



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:53 AM UTC

PDB ID : 3J7W / pdb_00003j7w
EMDB ID : EMD-6035
Title : Capsid Expansion Mechanism Of Bacteriophage T7 Revealed By Multi-State Atomic Models Derived From Cryo-EM Reconstructions
Authors : Guo, F.; Liu, Z.; Fang, P.A.; Zhang, Q.; Wright, E.T.; Wu, W.; Zhang, C.; Vago, F.; Ren, Y.; Jakata, J.; Chiu, W.; Serwer, P.; Jiang, W.
Deposited on : 2014-08-12
Resolution : 3.50 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

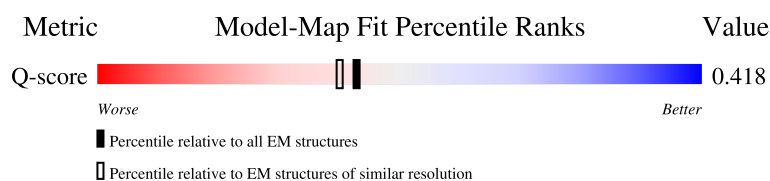
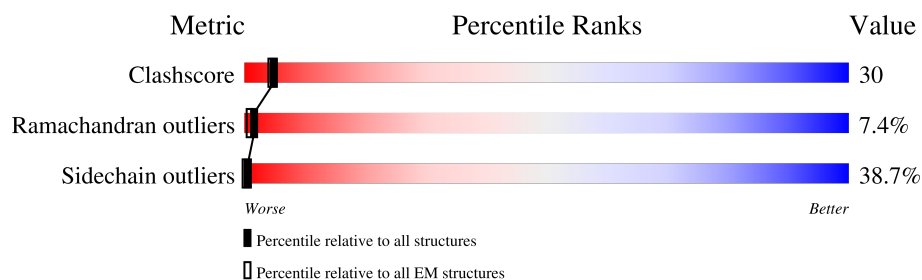
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	345	
1	B	345	
1	C	345	
1	D	345	

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Mol	Chain	Length	Quality of chain
1	E	345	10% 43% 40% 14% ••
1	F	345	9% 42% 38% 17% ••
1	G	345	17% 42% 38% 17% ••

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17829 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.

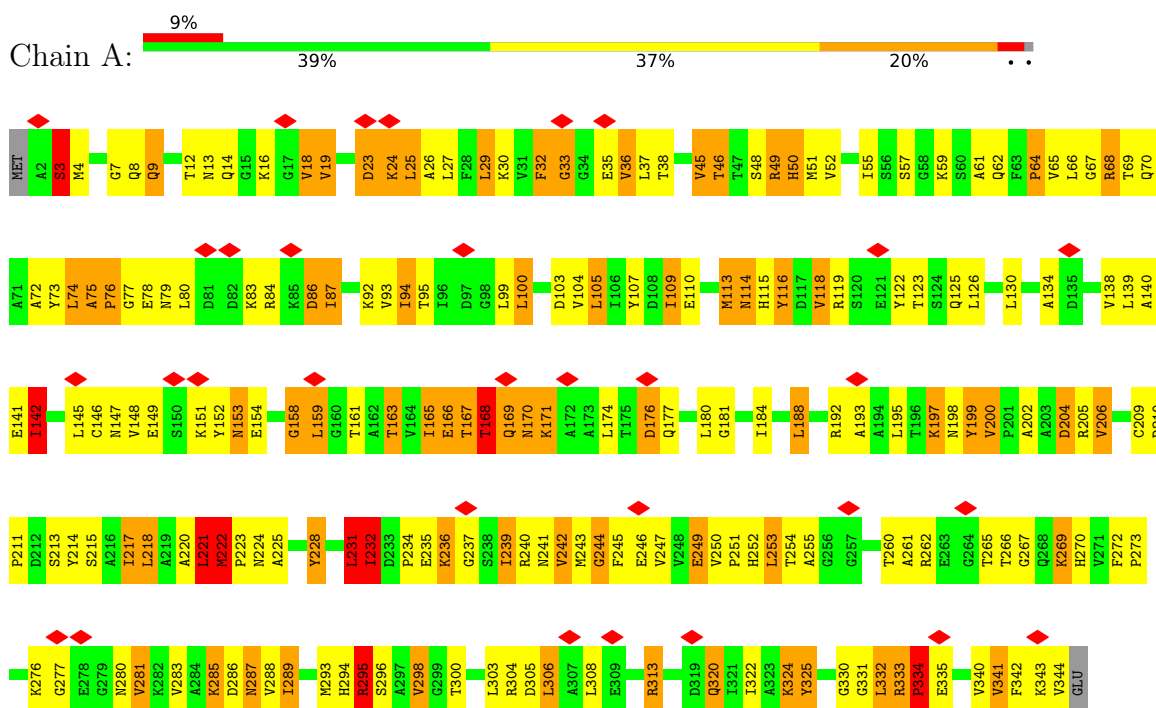
- Molecule 1 is a protein called Major capsid protein 10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	B	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	C	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	D	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	E	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	F	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		
1	G	343	Total	C	N	O	S	0	0
			2547	1593	452	491	11		

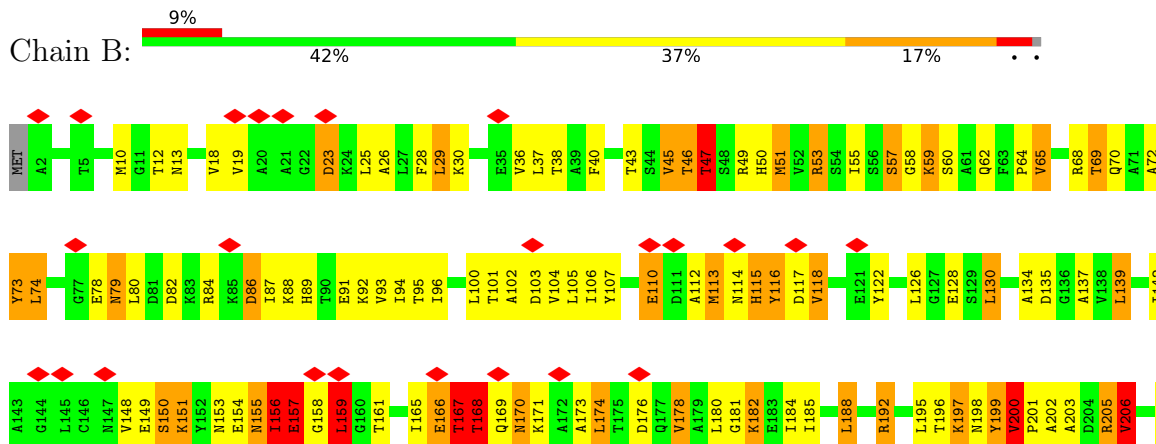
3 Residue-property plots

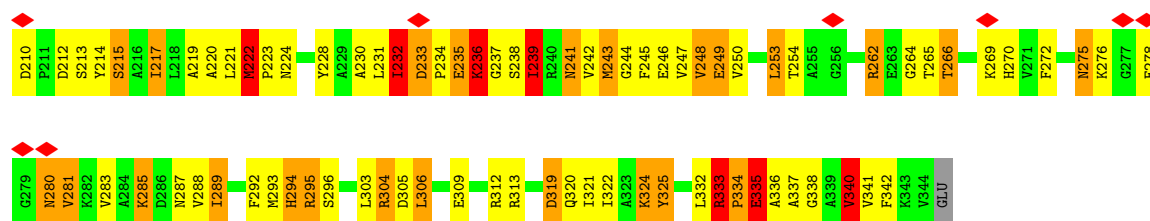
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

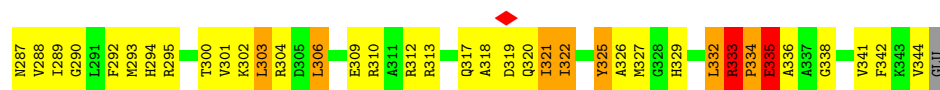
• Molecule 1: Major capsid protein 10A



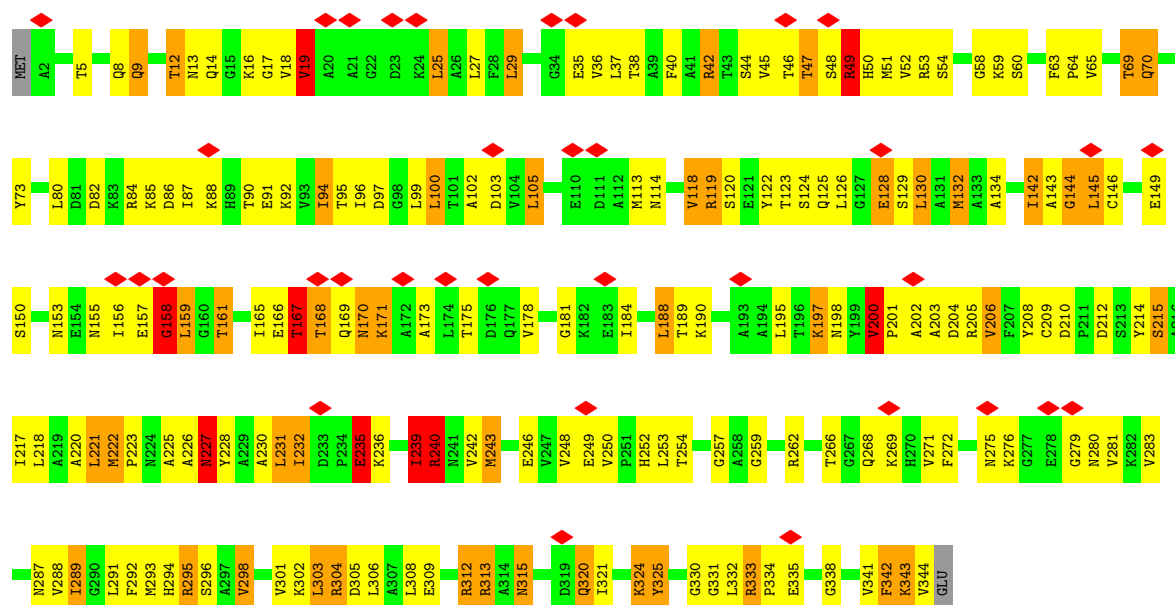
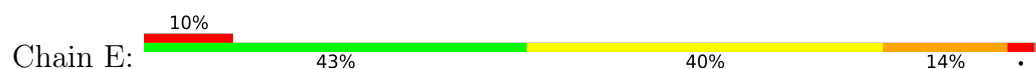
• Molecule 1: Major capsid protein 10A



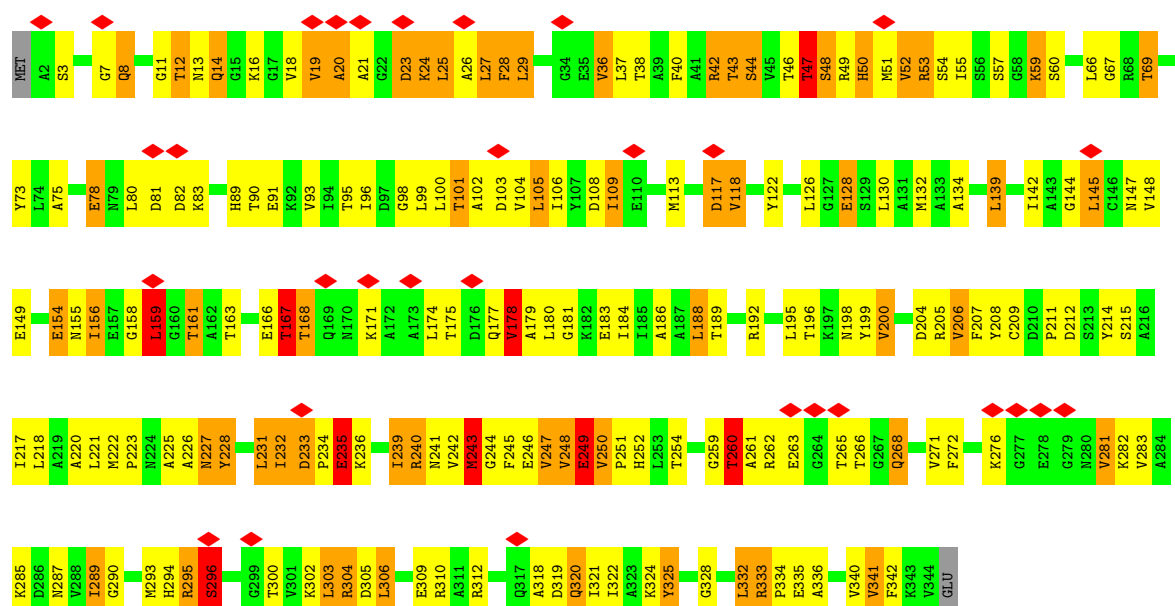
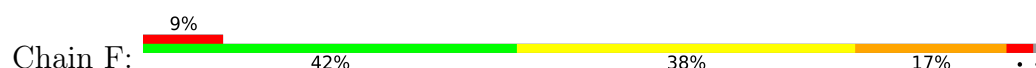




• Molecule 1: Major capsid protein 10A

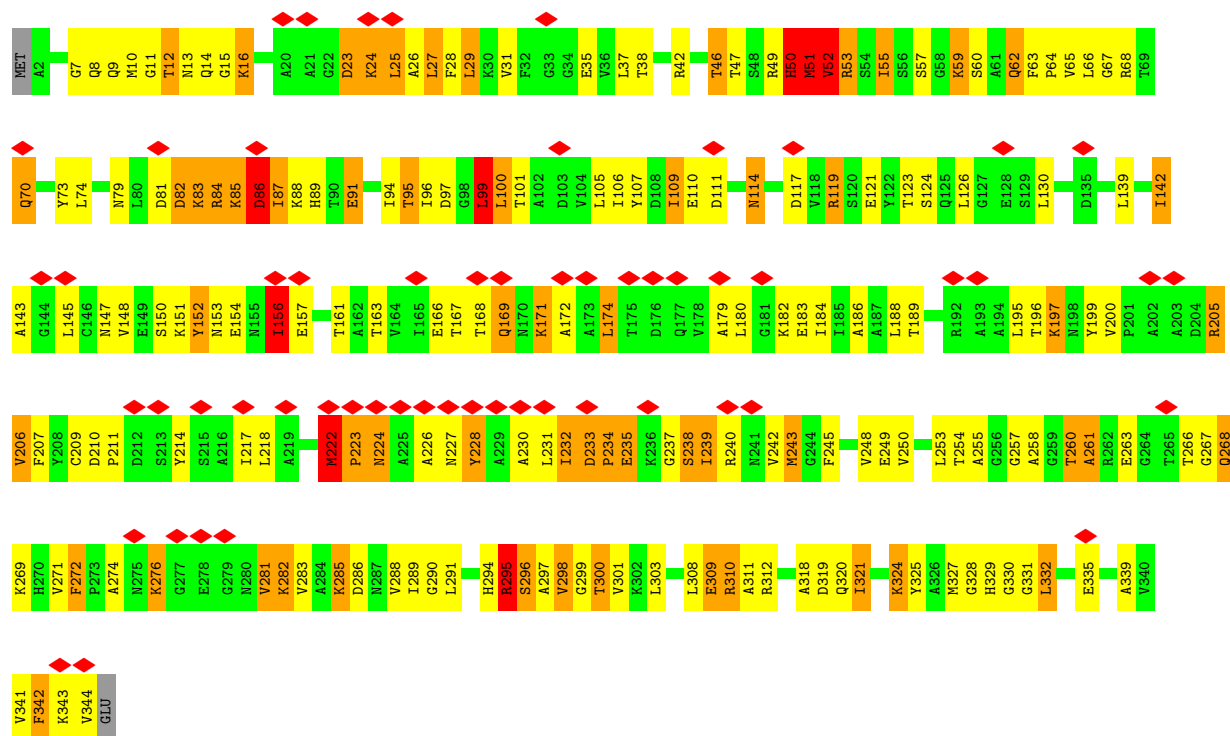


• Molecule 1: Major capsid protein 10A



• Molecule 1: Major capsid protein 10A

Chain G: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	43417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	57727	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	26.777	Depositor
Minimum map value	-25.608	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	1.187	Depositor
Recommended contour level	4.3	Depositor
Map size ($\text{\AA}$)	880.0, 880.0, 880.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.45	1/2582 (0.0%)	1.00	8/3491 (0.2%)
1	B	0.46	2/2582 (0.1%)	0.99	6/3491 (0.2%)
1	C	0.46	2/2582 (0.1%)	1.00	8/3491 (0.2%)
1	D	0.46	2/2582 (0.1%)	0.95	8/3491 (0.2%)
1	E	0.43	0/2582	0.95	2/3491 (0.1%)
1	F	0.43	0/2582	0.96	7/3491 (0.2%)
1	G	0.44	2/2582 (0.1%)	1.00	10/3491 (0.3%)
All	All	0.45	9/18074 (0.0%)	0.98	49/24437 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	333	ARG	C-N	7.77	1.40	1.33
1	G	222	MET	C-N	5.95	1.41	1.33
1	B	333	ARG	C-N	5.92	1.41	1.33
1	D	222	MET	C-N	5.76	1.41	1.33
1	C	334	PRO	N-CD	5.41	1.55	1.47
1	A	334	PRO	N-CD	5.38	1.55	1.47
1	B	334	PRO	N-CD	5.23	1.55	1.47
1	G	223	PRO	N-CD	5.08	1.54	1.47
1	D	223	PRO	N-CD	5.01	1.54	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	GLY	N-CA-C	-8.78	102.82	115.64
1	G	114	ASN	N-CA-C	8.63	121.64	111.71
1	F	248	VAL	N-CA-C	7.83	118.63	110.72
1	E	158	GLY	CA-C-N	7.32	134.87	121.70
1	E	158	GLY	C-N-CA	7.32	134.87	121.70
1	B	333	ARG	CA-C-N	-6.88	112.90	119.85
1	B	333	ARG	C-N-CA	-6.88	112.90	119.85
1	A	197	LYS	N-CA-C	-6.83	100.17	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	222	MET	CA-C-N	-6.83	112.73	119.76
1	G	222	MET	C-N-CA	-6.83	112.73	119.76
1	C	222	MET	CA-C-N	-6.75	112.82	119.64
1	C	222	MET	C-N-CA	-6.75	112.82	119.64
1	D	222	MET	CA-C-N	-6.70	112.86	119.76
1	D	222	MET	C-N-CA	-6.70	112.86	119.76
1	G	27	LEU	N-CA-C	-6.68	104.76	113.17
1	A	75	ALA	CA-C-N	6.58	128.07	119.84
1	A	75	ALA	C-N-CA	6.58	128.07	119.84
1	A	67	GLY	N-CA-C	6.43	119.96	110.63
1	G	67	GLY	N-CA-C	6.33	119.80	110.63
1	C	333	ARG	CA-C-N	-6.31	113.26	120.89
1	C	333	ARG	C-N-CA	-6.31	113.26	120.89
1	D	335	GLU	N-CA-C	-6.29	104.05	111.03
1	D	237	GLY	N-CA-C	6.20	121.49	114.67
1	D	67	GLY	N-CA-C	6.15	120.07	110.91
1	B	159	LEU	N-CA-C	6.06	118.81	108.02
1	F	159	LEU	N-CA-C	6.05	117.98	108.96
1	F	260	THR	CB-CA-C	-5.97	109.11	117.23
1	D	58	GLY	N-CA-C	5.89	120.14	112.25
1	F	93	VAL	N-CA-C	5.88	116.41	108.17
1	C	271	VAL	N-CA-C	5.70	117.28	108.44
1	G	51	MET	CB-CA-C	-5.70	110.02	116.63
1	C	235	GLU	CB-CA-C	-5.69	109.99	116.54
1	G	99	LEU	N-CA-C	5.67	116.40	108.00
1	A	231	LEU	N-CA-C	5.63	117.28	111.03
1	G	206	VAL	N-CA-C	5.61	115.75	108.35
1	A	221	LEU	N-CA-C	-5.56	103.35	110.53
1	D	176	ASP	N-CA-C	-5.51	105.54	114.09
1	B	222	MET	CA-C-N	-5.49	112.97	119.84
1	B	222	MET	C-N-CA	-5.49	112.97	119.84
1	G	50	HIS	N-CA-C	5.38	118.17	109.40
1	A	158	GLY	N-CA-C	-5.35	100.49	113.18
1	G	79	ASN	N-CA-C	5.29	117.35	109.25
1	D	46	THR	CB-CA-C	-5.23	110.12	117.23
1	B	340	VAL	CB-CA-C	5.15	118.03	110.98
1	F	296	SER	N-CA-C	-5.12	105.69	112.24
1	C	335	GLU	N-CA-C	-5.04	105.79	111.28
1	F	289	ILE	N-CA-C	-5.04	107.23	111.56
1	F	249	GLU	N-CA-C	5.03	118.57	111.52
1	A	16	LYS	N-CA-C	5.02	116.44	111.07

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	2547	0	2571	193	0
1	B	2547	0	2573	178	0
1	C	2547	0	2573	182	0
1	D	2547	0	2573	139	0
1	E	2547	0	2573	125	0
1	F	2547	0	2573	172	0
1	G	2547	0	2573	186	0
All	All	17829	0	18009	1068	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 30.

