



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 6TNZ / pdb_00006tnz
EMDB ID : EMD-10540
Title : Human polymerase delta-FEN1-PCNA toolbelt
Authors : Lancey, C.; Hamdan, S.M.; De Biasio, A.
Deposited on : 2019-12-10
Resolution : 4.05 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:

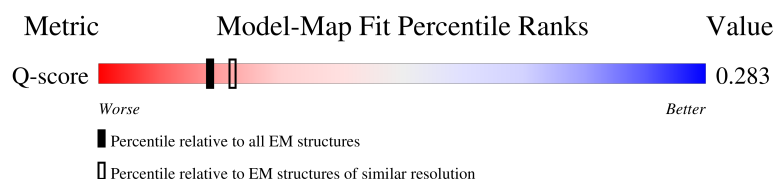
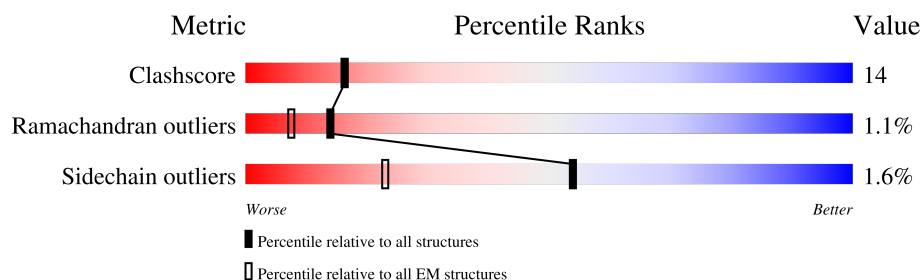
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.05 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	6569 (3.55 - 4.55)

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	1107	 6% 79% 12% 9%
2	B	469	 79% 13% 8%
3	C	474	 28% 70%
4	D	137	 36% 11% 52%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	264	
5	F	264	
5	G	264	
6	H	380	
7	P	25	
8	T	38	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SF4	A	1202	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22008 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 DNA polymerase delta catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total	C	N	O	S	1	0
			7926	5028	1405	1447	46		

- Molecule 2 is a protein called DNA polymerase delta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3304	2103	553	630	18		

- Molecule 3 is a protein called DNA polymerase delta subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	143	Total	C	N	O	S	0	0
			1130	715	196	214	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	initiating methionine	UNP Q15054
C	-6	TRP	-	expression tag	UNP Q15054
C	-5	SER	-	expression tag	UNP Q15054
C	-4	HIS	-	expression tag	UNP Q15054
C	-3	PRO	-	expression tag	UNP Q15054
C	-2	GLN	-	expression tag	UNP Q15054
C	-1	PHE	-	expression tag	UNP Q15054
C	0	GLU	-	expression tag	UNP Q15054
C	1	LYS	-	expression tag	UNP Q15054

- Molecule 4 is a protein called DNA polymerase delta subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			554	359	97	94	4		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	MET	-	initiating methionine	UNP Q9HCU8
D	-28	HIS	-	expression tag	UNP Q9HCU8
D	-27	HIS	-	expression tag	UNP Q9HCU8
D	-26	HIS	-	expression tag	UNP Q9HCU8
D	-25	HIS	-	expression tag	UNP Q9HCU8
D	-24	HIS	-	expression tag	UNP Q9HCU8
D	-23	HIS	-	expression tag	UNP Q9HCU8
D	-22	SER	-	expression tag	UNP Q9HCU8
D	-21	ARG	-	expression tag	UNP Q9HCU8
D	-20	ALA	-	expression tag	UNP Q9HCU8
D	-19	TRP	-	expression tag	UNP Q9HCU8
D	-18	ARG	-	expression tag	UNP Q9HCU8
D	-17	HIS	-	expression tag	UNP Q9HCU8
D	-16	PRO	-	expression tag	UNP Q9HCU8
D	-15	GLN	-	expression tag	UNP Q9HCU8
D	-14	PHE	-	expression tag	UNP Q9HCU8
D	-13	GLY	-	expression tag	UNP Q9HCU8
D	-12	GLY	-	expression tag	UNP Q9HCU8
D	-11	HIS	-	expression tag	UNP Q9HCU8
D	-10	HIS	-	expression tag	UNP Q9HCU8
D	-9	HIS	-	expression tag	UNP Q9HCU8
D	-8	HIS	-	expression tag	UNP Q9HCU8
D	-7	HIS	-	expression tag	UNP Q9HCU8
D	-6	HIS	-	expression tag	UNP Q9HCU8
D	-5	GLU	-	expression tag	UNP Q9HCU8
D	-4	ASN	-	expression tag	UNP Q9HCU8
D	-3	LEU	-	expression tag	UNP Q9HCU8
D	-2	TYR	-	expression tag	UNP Q9HCU8
D	-1	PHE	-	expression tag	UNP Q9HCU8
D	0	GLN	-	expression tag	UNP Q9HCU8
D	1	SER	-	expression tag	UNP Q9HCU8

