2.18	0.50
1:A:296:GLU:C	1:A:297:PHE:CD2	2.85	0.50
1:B:362:THR:CG2	1:B:363:THR:HG23	2.42	0.49
1:A:29:ASP:HB3	1:A:30:PRO:HD2	1.94	0.49
1:A:124:ILE:HG12	1:A:149:ILE:HG12	1.94	0.49
1:C:362:THR:CG2	1:C:363:THR:HG23	2.42	0.49
1:A:118:PHE:CD1	1:A:118:PHE:N	2.81	0.49
1:B:343:THR:CB	1:A:435:TYR:HB2	2.39	0.49
1:A:220:VAL:HG12	1:A:222:ALA:HB3	1.93	0.49
1:A:486:LEU:N	1:A:486:LEU:HD12	2.26	0.49
1:C:50:ASN:ND2	1:C:217:LEU:O	2.46	0.49
1:C:362:THR:CA	1:C:363:THR:CB	2.89	0.49
1:A:362:THR:CG2	1:A:363:THR:HG23	2.42	0.49
1:C:486:LEU:HD12	1:C:486:LEU:N	2.26	0.49
1:C:519:SER:HB3	1:C:520:TRP:O	2.13	0.49
1:A:110:ARG:HA	1:A:158:ILE:O	2.13	0.49
1:A:351:LYS:HD2	1:A:386:LEU:HB3	1.94	0.49
1:C:362:THR:CA	1:C:363:THR:CG2	2.63	0.49
1:B:220:VAL:CG1	1:B:221:PRO:CD	2.75	0.49
1:B:226:ALA:C	1:B:228:ARG:NH1	2.71	0.49
1:B:351:LYS:HD2	1:B:386:LEU:HB3	1.94	0.49
1:B:519:SER:HB3	1:B:520:TRP:O	2.12	0.49
1:C:474:LEU:O	1:C:518:VAL:HA	2.12	0.49
1:A:281:ILE:HD11	1:C:540:LYS:HZ3	1.76	0.49
1:A:442:ALA:O	1:A:443:ASP:HB3	2.06	0.49
1:A:474:LEU:O	1:A:518:VAL:HA	2.12	0.49
1:B:125:VAL:HG12	1:B:182:LEU:HD22	1.95	0.48
1:B:474:LEU:O	1:B:518:VAL:HA	2.12	0.48
1:A:519:SER:HB3	1:A:520:TRP:O	2.12	0.48
1:C:123:ILE:CD1	1:C:184:CYS:SG	2.90	0.48
1:C:119:THR:HG22	1:C:192:THR:HG22	1.95	0.48
1:C:164:ASP:OD1	1:C:171:HIS:HE1	1.96	0.48
1:A:223:ALA:O	1:A:224:ALA:HB3	2.11	0.48
1:A:238:ARG:HD2	1:A:511:THR:OG1	2.14	0.48
1:C:238:ARG:HD2	1:C:511:THR:OG1	2.14	0.48
1:C:296:GLU:C	1:C:297:PHE:CD2	2.85	0.48
1:C:367:GLN:HE21	1:C:367:GLN:CA	2.24	0.48
1:B:387:VAL:CG2	1:B:391:VAL:HG12	2.44	0.48
1:B:362:THR:CA	1:B:363:THR:CG2	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD23	1:A:520:TRP:N	2.19	0.48
1:A:353:THR:OG1	1:A:387:VAL:HG12	2.14	0.48
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.96	0.48
1:B:12:VAL:HB	1:C:149:ILE:O	2.14	0.48
1:B:85:LEU:HB3	1:B:179:THR:HB	1.96	0.48
1:B:125:VAL:CG1	1:B:182:LEU:HD22	2.43	0.48
1:C:123:ILE:HG12	1:C:124:ILE:N	2.28	0.47
1:B:353:THR:OG1	1:B:387:VAL:HG12	2.14	0.47
1:B:362:THR:CA	1:B:363:THR:CB	2.89	0.47
1:C:351:LYS:HD2	1:C:386:LEU:HB3	1.94	0.47
1:B:238:ARG:HD2	1:B:511:THR:OG1	2.14	0.47
1:A:47:GLY:N	1:C:165:VAL:CG1	2.74	0.47
1:A:105:GLY:O	1:A:164:ASP:HB2	2.14	0.47
1:A:118:PHE:N	1:A:118:PHE:HD1	2.12	0.47
1:A:425:PRO:HD2	1:C:425:PRO:HG3	1.73	0.47
1:A:523:ARG:O	1:A:523:ARG:HG2	2.07	0.47
1:B:223:ALA:O	1:B:224:ALA:CB	2.60	0.47
1:B:18:ALA:HB2	1:C:153:ARG:HH12	1.67	0.47
1:A:387:VAL:CG2	1:A:391:VAL:HG12	2.44	0.47
1:C:82:ASP:O	1:C:83:LEU:HD23	2.15	0.47
1:A:101:ASN:CB	1:C:131:GLY:O	2.62	0.47
1:A:220:VAL:HG13	1:A:221:PRO:HD2	1.97	0.47
1:C:364:ASN:N	1:C:365:ALA:HB3	2.20	0.47
1:B:337:ILE:HD13	1:B:357:MET:CE	2.45	0.47
1:B:392:ARG:CZ	1:A:248:PRO:CD	2.93	0.47
1:A:337:ILE:HD13	1:A:357:MET:CE	2.45	0.47
1:C:353:THR:OG1	1:C:387:VAL:HG12	2.14	0.47
1:B:445:ALA:CA	1:A:350:LEU:CG	2.45	0.47
1:B:532:SER:C	1:B:534:ALA:H	2.22	0.47
1:C:297:PHE:CE2	1:C:302:GLY:HA3	2.50	0.47
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.30	0.47
1:B:367:GLN:NE2	1:B:375:PHE:HD2	2.13	0.47
1:C:387:VAL:CG2	1:C:391:VAL:HG12	2.44	0.47
1:B:77:GLY:O	1:B:185:MET:HE2	2.15	0.46
1:B:10:SER:HA	1:C:147:HIS:O	2.15	0.46
1:B:98:GLN:HB2	1:A:95:HIS:CE1	2.50	0.46
1:A:297:PHE:CE2	1:A:302:GLY:HA3	2.50	0.46
1:A:220:VAL:CG1	1:A:222:ALA:HB2	2.46	0.46
1:A:367:GLN:NE2	1:A:375:PHE:HD2	2.14	0.46
1:A:162:LEU:HD13	1:A:182:LEU:HG	1.97	0.46
1:A:230:VAL:CG1	1:A:473:LEU:HD11	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ILE:HD13	1:C:357:MET:CE	2.45	0.46
1:C:71:SER:HA	1:C:201:VAL:HG12	1.97	0.46
1:B:238:ARG:NH1	1:B:512:ASP:HB3	2.31	0.46
1:A:127:CYS:HB3	1:A:180:MET:HE3	1.97	0.46
1:C:484:GLN:C	1:C:485:LEU:HD12	2.29	0.46
1:B:297:PHE:CE2	1:B:302:GLY:HA3	2.50	0.46
1:A:397:SER:HB2	1:A:439:ILE:CG2	2.46	0.46
1:C:238:ARG:NH1	1:C:512:ASP:HB3	2.31	0.46
1:A:110:ARG:NH1	1:A:159:GLU:OE1	2.49	0.45
1:A:238:ARG:H	1:A:238:ARG:HG2	1.63	0.45
1:A:484:GLN:C	1:A:485:LEU:HD12	2.29	0.45
1:C:297:PHE:CE2	1:C:302:GLY:CA	3.00	0.45
1:B:364:ASN:N	1:B:365:ALA:HB3	2.20	0.45
1:A:71:SER:HB2	1:A:72:PRO:HD2	1.98	0.45
1:A:539:LEU:HD12	1:A:539:LEU:HA	1.69	0.45
1:C:229:MET:CG	1:C:230:VAL:N	2.59	0.45
1:C:367:GLN:NE2	1:C:375:PHE:HD2	2.14	0.45
1:A:101:ASN:ND2	1:C:131:GLY:HA3	2.28	0.45
1:A:464:ASN:O	1:A:465:ALA:C	2.59	0.45
1:A:272:ASP:CG	1:C:537:ARG:CZ	2.89	0.45
1:B:18:ALA:HB2	1:C:153:ARG:HH11	1.79	0.45
1:B:104:VAL:HG13	1:B:170:PHE:HA	1.99	0.45
1:B:297:PHE:CE2	1:B:302:GLY:CA	3.00	0.45
1:B:352:VAL:HG13	1:B:352:VAL:O	2.17	0.45
1:B:397:SER:HB2	1:B:439:ILE:CG2	2.46	0.45
1:A:297:PHE:CE2	1:A:302:GLY:CA	3.00	0.45
1:C:77:GLY:O	1:C:185:MET:HE2	2.17	0.45
1:B:241:THR:CB	1:A:282:SER:HG	2.26	0.45
1:B:350:LEU:H	1:A:445:ALA:CB	2.30	0.45
1:B:464:ASN:O	1:B:465:ALA:C	2.59	0.45
1:C:352:VAL:HG13	1:C:352:VAL:O	2.17	0.45
1:B:437:ARG:HE	1:A:352:VAL:HB	1.77	0.45
1:A:107:MET:HE2	1:A:107:MET:HB3	1.89	0.45
1:A:169:LEU:CD1	1:C:168:VAL:O	2.52	0.45
1:A:224:ALA:O	1:A:225:ALA:HB2	2.17	0.45
1:B:269:VAL:CG2	1:B:270:HIS:N	2.80	0.45
1:B:352:VAL:CG1	1:A:437:ARG:HE	2.30	0.45
1:A:367:GLN:HE21	1:A:367:GLN:CA	2.24	0.45
1:C:194:GLY:C	1:C:196:THR:H	2.25	0.45
1:C:397:SER:HB2	1:C:439:ILE:CG2	2.46	0.45
1:A:227:ALA:HA	1:A:228:ARG:CZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:VAL:HG13	1:A:352:VAL:O	2.17	0.45
1:B:62:GLN:HB3	1:C:140:ALA:CB	2.47	0.44
1:B:90:ASN:HB3	1:B:93:LEU:HD12	1.98	0.44
1:C:192:THR:HG21	1:C:200:PHE:CD2	2.53	0.44
1:B:37:ALA:O	1:B:166:ARG:NH2	2.51	0.44
1:B:343:THR:C	1:A:435:TYR:CE2	2.95	0.44
1:B:530:VAL:HB	1:B:531:GLY:H	0.78	0.44
1:B:62:GLN:CB	1:C:140:ALA:HA	2.48	0.44
1:B:107:MET:CE	1:B:208:THR:HB	2.46	0.44
1:A:31:LEU:HD12	1:A:161:PRO:HG2	1.98	0.44
1:A:71:SER:H	1:A:74:ASN:ND2	2.14	0.44
1:A:238:ARG:NH1	1:A:512:ASP:HB3	2.31	0.44
1:B:362:THR:CB	1:B:363:THR:OG1	2.66	0.44
1:B:473:LEU:HD23	1:B:520:TRP:N	2.19	0.44
1:A:440:ASP:CB	1:A:443:ASP:O	2.53	0.44
1:A:362:THR:CG2	1:A:363:THR:CG2	2.89	0.44