All (1068) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:CB	1:A:335:GLU:HG2	1.27	1.63
1:B:74:LEU:HD22	1:B:80:LEU:CD2	1.35	1.53
1:A:159:LEU:HB2	1:A:335:GLU:CD	1.33	1.51
1:C:159:LEU:CD1	1:C:335:GLU:HA	1.41	1.48
1:A:159:LEU:CB	1:A:335:GLU:CG	1.94	1.44
1:A:159:LEU:CD2	1:A:335:GLU:HB3	1.47	1.41
1:C:159:LEU:HD13	1:C:335:GLU:CA	1.52	1.39
1:D:117:ASP:HA	1:D:118:VAL:CB	1.39	1.37
1:D:117:ASP:HA	1:D:118:VAL:CG1	1.57	1.35
1:C:296:SER:N	1:C:297:ALA:HB3	1.37	1.34
1:F:27:LEU:HD12	1:F:28:PHE:N	1.42	1.34
1:B:236:LYS:HA	1:C:243:MET:O	1.25	1.33
1:F:27:LEU:HD12	1:F:27:LEU:C	1.52	1.33
1:B:334:PRO:HA	1:B:335:GLU:O	1.27	1.32
1:B:74:LEU:CD2	1:B:80:LEU:HD21	1.62	1.29
1:B:236:LYS:CA	1:C:243:MET:O	1.81	1.29
1:D:117:ASP:CB	1:D:118:VAL:HG12	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD22	1:A:335:GLU:CB	1.63	1.26
1:G:85:LYS:HA	1:G:85:LYS:CE	1.50	1.25
1:A:159:LEU:HB2	1:A:335:GLU:CG	1.56	1.24
1:C:295:ARG:C	1:C:297:ALA:HB3	1.63	1.21
1:B:74:LEU:CD2	1:B:80:LEU:CD2	2.19	1.19
1:F:25:LEU:N	1:F:26:ALA:HB3	1.57	1.17
1:A:159:LEU:HB3	1:A:335:GLU:CG	1.63	1.17
1:B:40:PHE:CE1	1:C:333:ARG:NH2	2.14	1.14
1:G:85:LYS:HA	1:G:85:LYS:HE2	1.28	1.13
1:A:159:LEU:HB2	1:A:335:GLU:OE2	1.46	1.12
1:B:40:PHE:CZ	1:C:333:ARG:NH2	2.17	1.12
1:D:117:ASP:HB2	1:D:118:VAL:HG12	1.31	1.12
1:D:117:ASP:CA	1:D:118:VAL:HG12	1.79	1.12
1:G:51:MET:O	1:G:52:VAL:HG13	1.49	1.11
1:G:85:LYS:HA	1:G:85:LYS:HE3	1.22	1.11
1:A:159:LEU:CB	1:A:335:GLU:CD	2.18	1.10
1:G:298:VAL:HG13	1:G:331:GLY:HA2	1.25	1.10
1:B:74:LEU:HD22	1:B:80:LEU:HD23	1.23	1.10
1:G:51:MET:HG3	1:G:299:GLY:HA3	1.31	1.10
1:G:53:ARG:CG	1:G:53:ARG:HH11	1.64	1.10
1:D:117:ASP:CA	1:D:118:VAL:CB	2.30	1.10
1:G:300:THR:CG2	1:G:329:HIS:ND1	2.14	1.09
1:B:114:ASN:C	1:B:115:HIS:CD2	2.30	1.09
1:G:29:LEU:H	1:G:29:LEU:HD22	0.94	1.09
1:D:117:ASP:CA	1:D:118:VAL:CG1	2.30	1.09
1:D:222:MET:HG3	1:D:223:PRO:HD2	1.24	1.09
1:G:222:MET:HB3	1:G:223:PRO:HD2	1.33	1.08
1:B:45:VAL:HG12	1:B:46:THR:H	1.19	1.08
1:D:117:ASP:CA	1:D:118:VAL:HB	1.82	1.06
1:F:27:LEU:CD1	1:F:28:PHE:N	2.17	1.06
1:G:85:LYS:HE2	1:G:85:LYS:CA	1.86	1.04
1:G:85:LYS:CE	1:G:85:LYS:CA	2.30	1.03
1:G:51:MET:C	1:G:52:VAL:HG13	1.83	1.02
1:A:332:LEU:O	1:A:332:LEU:HD22	1.60	1.02
1:B:45:VAL:HG12	1:B:46:THR:N	1.74	1.01
1:G:168:THR:O	1:G:168:THR:HG22	1.59	1.01
1:D:117:ASP:HA	1:D:118:VAL:HB	1.04	1.00
1:G:29:LEU:H	1:G:29:LEU:CD2	1.74	1.00
1:G:295:ARG:O	1:G:296:SER:OG	1.76	1.00
1:B:222:MET:HE1	1:C:243:MET:CE	1.92	0.99
1:F:24:LYS:HZ3	1:F:24:LYS:HB3	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:THR:HG21	1:G:329:HIS:CE1	1.96	0.99
1:B:74:LEU:HD22	1:B:80:LEU:HD21	1.00	0.98
1:C:295:ARG:C	1:C:297:ALA:CB	2.36	0.98
1:A:168:THR:HG23	1:A:169:GLN:N	1.79	0.97
1:G:222:MET:HB3	1:G:223:PRO:CD	1.93	0.97
1:F:25:LEU:HD13	1:F:25:LEU:O	1.63	0.97
1:C:296:SER:HA	1:C:298:VAL:H	1.30	0.96
1:B:222:MET:HE1	1:C:243:MET:HE1	1.46	0.96
1:F:25:LEU:O	1:F:25:LEU:HD22	1.63	0.96
1:G:169:GLN:NE2	1:G:174:LEU:HD21	1.79	0.96
1:B:236:LYS:N	1:C:243:MET:O	1.98	0.95
1:G:29:LEU:HD22	1:G:29:LEU:N	1.76	0.95
1:C:296:SER:N	1:C:297:ALA:CB	2.30	0.95
1:F:25:LEU:N	1:F:26:ALA:CB	2.30	0.94
1:F:25:LEU:H	1:F:26:ALA:HB3	1.24	0.94
1:D:229:ALA:HB2	1:E:228:TYR:CZ	2.03	0.93
1:A:146:CYS:SG	1:A:334:PRO:HB3	2.09	0.92
1:B:116:TYR:N	1:B:116:TYR:HD2	1.68	0.92
1:G:53:ARG:HH11	1:G:53:ARG:HG3	1.32	0.92
1:C:159:LEU:HD12	1:C:335:GLU:HA	1.50	0.92
1:C:159:LEU:HD13	1:C:335:GLU:HA	0.91	0.91
1:C:161:THR:HG22	1:C:334:PRO:O	1.70	0.91
1:A:332:LEU:HD13	1:A:332:LEU:H	1.35	0.90
1:B:37:LEU:HB2	1:C:65:VAL:HG12	1.54	0.90
1:A:159:LEU:HD13	1:A:335:GLU:OE1	1.73	0.89
1:A:250:VAL:HG23	1:A:253:LEU:HG	1.53	0.89
1:G:300:THR:HG21	1:G:329:HIS:ND1	1.86	0.89
1:F:249:GLU:O	1:F:249:GLU:HG2	1.69	0.89
1:G:29:LEU:HD23	1:G:29:LEU:O	1.73	0.88
1:D:116:TYR:O	1:D:118:VAL:HB	1.71	0.88
1:G:51:MET:CG	1:G:299:GLY:HA3	2.03	0.88
1:G:85:LYS:HE2	1:G:85:LYS:O	1.73	0.88
1:D:117:ASP:CB	1:D:118:VAL:CG1	2.50	0.87
1:A:254:THR:HG22	1:A:255:ALA:H	1.39	0.86
1:G:85:LYS:HE2	1:G:85:LYS:C	1.99	0.86
1:C:242:VAL:HG12	1:C:243:MET:HE2	1.56	0.86
1:G:298:VAL:CG1	1:G:330:GLY:O	2.23	0.86
1:D:227:ASN:O	1:D:228:TYR:CG	2.30	0.85
1:D:222:MET:HG3	1:D:223:PRO:CD	2.08	0.84
1:D:227:ASN:O	1:D:228:TYR:CD2	2.30	0.84
1:G:297:ALA:O	1:G:332:LEU:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:MET:CE	1:C:243:MET:HE1	2.07	0.84
1:B:114:ASN:O	1:B:115:HIS:CG	2.30	0.83
1:B:114:ASN:O	1:B:116:TYR:CE2	2.30	0.83
1:B:334:PRO:CA	1:B:335:GLU:O	2.20	0.83
1:A:159:LEU:CD2	1:A:335:GLU:CB	2.36	0.83
1:F:27:LEU:HD12	1:F:28:PHE:CA	2.06	0.83
1:C:159:LEU:HD13	1:C:335:GLU:CB	2.07	0.83
1:F:24:LYS:HB3	1:F:24:LYS:NZ	1.92	0.83
1:G:298:VAL:HG12	1:G:330:GLY:O	1.80	0.82
1:G:53:ARG:HH11	1:G:53:ARG:HG2	1.42	0.82
1:G:294:HIS:CE1	1:G:296:SER:OG	2.32	0.82
1:G:25:LEU:HB2	1:G:26:ALA:HB2	1.62	0.82
1:F:27:LEU:C	1:F:27:LEU:CD1	2.30	0.81
1:B:206:VAL:HG23	1:B:246:GLU:HB3	1.61	0.81
1:A:273:PRO:HG2	1:A:281:VAL:HG11	1.63	0.81
1:C:159:LEU:CD1	1:C:335:GLU:CA	2.29	0.81
1:B:114:ASN:O	1:B:115:HIS:CD2	2.34	0.80
1:F:249:GLU:O	1:F:249:GLU:CG	2.30	0.80
1:A:332:LEU:HD23	1:A:333:ARG:HG2	1.64	0.80
1:G:168:THR:O	1:G:168:THR:CG2	2.30	0.80
1:B:116:TYR:N	1:B:116:TYR:CD2	2.42	0.79
1:G:230:ALA:HB1	1:G:231:LEU:HD23	1.63	0.79
1:F:24:LYS:O	1:F:25:LEU:CD1	2.30	0.79
1:F:25:LEU:O	1:F:25:LEU:CD1	2.30	0.79
1:F:25:LEU:O	1:F:25:LEU:CD2	2.30	0.79
1:F:208:TYR:CD2	1:F:248:VAL:HG21	2.17	0.79
1:G:51:MET:O	1:G:52:VAL:CG1	2.30	0.79
1:G:51:MET:C	1:G:52:VAL:CG1	2.55	0.79
1:F:25:LEU:CA	1:F:26:ALA:HB3	2.14	0.78
1:G:295:ARG:C	1:G:296:SER:OG	2.24	0.78
1:A:159:LEU:HD13	1:A:335:GLU:CD	2.09	0.78
1:G:51:MET:HG3	1:G:299:GLY:CA	2.14	0.78
1:G:171:LYS:HD3	1:G:172:ALA:H	1.48	0.78
1:A:332:LEU:CD2	1:A:333:ARG:HG2	2.14	0.77
1:A:168:THR:CG2	1:A:169:GLN:N	2.48	0.77
1:G:297:ALA:O	1:G:332:LEU:HD22	1.84	0.77
1:G:300:THR:CG2	1:G:329:HIS:CE1	2.63	0.77
1:A:332:LEU:O	1:A:333:ARG:HG3	1.86	0.76
1:B:114:ASN:O	1:B:116:TYR:HE2	1.65	0.76
1:G:51:MET:CG	1:G:299:GLY:CA	2.62	0.76
1:A:159:LEU:HD21	1:A:198:ASN:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:PRO:HA	1:B:335:GLU:C	2.10	0.76
1:B:45:VAL:HG12	1:B:46:THR:HG22	1.66	0.76
1:B:114:ASN:C	1:B:115:HIS:CG	2.64	0.76
1:A:168:THR:HG23	1:A:169:GLN:H	1.46	0.75
1:G:298:VAL:HG13	1:G:331:GLY:CA	2.13	0.75
1:C:203:ALA:HA	1:C:205:ARG:HD2	1.69	0.75
1:C:159:LEU:HB2	1:C:335:GLU:HG3	1.67	0.75
1:F:159:LEU:HB3	1:F:335:GLU:HB2	1.68	0.75
1:G:294:HIS:ND1	1:G:296:SER:OG	2.19	0.75
1:B:74:LEU:HD11	1:B:78:GLU:O	1.87	0.75
1:B:294:HIS:H	1:B:336:ALA:HB1	1.51	0.75
1:A:221:LEU:O	1:A:222:MET:HB2	1.86	0.75
1:G:85:LYS:O	1:G:86:ASP:CG	2.30	0.74
1:B:159:LEU:HD11	1:B:335:GLU:H	1.51	0.74
1:D:218:LEU:HD23	1:D:232:ILE:HD11	1.67	0.74
1:D:36:VAL:HG12	1:E:64:PRO:HG2	1.68	0.74
1:A:159:LEU:HB3	1:A:335:GLU:HG2	0.74	0.74
1:A:332:LEU:HD13	1:A:332:LEU:N	2.02	0.74
1:F:248:VAL:O	1:F:249:GLU:CD	2.30	0.74
1:G:294:HIS:ND1	1:G:295:ARG:O	2.20	0.73
1:A:142:ILE:HB	1:A:298:VAL:HG21	1.70	0.73
1:B:46:THR:O	1:B:47:THR:HB	1.88	0.73
1:D:287:ASN:HB3	1:D:341:VAL:HG13	1.69	0.73
1:G:51:MET:CB	1:G:299:GLY:HA2	2.19	0.73
1:C:154:GLU:HB3	1:C:334:PRO:CD	2.18	0.72
1:C:37:LEU:HD21	1:D:332:LEU:HD23	1.71	0.72
1:B:45:VAL:CG1	1:B:46:THR:H	1.93	0.72
1:B:74:LEU:CD2	1:B:80:LEU:HD23	2.07	0.72
1:D:226:ALA:C	1:D:227:ASN:OD1	2.33	0.72
1:F:103:ASP:OD1	1:F:262:ARG:NH2	2.23	0.71
1:G:86:ASP:C	1:G:86:ASP:OD2	2.32	0.71
1:C:332:LEU:O	1:C:333:ARG:HB3	1.90	0.71
1:A:159:LEU:HD22	1:A:335:GLU:HB3	0.73	0.71
1:F:24:LYS:O	1:F:25:LEU:HD13	1.91	0.71
1:B:45:VAL:HG12	1:B:46:THR:CG2	2.21	0.70
1:C:336:ALA:O	1:C:337:ALA:CB	2.38	0.70
1:A:239:ILE:HD11	1:A:247:VAL:HB	1.73	0.70
1:B:222:MET:HE1	1:C:243:MET:HE2	1.71	0.70
1:D:312:ARG:HG2	1:D:319:ASP:HB3	1.73	0.70
1:A:215:SER:OG	1:B:192:ARG:NH1	2.25	0.70
1:C:184:ILE:HD12	1:C:289:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:HD1	1:F:259:GLY:HA2	1.56	0.69
1:A:146:CYS:SG	1:A:334:PRO:CB	2.81	0.69
1:C:332:LEU:O	1:C:333:ARG:CB	2.41	0.69
1:G:29:LEU:CD2	1:G:29:LEU:N	2.42	0.69
1:G:254:THR:HG23	1:G:272:PHE:HD2	1.55	0.69
1:D:159:LEU:HD22	1:D:335:GLU:HG2	1.75	0.69
1:D:223:PRO:HG3	1:E:230:ALA:CB	2.23	0.69
1:F:42:ARG:NH1	1:F:128:GLU:OE1	2.24	0.69
1:C:174:LEU:O	1:C:176:ASP:N	2.26	0.69
1:F:47:THR:OG1	1:F:48:SER:N	2.25	0.69
1:E:333:ARG:NH1	1:E:335:GLU:OE1	2.25	0.68
1:D:96:ILE:HD13	1:D:303:LEU:HD11	1.76	0.68
1:F:27:LEU:O	1:F:28:PHE:CG	2.46	0.68
1:E:96:ILE:HD11	1:E:303:LEU:HB3	1.75	0.68
1:E:242:VAL:HG12	1:E:243:MET:HG2	1.75	0.68
1:F:24:LYS:O	1:F:25:LEU:HD12	1.93	0.68
1:F:25:LEU:O	1:F:25:LEU:CG	2.42	0.68
1:A:204:ASP:OD1	1:A:294:HIS:CD2	2.47	0.67
1:E:17:GLY:O	1:E:19:VAL:N	2.26	0.67
1:F:312:ARG:HG2	1:F:319:ASP:HB3	1.76	0.67
1:A:332:LEU:O	1:A:333:ARG:CG	2.42	0.67
1:B:45:VAL:CG1	1:B:46:THR:N	2.48	0.67
1:A:250:VAL:CG2	1:A:253:LEU:HG	2.23	0.67
1:C:154:GLU:HB3	1:C:334:PRO:HD3	1.76	0.67
1:F:25:LEU:HD13	1:F:25:LEU:C	2.19	0.67
1:G:26:ALA:HB1	1:G:28:PHE:H	1.59	0.67
1:B:222:MET:SD	1:C:243:MET:HE1	2.34	0.67
1:E:150:SER:OG	1:E:280:ASN:ND2	2.27	0.67
1:B:289:ILE:HG12	1:B:340:VAL:O	1.95	0.67
1:E:202:ALA:HA	1:E:205:ARG:HH12	1.60	0.67
1:C:157:GLU:HB2	1:C:159:LEU:HB3	1.77	0.67
1:G:254:THR:HG22	1:G:255:ALA:H	1.61	0.66
1:D:241:ASN:OD1	1:D:241:ASN:N	2.25	0.66
1:D:51:MET:SD	1:D:53:ARG:NH1	2.68	0.66
1:E:25:LEU:HD22	1:F:59:LYS:HE3	1.77	0.66
1:E:259:GLY:HA2	1:F:73:TYR:HD1	1.59	0.66
1:B:51:MET:HE1	1:B:53:ARG:HD2	1.78	0.66
1:C:48:SER:O	1:C:49:ARG:HD2	1.96	0.66
1:E:227:ASN:H	1:F:227:ASN:HD22	1.41	0.66
1:G:171:LYS:HD3	1:G:172:ALA:N	2.11	0.66
1:B:36:VAL:HG22	1:C:64:PRO:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LYS:HD2	1:F:60:SER:HB2	1.78	0.66
1:B:137:ALA:HB1	1:B:270:HIS:HD2	1.61	0.66
1:A:30:LYS:HG2	1:B:60:SER:HB3	1.77	0.65
1:G:111:ASP:OD1	1:G:119:ARG:NH1	2.28	0.65
1:A:92:LYS:NZ	1:A:333:ARG:H	1.95	0.65
1:A:159:LEU:HD23	1:A:335:GLU:HB3	1.68	0.65
1:G:53:ARG:HG2	1:G:53:ARG:NH1	2.05	0.65
1:F:50:HIS:HB3	1:F:52:VAL:HG12	1.79	0.65
1:G:52:VAL:O	1:G:52:VAL:HG23	1.95	0.65
1:B:115:HIS:CD2	1:B:115:HIS:N	2.64	0.65
1:D:209:CYS:SG	1:D:210:ASP:N	2.69	0.65
1:E:97:ASP:OD2	1:E:269:LYS:NZ	2.28	0.65
1:A:35:GLU:OE2	1:B:53:ARG:NH1	2.30	0.65
1:A:87:ILE:HD11	1:F:104:VAL:HG12	1.79	0.65
1:C:50:HIS:HE1	1:C:298:VAL:C	2.05	0.64
1:F:43:THR:OG1	1:F:44:SER:N	2.30	0.64
1:F:276:LYS:HG3	1:F:282:LYS:HA	1.77	0.64
1:G:166:GLU:OE1	1:G:342:PHE:HB3	1.97	0.64
1:A:197:LYS:O	1:A:198:ASN:HB2	1.98	0.64
1:B:107:TYR:HB2	1:B:110:GLU:HG2	1.78	0.64
1:F:199:TYR:O	1:F:200:VAL:HB	1.97	0.64
1:D:140:ALA:HA	1:D:272:PHE:HE1	1.63	0.64
1:B:116:TYR:HD2	1:B:116:TYR:H	1.45	0.63
1:E:49:ARG:NH1	1:E:246:GLU:OE2	2.31	0.63
1:E:257:GLY:HA3	1:E:268:GLN:HG2	1.78	0.63
1:G:42:ARG:H	1:G:42:ARG:HD3	1.62	0.63
1:D:310:ARG:HH21	1:D:321:ILE:HD11	1.64	0.63
1:G:169:GLN:HE21	1:G:174:LEU:HD21	1.60	0.63
1:A:159:LEU:CD1	1:A:335:GLU:CD	2.71	0.63
1:E:259:GLY:HA2	1:F:73:TYR:CD1	2.34	0.63
1:F:304:ARG:HG2	1:F:304:ARG:HH11	1.64	0.63
1:C:161:THR:OG1	1:C:162:ALA:N	2.27	0.62
1:C:286:ASP:OD2	1:C:287:ASN:N	2.32	0.62
1:C:296:SER:H	1:C:297:ALA:HB3	1.51	0.62
1:C:66:LEU:HB3	1:C:89:HIS:HB3	1.82	0.62
1:D:262:ARG:O	1:E:70:GLN:NE2	2.31	0.62
1:F:53:ARG:HH11	1:F:53:ARG:HB3	1.63	0.62
1:C:232:ILE:HG22	1:C:233:ASP:H	1.64	0.62
1:G:70:GLN:HA	1:G:70:GLN:HE21	1.64	0.62
1:A:140:ALA:HA	1:A:272:PHE:HE1	1.65	0.62
1:C:296:SER:CA	1:C:298:VAL:H	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ILE:HD12	1:F:289:ILE:HG21	1.82	0.62
1:A:214:TYR:HE1	1:A:239:ILE:HD12	1.65	0.62
1:B:69:THR:OG1	1:B:70:GLN:N	2.31	0.62
1:C:147:ASN:HD21	1:C:163:THR:HG21	1.65	0.62
1:F:161:THR:HG22	1:F:334:PRO:HB2	1.82	0.62
1:B:59:LYS:HE3	1:B:60:SER:H	1.65	0.61
1:F:243:MET:SD	1:F:243:MET:N	2.73	0.61
1:A:55:ILE:HD13	1:A:61:ALA:HB2	1.82	0.61
1:F:102:ALA:HB1	1:F:126:LEU:HD22	1.81	0.61
1:F:166:GLU:HG3	1:F:167:THR:O	2.01	0.61
1:B:156:ILE:HG23	1:B:157:GLU:H	1.66	0.61
1:G:300:THR:HG22	1:G:329:HIS:ND1	2.12	0.61
1:A:3:SER:OG	1:A:4:MET:N	2.29	0.61
1:E:69:THR:OG1	1:E:70:GLN:N	2.31	0.61
1:E:53:ARG:O	1:E:301:VAL:HA	2.01	0.61
1:F:105:LEU:HA	1:F:320:GLN:HB2	1.83	0.61
1:G:166:GLU:OE2	1:G:183:GLU:HB3	2.01	0.61
1:C:295:ARG:CA	1:C:297:ALA:HB3	2.30	0.61
1:A:161:THR:HB	1:A:334:PRO:O	2.01	0.60
1:A:204:ASP:OD2	1:A:295:ARG:HG2	2.02	0.60
1:F:287:ASN:HB3	1:F:341:VAL:HG13	1.82	0.60
1:G:254:THR:HG23	1:G:272:PHE:CD2	2.35	0.60
1:A:107:TYR:HB2	1:A:110:GLU:HG2	1.82	0.60
1:B:37:LEU:HD12	1:C:333:ARG:HH12	1.66	0.60
1:A:204:ASP:CG	1:A:204:ASP:O	2.44	0.60
1:D:169:GLN:O	1:D:170:ASN:ND2	2.21	0.60
1:G:207:PHE:CZ	1:G:290:GLY:HA3	2.37	0.60
1:G:312:ARG:HG2	1:G:319:ASP:HB3	1.84	0.60
1:A:159:LEU:CG	1:A:335:GLU:CD	2.74	0.60
1:E:231:LEU:HD23	1:E:232:ILE:HG23	1.82	0.60
1:A:221:LEU:HB3	1:A:232:ILE:HG21	1.84	0.60
1:D:142:ILE:HG23	1:D:143:ALA:H	1.66	0.60
1:F:305:ASP:CG	1:F:306:LEU:H	2.09	0.60
1:G:257:GLY:HA3	1:G:268:GLN:HB3	1.84	0.60
1:B:102:ALA:HB1	1:B:126:LEU:HD22	1.83	0.60
1:B:178:VAL:HG12	1:B:182:LYS:HE2	1.84	0.60
1:C:296:SER:HA	1:C:298:VAL:N	2.09	0.60
1:G:51:MET:HB2	1:G:299:GLY:HA2	1.84	0.60
1:E:304:ARG:HA	1:E:304:ARG:HH11	1.66	0.60
1:B:37:LEU:HD12	1:C:333:ARG:NH1	2.16	0.59
1:D:333:ARG:HG3	1:D:335:GLU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ILE:HG21	1:E:239:ILE:HA	1.84	0.59
1:B:232:ILE:HB	1:B:239:ILE:HA	1.84	0.59
1:C:40:PHE:HE2	1:D:335:GLU:HG3	1.67	0.59
1:D:157:GLU:OE2	1:D:158:GLY:N	2.35	0.59
1:D:169:GLN:C	1:D:170:ASN:HD22	2.10	0.59
1:G:169:GLN:NE2	1:G:174:LEU:CD2	2.62	0.59
1:A:294:HIS:O	1:A:295:ARG:HB3	2.01	0.59
1:C:50:HIS:HE1	1:C:298:VAL:O	1.85	0.59
1:F:305:ASP:O	1:F:325:TYR:HB2	2.03	0.59
1:G:51:MET:O	1:G:52:VAL:HG22	2.01	0.59
1:C:116:TYR:HD1	1:C:118:VAL:HG22	1.67	0.59
1:D:100:LEU:HB3	1:D:130:LEU:HD11	1.84	0.59
1:E:166:GLU:HB3	1:E:342:PHE:HA	1.84	0.59
1:B:289:ILE:HD12	1:B:342:PHE:CE1	2.38	0.59
1:A:99:LEU:HD11	1:A:324:LYS:HB2	1.84	0.59
1:F:208:TYR:CE2	1:F:248:VAL:HG21	2.38	0.59
1:G:142:ILE:HB	1:G:298:VAL:HG21	1.85	0.59
1:D:142:ILE:HD11	1:D:293:MET:HB3	1.83	0.59
1:G:184:ILE:HD12	1:G:289:ILE:HG21	1.84	0.58
1:A:167:THR:O	1:A:168:THR:HB	2.03	0.58
1:B:46:THR:HG21	1:B:139:LEU:HG	1.85	0.58
1:C:143:ALA:HB2	1:C:291:LEU:HD13	1.84	0.58
1:D:116:TYR:O	1:D:118:VAL:CB	2.49	0.58
1:A:243:MET:O	1:A:245:PHE:N	2.36	0.58
1:C:166:GLU:HB3	1:C:342:PHE:HA	1.85	0.58
1:G:205:ARG:HB2	1:G:245:PHE:CD2	2.39	0.58
1:G:49:ARG:O	1:G:295:ARG:NH1	2.37	0.58
1:A:241:ASN:ND2	1:A:245:PHE:O	2.37	0.58
1:E:235:GLU:HG2	1:F:241:ASN:HB2	1.85	0.58
1:A:134:ALA:HB2	1:A:325:TYR:OH	2.04	0.58
1:F:186:ALA:O	1:F:189:THR:OG1	2.20	0.58
1:B:114:ASN:O	1:B:116:TYR:CD2	2.56	0.58
1:G:11:GLY:O	1:G:24:LYS:HB2	2.04	0.58
1:B:202:ALA:HB2	1:B:205:ARG:HH11	1.68	0.58
1:D:45:VAL:N	1:D:135:ASP:OD2	2.37	0.58
1:G:230:ALA:HB1	1:G:231:LEU:HA	1.85	0.58
1:B:262:ARG:HD2	1:C:84:ARG:HA	1.85	0.57
1:C:155:ASN:OD1	1:C:156:ILE:N	2.33	0.57
1:C:168:THR:OG1	1:C:169:GLN:N	2.37	0.57
1:D:260:THR:H	1:E:73:TYR:HB2	1.67	0.57
1:F:148:VAL:HG22	1:F:281:VAL:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:ILE:HD11	1:F:342:PHE:HD2	1.69	0.57
1:A:104:VAL:HG23	1:A:126:LEU:HD21	1.86	0.57
1:B:23:ASP:OD2	1:B:23:ASP:N	2.37	0.57
1:D:116:TYR:C	1:D:118:VAL:HB	2.29	0.57
1:F:149:GLU:CD	1:F:149:GLU:H	2.11	0.57
1:A:167:THR:O	1:A:168:THR:CB	2.52	0.57
1:G:300:THR:HG23	1:G:329:HIS:ND1	2.13	0.57
1:B:167:THR:OG1	1:B:168:THR:N	2.35	0.57
1:D:332:LEU:O	1:D:333:ARG:HB2	2.03	0.57
1:E:231:LEU:H	1:E:231:LEU:HD22	1.69	0.57
1:F:232:ILE:HG12	1:F:233:ASP:N	2.19	0.57
1:F:47:THR:O	1:F:49:ARG:N	2.38	0.57
1:A:23:ASP:HA	1:A:24:LYS:HG2	1.85	0.57
1:F:207:PHE:HB2	1:F:245:PHE:HD1	1.69	0.57
1:C:51:MET:HG2	1:C:296:SER:HB2	1.87	0.57