- Molecule 5 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	251	Total	C	N	O	S	0	0
			1924	1211	314	383	16		
5	F	249	Total	C	N	O	S	0	0
			1913	1205	312	380	16		
5	G	249	Total	C	N	O	S	0	0
			1913	1204	314	379	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P12004
E	-1	PRO	-	expression tag	UNP P12004
E	0	HIS	-	expression tag	UNP P12004
F	-2	GLY	-	expression tag	UNP P12004
F	-1	PRO	-	expression tag	UNP P12004
F	0	HIS	-	expression tag	UNP P12004
G	-2	GLY	-	expression tag	UNP P12004
G	-1	PRO	-	expression tag	UNP P12004
G	0	HIS	-	expression tag	UNP P12004

- Molecule 6 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	306	Total	C	N	O	S	0	0
			2282	1436	396	437	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	181	ALA	ASP	conflict	UNP P39748

- Molecule 7 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	23	Total	C	N	O	P	0	0
			469	225	84	137	23		

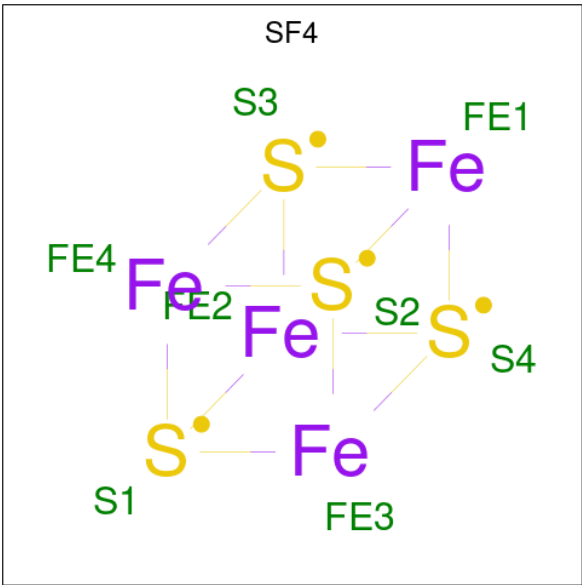
- Molecule 8 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	27	Total	C	N	O	P	0	0
			555	266	100	162	27		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

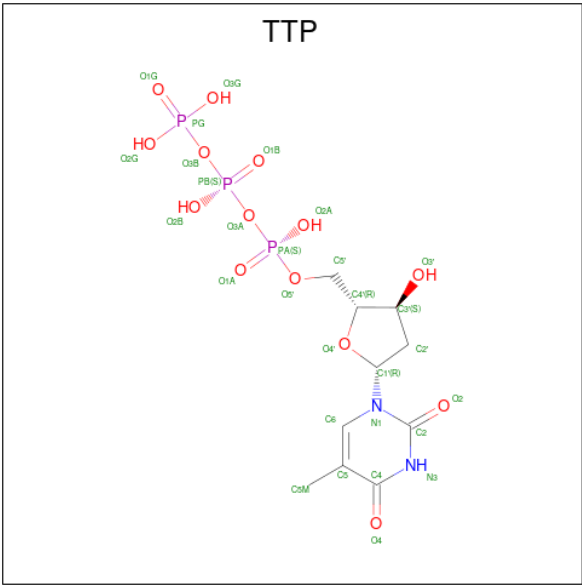
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Zn	0
			1	1	