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.82	0.44
1:A:532:SER:C	1:A:534:ALA:N	2.48	0.44
1:C:297:PHE:CB	1:C:300:GLY:HA2	2.48	0.44
1:C:362:THR:CB	1:C:363:THR:OG1	2.66	0.44
1:B:13:ASP:HB2	1:B:155:LEU:HD22	2.00	0.44
1:B:392:ARG:NH1	1:A:248:PRO:HG2	2.32	0.44
1:B:446:ALA:HB3	1:A:350:LEU:CD2	2.03	0.44
1:A:122:LYS:HZ2	1:A:151:ASP:HB2	1.83	0.44
1:A:328:TYR:OH	1:A:374:VAL:HG11	2.18	0.44
1:A:337:ILE:HD13	1:A:357:MET:HE1	1.99	0.44
1:A:424:LEU:HD12	1:C:425:PRO:HB2	1.98	0.44
1:A:523:ARG:CD	1:C:526:GLN:HE21	1.78	0.44
1:A:540:LYS:HB3	1:A:540:LYS:HE3	1.71	0.44
1:C:269:VAL:HG22	1:C:270:HIS:O	2.18	0.44
1:C:328:TYR:OH	1:C:374:VAL:HG11	2.18	0.44
1:B:200:PHE:HD1	1:C:191:ARG:CD	2.27	0.44
1:B:269:VAL:HG22	1:B:270:HIS:O	2.18	0.44
1:B:343:THR:OG1	1:A:435:TYR:HB2	2.18	0.44
1:B:435:TYR:CZ	1:A:343:THR:C	2.95	0.44
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.78	0.44
1:B:535:THR:C	1:B:537:ARG:NH1	2.73	0.43
1:A:169:LEU:HD21	1:C:169:LEU:HG	2.00	0.43
1:A:269:VAL:CG2	1:A:270:HIS:N	2.80	0.43
1:C:337:ILE:HD13	1:C:357:MET:HE1	1.99	0.43
1:B:226:ALA:HB1	1:B:228:ARG:NH2	2.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:MET:HB3	1:B:539:LEU:H	1.52	0.43
1:A:33:MET:HE1	1:A:180:MET:HE1	2.00	0.43
1:A:100:TYR:HA	1:A:218:PHE:O	2.18	0.43
1:C:464:ASN:O	1:C:465:ALA:C	2.59	0.43
1:B:21:LEU:HB3	1:B:117:ALA:HB1	2.00	0.43
1:B:62:GLN:CB	1:C:140:ALA:CB	2.96	0.43
1:B:490:LYS:HG3	1:B:527:LEU:HD21	2.00	0.43
1:B:22:VAL:HG12	1:B:153:ARG:HD2	1.99	0.43
1:B:328:TYR:OH	1:B:374:VAL:HG11	2.18	0.43
1:B:337:ILE:HD13	1:B:357:MET:HE1	1.99	0.43
1:A:439:ILE:HB	1:A:440:ASP:O	2.19	0.43
1:A:269:VAL:HG22	1:A:270:HIS:O	2.18	0.43
1:A:362:THR:CB	1:A:363:THR:OG1	2.66	0.43
1:B:64:PRO:HG3	1:B:88:HIS:O	2.19	0.43
1:A:297:PHE:CB	1:A:300:GLY:HA2	2.48	0.43
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.79	0.43
1:C:238:ARG:H	1:C:238:ARG:HG2	1.63	0.43
1:B:82:ASP:OD1	1:B:181:ARG:HD2	2.18	0.43
1:B:219:LEU:HD23	1:B:219:LEU:HA	1.92	0.43
1:B:439:ILE:HB	1:B:440:ASP:O	2.19	0.43
1:C:226:ALA:O	1:C:227:ALA:HB2	2.19	0.43
1:C:439:ILE:HB	1:C:440:ASP:O	2.19	0.43
1:B:53:ASP:HA	1:B:54:PRO:HD2	1.89	0.43
1:A:45:THR:CB	1:C:166:ARG:CB	2.94	0.43
1:A:61:VAL:HG12	1:A:62:GLN:N	2.33	0.43
1:A:501:TYR:CZ	1:A:503:GLY:HA3	2.54	0.42
1:C:364:ASN:C	1:C:364:ASN:HD22	2.27	0.42
1:C:109:VAL:HG22	1:C:208:THR:HG22	2.02	0.42
1:C:469:GLN:O	1:C:470:SER:HB2	2.20	0.42
1:C:501:TYR:CZ	1:C:503:GLY:HA3	2.54	0.42
1:B:39:SER:OG	1:B:215:ASN:HB2	2.19	0.42
1:B:248:PRO:HD2	1:A:392:ARG:CZ	2.46	0.42
1:B:364:ASN:C	1:B:364:ASN:HD22	2.27	0.42
1:A:31:LEU:HD22	1:A:146:PRO:HB2	2.01	0.42
1:C:90:ASN:HA	1:C:91:PRO:HD2	1.79	0.42
1:C:269:VAL:CG2	1:C:270:HIS:N	2.80	0.42
1:B:293:ALA:HB3	1:B:388:ASP:HA	2.02	0.42
1:B:352:VAL:CG1	1:A:444:ALA:HB3	2.42	0.42
1:B:501:TYR:CZ	1:B:503:GLY:HA3	2.54	0.42
1:A:42:ALA:HB2	1:A:170:PHE:HB3	2.02	0.42
1:A:438:GLN:O	1:A:438:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:GLN:O	1:B:470:SER:HB2	2.20	0.42
1:A:281:ILE:HD12	1:A:281:ILE:HG23	1.74	0.42
1:C:539:LEU:HD12	1:C:539:LEU:HA	1.79	0.42
1:C:438:GLN:O	1:C:438:GLN:HG2	2.20	0.42
1:A:119:THR:CG2	1:A:200:PHE:CE2	3.03	0.42
1:B:71:SER:N	1:B:74:ASN:HD22	2.16	0.42
1:A:220:VAL:HG13	1:A:222:ALA:H	1.84	0.42
1:A:364:ASN:C	1:A:364:ASN:HD22	2.27	0.41
1:B:438:GLN:O	1:B:438:GLN:HG2	2.20	0.41
1:A:368:ALA:HA	1:A:369:PRO:HD2	1.80	0.41
1:B:14:GLY:O	1:B:15:ALA:C	2.63	0.41
1:A:474:LEU:O	1:A:518:VAL:CB	2.68	0.41
1:B:36:VAL:HG11	1:B:164:ASP:O	2.21	0.41
1:B:297:PHE:CB	1:B:300:GLY:HA2	2.48	0.41
1:A:218:PHE:CD1	1:C:129:PRO:CB	3.04	0.41
1:A:269:VAL:O	1:A:495:GLY:HA3	2.21	0.41
1:B:230:VAL:HB	1:B:466:PHE:CD2	2.55	0.41
1:B:392:ARG:CZ	1:A:248:PRO:CG	2.99	0.41
1:B:444:ALA:CB	1:A:352:VAL:HG11	2.51	0.41
1:C:83:LEU:O	1:C:181:ARG:HA	2.20	0.41
1:B:303:GLU:O	1:B:378:VAL:CG2	2.55	0.41
1:B:474:LEU:O	1:B:518:VAL:CB	2.68	0.41
1:A:295:TYR:HE2	1:A:388:ASP:HB3	1.85	0.41
1:B:281:ILE:HD12	1:B:281:ILE:HG23	1.74	0.41
1:A:122:LYS:HZ3	1:A:151:ASP:HB2	1.85	0.41
1:A:220:VAL:HG21	1:C:132:PHE:HD1	1.82	0.41
1:A:387:VAL:HG22	1:A:388:ASP:N	2.36	0.41
1:C:474:LEU:O	1:C:518:VAL:HB	2.21	0.41
1:B:71:SER:HB2	1:B:201:VAL:HG12	2.02	0.41
1:B:175:ARG:O	1:B:175:ARG:HG2	2.20	0.41
1:B:269:VAL:O	1:B:495:GLY:HA3	2.20	0.41
1:A:170:PHE:CD2	1:C:167:ASN:O	2.74	0.41
1:A:474:LEU:O	1:A:518:VAL:HB	2.21	0.41
1:B:116:ASN:C	1:B:118:PHE:N	2.79	0.41
1:A:293:ALA:HB3	1:A:388:ASP:HA	2.02	0.41
1:A:401:PHE:CG	1:A:436:MET:HE1	2.56	0.41
1:A:440:ASP:OD2	1:A:441:THR:HB	2.21	0.41
1:A:469:GLN:O	1:A:470:SER:HB2	2.20	0.41
1:C:269:VAL:O	1:C:495:GLY:HA3	2.21	0.41
1:C:356:GLU:HG2	1:C:379:THR:HG21	1.85	0.41
1:C:368:ALA:HA	1:C:369:PRO:HD2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LEU:O	1:C:518:VAL:CB	2.68	0.41
1:B:474:LEU:O	1:B:518:VAL:HB	2.21	0.41
1:A:53:ASP:HA	1:A:54:PRO:HD2	1.88	0.41
1:A:170:PHE:C	1:C:167:ASN:ND2	2.75	0.41
1:A:221:PRO:O	1:A:222:ALA:C	2.64	0.41
1:C:293:ALA:HB3	1:C:388:ASP:HA	2.02	0.41
1:C:401:PHE:CG	1:C:436:MET:HE1	2.56	0.41
1:B:200:PHE:CD1	1:C:191:ARG:HD3	2.54	0.40
1:B:387:VAL:HG22	1:B:391:VAL:HG11	2.03	0.40
1:B:445:ALA:HA	1:A:350:LEU:H	1.55	0.40
1:A:301:THR:O	1:A:303:GLU:N	2.54	0.40
1:C:295:TYR:HE2	1:C:388:ASP:HB3	1.85	0.40
1:C:361:PRO:HA	1:C:407:GLU:HB2	2.03	0.40
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.78	0.40
1:B:538:MET:O	1:B:539:LEU:HB3	2.17	0.40
1:A:81:PHE:CZ	1:A:184:CYS:HB2	2.57	0.40
1:A:387:VAL:HG22	1:A:391:VAL:HG11	2.03	0.40
1:C:301:THR:O	1:C:303:GLU:N	2.54	0.40
1:B:95:HIS:HE1	1:A:95:HIS:O	2.04	0.40
1:B:301:THR:O	1:B:303:GLU:N	2.54	0.40
1:B:481:LEU:HA	1:B:481:LEU:HD12	1.82	0.40
1:C:281:ILE:HG23	1:C:281:ILE:HD12	1.74	0.40
1:B:401:PHE:CG	1:B:436:MET:HE1	2.56	0.40
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	504/531 (95%)	446 (88%)	38 (8%)	20 (4%)	2 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	523/531 (98%)	458 (88%)	41 (8%)	24 (5%)	2	17
1	C	504/531 (95%)	446 (88%)	38 (8%)	20 (4%)	2	18
All	All	1531/1593 (96%)	1350 (88%)	117 (8%)	64 (4%)	3	17