1:C:142:ILE:HB	1:C:298:VAL:HG21	1.87	0.57
1:D:300:THR:HG22	1:D:329:HIS:ND1	2.19	0.57
1:F:231:LEU:HD23	1:F:232:ILE:HG22	1.86	0.57
1:F:294:HIS:HB3	1:F:336:ALA:HB1	1.87	0.57
1:G:53:ARG:HG3	1:G:53:ARG:NH1	2.09	0.57
1:D:243:MET:O	1:D:245:PHE:N	2.38	0.57
1:G:7:GLY:O	1:G:9:GLN:N	2.35	0.57
1:A:305:ASP:CG	1:A:306:LEU:H	2.12	0.57
1:G:209:CYS:SG	1:G:210:ASP:N	2.77	0.57
1:D:212:ASP:OD1	1:D:212:ASP:N	2.36	0.56
1:B:232:ILE:HG12	1:B:233:ASP:N	2.20	0.56
1:D:223:PRO:HG3	1:E:230:ALA:HB2	1.88	0.56
1:E:49:ARG:HE	1:E:206:VAL:HG21	1.70	0.56
1:A:181:GLY:HA3	1:A:220:ALA:HB2	1.88	0.56
1:B:235:GLU:O	1:B:236:LYS:HB3	2.06	0.56
1:B:254:THR:HG21	1:B:285:LYS:HE3	1.86	0.56
1:D:166:GLU:HB2	1:D:342:PHE:HA	1.88	0.56
1:A:139:LEU:CD2	1:A:253:LEU:CD2	2.83	0.56
1:E:181:GLY:HA3	1:E:220:ALA:HB2	1.86	0.56
1:D:102:ALA:HB1	1:D:126:LEU:HD12	1.87	0.56
1:A:231:LEU:HD23	1:A:232:ILE:H	1.70	0.55
1:A:332:LEU:N	1:A:332:LEU:CD1	2.69	0.55
1:D:148:VAL:HG13	1:D:281:VAL:HB	1.87	0.55
1:D:227:ASN:OD1	1:D:227:ASN:N	2.35	0.55
1:F:117:ASP:OD1	1:F:117:ASP:N	2.34	0.55
1:E:159:LEU:HD23	1:E:335:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:HB2	1:B:325:TYR:OH	2.05	0.55
1:C:257:GLY:HA3	1:C:268:GLN:HB2	1.89	0.55
1:C:327:MET:HE3	1:C:329:HIS:HE1	1.71	0.55
1:F:96:ILE:HA	1:F:328:GLY:HA3	1.89	0.55
1:A:103:ASP:H	1:A:262:ARG:HH22	1.55	0.55
1:A:214:TYR:CE1	1:A:239:ILE:HD12	2.42	0.55
1:A:254:THR:HG23	1:A:272:PHE:HB2	1.89	0.55
1:D:155:ASN:CG	1:D:156:ILE:H	2.14	0.55
1:F:75:ALA:HB3	1:F:78:GLU:HG3	1.89	0.55
1:G:169:GLN:HG3	1:G:174:LEU:HD11	1.88	0.55
1:A:163:THR:O	1:A:163:THR:OG1	2.25	0.55
1:D:229:ALA:HB2	1:E:228:TYR:CE1	2.41	0.55
1:A:75:ALA:HB1	1:A:76:PRO:HD2	1.89	0.55
1:E:102:ALA:HB1	1:E:126:LEU:HD22	1.87	0.55
1:E:294:HIS:ND1	1:E:295:ARG:O	2.39	0.55
1:F:19:VAL:O	1:F:21:ALA:N	2.37	0.55
1:F:205:ARG:HB2	1:F:244:GLY:O	2.07	0.55
1:A:29:LEU:HD13	1:A:29:LEU:H	1.72	0.55
1:E:120:SER:O	1:E:123:THR:OG1	2.22	0.55
1:F:333:ARG:HH11	1:F:333:ARG:HB2	1.72	0.55
1:B:114:ASN:C	1:B:115:HIS:HD2	2.10	0.55
1:D:259:GLY:HA2	1:E:73:TYR:HD1	1.71	0.55
1:D:293:MET:HA	1:D:336:ALA:O	2.07	0.55
1:E:113:MET:O	1:E:114:ASN:ND2	2.40	0.55
1:F:294:HIS:O	1:F:295:ARG:HB3	2.07	0.55
1:A:166:GLU:OE1	1:A:167:THR:O	2.25	0.54
1:B:313:ARG:NH2	1:C:81:ASP:OD2	2.41	0.54
1:C:265:THR:HG22	1:C:266:THR:H	1.72	0.54
1:F:179:ALA:O	1:F:183:GLU:HG2	2.06	0.54
1:A:73:TYR:CD1	1:F:259:GLY:HA2	2.40	0.54
1:A:332:LEU:HD22	1:A:332:LEU:C	2.31	0.54
1:B:150:SER:O	1:B:151:LYS:HG2	2.08	0.54
1:E:289:ILE:HD11	1:E:342:PHE:CE2	2.42	0.54
1:A:262:ARG:O	1:B:70:GLN:NE2	2.41	0.54
1:B:65:VAL:HG13	1:B:91:GLU:HA	1.89	0.54
1:B:181:GLY:HA3	1:B:220:ALA:HB2	1.89	0.54
1:D:14:GLN:HE21	1:D:14:GLN:HA	1.71	0.54
1:B:224:ASN:HB3	1:C:182:LYS:HE2	1.90	0.54
1:C:298:VAL:HG12	1:C:299:GLY:N	2.23	0.54
1:D:302:LYS:HG2	1:D:327:MET:HE2	1.90	0.54
1:G:50:HIS:HA	1:G:295:ARG:HH11	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:TYR:OH	1:B:237:GLY:O	2.22	0.54
1:D:159:LEU:HB3	1:D:335:GLU:HA	1.89	0.54
1:G:85:LYS:HE3	1:G:85:LYS:CA	2.15	0.54
1:G:148:VAL:HG22	1:G:282:LYS:H	1.73	0.54
1:D:26:ALA:O	1:D:27:LEU:HB3	2.08	0.54
1:D:184:ILE:HD12	1:D:289:ILE:HG21	1.89	0.54
1:D:306:LEU:HD23	1:D:325:TYR:HB3	1.90	0.54
1:E:236:LYS:H	1:F:243:MET:HA	1.72	0.54
1:B:122:TYR:CD1	1:C:87:ILE:HD12	2.43	0.54
1:F:231:LEU:HD23	1:F:232:ILE:H	1.73	0.54
1:F:304:ARG:HH11	1:F:304:ARG:CG	2.21	0.54
1:G:169:GLN:HE21	1:G:174:LEU:CG	2.20	0.54
1:B:234:PRO:HB2	1:C:231:LEU:HD21	1.90	0.53
1:G:166:GLU:OE2	1:G:183:GLU:CB	2.56	0.53
1:G:169:GLN:HE21	1:G:174:LEU:CD2	2.20	0.53
1:A:197:LYS:HB3	1:F:211:PRO:HG3	1.88	0.53
1:A:254:THR:HG22	1:A:255:ALA:N	2.17	0.53
1:G:224:ASN:N	1:G:224:ASN:HD22	2.07	0.53
1:A:32:PHE:CG	1:A:33:GLY:N	2.76	0.53
1:A:252:HIS:H	1:A:252:HIS:CD2	2.26	0.53
1:C:222:MET:C	1:D:228:TYR:HH	2.16	0.53
1:C:138:VAL:O	1:C:141:GLU:HG2	2.08	0.53
1:F:214:TYR:HB2	1:F:249:GLU:HB2	1.89	0.53
1:A:72:ALA:O	1:F:100:LEU:HD23	2.09	0.53
1:E:206:VAL:HG23	1:E:246:GLU:HB3	1.90	0.53
1:G:274:ALA:HA	1:G:285:LYS:HG2	1.91	0.53
1:A:193:ALA:HB2	1:F:215:SER:HB2	1.91	0.53
1:D:218:LEU:HD22	1:E:243:MET:HE1	1.90	0.53
1:E:228:TYR:HD1	1:E:230:ALA:H	1.57	0.53
1:G:51:MET:CB	1:G:299:GLY:CA	2.86	0.53
1:C:108:ASP:OD1	1:C:108:ASP:N	2.41	0.53
1:C:148:VAL:HG12	1:C:283:VAL:HG13	1.91	0.53
1:C:159:LEU:HD13	1:C:335:GLU:N	2.16	0.53
1:E:202:ALA:HA	1:E:205:ARG:NH1	2.22	0.53
1:F:19:VAL:HG22	1:F:20:ALA:H	1.73	0.53
1:F:24:LYS:O	1:F:24:LYS:HD2	2.09	0.53
1:C:336:ALA:O	1:C:337:ALA:HB2	2.08	0.53
1:A:113:MET:O	1:A:114:ASN:ND2	2.32	0.52
1:B:170:ASN:OD1	1:B:170:ASN:N	2.42	0.52
1:E:252:HIS:CD2	1:E:252:HIS:H	2.28	0.52
1:E:276:LYS:HA	1:E:281:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ASP:OD2	1:F:26:ALA:HB2	2.09	0.52
1:F:208:TYR:CD2	1:F:248:VAL:CG2	2.90	0.52
1:A:159:LEU:HB3	1:A:335:GLU:CB	2.36	0.52
1:B:45:VAL:HB	1:B:135:ASP:OD1	2.10	0.52
1:C:33:GLY:HA3	1:D:63:PHE:CE1	2.43	0.52
1:A:158:GLY:O	1:A:159:LEU:HD12	2.08	0.52
1:F:27:LEU:HD12	1:F:28:PHE:HA	1.91	0.52
1:A:221:LEU:HD23	1:A:232:ILE:HB	1.91	0.52
1:B:205:ARG:HA	1:B:294:HIS:HA	1.91	0.52
1:C:103:ASP:H	1:C:262:ARG:NH2	2.06	0.52
1:D:60:SER:HB3	1:D:95:THR:HG22	1.91	0.52
1:F:132:MET:HG3	1:F:252:HIS:CE1	2.44	0.52
1:A:50:HIS:CE1	1:A:300:THR:HG23	2.45	0.52
1:B:79:ASN:N	1:B:79:ASN:HD22	2.07	0.52
1:B:305:ASP:O	1:B:325:TYR:HB2	2.09	0.52
1:E:155:ASN:OD1	1:E:156:ILE:N	2.40	0.52
1:C:224:ASN:N	1:C:224:ASN:HD22	2.08	0.52
1:C:242:VAL:HG12	1:C:243:MET:CE	2.35	0.52
1:F:207:PHE:O	1:F:248:VAL:HG22	2.10	0.52
1:A:167:THR:CG2	1:A:168:THR:N	2.73	0.51
1:B:166:GLU:HB2	1:B:341:VAL:O	2.10	0.51
1:D:265:THR:OG1	1:D:268:GLN:OE1	2.27	0.51
1:E:42:ARG:HB3	1:F:199:TYR:CE1	2.45	0.51
1:E:105:LEU:HA	1:E:320:GLN:HB2	1.91	0.51
1:E:343:LYS:HD3	1:E:344:VAL:HG23	1.92	0.51
1:G:156:ILE:HG13	1:G:157:GLU:H	1.75	0.51
1:B:224:ASN:HA	1:C:226:ALA:HA	1.92	0.51
1:C:159:LEU:HB2	1:C:335:GLU:CG	2.36	0.51
1:C:169:GLN:HB3	1:C:343:LYS:HE2	1.92	0.51
1:D:30:LYS:HB3	1:E:60:SER:HB3	1.91	0.51
1:D:223:PRO:HB3	1:E:228:TYR:CE1	2.44	0.51
1:F:27:LEU:HD22	1:G:91:GLU:HB3	1.93	0.51
1:E:239:ILE:HG22	1:E:240:ARG:N	2.25	0.51
1:A:222:MET:HG3	1:A:223:PRO:HD2	1.92	0.51
1:B:319:ASP:OD2	1:B:319:ASP:N	2.44	0.51
1:C:91:GLU:N	1:C:91:GLU:OE1	2.44	0.51
1:C:244:GLY:O	1:C:245:PHE:CD1	2.63	0.51
1:E:253:LEU:HD23	1:E:254:THR:N	2.26	0.51
1:F:24:LYS:NZ	1:F:24:LYS:CB	2.63	0.51
1:G:85:LYS:O	1:G:86:ASP:CB	2.59	0.51
1:A:210:ASP:HB2	1:A:211:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HB3	1:A:342:PHE:HE2	1.74	0.51
1:A:325:TYR:C	1:A:325:TYR:CD2	2.89	0.51
1:B:46:THR:HG21	1:B:139:LEU:CG	2.40	0.51
1:G:151:LYS:O	1:G:153:ASN:N	2.43	0.51
1:G:180:LEU:O	1:G:184:ILE:HG12	2.10	0.51
1:A:205:ARG:HB2	1:A:244:GLY:O	2.11	0.51
1:F:174:LEU:HD11	1:F:180:LEU:HD13	1.92	0.51
1:F:207:PHE:HE2	1:F:209:CYS:HB3	1.75	0.51
1:B:46:THR:O	1:B:47:THR:CB	2.58	0.51
1:E:102:ALA:HA	1:E:262:ARG:HH22	1.76	0.51
1:A:209:CYS:SG	1:A:213:SER:HB2	2.50	0.51
1:E:214:TYR:CZ	1:E:239:ILE:HG13	2.45	0.51
1:A:7:GLY:C	1:A:9:GLN:H	2.17	0.51
1:B:29:LEU:HD13	1:B:29:LEU:H	1.76	0.51
1:C:179:ALA:O	1:C:183:GLU:HG2	2.11	0.51
1:A:35:GLU:OE2	1:B:53:ARG:HD3	2.10	0.50
1:B:171:LYS:HB3	1:B:342:PHE:CD1	2.46	0.50
1:C:306:LEU:HA	1:C:325:TYR:HB3	1.92	0.50
1:D:294:HIS:O	1:D:294:HIS:ND1	2.44	0.50
1:G:26:ALA:HB1	1:G:28:PHE:HB2	1.92	0.50
1:G:147:ASN:HD21	1:G:339:ALA:HB3	1.76	0.50
1:B:45:VAL:HG21	1:B:250:VAL:HG23	1.93	0.50
1:E:289:ILE:HD11	1:E:342:PHE:CD2	2.46	0.50
1:C:74:LEU:HG	1:C:80:LEU:HB2	1.93	0.50
1:E:312:ARG:HB2	1:E:312:ARG:CZ	2.39	0.50
1:F:227:ASN:OD1	1:F:227:ASN:N	2.45	0.50
1:A:325:TYR:C	1:A:325:TYR:HD2	2.20	0.50
1:G:207:PHE:HE2	1:G:209:CYS:HB2	1.75	0.50
1:E:128:GLU:HG3	1:E:129:SER:N	2.26	0.50
1:F:181:GLY:HA3	1:F:220:ALA:HB2	1.92	0.50
1:C:96:ILE:HA	1:C:328:GLY:HA3	1.93	0.50
1:C:148:VAL:HB	1:C:281:VAL:HG22	1.93	0.50
1:G:171:LYS:HB3	1:G:342:PHE:CZ	2.46	0.50
1:G:224:ASN:HD22	1:G:224:ASN:H	1.59	0.50
1:B:49:ARG:NH2	1:B:248:VAL:HG11	2.26	0.50
1:B:214:TYR:CG	1:B:249:GLU:HG2	2.47	0.50
1:A:100:LEU:HD21	1:A:325:TYR:HE2	1.76	0.50
1:B:241:ASN:OD1	1:B:241:ASN:N	2.22	0.50
1:C:138:VAL:O	1:C:142:ILE:HG22	2.12	0.50
1:D:35:GLU:CD	1:E:53:ARG:HE	2.20	0.50
1:F:134:ALA:HB2	1:F:325:TYR:OH	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ASN:CG	1:F:156:ILE:H	2.18	0.50
1:G:51:MET:CG	1:G:299:GLY:HA2	2.39	0.50
1:A:94:ILE:HD13	1:A:95:THR:H	1.76	0.49
1:B:122:TYR:HD1	1:C:87:ILE:HD12	1.76	0.49
1:B:155:ASN:HD22	1:B:156:ILE:N	2.10	0.49
1:B:159:LEU:HD11	1:B:335:GLU:N	2.24	0.49
1:C:297:ALA:C	1:C:298:VAL:HG23	2.37	0.49
1:D:45:VAL:HG13	1:D:46:THR:HG23	1.92	0.49
1:D:200:VAL:HG11	1:D:335:GLU:OE2	2.11	0.49
1:F:207:PHE:CD2	1:F:247:VAL:HG12	2.47	0.49
1:F:248:VAL:O	1:F:249:GLU:OE2	2.30	0.49
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.78	0.49
1:C:295:ARG:CA	1:C:297:ALA:CB	2.87	0.49
1:D:180:LEU:O	1:D:184:ILE:HG12	2.12	0.49
1:G:171:LYS:CD	1:G:171:LYS:H	2.25	0.49
1:G:294:HIS:O	1:G:295:ARG:HB3	2.11	0.49
1:B:294:HIS:HB3	1:B:336:ALA:CB	2.42	0.49
1:E:170:ASN:HD21	1:E:173:ALA:HB3	1.77	0.49
1:E:171:LYS:HE2	1:E:342:PHE:CZ	2.47	0.49
1:F:159:LEU:HB3	1:F:335:GLU:CB	2.40	0.49
1:F:249:GLU:O	1:F:249:GLU:OE2	2.30	0.49
1:G:186:ALA:O	1:G:189:THR:OG1	2.23	0.49
1:C:12:THR:HG23	1:C:14:GLN:HG2	1.94	0.49
1:B:57:SER:OG	1:B:58:GLY:N	2.45	0.49
1:B:333:ARG:CG	1:B:333:ARG:HH11	2.26	0.49
1:A:45:VAL:HG22	1:A:49:ARG:HH12	1.77	0.49
1:D:87:ILE:HD13	1:D:87:ILE:H	1.77	0.49
1:D:292:PHE:CZ	1:D:338:GLY:HA3	2.46	0.49
1:G:168:THR:O	1:G:169:GLN:OE1	2.30	0.49
1:G:298:VAL:HG13	1:G:330:GLY:O	2.07	0.49
1:C:45:VAL:O	1:C:135:ASP:OD2	2.30	0.49
1:B:199:TYR:O	1:B:200:VAL:HG13	2.12	0.49
1:B:254:THR:HG22	1:B:272:PHE:CD2	2.47	0.49
1:C:276:LYS:HB2	1:C:284:ALA:HB2	1.94	0.49
1:C:343:LYS:HG2	1:C:344:VAL:H	1.77	0.49
1:D:223:PRO:HG3	1:E:230:ALA:HB1	1.93	0.49
1:E:218:LEU:O	1:E:222:MET:HG2	2.13	0.49
1:E:313:ARG:NH2	1:F:81:ASP:OD1	2.46	0.49
1:F:295:ARG:HG3	1:F:296:SER:N	2.26	0.49
1:A:214:TYR:CD2	1:A:249:GLU:HG2	2.48	0.49
1:C:189:THR:OG1	1:C:190:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ILE:HG12	1:C:342:PHE:CE2	2.48	0.49
1:E:325:TYR:C	1:E:325:TYR:HD2	2.21	0.49
1:G:167:THR:O	1:G:169:GLN:OE1	2.30	0.49
1:A:49:ARG:O	1:A:295:ARG:HD3	2.12	0.49
1:F:46:THR:HB	1:F:47:THR:HA	1.94	0.49
1:G:25:LEU:HD13	1:G:25:LEU:H	1.76	0.49
1:G:55:ILE:HG23	1:G:301:VAL:HG13	1.95	0.49
1:D:13:ASN:HA	1:D:27:LEU:HD22	1.94	0.48
1:F:154:GLU:HG3	1:F:159:LEU:HD21	1.95	0.48
1:A:36:VAL:HG13	1:B:64:PRO:HG2	1.94	0.48
1:C:294:HIS:HD2	1:C:295:ARG:O	1.96	0.48
1:G:214:TYR:CE1	1:G:239:ILE:HD11	2.47	0.48
1:G:227:ASN:O	1:G:228:TYR:HB2	2.13	0.48
1:B:292:PHE:CZ	1:B:338:GLY:HA3	2.49	0.48
1:C:66:LEU:CB	1:C:89:HIS:HB3	2.43	0.48
1:D:279:GLY:C	1:D:281:VAL:H	2.21	0.48
1:D:325:TYR:C	1:D:325:TYR:CD2	2.91	0.48
1:F:154:GLU:HG3	1:F:159:LEU:HD11	1.95	0.48
1:F:207:PHE:CZ	1:F:290:GLY:HA3	2.48	0.48
1:F:304:ARG:HG2	1:F:304:ARG:NH1	2.26	0.48
1:G:295:ARG:C	1:G:297:ALA:H	2.21	0.48
1:A:72:ALA:HB2	1:F:262:ARG:CZ	2.43	0.48
1:B:236:LYS:HA	1:C:243:MET:C	2.22	0.48
1:E:144:GLY:O	1:E:146:CYS:N	2.47	0.48
1:F:8:GLN:OE1	1:G:87:ILE:HB	2.13	0.48
1:A:228:TYR:CE1	1:F:223:PRO:HA	2.49	0.48
1:C:222:MET:C	1:D:228:TYR:OH	2.56	0.48
1:G:169:GLN:HE22	1:G:174:LEU:HD21	1.71	0.48
1:A:228:TYR:HE1	1:F:223:PRO:HA	1.79	0.48
1:B:180:LEU:O	1:B:184:ILE:HG12	2.13	0.48
1:D:122:TYR:HE1	1:E:87:ILE:HG13	1.78	0.48
1:E:100:LEU:HB3	1:E:130:LEU:HD11	1.95	0.48
1:E:305:ASP:O	1:E:325:TYR:HB2	2.13	0.48
1:B:231:LEU:HD23	1:B:231:LEU:H	1.78	0.48
1:C:19:VAL:O	1:C:21:ALA:N	2.47	0.48
1:D:186:ALA:O	1:D:189:THR:OG1	2.26	0.48
1:E:325:TYR:C	1:E:325:TYR:CD2	2.92	0.48
1:G:143:ALA:HB3	1:G:272:PHE:CZ	2.49	0.48
1:G:148:VAL:HG13	1:G:281:VAL:HA	1.94	0.48
1:A:269:LYS:HB3	1:A:270:HIS:CD2	2.49	0.48
1:B:289:ILE:HD11	1:B:341:VAL:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.77	0.48
1:D:243:MET:HB2	1:D:245:PHE:CD1	2.48	0.48
1:E:315:ASN:HD22	1:E:315:ASN:N	2.10	0.48
1:A:46:THR:H	1:A:49:ARG:HH11	1.62	0.48
1:B:289:ILE:HD13	1:B:289:ILE:N	2.29	0.48
1:D:117:ASP:O	1:D:117:ASP:OD2	2.30	0.48
1:F:180:LEU:O	1:F:184:ILE:HG12	2.13	0.48
1:A:50:HIS:HE1	1:A:300:THR:HG23	1.78	0.47
1:A:217:ILE:HD13	1:A:217:ILE:HA	1.75	0.47
1:A:241:ASN:HB2	1:F:235:GLU:HG3	1.95	0.47
1:B:243:MET:O	1:B:245:PHE:N	2.47	0.47
1:D:207:PHE:CZ	1:D:290:GLY:HA3	2.49	0.47
1:G:300:THR:CG2	1:G:329:HIS:CG	2.95	0.47
1:A:159:LEU:CG	1:A:335:GLU:CG	2.83	0.47
1:C:103:ASP:OD1	1:C:262:ARG:NH2	2.48	0.47
1:C:164:VAL:HG12	1:C:340:VAL:HG12	1.96	0.47
1:G:23:ASP:OD2	1:G:23:ASP:N	2.44	0.47
1:A:165:ILE:HD13	1:A:166:GLU:H	1.78	0.47
1:A:202:ALA:HA	1:A:205:ARG:HH12	1.80	0.47
1:B:305:ASP:CG	1:B:306:LEU:H	2.20	0.47
1:C:116:TYR:CD1	1:C:118:VAL:HG22	2.48	0.47
1:A:139:LEU:HD21	1:A:253:LEU:CD2	2.44	0.47
1:A:170:ASN:OD1	1:A:170:ASN:N	2.45	0.47
1:B:197:LYS:HE3	1:B:197:LYS:HB2	1.79	0.47
1:C:180:LEU:O	1:C:184:ILE:HG12	2.13	0.47
1:F:167:THR:HG22	1:F:168:THR:H	1.80	0.47
1:G:51:MET:O	1:G:52:VAL:CB	2.62	0.47
1:A:105:LEU:HA	1:A:320:GLN:HB2	1.95	0.47
1:A:242:VAL:O	1:F:235:GLU:HA	2.13	0.47
1:B:209:CYS:SG	1:B:213:SER:HB2	2.54	0.47
1:B:253:LEU:HD13	1:B:253:LEU:HA	1.71	0.47
1:C:294:HIS:HD2	1:C:295:ARG:HG3	1.80	0.47
1:C:297:ALA:O	1:C:298:VAL:CG2	2.62	0.47
1:D:99:LEU:HD12	1:D:326:ALA:HB2	1.96	0.47
1:E:289:ILE:CD1	1:E:289:ILE:N	2.78	0.47
1:F:171:LYS:O	1:F:174:LEU:HG	2.14	0.47
1:A:159:LEU:HD11	1:A:198:ASN:HB3	1.95	0.47
1:A:218:LEU:HD21	1:A:237:GLY:O	2.14	0.47
1:A:231:LEU:HD22	1:A:231:LEU:H	1.80	0.47
1:C:195:LEU:O	1:C:200:VAL:HG13	2.14	0.47
1:G:161:THR:HA	1:G:335:GLU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:CD2	1:A:335:GLU:CG	2.88	0.47
1:A:195:LEU:HD22	1:A:205:ARG:HE	1.80	0.47
1:A:287:ASN:HD22	1:A:287:ASN:H	1.61	0.47
1:B:64:PRO:HA	1:B:91:GLU:HB2	1.97	0.47
1:B:304:ARG:HH11	1:B:304:ARG:HA	1.80	0.47
1:C:37:LEU:HB2	1:D:65:VAL:HG12	1.95	0.47
1:D:68:ARG:O	1:D:69:THR:OG1	2.27	0.47
1:D:229:ALA:HB2	1:E:228:TYR:CE2	2.49	0.47
1:E:170:ASN:HB3	1:E:344:VAL:HB	1.96	0.47
1:E:252:HIS:H	1:E:252:HIS:HD2	1.61	0.47
1:E:279:GLY:O	1:E:281:VAL:HG12	2.14	0.47
1:F:178:VAL:O	1:F:180:LEU:N	2.42	0.47
1:F:207:PHE:HB2	1:F:245:PHE:CD1	2.50	0.47
1:G:83:LYS:H	1:G:83:LYS:HD3	1.79	0.47
1:B:215:SER:HB2	1:C:193:ALA:HB2	1.97	0.47
1:C:84:ARG:C	1:C:85:LYS:HD3	2.40	0.47
1:C:118:VAL:O	1:C:120:SER:N	2.42	0.47
1:E:94:ILE:HB	1:E:330:GLY:HA3	1.97	0.47
1:G:50:HIS:O	1:G:50:HIS:ND1	2.48	0.47
1:A:139:LEU:HD22	1:A:253:LEU:CD2	2.45	0.47
1:B:59:LYS:HB3	1:B:59:LYS:HE2	1.45	0.47
1:C:50:HIS:O	1:C:51:MET:C	2.58	0.47
1:D:43:THR:HB	1:D:44:SER:H	1.41	0.47
1:E:47:THR:HA	1:E:48:SER:HA	1.59	0.47
1:E:169:GLN:HG3	1:E:170:ASN:ND2	2.30	0.47
1:G:59:LYS:HD2	1:G:60:SER:OG	2.15	0.47
1:A:72:ALA:O	1:F:100:LEU:HA	2.15	0.47
1:B:64:PRO:HA	1:B:91:GLU:CB	2.45	0.47
1:C:244:GLY:O	1:C:245:PHE:CG	2.68	0.47
1:F:268:GLN:HE21	1:F:268:GLN:HB2	1.50	0.47
1:C:239:ILE:O	1:C:240:ARG:HB2	2.15	0.46
1:D:333:ARG:C	1:D:335:GLU:H	2.23	0.46
1:E:126:LEU:HD23	1:F:69:THR:HG21	1.96	0.46
1:F:51:MET:HG3	1:F:296:SER:HA	1.97	0.46
1:F:147:ASN:HB2	1:F:283:VAL:HG11	1.98	0.46
1:G:325:TYR:CD2	1:G:327:MET:HG3	2.50	0.46
1:A:159:LEU:CB	1:A:335:GLU:OE2	2.39	0.46
1:A:209:CYS:SG	1:A:210:ASP:N	2.87	0.46
1:B:169:GLN:HB2	1:B:173:ALA:HB3	1.97	0.46
1:C:152:TYR:O	1:C:153:ASN:ND2	2.48	0.46
1:C:200:VAL:HG23	1:C:294:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:HE3	1:C:223:PRO:HD3	1.95	0.46
1:D:40:PHE:CZ	1:E:200:VAL:HG23	2.51	0.46
1:G:289:ILE:HD11	1:G:342:PHE:CG	2.50	0.46
1:G:300:THR:HG22	1:G:329:HIS:CG	2.49	0.46
1:A:298:VAL:HG22	1:A:331:GLY:HA2	1.97	0.46
1:C:294:HIS:CD2	1:C:295:ARG:HG3	2.50	0.46