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



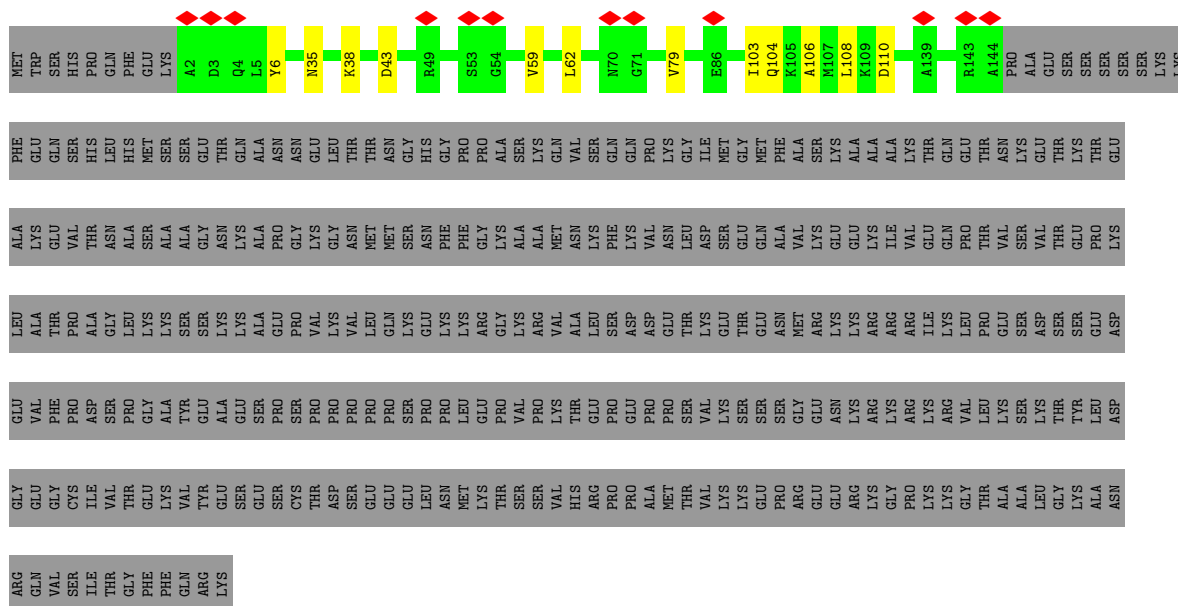
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	Fe	S	0
			8	4	4	

- Molecule 11 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).

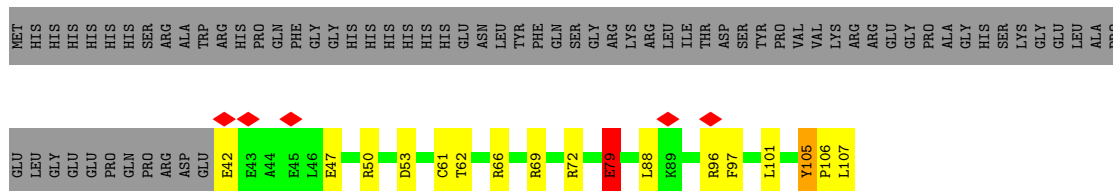
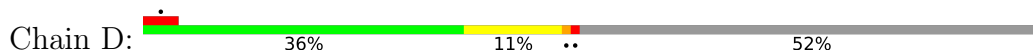


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			29	10	2	14	3	

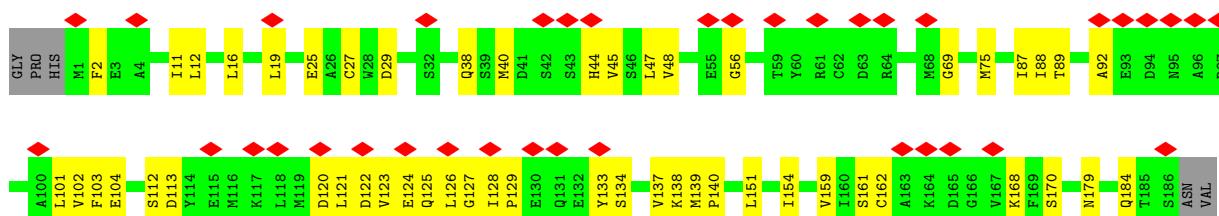
- Molecule 3: DNA polymerase delta subunit 3