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ALA
1	B	223	ALA
1	B	302	GLY
1	B	362	THR
1	B	363	THR
1	B	365	ALA
1	B	367	GLN
1	B	379	THR
1	B	439	ILE
1	B	440	ASP
1	B	443	ASP
1	B	518	VAL
1	B	520	TRP
1	B	531	GLY
1	B	539	LEU
1	A	222	ALA
1	A	224	ALA
1	A	302	GLY
1	A	362	THR
1	A	363	THR
1	A	365	ALA
1	A	367	GLN
1	A	379	THR
1	A	439	ILE
1	A	440	ASP
1	A	443	ASP
1	A	518	VAL
1	A	520	TRP
1	A	530	VAL
1	A	533	LEU
1	A	536	GLY
1	C	221	PRO
1	C	224	ALA
1	C	302	GLY

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Mol	Chain	Res	Type
1	C	362	THR
1	C	363	THR
1	C	365	ALA
1	C	367	GLN
1	C	379	THR
1	C	439	ILE
1	C	440	ASP
1	C	443	ASP
1	C	518	VAL
1	C	520	TRP
1	B	224	ALA
1	B	536	GLY
1	A	196	THR
1	A	225	ALA
1	C	173	ASN
1	C	196	THR
1	C	227	ALA
1	B	40	SER
1	B	196	THR
1	B	537	ARG
1	B	530	VAL
1	C	43	VAL
1	B	519	SER
1	B	521	VAL
1	A	519	SER
1	A	521	VAL
1	C	519	SER
1	C	521	VAL
1	B	221	PRO
1	C	57	ILE