1:D:224:ASN:C	1:D:226:ALA:H	2.22	0.46
1:E:292:PHE:CZ	1:E:338:GLY:HA3	2.51	0.46
1:G:64:PRO:HA	1:G:91:GLU:HA	1.98	0.46
1:G:243:MET:HE2	1:G:243:MET:HB2	1.77	0.46
1:A:184:ILE:O	1:A:188:LEU:HB2	2.16	0.46
1:A:295:ARG:HD2	1:A:296:SER:H	1.81	0.46
1:B:205:ARG:HG2	1:B:245:PHE:CE1	2.51	0.46
1:C:336:ALA:O	1:C:337:ALA:HB3	2.13	0.46
1:D:45:VAL:HG11	1:D:250:VAL:HG11	1.97	0.46
1:D:102:ALA:O	1:D:322:ILE:HG12	2.16	0.46
1:F:27:LEU:CD1	1:F:28:PHE:CA	2.81	0.46
1:B:157:GLU:OE2	1:B:159:LEU:HB2	2.15	0.46
1:B:159:LEU:CD1	1:B:335:GLU:H	2.22	0.46
1:D:191:ALA:HB1	1:D:292:PHE:CZ	2.51	0.46
1:F:7:GLY:O	1:F:8:GLN:HB3	2.15	0.46
1:F:239:ILE:O	1:F:240:ARG:HB2	2.15	0.46
1:G:214:TYR:HE1	1:G:239:ILE:HD11	1.80	0.46
1:A:200:VAL:HG22	1:F:40:PHE:CE1	2.51	0.46
1:B:74:LEU:CD1	1:B:78:GLU:O	2.59	0.46
1:E:157:GLU:O	1:E:159:LEU:HD12	2.15	0.46
1:G:12:THR:OG1	1:G:13:ASN:N	2.49	0.46
1:F:171:LYS:HB2	1:F:342:PHE:CE1	2.51	0.46
1:A:153:ASN:N	1:A:153:ASN:OD1	2.47	0.46
1:A:171:LYS:H	1:A:171:LYS:HG2	1.55	0.46
1:B:234:PRO:O	1:C:231:LEU:HD21	2.14	0.46
1:G:53:ARG:CG	1:G:53:ARG:NH1	2.36	0.46
1:G:86:ASP:O	1:G:87:ILE:HD13	2.16	0.46
1:D:206:VAL:HG23	1:D:246:GLU:HB2	1.98	0.46
1:D:260:THR:HB	1:D:261:ALA:H	1.52	0.46
1:F:225:ALA:HA	1:F:226:ALA:HA	1.51	0.46
1:G:228:TYR:CD2	1:G:230:ALA:HB3	2.51	0.46
1:C:327:MET:HE3	1:C:329:HIS:CE1	2.50	0.45
1:E:42:ARG:NE	1:E:128:GLU:OE1	2.38	0.45
1:E:170:ASN:C	1:E:170:ASN:HD22	2.23	0.45
1:E:239:ILE:HG22	1:E:240:ARG:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ARG:HA	1:E:304:ARG:HD3	1.63	0.45
1:E:167:THR:O	1:E:168:THR:HG22	2.17	0.45
1:G:205:ARG:O	1:G:245:PHE:HA	2.17	0.45
1:B:265:THR:HG22	1:B:266:THR:H	1.82	0.45
1:F:109:ILE:HG12	1:G:99:LEU:HD23	1.99	0.45
1:G:166:GLU:HB3	1:G:342:PHE:HB3	1.99	0.45
1:A:166:GLU:HB2	1:A:341:VAL:O	2.17	0.45
1:A:254:THR:HG21	1:A:285:LYS:HE2	1.98	0.45
1:C:252:HIS:ND1	1:C:252:HIS:O	2.49	0.45
1:C:289:ILE:HD12	1:C:289:ILE:HA	1.68	0.45
1:D:45:VAL:HG22	1:D:46:THR:H	1.81	0.45
1:D:253:LEU:O	1:D:254:THR:HB	2.16	0.45
1:G:27:LEU:O	1:G:27:LEU:HG	2.16	0.45
1:B:322:ILE:HD11	1:C:80:LEU:HD11	1.98	0.45
1:D:46:THR:OG1	1:D:47:THR:N	2.49	0.45
1:D:254:THR:HG21	1:D:285:LYS:HD3	1.97	0.45
1:E:103:ASP:OD1	1:E:262:ARG:NH1	2.49	0.45
1:F:144:GLY:O	1:F:148:VAL:HB	2.16	0.45
1:C:221:LEU:HD13	1:C:221:LEU:HA	1.71	0.45
1:D:76:PRO:HA	1:D:77:GLY:HA2	1.55	0.45
1:E:29:LEU:HD22	1:E:29:LEU:H	1.82	0.45
1:E:171:LYS:HE2	1:E:342:PHE:CE1	2.52	0.45
1:E:298:VAL:HG12	1:E:331:GLY:HA2	1.98	0.45
1:F:14:GLN:HB3	1:G:88:LYS:HE2	1.99	0.45
1:G:81:ASP:OD2	1:G:84:ARG:NH1	2.34	0.45
1:G:106:ILE:O	1:G:318:ALA:HB1	2.16	0.45
1:G:195:LEU:HD23	1:G:205:ARG:HE	1.81	0.45
1:G:276:LYS:HE2	1:G:343:LYS:HG2	1.97	0.45
1:A:105:LEU:HD13	1:A:320:GLN:HB2	1.99	0.45
1:A:141:GLU:OE2	1:A:330:GLY:HA2	2.17	0.45
1:C:69:THR:OG1	1:C:70:GLN:N	2.49	0.45
1:C:305:ASP:CG	1:C:306:LEU:N	2.74	0.45
1:E:158:GLY:N	1:E:159:LEU:HB2	2.32	0.45
1:G:171:LYS:CD	1:G:171:LYS:N	2.78	0.45
1:A:86:ASP:OD2	1:A:86:ASP:N	2.45	0.45
1:A:332:LEU:O	1:A:332:LEU:CD2	2.48	0.45
1:D:103:ASP:N	1:D:103:ASP:OD2	2.50	0.45
1:F:98:GLY:HA2	1:F:99:LEU:HA	1.63	0.45
1:G:234:PRO:O	1:G:235:GLU:HB3	2.16	0.45
1:A:119:ARG:O	1:A:122:TYR:HB2	2.16	0.45
1:A:240:ARG:H	1:A:240:ARG:HG2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:HD22	1:A:287:ASN:N	2.13	0.45
1:D:105:LEU:HA	1:D:320:GLN:HB2	1.97	0.45
1:E:215:SER:HB2	1:F:192:ARG:HH12	1.82	0.45
1:E:236:LYS:N	1:F:243:MET:HA	2.32	0.45
1:G:147:ASN:ND2	1:G:339:ALA:HB3	2.32	0.45
1:A:139:LEU:HD11	1:A:253:LEU:HD21	1.99	0.45
1:A:184:ILE:HD11	1:A:289:ILE:HG21	1.98	0.45
1:A:254:THR:O	1:A:255:ALA:C	2.59	0.45
1:B:45:VAL:CG1	1:B:46:THR:HG22	2.42	0.45
1:B:157:GLU:HB2	1:B:158:GLY:H	1.56	0.45
1:B:280:ASN:N	1:B:280:ASN:HD22	2.15	0.45
1:C:215:SER:OG	1:D:193:ALA:HB2	2.16	0.45
1:D:289:ILE:HD11	1:D:342:PHE:CD2	2.52	0.45
1:B:46:THR:HG21	1:B:139:LEU:CD2	2.47	0.44
1:B:287:ASN:O	1:B:287:ASN:ND2	2.49	0.44
1:C:96:ILE:HG12	1:C:328:GLY:N	2.32	0.44
1:E:9:GLN:O	1:E:12:THR:HG22	2.17	0.44
1:E:49:ARG:HD3	1:E:208:TYR:OH	2.16	0.44
1:A:223:PRO:HG3	1:B:230:ALA:HB2	1.99	0.44
1:B:275:ASN:C	1:B:275:ASN:HD22	2.24	0.44
1:C:295:ARG:C	1:C:297:ALA:HB2	2.34	0.44
1:A:139:LEU:HD22	1:A:253:LEU:HD22	1.98	0.44
1:B:13:ASN:HB3	1:B:18:VAL:HG11	2.00	0.44
1:A:7:GLY:HA3	1:A:9:GLN:HE21	1.83	0.44
1:C:89:HIS:N	1:C:89:HIS:CD2	2.85	0.44
1:C:207:PHE:CE2	1:C:209:CYS:HB2	2.52	0.44
1:C:244:GLY:C	1:C:245:PHE:CD1	2.95	0.44
1:D:68:ARG:HA	1:D:68:ARG:HD3	1.67	0.44
1:E:143:ALA:HB2	1:E:291:LEU:HD13	2.00	0.44
1:F:106:ILE:O	1:F:318:ALA:HB1	2.17	0.44
1:C:159:LEU:HD13	1:C:335:GLU:HB2	1.97	0.44
1:C:185:ILE:O	1:C:189:THR:HG23	2.18	0.44
1:G:15:GLY:O	1:G:16:LYS:HD2	2.18	0.44
1:G:51:MET:O	1:G:52:VAL:CG2	2.66	0.44
1:G:82:ASP:OD1	1:G:83:LYS:HG3	2.18	0.44
1:B:46:THR:HG21	1:B:139:LEU:HD21	2.00	0.44
1:B:293:MET:HA	1:B:336:ALA:O	2.17	0.44
1:E:197:LYS:HE3	1:E:197:LYS:HB2	1.71	0.44
1:E:295:ARG:O	1:E:296:SER:OG	2.35	0.44
1:G:96:ILE:HG22	1:G:328:GLY:HA3	1.98	0.44
1:G:260:THR:HG23	1:G:261:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:309:GLU:OE1	1:G:311:ALA:HB2	2.18	0.44
1:A:139:LEU:CD2	1:A:253:LEU:HD22	2.48	0.44
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.30	0.44
1:D:107:TYR:HD1	1:D:318:ALA:HB2	1.83	0.44
1:F:222:MET:SD	1:F:223:PRO:HD2	2.58	0.44
1:B:101:THR:HG22	1:B:324:LYS:HB3	1.99	0.44
1:C:188:LEU:HD13	1:C:242:VAL:HG21	1.99	0.44
1:C:239:ILE:HB	1:C:240:ARG:H	1.56	0.44
1:F:156:ILE:C	1:F:158:GLY:H	2.26	0.44
1:F:252:HIS:H	1:F:252:HIS:CD2	2.36	0.44
1:C:254:THR:HG23	1:C:272:PHE:CD2	2.53	0.43
1:F:145:LEU:HD22	1:F:145:LEU:HA	1.84	0.43
1:F:250:VAL:HA	1:F:251:PRO:HD3	1.77	0.43
1:G:276:LYS:HB3	1:G:276:LYS:HE3	1.62	0.43
1:C:204:ASP:OD2	1:C:295:ARG:HG2	2.18	0.43
1:E:161:THR:HB	1:E:334:PRO:O	2.18	0.43
1:F:198:ASN:HB3	1:F:335:GLU:HG2	2.01	0.43
1:G:156:ILE:HD12	1:G:156:ILE:HA	1.84	0.43
1:G:285:LYS:HB3	1:G:285:LYS:HE2	1.91	0.43
1:A:74:LEU:HG	1:F:101:THR:HG21	2.01	0.43
1:B:161:THR:HB	1:B:337:ALA:O	2.18	0.43
1:C:33:GLY:HA3	1:D:63:PHE:HE1	1.82	0.43
1:F:282:LYS:HB3	1:F:282:LYS:HE2	1.79	0.43
1:G:46:THR:CB	1:G:47:THR:HA	2.47	0.43
1:G:197:LYS:HB2	1:G:197:LYS:HE3	1.64	0.43
1:A:65:VAL:HG22	1:F:37:LEU:HB3	2.01	0.43
1:A:70:GLN:NE2	1:F:262:ARG:O	2.51	0.43
1:B:205:ARG:HB3	1:B:206:VAL:H	1.54	0.43
1:C:223:PRO:HG2	1:D:221:LEU:HD11	2.00	0.43
1:E:217:ILE:O	1:E:221:LEU:HD22	2.18	0.43
1:F:96:ILE:HD12	1:F:303:LEU:HD11	1.99	0.43
1:F:260:THR:HB	1:F:261:ALA:H	1.55	0.43
1:G:26:ALA:HB1	1:G:28:PHE:N	2.31	0.43
1:B:25:LEU:HA	1:B:26:ALA:HA	1.58	0.43
1:B:159:LEU:HD13	1:B:159:LEU:HA	1.72	0.43
1:B:214:TYR:CE1	1:B:239:ILE:HD12	2.53	0.43
1:C:29:LEU:HD22	1:C:29:LEU:H	1.83	0.43
1:C:176:ASP:C	1:C:178:VAL:H	2.26	0.43
1:E:70:GLN:HE21	1:E:70:GLN:HB3	1.66	0.43
1:E:100:LEU:O	1:E:324:LYS:HA	2.19	0.43
1:A:206:VAL:HG22	1:A:246:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG13	1:B:281:VAL:HA	2.00	0.43
1:B:249:GLU:H	1:B:249:GLU:HG3	1.57	0.43
1:G:60:SER:OG	1:G:95:THR:HA	2.19	0.43
1:A:25:LEU:HA	1:A:26:ALA:HA	1.72	0.43
1:A:100:LEU:HB3	1:B:73:TYR:CD2	2.53	0.43
1:B:174:LEU:HD21	1:B:180:LEU:HD13	2.00	0.43
1:C:42:ARG:NE	1:C:128:GLU:OE1	2.31	0.43
1:D:228:TYR:C	1:D:228:TYR:CD1	2.97	0.43
1:D:294:HIS:O	1:D:294:HIS:CG	2.72	0.43
1:E:228:TYR:HA	1:F:228:TYR:CG	2.53	0.43
1:F:27:LEU:CD1	1:F:28:PHE:HA	2.49	0.43
1:A:46:THR:O	1:A:50:HIS:HD2	2.02	0.43
1:A:199:TYR:O	1:A:200:VAL:HB	2.19	0.43
1:A:243:MET:SD	1:A:243:MET:N	2.91	0.43
1:B:232:ILE:HG21	1:B:239:ILE:HG12	2.00	0.43
1:E:113:MET:HE3	1:E:113:MET:HB2	1.90	0.43
1:A:109:ILE:HG23	1:A:113:MET:HE3	2.00	0.43
1:B:100:LEU:HG	1:C:73:TYR:CD2	2.53	0.43
1:C:239:ILE:HG13	1:C:247:VAL:HG21	2.01	0.43
1:D:333:ARG:C	1:D:335:GLU:N	2.74	0.43
1:E:37:LEU:HD11	1:F:333:ARG:NH1	2.34	0.43
1:E:134:ALA:HB2	1:E:325:TYR:OH	2.19	0.43
1:F:25:LEU:CD1	1:F:25:LEU:C	2.89	0.43
1:G:232:ILE:HG22	1:G:233:ASP:H	1.84	0.43
1:G:253:LEU:HD23	1:G:254:THR:H	1.84	0.43
1:B:312:ARG:HA	1:B:319:ASP:HB3	2.01	0.43
1:E:293:MET:HG3	1:E:295:ARG:H	1.84	0.43
1:D:168:THR:HG21	1:D:174:LEU:HD23	2.00	0.42
1:D:241:ASN:HB3	1:D:245:PHE:O	2.18	0.42
1:F:139:LEU:HD13	1:F:139:LEU:HA	1.87	0.42
1:F:178:VAL:HG13	1:F:179:ALA:N	2.34	0.42
1:F:254:THR:HA	1:F:272:PHE:CD1	2.54	0.42
1:G:210:ASP:HB2	1:G:211:PRO:HD2	2.01	0.42
1:G:235:GLU:HG2	1:G:235:GLU:O	2.18	0.42
1:G:260:THR:HG21	1:G:266:THR:OG1	2.18	0.42
1:A:224:ASN:HA	1:A:225:ALA:HA	1.66	0.42
1:C:145:LEU:O	1:C:149:GLU:HG3	2.19	0.42
1:D:304:ARG:HH11	1:D:304:ARG:HA	1.83	0.42
1:G:59:LYS:HE2	1:G:59:LYS:HB3	1.27	0.42
1:G:150:SER:C	1:G:152:TYR:H	2.26	0.42
1:G:179:ALA:O	1:G:183:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:CG	1:B:333:ARG:NH1	2.82	0.42
1:C:31:VAL:O	1:C:32:PHE:HB3	2.19	0.42
1:C:147:ASN:ND2	1:C:163:THR:HG21	2.33	0.42
1:C:222:MET:HB3	1:C:223:PRO:CD	2.50	0.42
1:A:45:VAL:HG22	1:A:49:ARG:NH1	2.34	0.42
1:A:262:ARG:HD3	1:B:72:ALA:HB2	2.01	0.42
1:C:42:ARG:HG3	1:D:199:TYR:CE1	2.55	0.42
1:D:282:LYS:H	1:D:282:LYS:HG2	1.60	0.42
1:G:86:ASP:OD2	1:G:87:ILE:N	2.51	0.42
1:G:99:LEU:HB3	1:G:100:LEU:H	1.41	0.42
1:B:236:LYS:HE2	1:B:238:SER:HB3	2.01	0.42
1:C:68:ARG:HD3	1:C:68:ARG:HA	1.76	0.42
1:C:325:TYR:CE2	1:C:327:MET:HE2	2.55	0.42
1:F:148:VAL:HG13	1:F:281:VAL:HB	2.02	0.42
1:A:24:LYS:HD3	1:A:25:LEU:H	1.84	0.42
1:A:158:GLY:C	1:A:335:GLU:OE2	2.63	0.42
1:A:242:VAL:C	1:F:235:GLU:HA	2.45	0.42
1:C:40:PHE:CE2	1:D:335:GLU:HG3	2.51	0.42
1:C:188:LEU:HA	1:C:188:LEU:HD23	1.84	0.42
1:D:57:SER:OG	1:D:58:GLY:N	2.49	0.42
1:D:151:LYS:HG3	1:D:152:TYR:CD2	2.54	0.42
1:D:155:ASN:CG	1:D:156:ILE:N	2.78	0.42
1:E:64:PRO:HA	1:E:91:GLU:CB	2.48	0.42
1:G:46:THR:HB	1:G:47:THR:HA	2.01	0.42
1:A:49:ARG:NH2	1:A:246:GLU:OE1	2.28	0.42
1:A:64:PRO:HG2	1:F:36:VAL:HG22	2.01	0.42
1:A:75:ALA:O	1:A:77:GLY:N	2.52	0.42
1:B:171:LYS:HB2	1:B:171:LYS:HE2	1.90	0.42
1:C:100:LEU:HB3	1:D:73:TYR:CD2	2.55	0.42
1:E:130:LEU:HD13	1:E:130:LEU:HA	1.78	0.42
1:F:53:ARG:HB3	1:F:53:ARG:NH1	2.30	0.42
1:F:206:VAL:HG23	1:F:246:GLU:HB2	2.00	0.42
1:G:100:LEU:HD21	1:G:258:ALA:O	2.20	0.42
1:G:205:ARG:HB2	1:G:245:PHE:HD2	1.84	0.42
1:A:139:LEU:HD21	1:A:253:LEU:HD21	2.01	0.42
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.35	0.42
1:B:46:THR:HG23	1:B:135:ASP:OD2	2.19	0.42
1:B:185:ILE:HD13	1:B:185:ILE:HA	1.93	0.42
1:C:7:GLY:O	1:C:8:GLN:HB2	2.19	0.42
1:A:197:LYS:O	1:A:198:ASN:CB	2.67	0.42
1:B:202:ALA:HB2	1:B:205:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.80	0.42
1:D:56:SER:OG	1:D:57:SER:N	2.53	0.42
1:D:310:ARG:NH2	1:D:321:ILE:HD11	2.31	0.42
1:E:158:GLY:CA	1:E:159:LEU:HB2	2.50	0.42
1:G:107:TYR:HA	1:G:318:ALA:HB1	2.01	0.42
1:B:113:MET:O	1:B:113:MET:HG2	2.20	0.42
1:B:215:SER:CB	1:C:193:ALA:HB2	2.49	0.42
1:C:227:ASN:HB3	1:C:228:TYR:H	1.57	0.42
1:C:262:ARG:NH1	1:D:72:ALA:HB2	2.35	0.42
1:E:37:LEU:HD21	1:F:332:LEU:HD23	2.02	0.42
1:A:24:LYS:HG2	1:A:24:LYS:HZ2	1.71	0.41
1:A:94:ILE:HD13	1:A:95:THR:N	2.35	0.41
1:B:156:ILE:HG23	1:B:157:GLU:N	2.34	0.41
1:B:185:ILE:HG12	1:B:217:ILE:HD11	2.01	0.41
1:B:217:ILE:HD13	1:B:217:ILE:HA	1.69	0.41
1:B:294:HIS:HB3	1:B:336:ALA:HB2	2.01	0.41
1:B:304:ARG:HH11	1:B:304:ARG:CA	2.33	0.41
1:E:225:ALA:HA	1:E:226:ALA:HA	1.78	0.41
1:G:310:ARG:HB3	1:G:321:ILE:HG13	2.01	0.41
1:A:176:ASP:O	1:A:177:GLN:HB3	2.21	0.41
1:A:250:VAL:HA	1:A:251:PRO:HD2	1.88	0.41
1:B:219:ALA:HB2	1:C:189:THR:HG21	2.02	0.41
1:C:312:ARG:HG2	1:C:319:ASP:HB3	2.02	0.41
1:E:50:HIS:CG	1:E:51:MET:N	2.88	0.41
1:G:99:LEU:HA	1:G:99:LEU:HD22	1.74	0.41
1:B:285:LYS:HE2	1:B:285:LYS:O	2.20	0.41
1:C:211:PRO:O	1:C:214:TYR:HB3	2.20	0.41
1:D:14:GLN:O	1:D:14:GLN:HG3	2.19	0.41
1:D:92:LYS:HD3	1:D:332:LEU:HA	2.02	0.41
1:G:143:ALA:HB3	1:G:272:PHE:HZ	1.85	0.41
1:G:207:PHE:N	1:G:245:PHE:HB3	2.35	0.41
1:G:286:ASP:OD1	1:G:286:ASP:N	2.53	0.41
1:C:304:ARG:HA	1:C:304:ARG:HD3	1.60	0.41
1:D:108:ASP:HB2	1:D:317:GLN:O	2.19	0.41
1:A:7:GLY:O	1:A:8:GLN:HB3	2.19	0.41
1:A:13:ASN:OD1	1:A:18:VAL:HG11	2.20	0.41
1:A:100:LEU:HD22	1:B:73:TYR:CE2	2.56	0.41
1:D:224:ASN:C	1:D:226:ALA:N	2.77	0.41
1:E:42:ARG:HG3	1:E:132:MET:HE2	2.02	0.41
1:E:200:VAL:HG22	1:E:201:PRO:HD2	2.02	0.41
1:E:37:LEU:HD12	1:E:37:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG12	1:A:243:MET:H	1.85	0.41
1:A:332:LEU:CD2	1:A:332:LEU:C	2.93	0.41
1:E:188:LEU:HD13	1:E:188:LEU:HA	1.72	0.41
1:G:101:THR:HG23	1:G:324:LYS:HB3	2.02	0.41
1:A:165:ILE:HD13	1:A:166:GLU:N	2.36	0.41
1:B:65:VAL:O	1:B:89:HIS:HB2	2.21	0.41
1:C:241:ASN:ND2	1:C:246:GLU:OE2	2.53	0.41
1:G:211:PRO:HA	1:G:249:GLU:OE1	2.21	0.41
1:A:75:ALA:HB3	1:A:78:GLU:OE2	2.20	0.41
1:A:87:ILE:HG13	1:F:122:TYR:CE1	2.56	0.41
1:A:92:LYS:HZ1	1:A:333:ARG:H	1.67	0.41
1:C:91:GLU:H	1:C:91:GLU:CD	2.27	0.41
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.90	0.41
1:C:141:GLU:OE2	1:C:329:HIS:HB2	2.21	0.41
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.88	0.41
1:D:207:PHE:HE2	1:D:209:CYS:HB2	1.86	0.41
1:E:142:ILE:HB	1:E:298:VAL:HG11	2.02	0.41
1:E:195:LEU:HD21	1:E:205:ARG:HD3	2.03	0.41
1:E:253:LEU:O	1:E:254:THR:HB	2.21	0.41
1:F:11:GLY:O	1:F:12:THR:HB	2.21	0.41
1:F:25:LEU:HD23	1:F:28:PHE:CE1	2.56	0.41
1:F:177:GLN:O	1:F:178:VAL:HG12	2.21	0.41
1:G:150:SER:O	1:G:151:LYS:HB3	2.20	0.41
1:G:310:ARG:HE	1:G:321:ILE:HD11	1.85	0.41
1:B:201:PRO:HB2	1:B:203:ALA:HB3	2.03	0.41
1:B:295:ARG:HD2	1:B:296:SER:H	1.85	0.41
1:C:83:LYS:N	1:C:83:LYS:HD3	2.36	0.41
1:C:113:MET:N	1:C:113:MET:SD	2.90	0.41
1:C:192:ARG:HD2	1:C:243:MET:HB3	2.02	0.41
1:C:218:LEU:HD22	1:C:232:ILE:HG21	2.03	0.41
1:D:121:GLU:O	1:D:125:GLN:HG2	2.20	0.41
1:F:27:LEU:HD13	1:F:28:PHE:N	2.21	0.41
1:A:116:TYR:HE2	1:A:118:VAL:HG23	1.85	0.40
1:B:188:LEU:HD13	1:B:188:LEU:HA	1.91	0.40
1:C:50:HIS:ND1	1:C:51:MET:N	2.69	0.40
1:D:33:GLY:HA3	1:E:63:PHE:HE1	1.85	0.40
1:B:112:ALA:O	1:B:113:MET:HG2	2.21	0.40
1:B:233:ASP:HA	1:B:234:PRO:HD3	1.77	0.40
1:C:297:ALA:C	1:C:298:VAL:CG2	2.94	0.40
1:D:333:ARG:N	1:D:334:PRO:HD2	2.36	0.40
1:E:85:LYS:HA	1:E:85:LYS:HD3	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:PHE:HB3	1:F:29:LEU:H	1.71	0.40
1:F:147:ASN:HB2	1:F:283:VAL:CG1	2.51	0.40
1:F:188:LEU:HB3	1:F:242:VAL:HG11	2.03	0.40
1:A:148:VAL:HG13	1:A:281:VAL:HA	2.04	0.40
1:C:171:LYS:H	1:C:171:LYS:HG3	1.51	0.40
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.92	0.40
1:F:234:PRO:O	1:F:235:GLU:HB3	2.21	0.40
1:G:109:ILE:HD12	1:G:109:ILE:HA	1.94	0.40
1:G:343:LYS:HD3	1:G:344:VAL:O	2.20	0.40
1:A:147:ASN:HD22	1:A:147:ASN:N	2.19	0.40
1:B:295:ARG:HD2	1:B:296:SER:N	2.37	0.40
1:C:159:LEU:HD12	1:C:161:THR:H	1.87	0.40
1:D:228:TYR:HE1	1:D:230:ALA:HB3	1.86	0.40
1:E:227:ASN:OD1	1:E:227:ASN:N	2.55	0.40
1:F:254:THR:HG21	1:F:285:LYS:HE3	2.02	0.40
1:G:62:GLN:OE1	1:G:91:GLU:HG3	2.20	0.40
1:G:238:SER:C	1:G:239:ILE:HD12	2.47	0.40
1:A:223:PRO:HG3	1:B:230:ALA:CB	2.52	0.40
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.84	0.40
1:C:16:LYS:HE3	1:C:16:LYS:HB3	1.44	0.40
1:C:332:LEU:O	1:C:332:LEU:HD12	2.21	0.40
1:D:223:PRO:O	1:D:224:ASN:CB	2.70	0.40
1:E:125:GLN:NE2	1:F:67:GLY:O	2.55	0.40
1:F:25:LEU:HA	1:F:26:ALA:HB3	2.00	0.40
1:G:25:LEU:HB2	1:G:26:ALA:CB	2.44	0.40
1:G:231:LEU:HB3	1:G:233:ASP:HB2	2.03	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	341/345 (99%)	262 (77%)	51 (15%)	28 (8%)	0	8
1	B	341/345 (99%)	275 (81%)	40 (12%)	26 (8%)	1	8
1	C	341/345 (99%)	267 (78%)	48 (14%)	26 (8%)	1	8
1	D	341/345 (99%)	271 (80%)	46 (14%)	24 (7%)	1	10
1	E	341/345 (99%)	266 (78%)	50 (15%)	25 (7%)	1	9
1	F	341/345 (99%)	280 (82%)	38 (11%)	23 (7%)	1	11
1	G	341/345 (99%)	281 (82%)	36 (11%)	24 (7%)	1	10
All	All	2387/2415 (99%)	1902 (80%)	309 (13%)	176 (7%)	1	9