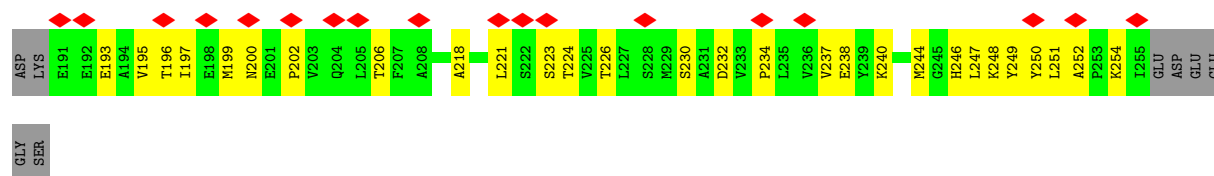


- Molecule 4: DNA polymerase delta subunit 4

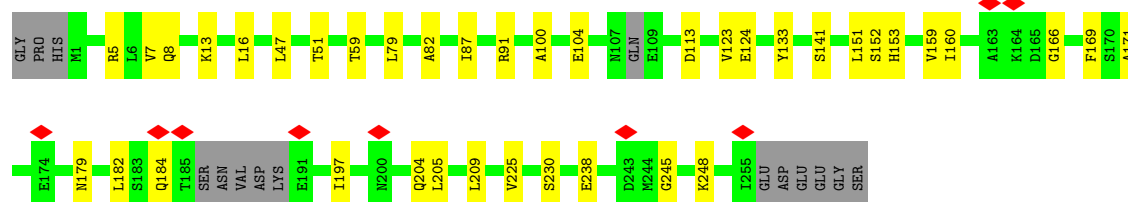
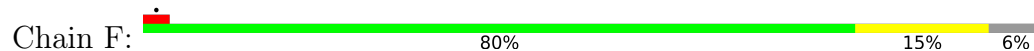


- Molecule 5: Proliferating cell nuclear antigen

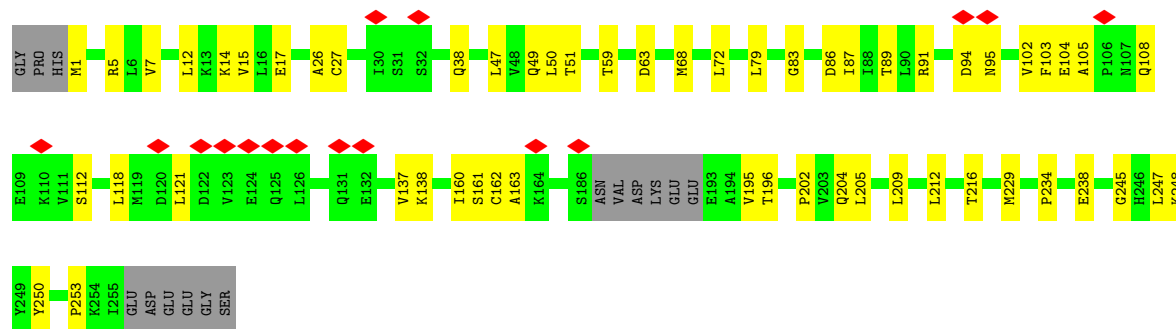
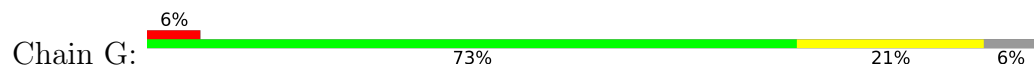




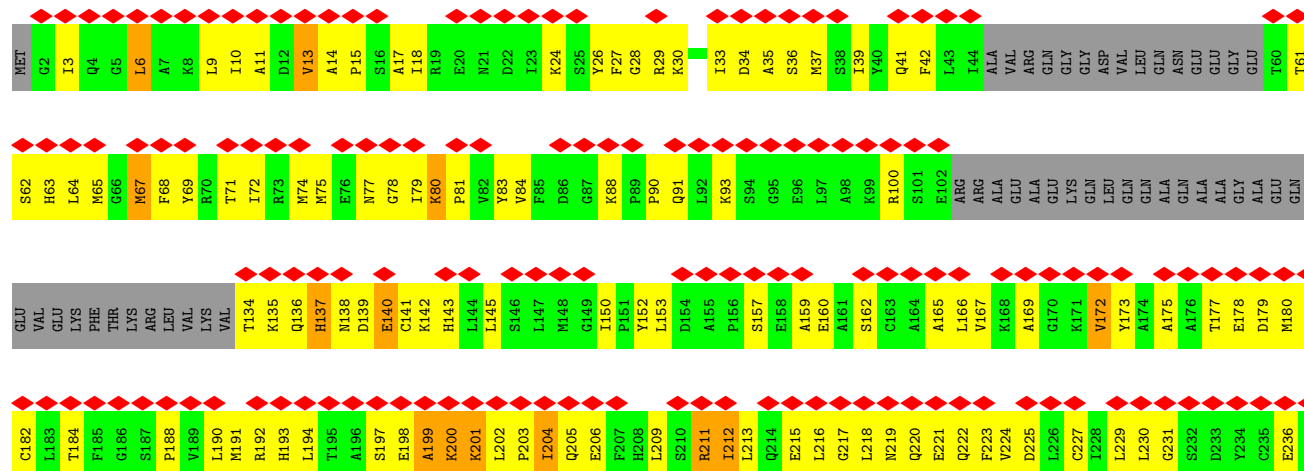
• Molecule 5: Proliferating cell nuclear antigen