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	418/434 (96%)	382 (91%)	36 (9%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	431/434 (99%)	399 (93%)	32 (7%)	13	33
1	C	418/434 (96%)	385 (92%)	33 (8%)	11	32
All	All	1267/1302 (97%)	1166 (92%)	101 (8%)	13	31

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	SER
1	B	84	SER
1	B	104	VAL
1	B	126	SER
1	B	139	ILE
1	B	141	GLN
1	B	153	ARG
1	B	182	LEU
1	B	220	VAL
1	B	228	ARG
1	B	230	VAL
1	B	237	PRO
1	B	259	PRO
1	B	296	GLU
1	B	352	VAL
1	B	356	GLU
1	B	357	MET
1	B	363	THR
1	B	364	ASN
1	B	366	ASP
1	B	367	GLN
1	B	378	VAL
1	B	424	LEU
1	B	439	ILE
1	B	471	GLU
1	B	485	LEU
1	B	508	THR
1	B	514	ILE
1	B	518	VAL
1	B	521	VAL
1	B	539	LEU
1	B	540	LYS
1	A	41	THR
1	A	45	THR

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Mol	Chain	Res	Type
1	A	84	SER
1	A	101	ASN
1	A	118	PHE
1	A	124	ILE
1	A	141	GLN
1	A	154	THR
1	A	179	THR
1	A	180	MET
1	A	181	ARG
1	A	191	ARG
1	A	220	VAL
1	A	228	ARG
1	A	230	VAL
1	A	237	PRO
1	A	259	PRO
1	A	296	GLU
1	A	352	VAL
1	A	356	GLU
1	A	357	MET
1	A	363	THR
1	A	364	ASN
1	A	366	ASP
1	A	367	GLN
1	A	378	VAL
1	A	424	LEU
1	A	439	ILE
1	A	471	GLU
1	A	485	LEU
1	A	508	THR
1	A	514	ILE
1	A	518	VAL
1	A	521	VAL
1	A	529	SER
1	A	540	LYS
1	C	31	LEU
1	C	57	ILE
1	C	101	ASN
1	C	104	VAL
1	C	107	MET
1	C	108	ARG
1	C	123	ILE
1	C	135	HIS

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Mol	Chain	Res	Type
1	C	136	ASN
1	C	152	VAL
1	C	230	VAL
1	C	237	PRO
1	C	259	PRO
1	C	296	GLU
1	C	352	VAL
1	C	356	GLU
1	C	357	MET
1	C	363	THR
1	C	364	ASN
1	C	366	ASP
1	C	367	GLN
1	C	378	VAL
1	C	424	LEU
1	C	439	ILE
1	C	471	GLU
1	C	485	LEU
1	C	508	THR
1	C	514	ILE
1	C	518	VAL
1	C	521	VAL
1	C	532	SER
1	C	533	LEU
1	C	540	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	B	74	ASN
1	B	135	HIS
1	B	171	HIS
1	B	177	GLN
1	B	263	GLN
1	B	364	ASN
1	B	367	GLN
1	B	371	GLN
1	B	464	ASN
1	B	469	GLN
1	B	526	GLN
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	95	HIS
1	A	101	ASN
1	A	106	ASN
1	A	171	HIS
1	A	263	GLN
1	A	364	ASN
1	A	367	GLN
1	A	371	GLN
1	A	464	ASN
1	A	469	GLN
1	A	526	GLN
1	C	50	ASN
1	C	59	ASN
1	C	74	ASN
1	C	171	HIS
1	C	263	GLN
1	C	364	ASN
1	C	367	GLN
1	C	371	GLN
1	C	464	ASN
1	C	469	GLN
1	C	526	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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.

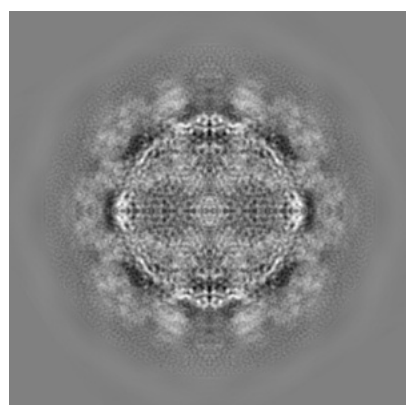
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7564. These allow visual inspection of the internal detail of the map and identification of artifacts.

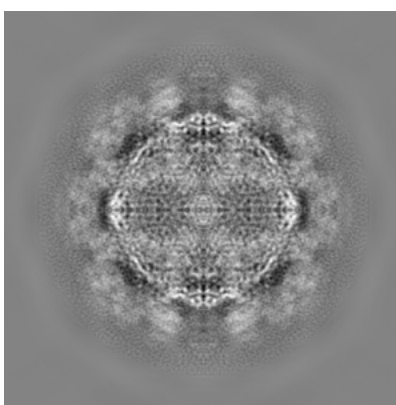
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

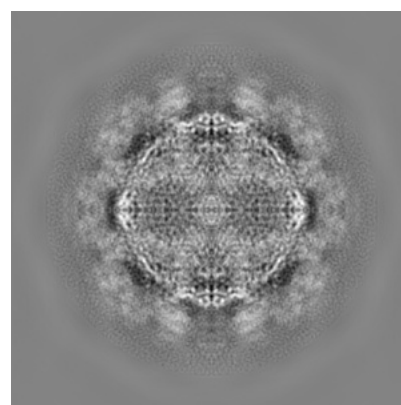
6.1.1 Primary map



X



Y

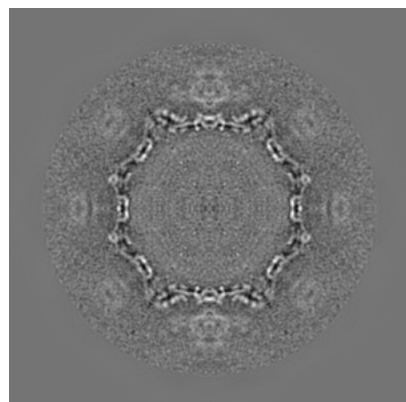


Z

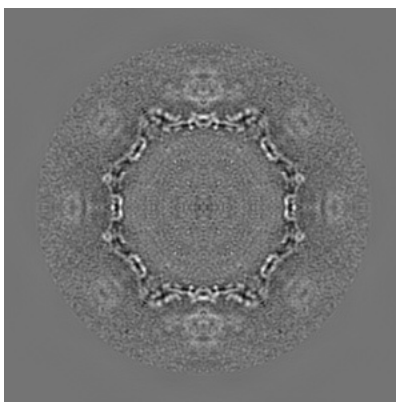
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