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	19	VAL
1	A	76	PRO
1	A	222	MET
1	A	236	LYS
1	A	244	GLY
1	A	277	GLY
1	A	288	VAL
1	A	295	ARG
1	B	47	THR
1	B	118	VAL
1	B	156	ILE
1	B	157	GLU
1	B	200	VAL
1	B	206	VAL
1	B	232	ILE
1	B	236	LYS
1	B	239	ILE
1	B	333	ARG
1	B	335	GLU
1	C	8	GLN
1	C	12	THR
1	C	51	MET
1	C	116	TYR
1	C	170	ASN
1	C	175	THR
1	C	240	ARG
1	C	288	VAL
1	C	295	ARG

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Mol	Chain	Res	Type
1	C	337	ALA
1	D	69	THR
1	D	118	VAL
1	D	142	ILE
1	D	148	VAL
1	D	333	ARG
1	D	334	PRO
1	E	18	VAL
1	E	19	VAL
1	E	49	ARG
1	E	159	LEU
1	E	239	ILE
1	E	288	VAL
1	F	8	GLN
1	F	12	THR
1	F	28	PHE
1	F	48	SER
1	F	118	VAL
1	F	178	VAL
1	F	240	ARG
1	F	266	THR
1	G	12	THR
1	G	52	VAL
1	G	100	LEU
1	G	117	ASP
1	G	156	ILE
1	G	222	MET
1	G	234	PRO
1	A	116	TYR
1	B	57	SER
1	B	228	TYR
1	B	235	GLU
1	B	244	GLY
1	B	288	VAL
1	C	58	GLY
1	C	118	VAL
1	C	201	PRO
1	C	266	THR
1	C	278	GLU
1	D	20	ALA
1	D	48	SER
1	D	149	GLU