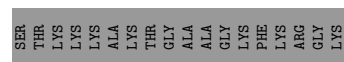


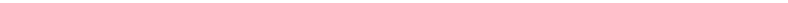
• Molecule 5: Proliferating cell nuclear antigen

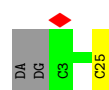


• Molecule 6: Flap endonuclease 1

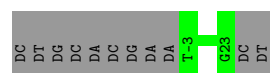




- Chain P:  88% 8%



- Chain T: 71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	57471	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0073	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, ZN, DOC, SF4

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	0.36	0/8094	0.70	11/10971 (0.1%)
2	B	0.38	0/3380	0.66	4/4604 (0.1%)
3	C	0.27	0/1149	0.57	0/1553
4	D	0.44	0/574	0.90	0/783
5	E	0.26	0/1949	0.59	0/2632
5	F	0.30	0/1937	0.61	0/2614
5	G	0.26	0/1938	0.58	0/2617
6	H	0.42	1/2322 (0.0%)	0.95	8/3141 (0.3%)
7	P	0.35	0/505	0.54	0/777
8	T	0.36	0/622	0.57	0/958
All	All	0.35	1/22470 (0.0%)	0.69	23/30650 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	338	GLY	N-CA	-5.54	1.37	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	ALA	N-CA-C	7.47	119.42	111.28
1	A	1098	ARG	N-CA-C	-6.99	103.74	111.36
6	H	241	ILE	N-CA-C	6.92	119.40	109.51
1	A	592	GLY	N-CA-C	6.65	118.98	110.20
1	A	1024	ALA	N-CA-C	6.58	118.45	111.28
6	H	266	ASN	N-CA-C	-6.31	105.95	113.21
6	H	211	ARG	N-CA-C	-6.04	106.04	113.41
1	A	82	PRO	CA-C-N	6.03	132.41	120.94
1	A	82	PRO	C-N-CA	6.03	132.41	120.94
2	B	331	PRO	N-CA-C	-5.77	101.15	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	331	PRO	CA-C-N	-5.66	114.01	122.39
2	B	331	PRO	C-N-CA	-5.66	114.01	122.39
6	H	212	ILE	N-CA-C	-5.53	104.93	110.30
1	A	1079	PHE	CA-C-N	5.46	131.97	121.54
1	A	1079	PHE	C-N-CA	5.46	131.97	121.54
1	A	1091	ASP	N-CA-C	5.41	117.26	111.36
1	A	1099	PHE	N-CA-C	-5.34	103.48	110.53
6	H	140	GLU	N-CA-C	-5.16	106.67	112.87
1	A	1022	GLN	N-CA-C	5.14	119.54	113.16
6	H	100	ARG	N-CA-C	-5.06	106.88	113.16
1	A	421	LEU	N-CA-C	5.06	118.94	112.87
6	H	80	LYS	CA-C-N	5.01	125.45	120.14
6	H	80	LYS	C-N-CA	5.01	125.45	120.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7926	0	7967	133	0
2	B	3304	0	3255	34	0
3	C	1130	0	1138	7	0
4	D	554	0	537	11	0
5	E	1924	0	1929	146	0
5	F	1913	0	1922	24	0
5	G	1913	0	1928	33	0
6	H	2282	0	2178	332	0
7	P	469	0	261	0	0
8	T	555	0	307	0	0
9	A	1	0	0	0	0
10	A	8	0	0	2	0
11	A	29	0	10	0	0
All	All	22008	0	21432	617	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 14.