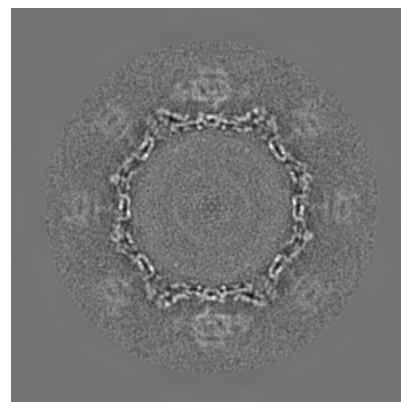
6.2.1 Primary map



X Index: 192



Y Index: 192

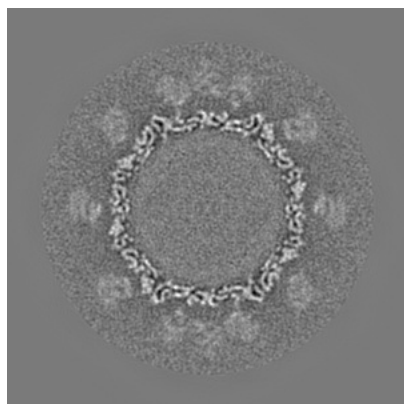


Z Index: 192

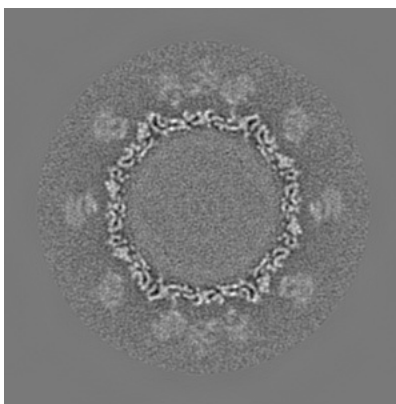
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

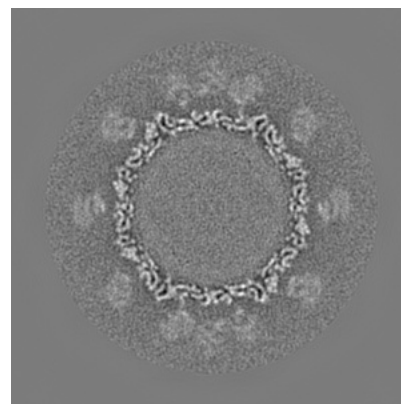
6.3.1 Primary map



X Index: 181



Y Index: 203

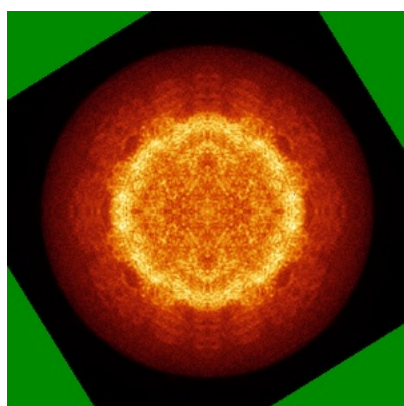


Z Index: 202

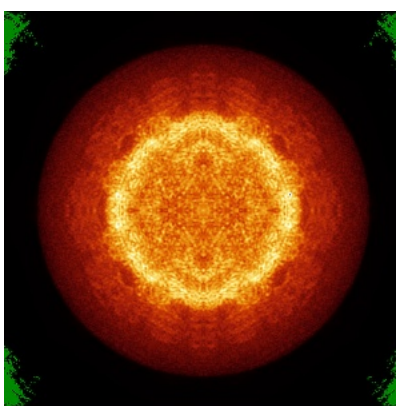
The images above show the largest variance slices of the map in three orthogonal directions.