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Mol	Chain	Res	Type
1	D	244	GLY
1	E	8	GLN
1	E	12	THR
1	F	19	VAL
1	F	57	SER
1	F	168	THR
1	F	243	MET
1	F	247	VAL
1	G	152	TYR
1	G	199	TYR
1	G	226	ALA
1	G	267	GLY
1	G	288	VAL
1	G	295	ARG
1	A	12	THR
1	A	33	GLY
1	A	57	SER
1	A	168	THR
1	A	261	ALA
1	B	86	ASP
1	C	19	VAL
1	C	161	THR
1	C	222	MET
1	C	228	TYR
1	C	239	ILE
1	D	12	THR
1	D	23	ASP
1	D	116	TYR
1	D	152	TYR
1	D	154	GLU
1	D	157	GLU
1	D	170	ASN
1	D	254	THR
1	D	288	VAL
1	E	13	ASN
1	E	118	VAL
1	E	119	ARG
1	E	145	LEU
1	E	227	ASN
1	F	23	ASP
1	F	175	THR
1	G	8	GLN

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Mol	Chain	Res	Type
1	G	174	LEU
1	G	228	TYR
1	G	232	ILE
1	G	238	SER
1	G	261	ALA
1	A	200	VAL
1	A	234	PRO
1	A	266	THR
1	A	267	GLY
1	A	280	ASN
1	B	12	THR
1	B	45	VAL
1	B	167	THR
1	B	266	THR
1	C	23	ASP
1	C	280	ASN
1	D	57	SER
1	D	224	ASN
1	E	167	THR
1	E	175	THR
1	E	203	ALA
1	E	235	GLU
1	E	266	THR
1	F	14	GLN
1	F	20	ALA
1	F	167	THR
1	F	200	VAL
1	F	239	ILE
1	G	233	ASP
1	G	260	THR
1	A	3	SER
1	B	74	LEU
1	B	168	THR
1	C	168	THR
1	C	242	VAL
1	D	88	LYS
1	E	58	GLY
1	E	240	ARG
1	F	235	GLU
1	G	86	ASP
1	G	239	ILE
1	A	68	ARG

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Mol	Chain	Res	Type
1	A	142	ILE
1	A	152	TYR
1	A	199	TYR
1	B	223	PRO
1	C	333	ARG
1	F	47	THR
1	B	242	VAL
1	B	264	GLY
1	A	64	PRO
1	A	232	ILE
1	E	144	GLY
1	F	206	VAL
1	G	237	GLY
1	C	279	GLY
1	D	45	VAL
1	E	158	GLY
1	E	223	PRO
1	A	242	VAL
1	E	333	ARG
1	D	200	VAL
1	E	200	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	259/261 (99%)	151 (58%)	108 (42%)	0	0
1	B	259/261 (99%)	145 (56%)	114 (44%)	0	0
1	C	259/261 (99%)	167 (64%)	92 (36%)	0	1
1	D	259/261 (99%)	167 (64%)	92 (36%)	0	1
1	E	259/261 (99%)	155 (60%)	104 (40%)	0	1
1	F	259/261 (99%)	167 (64%)	92 (36%)	0	1
1	G	259/261 (99%)	160 (62%)	99 (38%)	0	1
All	All	1813/1827 (99%)	1112 (61%)	701 (39%)	0	1

All (701) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	14	GLN
1	A	18	VAL
1	A	19	VAL
1	A	23	ASP
1	A	24	LYS
1	A	25	LEU
1	A	27	LEU
1	A	29	LEU
1	A	32	PHE
1	A	36	VAL
1	A	37	LEU
1	A	38	THR
1	A	45	VAL
1	A	46	THR
1	A	48	SER
1	A	49	ARG
1	A	50	HIS
1	A	51	MET
1	A	52	VAL
1	A	59	LYS
1	A	62	GLN
1	A	66	LEU
1	A	68	ARG
1	A	69	THR
1	A	74	LEU
1	A	79	ASN
1	A	80	LEU
1	A	83	LYS
1	A	84	ARG
1	A	86	ASP
1	A	87	ILE
1	A	93	VAL
1	A	94	ILE
1	A	100	LEU
1	A	105	LEU
1	A	109	ILE
1	A	113	MET
1	A	114	ASN
1	A	115	HIS
1	A	118	VAL
1	A	123	THR

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Mol	Chain	Res	Type
1	A	125	GLN
1	A	130	LEU
1	A	138	VAL
1	A	142	ILE
1	A	145	LEU
1	A	149	GLU
1	A	151	LYS
1	A	153	ASN
1	A	154	GLU
1	A	159	LEU
1	A	163	THR
1	A	165	ILE
1	A	166	GLU
1	A	167	THR
1	A	168	THR
1	A	169	GLN
1	A	170	ASN
1	A	171	LYS
1	A	174	LEU
1	A	176	ASP
1	A	180	LEU
1	A	188	LEU
1	A	192	ARG
1	A	204	ASP
1	A	206	VAL
1	A	217	ILE
1	A	218	LEU
1	A	221	LEU
1	A	222	MET
1	A	228	TYR
1	A	231	LEU
1	A	232	ILE
1	A	235	GLU
1	A	236	LYS
1	A	239	ILE
1	A	249	GLU
1	A	253	LEU
1	A	260	THR
1	A	265	THR
1	A	269	LYS
1	A	276	LYS
1	A	281	VAL

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Mol	Chain	Res	Type
1	A	283	VAL
1	A	285	LYS
1	A	286	ASP
1	A	287	ASN
1	A	289	ILE
1	A	293	MET
1	A	295	ARG
1	A	298	VAL
1	A	303	LEU
1	A	304	ARG
1	A	306	LEU
1	A	308	LEU
1	A	313	ARG
1	A	320	GLN
1	A	322	ILE
1	A	324	LYS
1	A	325	TYR
1	A	332	LEU
1	A	333	ARG
1	A	334	PRO
1	A	340	VAL
1	A	341	VAL
1	A	343	LYS
1	A	344	VAL
1	B	10	MET
1	B	19	VAL
1	B	23	ASP
1	B	28	PHE
1	B	29	LEU
1	B	30	LYS
1	B	38	THR
1	B	43	THR
1	B	46	THR
1	B	47	THR
1	B	50	HIS
1	B	51	MET
1	B	53	ARG
1	B	55	ILE
1	B	59	LYS
1	B	62	GLN
1	B	65	VAL
1	B	68	ARG

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Mol	Chain	Res	Type
1	B	69	THR
1	B	73	TYR
1	B	79	ASN
1	B	82	ASP
1	B	84	ARG
1	B	86	ASP
1	B	87	ILE
1	B	88	LYS
1	B	92	LYS
1	B	93	VAL
1	B	94	ILE
1	B	95	THR
1	B	96	ILE
1	B	103	ASP
1	B	104	VAL
1	B	105	LEU
1	B	106	ILE
1	B	110	GLU
1	B	113	MET
1	B	115	HIS
1	B	116	TYR
1	B	117	ASP
1	B	118	VAL
1	B	128	GLU
1	B	130	LEU
1	B	139	LEU
1	B	142	ILE
1	B	149	GLU
1	B	150	SER
1	B	151	LYS
1	B	153	ASN
1	B	154	GLU
1	B	155	ASN
1	B	156	ILE
1	B	157	GLU
1	B	159	LEU
1	B	165	ILE
1	B	166	GLU
1	B	167	THR
1	B	168	THR
1	B	170	ASN
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	176	ASP
1	B	178	VAL
1	B	182	LYS
1	B	188	LEU
1	B	192	ARG
1	B	195	LEU
1	B	196	THR
1	B	197	LYS
1	B	198	ASN
1	B	199	TYR
1	B	200	VAL
1	B	205	ARG
1	B	206	VAL
1	B	210	ASP
1	B	212	ASP
1	B	215	SER
1	B	217	ILE
1	B	221	LEU
1	B	222	MET
1	B	232	ILE
1	B	233	ASP
1	B	236	LYS
1	B	239	ILE
1	B	241	ASN
1	B	243	MET
1	B	247	VAL
1	B	248	VAL
1	B	249	GLU
1	B	253	LEU
1	B	262	ARG
1	B	269	LYS
1	B	275	ASN
1	B	276	LYS
1	B	278	GLU
1	B	280	ASN
1	B	281	VAL
1	B	283	VAL
1	B	285	LYS
1	B	289	ILE
1	B	294	HIS
1	B	295	ARG
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	304	ARG
1	B	306	LEU
1	B	309	GLU
1	B	319	ASP
1	B	320	GLN
1	B	321	ILE
1	B	324	LYS
1	B	325	TYR
1	B	332	LEU
1	B	333	ARG
1	B	335	GLU
1	B	340	VAL
1	C	16	LYS
1	C	25	LEU
1	C	27	LEU
1	C	29	LEU
1	C	31	VAL
1	C	32	PHE
1	C	36	VAL
1	C	37	LEU
1	C	46	THR
1	C	49	ARG
1	C	51	MET
1	C	55	ILE
1	C	59	LYS
1	C	62	GLN
1	C	69	THR
1	C	73	TYR
1	C	74	LEU
1	C	79	ASN
1	C	80	LEU
1	C	83	LYS
1	C	84	ARG
1	C	87	ILE
1	C	89	HIS
1	C	90	THR
1	C	92	LYS
1	C	94	ILE
1	C	96	ILE
1	C	100	LEU
1	C	101	THR
1	C	108	ASP

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Mol	Chain	Res	Type
1	C	109	ILE
1	C	113	MET
1	C	115	HIS
1	C	118	VAL
1	C	119	ARG
1	C	124	SER
1	C	130	LEU
1	C	132	MET
1	C	139	LEU
1	C	142	ILE
1	C	147	ASN
1	C	154	GLU
1	C	156	ILE
1	C	159	LEU
1	C	163	THR
1	C	165	ILE
1	C	171	LYS
1	C	174	LEU
1	C	175	THR
1	C	176	ASP
1	C	178	VAL
1	C	180	LEU
1	C	190	LYS
1	C	195	LEU
1	C	197	LYS
1	C	200	VAL
1	C	204	ASP
1	C	205	ARG
1	C	206	VAL
1	C	215	SER
1	C	217	ILE
1	C	218	LEU
1	C	224	ASN
1	C	232	ILE
1	C	236	LYS
1	C	243	MET
1	C	247	VAL
1	C	253	LEU
1	C	265	THR
1	C	269	LYS
1	C	271	VAL
1	C	275	ASN