All (617) 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)
5:E:234:PRO:HG2	6:H:344:PHE:CZ	1.31	1.58
1:A:861:VAL:CG1	1:A:985:ARG:HD3	1.40	1.48
5:E:27:CYS:SG	6:H:350:LEU:CG	2.02	1.47
1:A:688:GLY:HA2	1:A:691:LEU:CD2	1.43	1.46
1:A:861:VAL:HG11	1:A:985:ARG:NE	1.28	1.42
5:E:27:CYS:SG	6:H:350:LEU:HD12	1.60	1.41
1:A:861:VAL:CG1	1:A:985:ARG:CD	1.98	1.41
5:E:27:CYS:SG	6:H:350:LEU:CD1	2.10	1.40
5:E:129:PRO:CD	6:H:344:PHE:CD1	2.06	1.38
1:A:861:VAL:HG13	1:A:985:ARG:CD	1.52	1.34
5:E:40:MET:CE	5:E:126:LEU:HD21	1.58	1.33
5:E:252:ALA:HB2	6:H:340:LEU:CD2	1.62	1.27
5:E:27:CYS:SG	6:H:350:LEU:HG	1.66	1.23
5:E:234:PRO:HG2	6:H:344:PHE:CE2	1.72	1.22
5:E:234:PRO:CG	6:H:344:PHE:CZ	2.22	1.22
5:E:232:ASP:O	6:H:343:PHE:CE1	1.92	1.20
5:E:69:GLY:HA3	5:E:121:LEU:CD1	1.72	1.18
5:E:129:PRO:HD3	6:H:344:PHE:CD1	1.70	1.17
1:A:981:ALA:HB1	1:A:985:ARG:NH1	1.61	1.16
5:E:126:LEU:HA	6:H:347:THR:N	1.60	1.14
1:A:861:VAL:CG1	1:A:985:ARG:NE	2.09	1.14
6:H:28:GLY:HA2	6:H:335:SER:N	1.59	1.14
5:E:129:PRO:HD2	6:H:344:PHE:CD1	1.80	1.11
5:E:252:ALA:CB	6:H:340:LEU:HD23	1.83	1.09
1:A:688:GLY:O	1:A:691:LEU:HG	1.53	1.08
5:E:27:CYS:SG	6:H:350:LEU:CB	2.42	1.07
1:A:688:GLY:HA2	1:A:691:LEU:HD23	1.37	1.05
6:H:28:GLY:HA2	6:H:334:GLY:C	1.81	1.05
5:E:125:GLN:O	6:H:348:GLY:N	1.87	1.04
1:A:981:ALA:CB	1:A:985:ARG:HH12	1.70	1.04
5:E:129:PRO:HD2	6:H:344:PHE:CE1	1.91	1.04
5:E:126:LEU:CA	6:H:347:THR:H	1.70	1.03
5:E:69:GLY:HA3	5:E:121:LEU:HD11	1.37	1.03
5:E:40:MET:HE3	5:E:126:LEU:HD21	1.38	1.02
5:E:129:PRO:CD	6:H:344:PHE:HD1	1.52	1.02
1:A:688:GLY:HA2	1:A:691:LEU:HD21	1.06	1.01
1:A:688:GLY:CA	1:A:691:LEU:CD2	2.38	1.00
5:E:126:LEU:CB	6:H:346:VAL:HA	1.92	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:CYS:SG	6:H:350:LEU:HB3	2.01	1.00
1:A:981:ALA:HB1	1:A:985:ARG:HH12	0.83	0.99
5:E:252:ALA:HB2	6:H:340:LEU:HD23	0.99	0.98
6:H:27:PHE:CD2	6:H:77:ASN:O	2.16	0.97
6:H:330:LYS:HE2	6:H:330:LYS:HA	1.44	0.97
1:A:688:GLY:CA	1:A:691:LEU:HD21	1.96	0.96
5:E:126:LEU:HB3	6:H:346:VAL:HA	1.46	0.95
5:E:40:MET:CE	5:E:126:LEU:CD2	2.45	0.95
1:A:861:VAL:HG11	1:A:985:ARG:CD	1.81	0.95
1:A:1026:CYS:O	1:A:1030:GLN:HG3	1.67	0.95
6:H:29:ARG:HD3	6:H:173:TYR:CD2	2.01	0.94