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

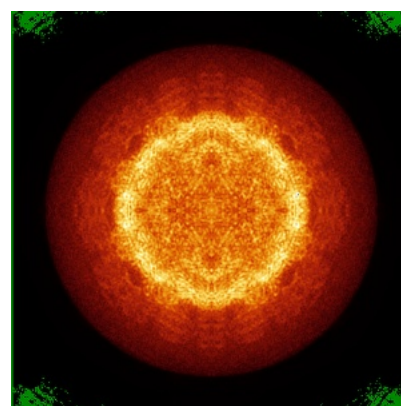
6.4.1 Primary map



X



Y

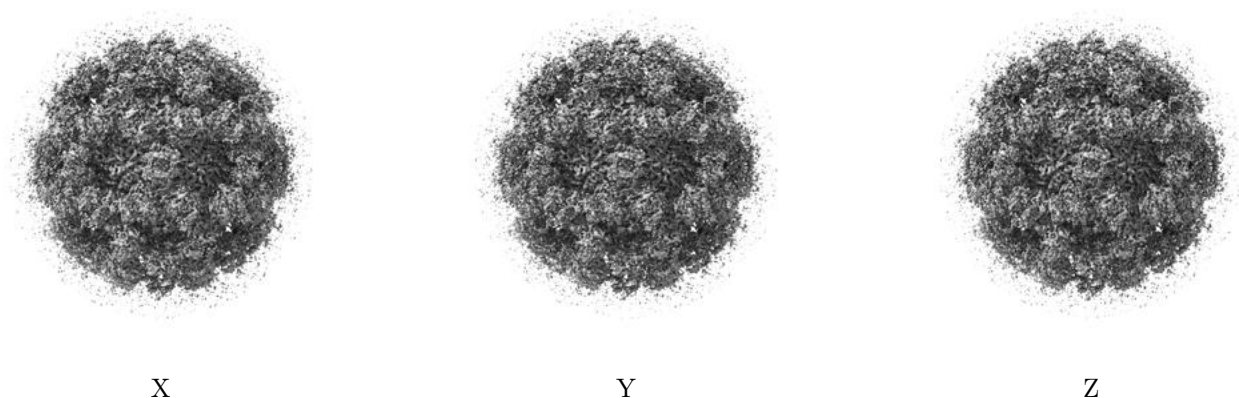


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

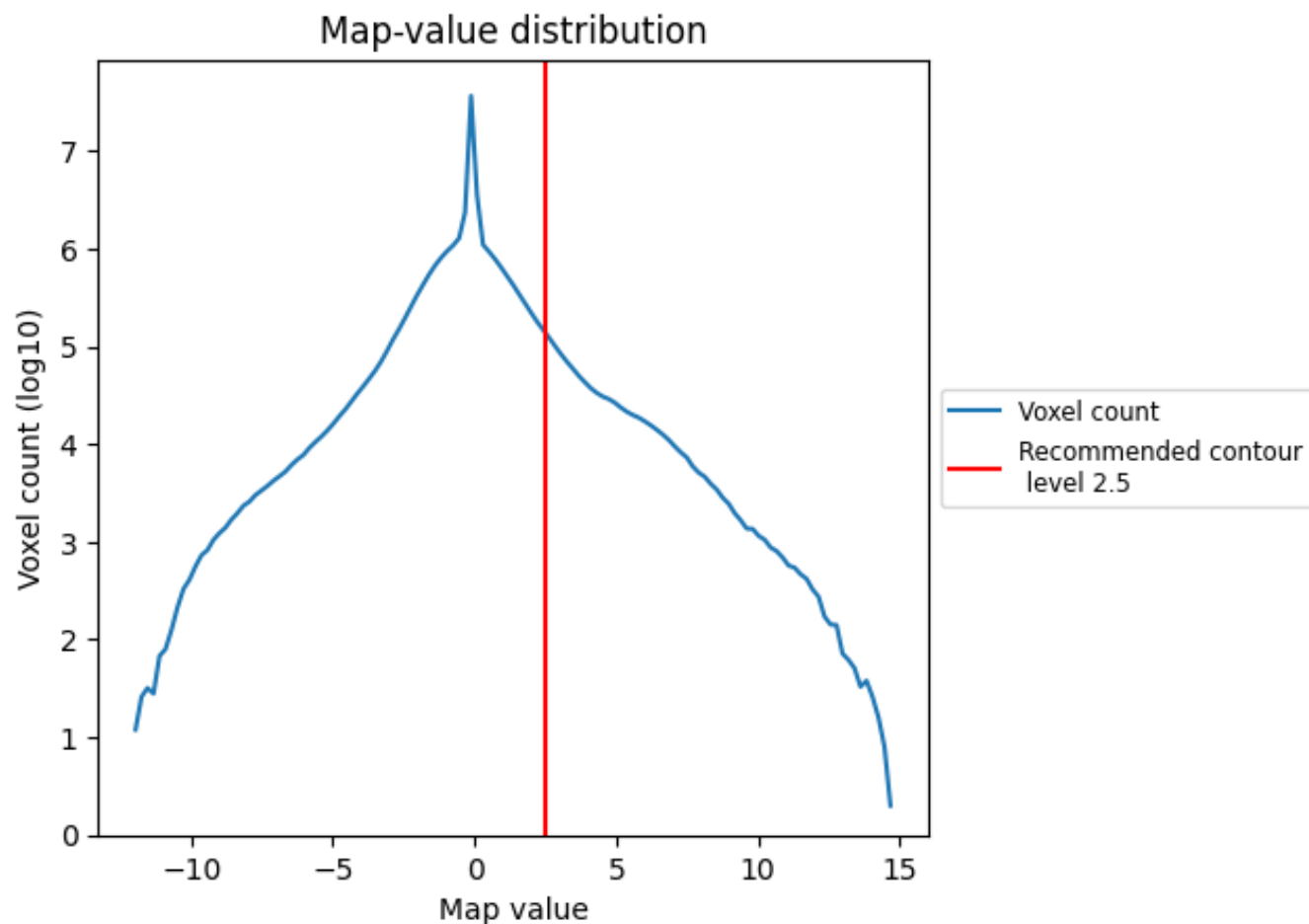
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

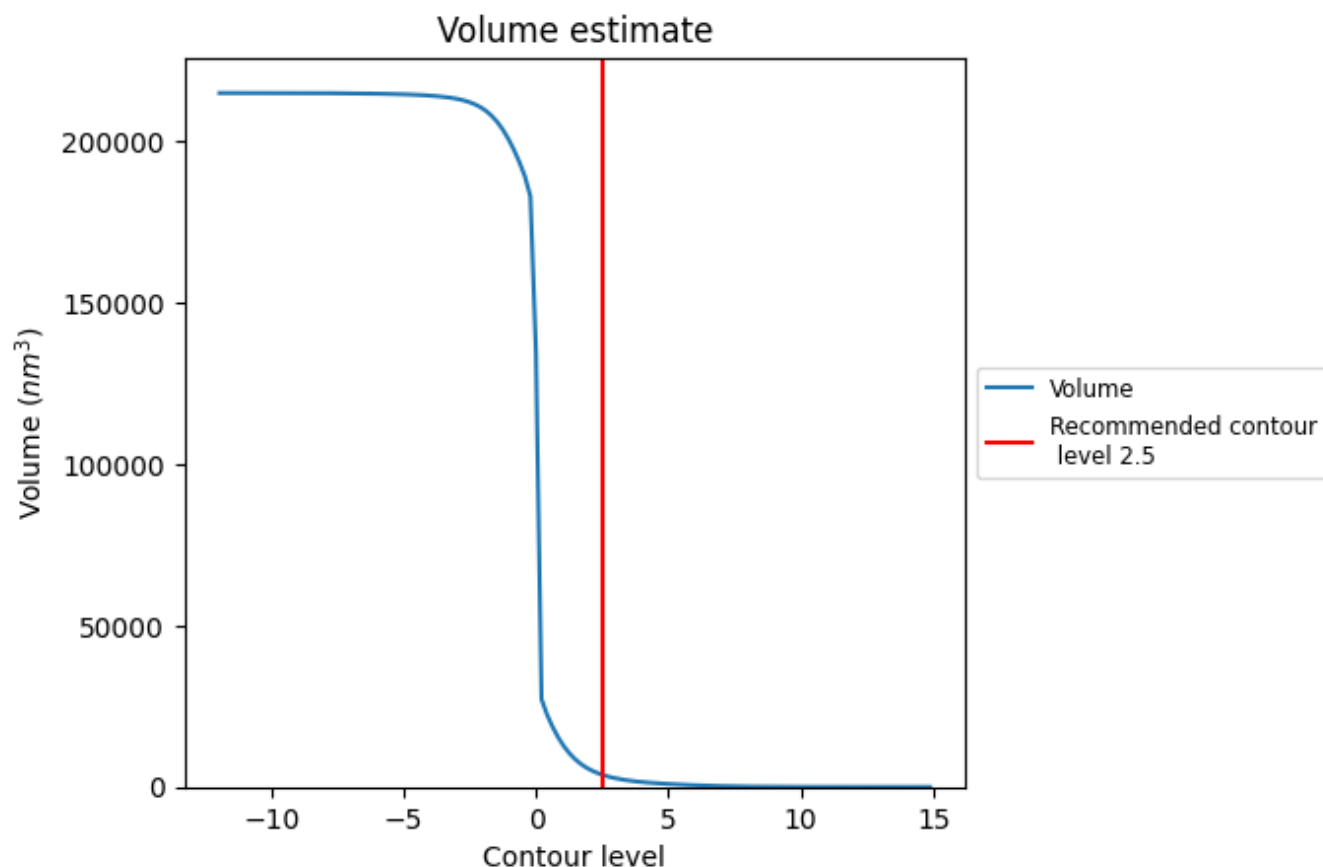
This section contains the results of statistical analysis of the map.

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.