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Mol	Chain	Res	Type
1	C	281	VAL
1	C	282	LYS
1	C	283	VAL
1	C	289	ILE
1	C	295	ARG
1	C	300	THR
1	C	301	VAL
1	C	303	LEU
1	C	304	ARG
1	C	305	ASP
1	C	306	LEU
1	C	309	GLU
1	C	313	ARG
1	C	320	GLN
1	C	324	LYS
1	C	327	MET
1	C	329	HIS
1	C	333	ARG
1	C	340	VAL
1	C	341	VAL
1	D	5	THR
1	D	9	GLN
1	D	10	MET
1	D	13	ASN
1	D	14	GLN
1	D	18	VAL
1	D	19	VAL
1	D	25	LEU
1	D	29	LEU
1	D	31	VAL
1	D	32	PHE
1	D	35	GLU
1	D	37	LEU
1	D	43	THR
1	D	52	VAL
1	D	53	ARG
1	D	55	ILE
1	D	60	SER
1	D	66	LEU
1	D	74	LEU
1	D	80	LEU
1	D	81	ASP

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Mol	Chain	Res	Type
1	D	87	ILE
1	D	90	THR
1	D	94	ILE
1	D	96	ILE
1	D	100	LEU
1	D	101	THR
1	D	105	LEU
1	D	108	ASP
1	D	109	ILE
1	D	113	MET
1	D	114	ASN
1	D	121	GLU
1	D	123	THR
1	D	126	LEU
1	D	130	LEU
1	D	132	MET
1	D	135	ASP
1	D	139	LEU
1	D	141	GLU
1	D	142	ILE
1	D	149	GLU
1	D	156	ILE
1	D	157	GLU
1	D	163	THR
1	D	165	ILE
1	D	166	GLU
1	D	167	THR
1	D	168	THR
1	D	170	ASN
1	D	171	LYS
1	D	175	THR
1	D	178	VAL
1	D	183	GLU
1	D	188	LEU
1	D	192	ARG
1	D	196	THR
1	D	200	VAL
1	D	205	ARG
1	D	209	CYS
1	D	212	ASP
1	D	218	LEU
1	D	221	LEU

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Mol	Chain	Res	Type
1	D	227	ASN
1	D	241	ASN
1	D	248	VAL
1	D	249	GLU
1	D	250	VAL
1	D	253	LEU
1	D	260	THR
1	D	266	THR
1	D	268	GLN
1	D	269	LYS
1	D	275	ASN
1	D	276	LYS
1	D	278	GLU
1	D	282	LYS
1	D	283	VAL
1	D	295	ARG
1	D	301	VAL
1	D	303	LEU
1	D	306	LEU
1	D	309	GLU
1	D	313	ARG
1	D	321	ILE
1	D	322	ILE
1	D	325	TYR
1	D	332	LEU
1	D	333	ARG
1	D	335	GLU
1	D	344	VAL
1	E	5	THR
1	E	9	GLN
1	E	14	GLN
1	E	16	LYS
1	E	19	VAL
1	E	25	LEU
1	E	27	LEU
1	E	29	LEU
1	E	35	GLU
1	E	36	VAL
1	E	38	THR
1	E	40	PHE
1	E	42	ARG
1	E	44	SER

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Mol	Chain	Res	Type
1	E	45	VAL
1	E	46	THR
1	E	47	THR
1	E	49	ARG
1	E	52	VAL
1	E	54	SER
1	E	59	LYS
1	E	65	VAL
1	E	69	THR
1	E	70	GLN
1	E	80	LEU
1	E	82	ASP
1	E	84	ARG
1	E	86	ASP
1	E	88	LYS
1	E	90	THR
1	E	92	LYS
1	E	94	ILE
1	E	95	THR
1	E	99	LEU
1	E	100	LEU
1	E	105	LEU
1	E	118	VAL
1	E	119	ARG
1	E	122	TYR
1	E	124	SER
1	E	128	GLU
1	E	130	LEU
1	E	132	MET
1	E	142	ILE
1	E	145	LEU
1	E	149	GLU
1	E	153	ASN
1	E	161	THR
1	E	165	ILE
1	E	167	THR
1	E	168	THR
1	E	170	ASN
1	E	171	LYS
1	E	178	VAL
1	E	184	ILE
1	E	188	LEU

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Mol	Chain	Res	Type
1	E	189	THR
1	E	190	LYS
1	E	197	LYS
1	E	198	ASN
1	E	200	VAL
1	E	204	ASP
1	E	206	VAL
1	E	209	CYS
1	E	210	ASP
1	E	212	ASP
1	E	215	SER
1	E	221	LEU
1	E	222	MET
1	E	227	ASN
1	E	231	LEU
1	E	232	ILE
1	E	235	GLU
1	E	239	ILE
1	E	240	ARG
1	E	243	MET
1	E	248	VAL
1	E	249	GLU
1	E	250	VAL
1	E	271	VAL
1	E	272	PHE
1	E	275	ASN
1	E	283	VAL
1	E	287	ASN
1	E	289	ILE
1	E	295	ARG
1	E	298	VAL
1	E	302	LYS
1	E	303	LEU
1	E	304	ARG
1	E	306	LEU
1	E	308	LEU
1	E	309	GLU
1	E	312	ARG
1	E	313	ARG
1	E	315	ASN
1	E	320	GLN
1	E	321	ILE

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Mol	Chain	Res	Type
1	E	324	LYS
1	E	325	TYR
1	E	332	LEU
1	E	341	VAL
1	E	342	PHE
1	E	343	LYS
1	F	3	SER
1	F	13	ASN
1	F	16	LYS
1	F	18	VAL
1	F	24	LYS
1	F	25	LEU
1	F	27	LEU
1	F	29	LEU
1	F	36	VAL
1	F	38	THR
1	F	42	ARG
1	F	43	THR
1	F	44	SER
1	F	47	THR
1	F	50	HIS
1	F	52	VAL
1	F	53	ARG
1	F	54	SER
1	F	55	ILE
1	F	59	LYS
1	F	66	LEU
1	F	69	THR
1	F	78	GLU
1	F	80	LEU
1	F	82	ASP
1	F	83	LYS
1	F	89	HIS
1	F	90	THR
1	F	91	GLU
1	F	95	THR
1	F	101	THR
1	F	105	LEU
1	F	108	ASP
1	F	109	ILE
1	F	113	MET
1	F	117	ASP

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Mol	Chain	Res	Type
1	F	118	VAL
1	F	128	GLU
1	F	130	LEU
1	F	139	LEU
1	F	142	ILE
1	F	145	LEU
1	F	154	GLU
1	F	156	ILE
1	F	159	LEU
1	F	161	THR
1	F	163	THR
1	F	167	THR
1	F	178	VAL
1	F	188	LEU
1	F	195	LEU
1	F	196	THR
1	F	204	ASP
1	F	212	ASP
1	F	217	ILE
1	F	218	LEU
1	F	221	LEU
1	F	227	ASN
1	F	228	TYR
1	F	231	LEU
1	F	232	ILE
1	F	233	ASP
1	F	235	GLU
1	F	236	LYS
1	F	243	MET
1	F	249	GLU
1	F	250	VAL
1	F	260	THR
1	F	263	GLU
1	F	265	THR
1	F	268	GLN
1	F	271	VAL
1	F	281	VAL
1	F	293	MET
1	F	295	ARG
1	F	296	SER
1	F	300	THR
1	F	302	LYS

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Mol	Chain	Res	Type
1	F	303	LEU
1	F	304	ARG
1	F	306	LEU
1	F	309	GLU
1	F	310	ARG
1	F	320	GLN
1	F	321	ILE
1	F	322	ILE
1	F	324	LYS
1	F	325	TYR
1	F	332	LEU
1	F	333	ARG
1	F	340	VAL
1	F	341	VAL
1	G	10	MET
1	G	14	GLN
1	G	16	LYS
1	G	23	ASP
1	G	24	LYS
1	G	25	LEU
1	G	29	LEU
1	G	31	VAL
1	G	35	GLU
1	G	37	LEU
1	G	38	THR
1	G	46	THR
1	G	50	HIS
1	G	51	MET
1	G	52	VAL
1	G	53	ARG
1	G	55	ILE
1	G	57	SER
1	G	59	LYS
1	G	62	GLN
1	G	63	PHE
1	G	65	VAL
1	G	66	LEU
1	G	68	ARG
1	G	70	GLN
1	G	73	TYR
1	G	74	LEU
1	G	82	ASP

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Mol	Chain	Res	Type
1	G	83	LYS
1	G	84	ARG
1	G	85	LYS
1	G	86	ASP
1	G	87	ILE
1	G	89	HIS
1	G	91	GLU
1	G	94	ILE
1	G	95	THR
1	G	97	ASP
1	G	99	LEU
1	G	105	LEU
1	G	109	ILE
1	G	110	GLU
1	G	114	ASN
1	G	119	ARG
1	G	121	GLU
1	G	123	THR
1	G	124	SER
1	G	126	LEU
1	G	130	LEU
1	G	139	LEU
1	G	142	ILE
1	G	145	LEU
1	G	154	GLU
1	G	156	ILE
1	G	163	THR
1	G	169	GLN
1	G	171	LYS
1	G	182	LYS
1	G	188	LEU
1	G	196	THR
1	G	197	LYS
1	G	200	VAL
1	G	205	ARG
1	G	206	VAL
1	G	217	ILE
1	G	218	LEU
1	G	222	MET
1	G	224	ASN
1	G	235	GLU
1	G	240	ARG

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Mol	Chain	Res	Type
1	G	242	VAL
1	G	243	MET
1	G	248	VAL
1	G	250	VAL
1	G	263	GLU
1	G	268	GLN
1	G	269	LYS
1	G	271	VAL
1	G	272	PHE
1	G	276	LYS
1	G	281	VAL
1	G	282	LYS
1	G	283	VAL
1	G	285	LYS
1	G	291	LEU
1	G	295	ARG
1	G	296	SER
1	G	298	VAL
1	G	300	THR
1	G	303	LEU
1	G	308	LEU
1	G	309	GLU
1	G	310	ARG
1	G	320	GLN
1	G	321	ILE
1	G	324	LYS
1	G	332	LEU
1	G	341	VAL
1	G	342	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	50	HIS
1	A	62	GLN
1	A	89	HIS
1	A	125	GLN
1	A	147	ASN
1	A	252	HIS
1	A	268	GLN
1	A	270	HIS

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Mol	Chain	Res	Type
1	A	287	ASN
1	A	315	ASN
1	A	320	GLN
1	B	13	ASN
1	B	79	ASN
1	B	115	HIS
1	B	125	GLN
1	B	155	ASN
1	B	177	GLN
1	B	224	ASN
1	B	270	HIS
1	B	275	ASN
1	B	280	ASN
1	B	287	ASN
1	C	50	HIS
1	C	125	GLN
1	C	147	ASN
1	C	153	ASN
1	C	268	GLN
1	C	275	ASN
1	C	315	ASN
1	C	320	GLN
1	C	329	HIS
1	D	14	GLN
1	D	50	HIS
1	D	89	HIS
1	D	153	ASN
1	D	252	HIS
1	D	315	ASN
1	E	13	ASN
1	E	50	HIS
1	E	89	HIS
1	E	114	ASN
1	E	125	GLN
1	E	170	ASN
1	E	224	ASN
1	E	275	ASN
1	E	280	ASN
1	E	315	ASN
1	F	155	ASN
1	F	169	GLN
1	F	227	ASN

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Mol	Chain	Res	Type
1	F	252	HIS
1	F	268	GLN
1	G	9	GLN
1	G	70	GLN
1	G	114	ASN
1	G	147	ASN
1	G	153	ASN
1	G	169	GLN
1	G	224	ASN
1	G	241	ASN
1	G	287	ASN
1	G	315	ASN

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.

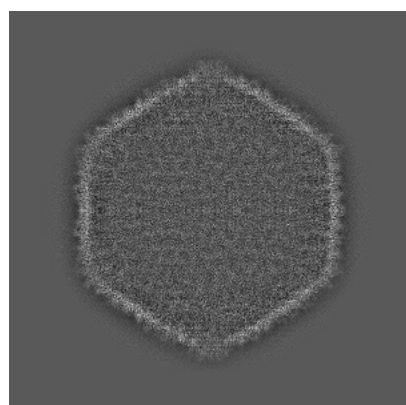
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6035. These allow visual inspection of the internal detail of the map and identification of artifacts.

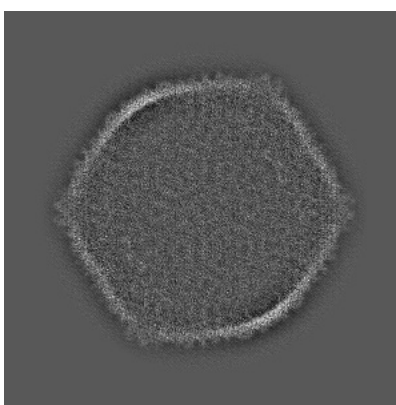
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

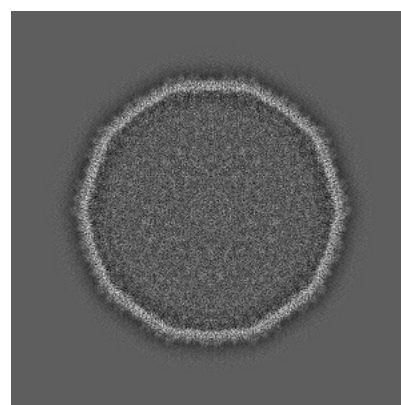
6.1.1 Primary map



X



Y

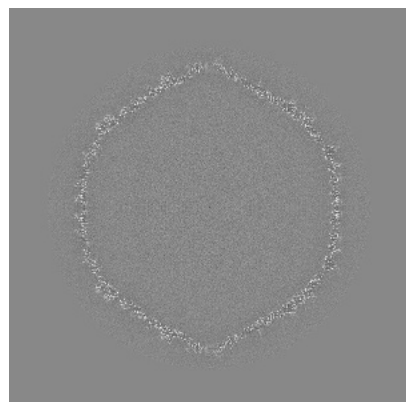


Z

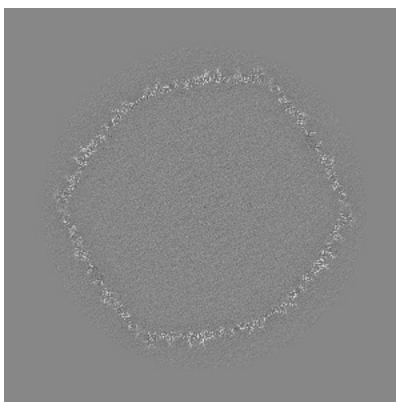
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

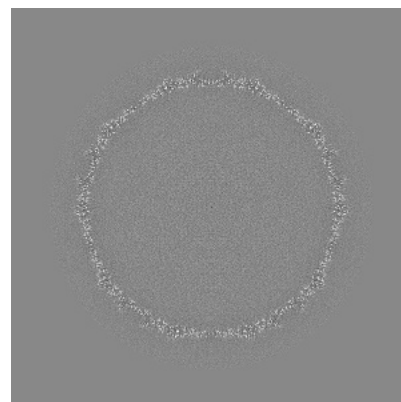
6.2.1 Primary map



X Index: 400



Y Index: 400

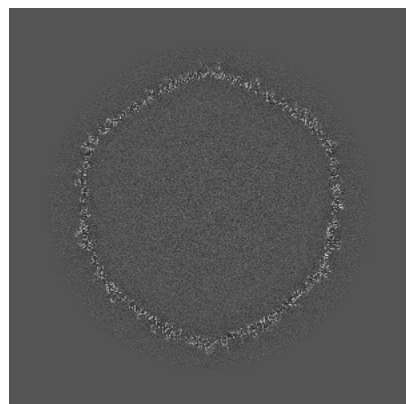


Z Index: 400

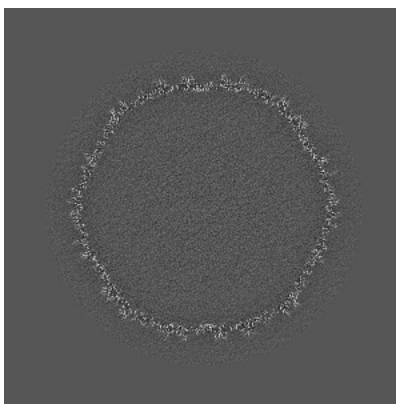
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

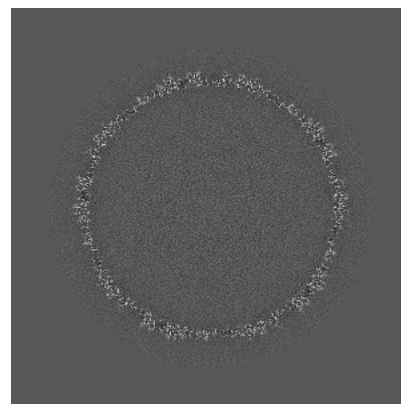
6.3.1 Primary map



X Index: 434



Y Index: 332

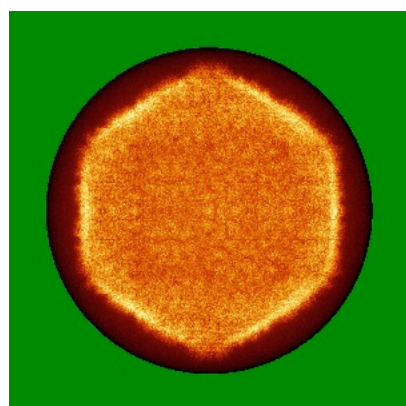


Z Index: 398

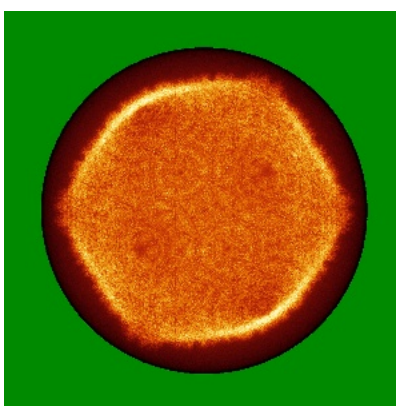
The images above show the largest variance slices of the map in three orthogonal directions.