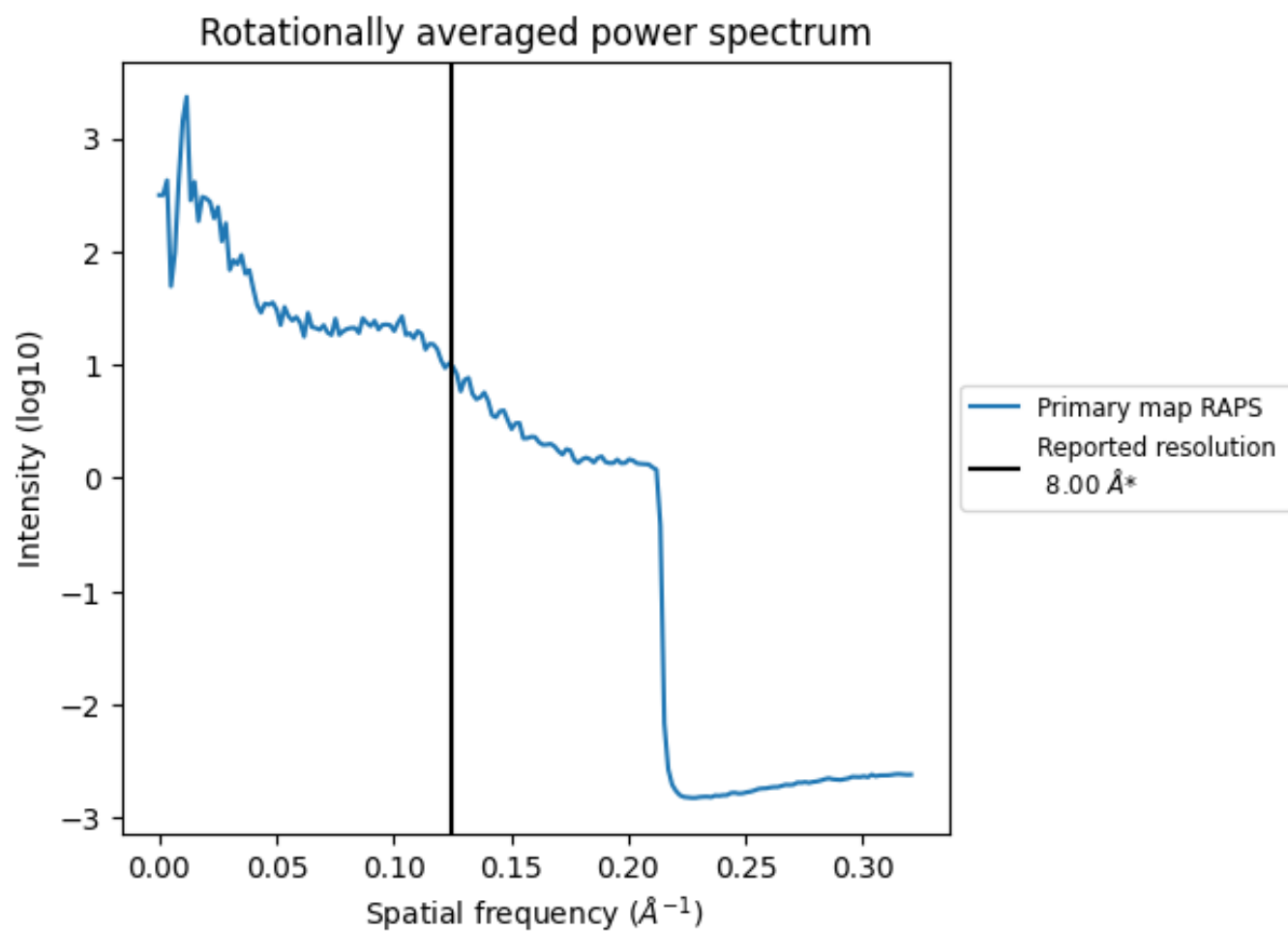
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3779 nm³; this corresponds to an approximate mass of 3414 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 0.125 Å⁻¹

8 Fourier-Shell correlation

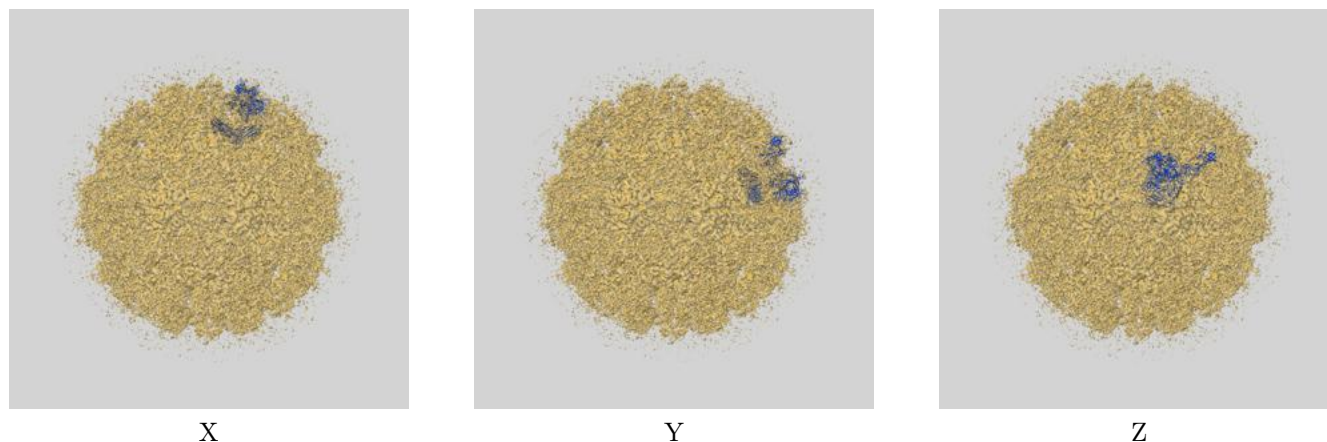
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

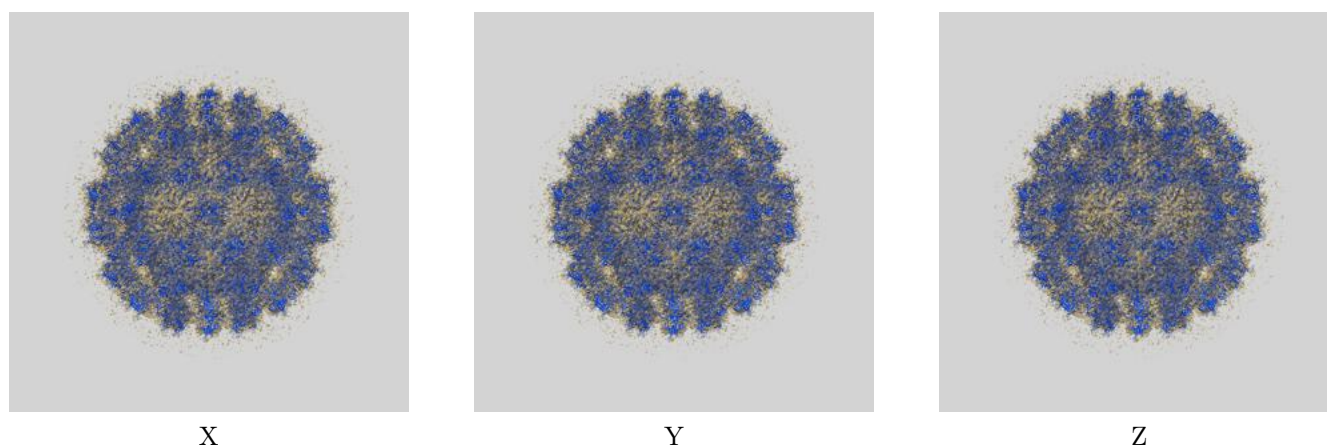
This section contains information regarding the fit between EMDB map EMD-7564 and PDB model 6CRJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

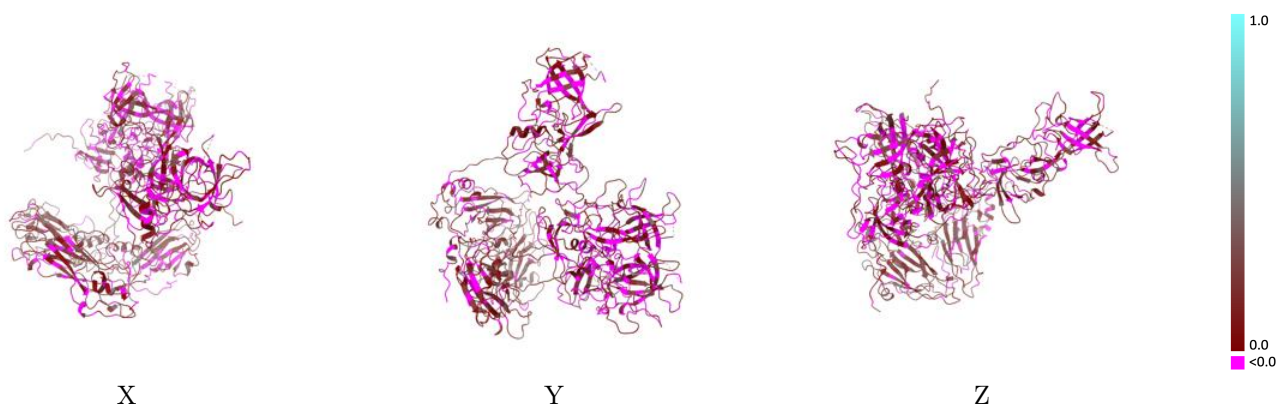


9.1.2 Map-model assembly overlay [i](#)



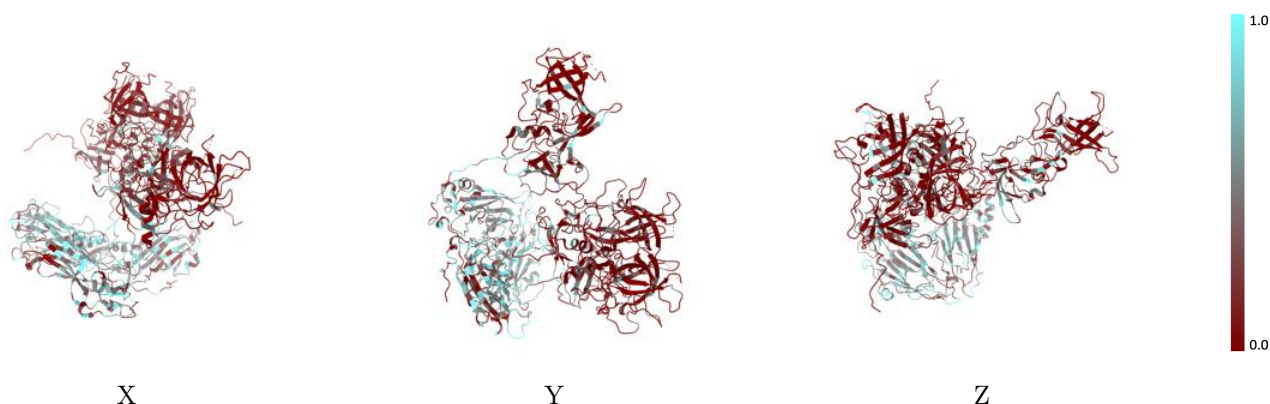
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



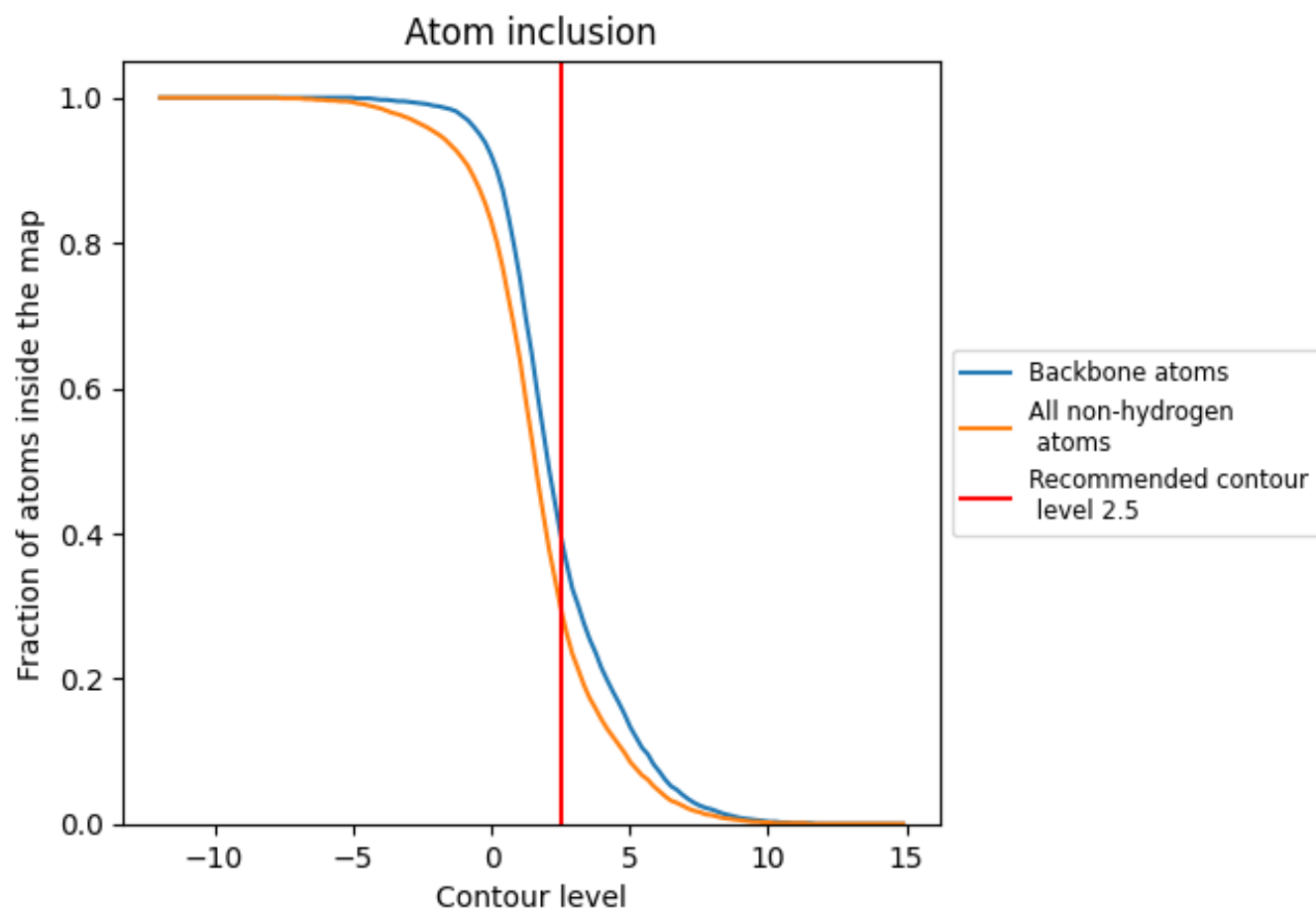
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 30% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2980	0.0810
A	0.2850	0.0760
B	0.2860	0.0800
C	0.3250	0.0860