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

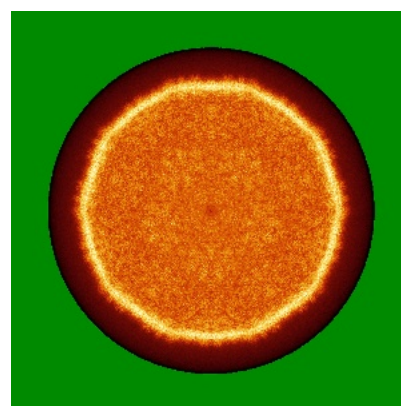
6.4.1 Primary map



X



Y



Z

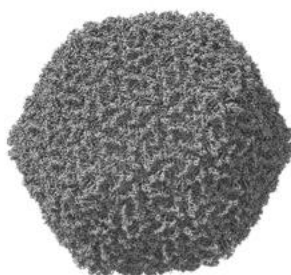
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

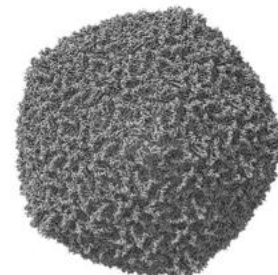
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

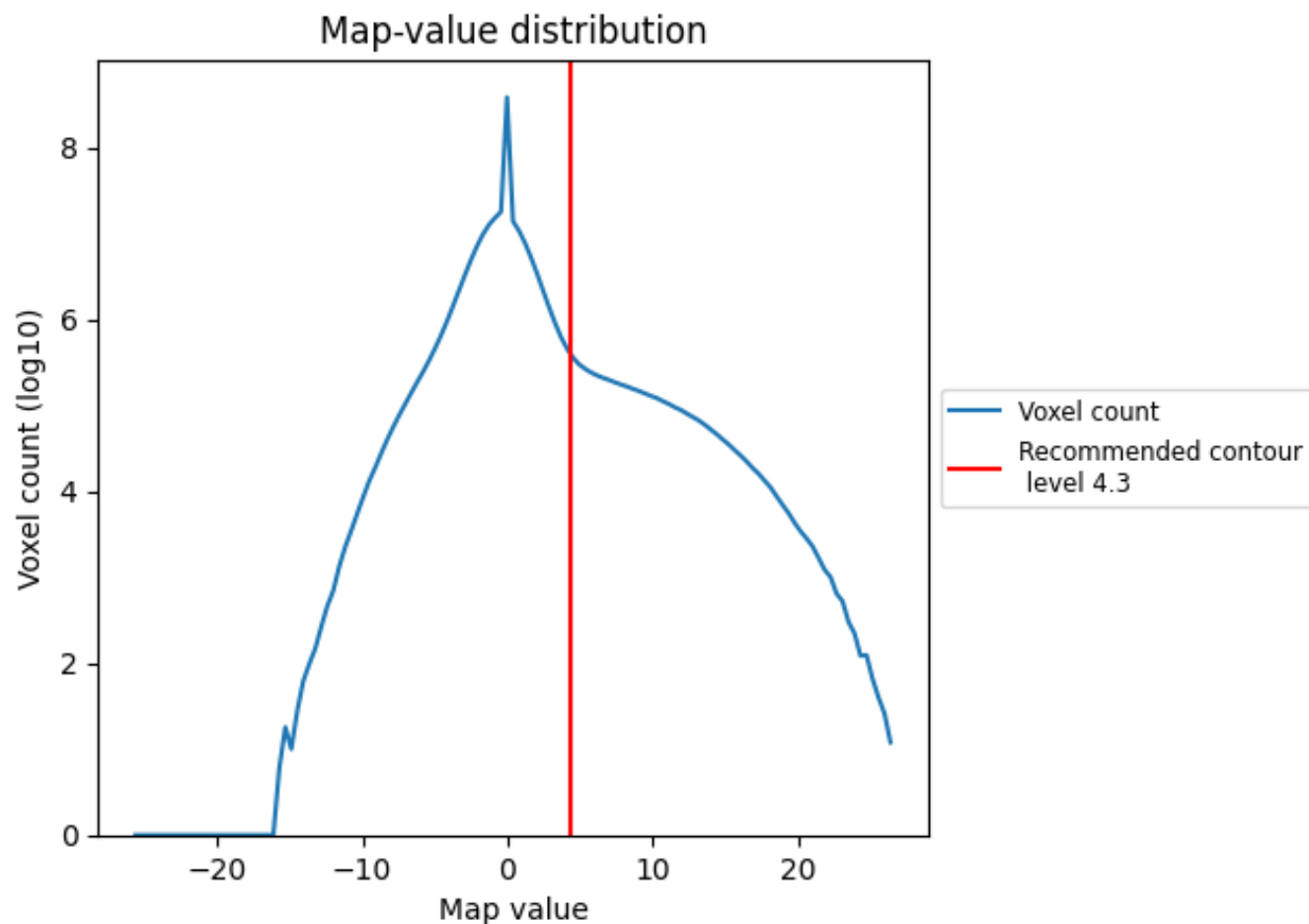
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

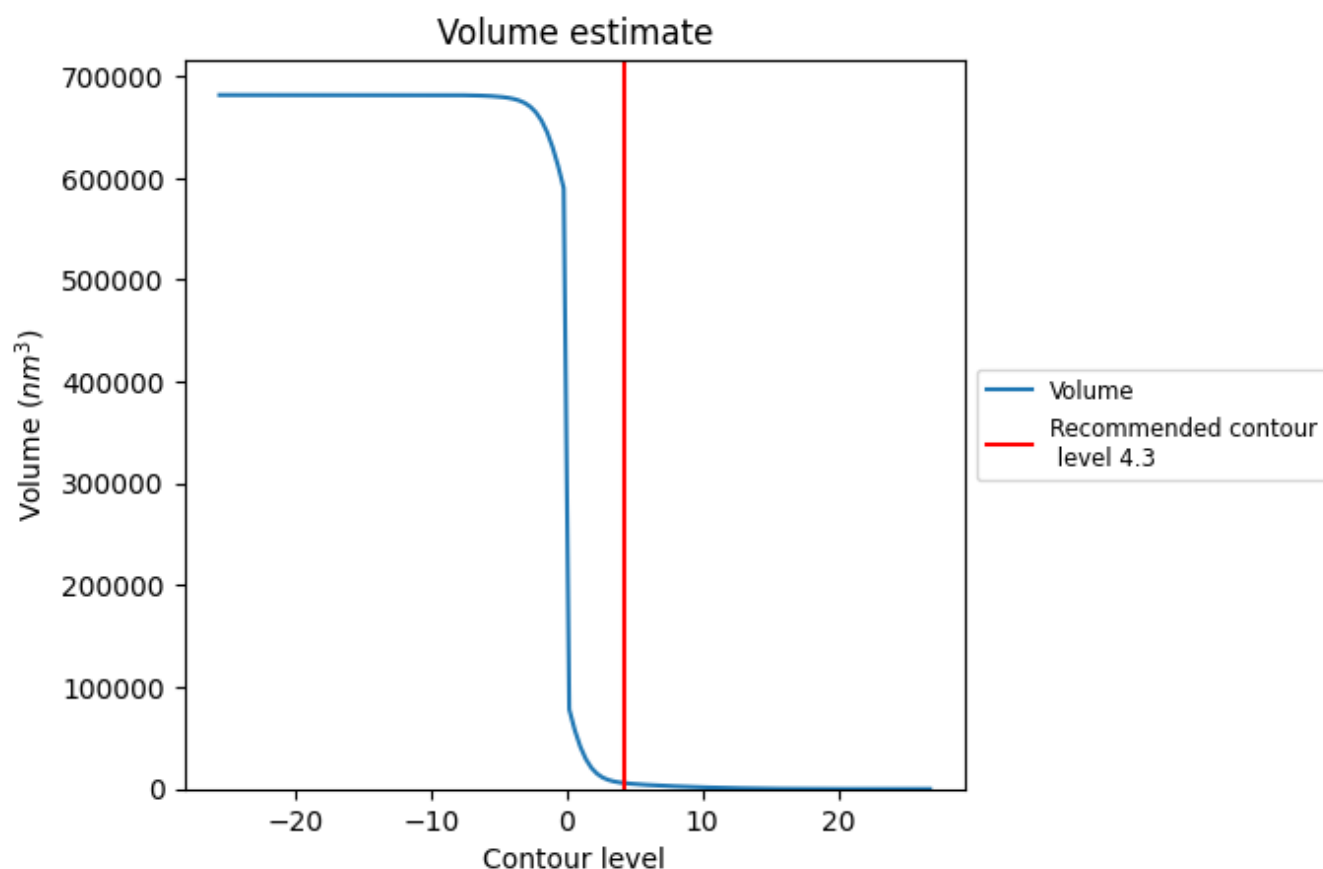
This section contains the results of statistical analysis of the map.

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.

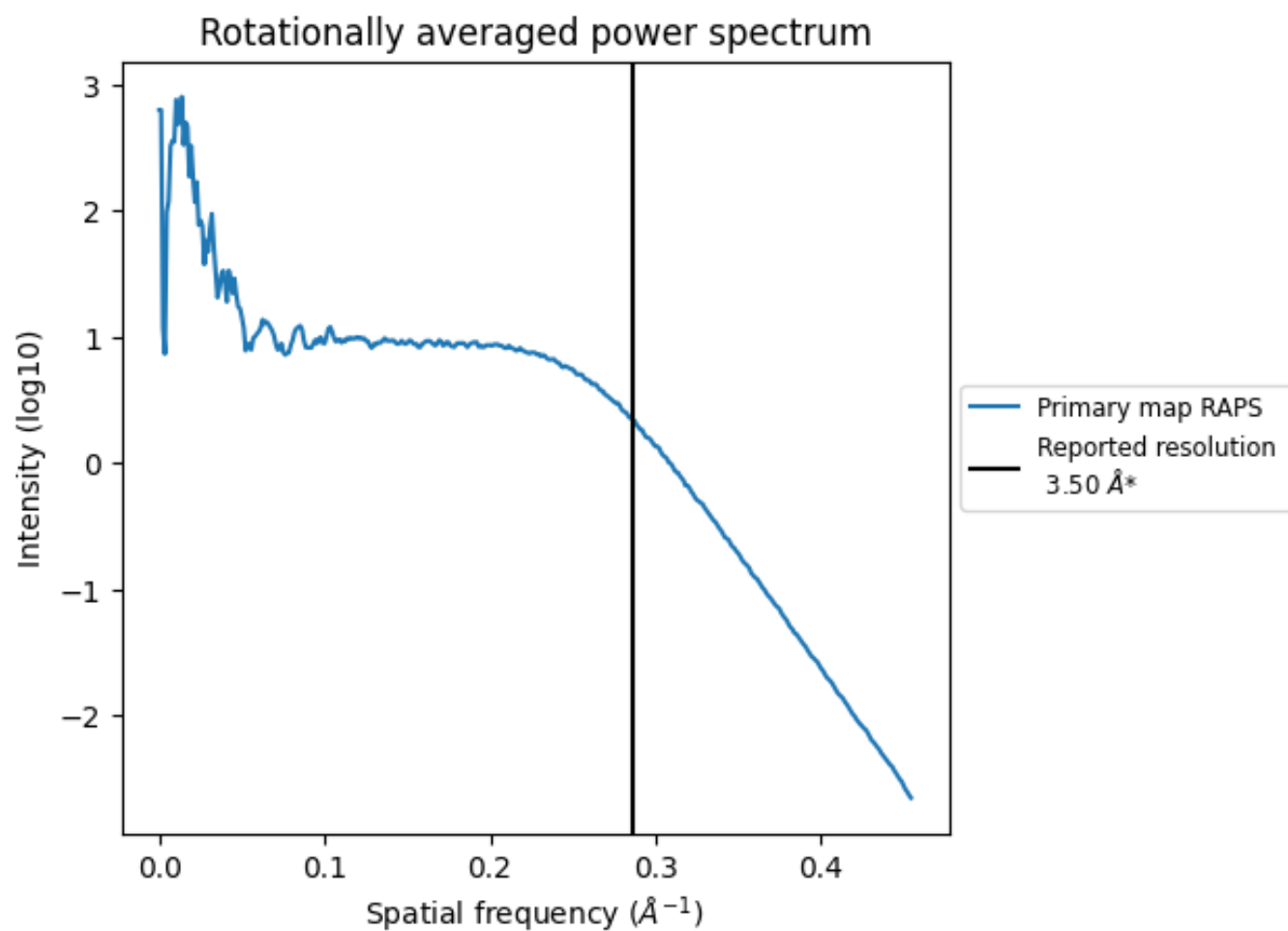
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5664 nm^3 ; this corresponds to an approximate mass of 5116 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 0.286 Å⁻¹

8 Fourier-Shell correlation ⓘ

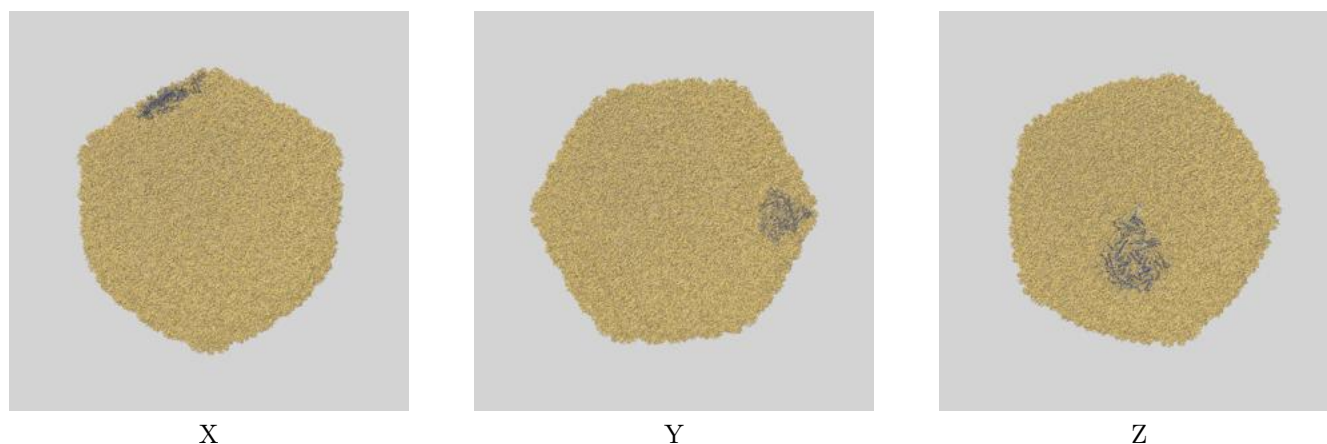
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

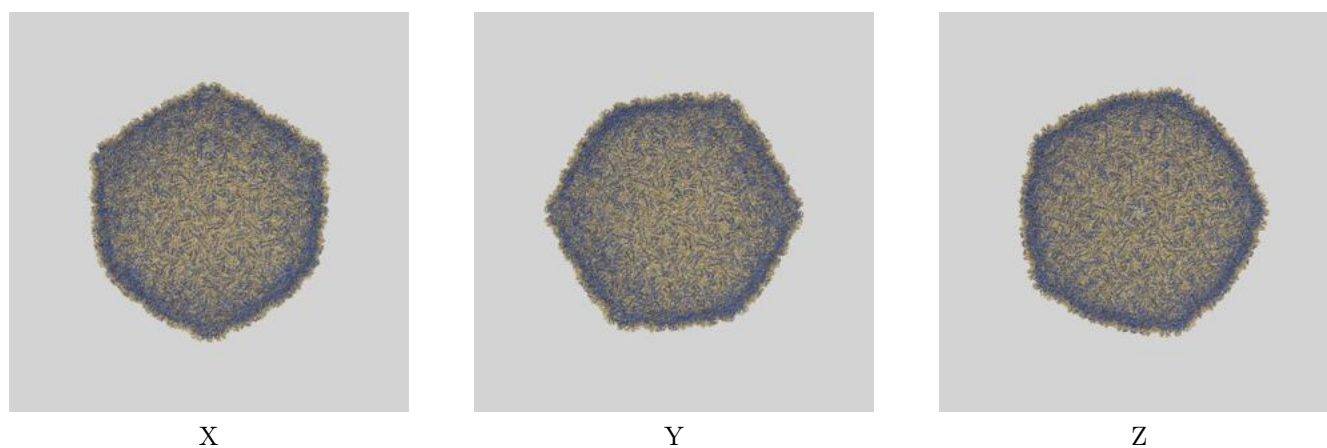
This section contains information regarding the fit between EMDB map EMD-6035 and PDB model 3J7W. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



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



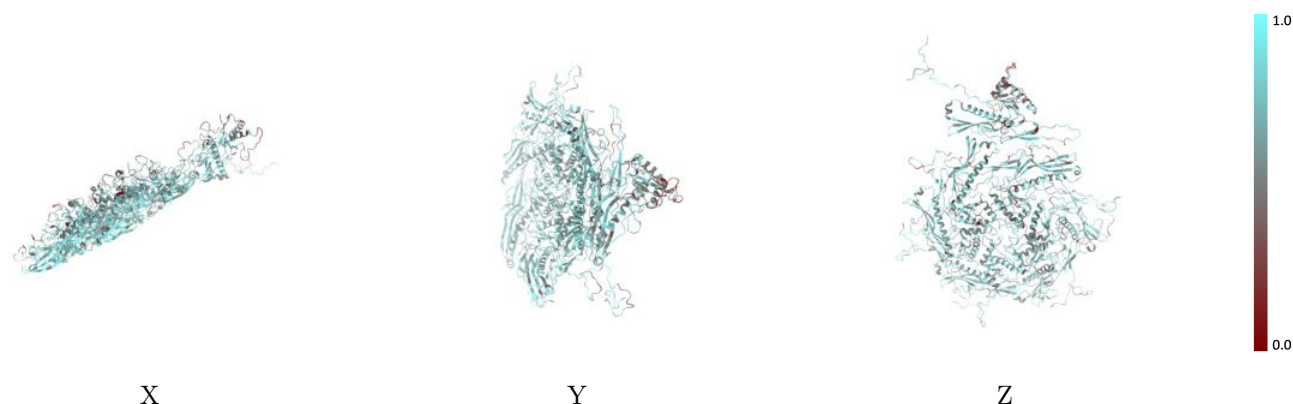
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



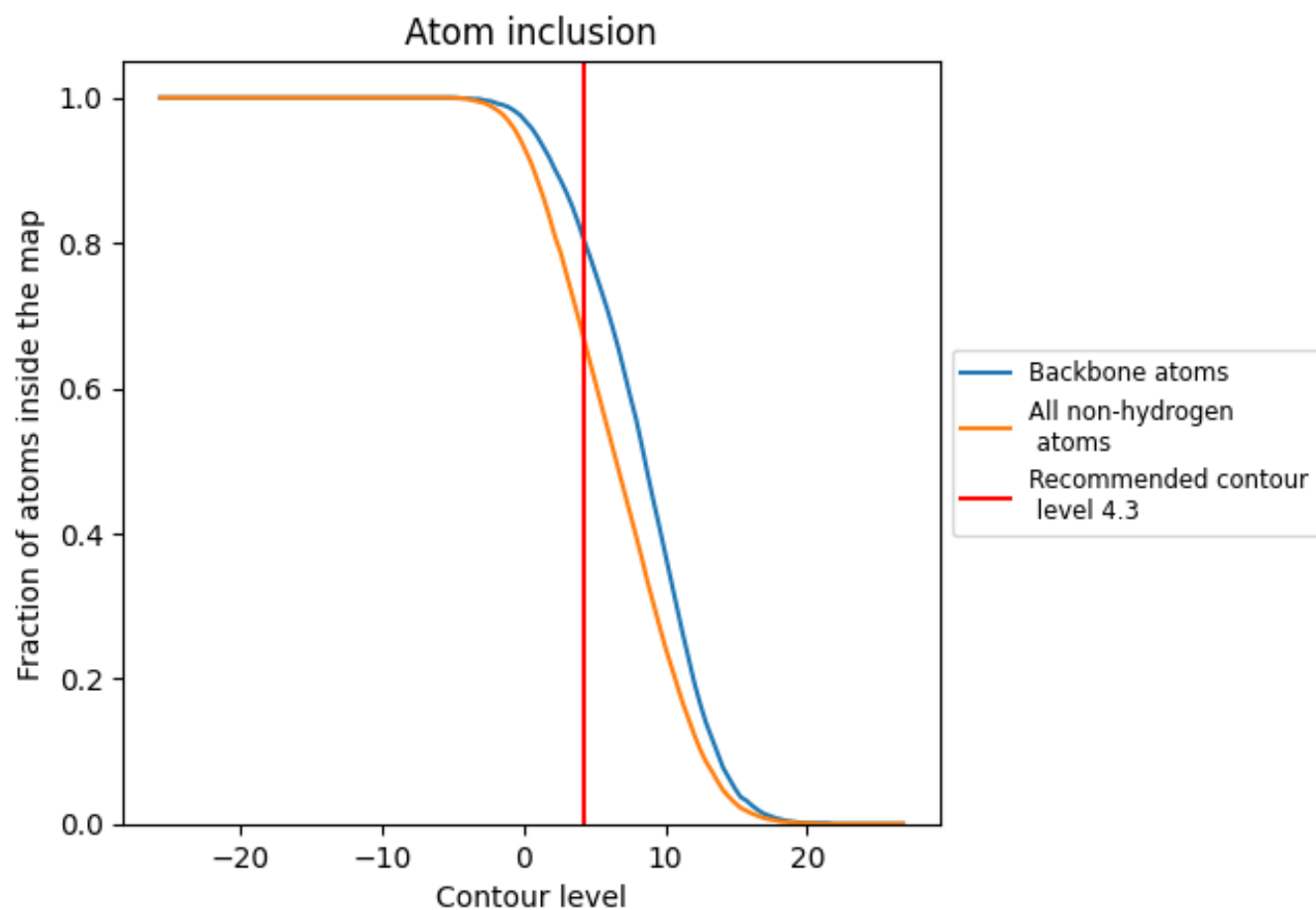
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.4180
A	0.6610	0.4210
B	0.6660	0.4170
C	0.6870	0.4180
D	0.6970	0.4320
E	0.6750	0.4300
F	0.6590	0.4100
G	0.6120	0.3990

1.0

0.0

<0.0