1:A:861:VAL:HG13	1:A:985:ARG:HD3	0.95	0.94
5:E:69:GLY:CA	5:E:121:LEU:CD1	2.45	0.93
5:E:69:GLY:CA	5:E:121:LEU:HD11	1.98	0.93
5:E:234:PRO:HG2	6:H:344:PHE:HZ	1.15	0.92
6:H:238:ILE:HG23	6:H:241:ILE:HD11	1.51	0.92
6:H:26:TYR:CE1	6:H:29:ARG:NH1	2.38	0.91
5:E:44:HIS:CD2	6:H:339:ARG:HD3	2.07	0.90
5:E:123:VAL:O	6:H:349:SER:HA	1.72	0.90
5:E:232:ASP:O	6:H:343:PHE:CZ	2.24	0.89
6:H:28:GLY:HA3	6:H:335:SER:HA	1.54	0.89
5:E:123:VAL:O	6:H:349:SER:CA	2.21	0.89
6:H:184:THR:HG22	6:H:227:CYS:SG	2.11	0.89
5:E:69:GLY:HA3	5:E:121:LEU:HD12	1.54	0.89
5:E:121:LEU:N	6:H:352:SER:OG	2.06	0.88
6:H:71:THR:HG21	6:H:150:ILE:HD13	1.53	0.87
6:H:28:GLY:CA	6:H:334:GLY:C	2.48	0.87
5:E:121:LEU:HB2	6:H:352:SER:H	1.39	0.85
5:E:252:ALA:CB	6:H:340:LEU:CD2	2.50	0.85
5:E:121:LEU:O	6:H:351:SER:HB3	1.75	0.85
1:A:164:LEU:HB3	1:A:190:VAL:HG11	1.59	0.85
5:E:40:MET:HE3	5:E:126:LEU:CD2	2.04	0.84
6:H:27:PHE:CD1	6:H:78:GLY:HA3	2.12	0.84
5:E:123:VAL:O	6:H:349:SER:CB	2.25	0.84
5:E:234:PRO:CG	6:H:344:PHE:HZ	1.75	0.83
5:E:121:LEU:O	6:H:351:SER:CB	2.27	0.83
5:E:40:MET:HE2	5:E:126:LEU:HD21	1.61	0.83
5:E:129:PRO:CG	6:H:344:PHE:HD1	1.92	0.83
6:H:254:LYS:H	6:H:254:LYS:HD2	1.41	0.82
5:E:120:ASP:HA	6:H:352:SER:OG	1.79	0.82
6:H:28:GLY:CA	6:H:335:SER:N	2.42	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:GLN:N	6:H:348:GLY:O	2.12	0.82
5:E:126:LEU:HA	6:H:347:THR:H	0.75	0.81
6:H:28:GLY:CA	6:H:335:SER:HA	2.11	0.81
5:E:121:LEU:O	6:H:351:SER:HA	1.82	0.80
5:E:121:LEU:O	6:H:351:SER:CA	2.29	0.79
5:E:120:ASP:HA	6:H:352:SER:HG	1.47	0.79
1:A:1038:GLN:HE22	2:B:273:VAL:HA	1.48	0.79
6:H:152:TYR:O	6:H:153:LEU:HD12	1.82	0.79
5:E:252:ALA:HB2	6:H:340:LEU:CG	2.13	0.79
6:H:152:TYR:C	6:H:153:LEU:HD12	2.08	0.79
1:A:188:LEU:HA	1:A:213:THR:O	1.82	0.77
1:A:861:VAL:HG11	1:A:985:ARG:HE	0.96	0.77
6:H:27:PHE:CE1	6:H:334:GLY:HA2	2.19	0.77
5:E:69:GLY:CA	5:E:121:LEU:HD12	2.13	0.77
5:E:125:GLN:O	6:H:347:THR:N	2.19	0.76
6:H:26:TYR:CD1	6:H:29:ARG:NH1	2.53	0.76
5:E:123:VAL:O	6:H:349:SER:HB3	1.85	0.76
5:E:40:MET:HE1	5:E:126:LEU:HD21	1.67	0.75
6:H:30:LYS:O	6:H:172:VAL:HG22	1.87	0.75
1:A:1078:ILE:HG13	10:A:1202:SF4:S1	2.26	0.75
5:E:125:GLN:OE1	6:H:350:LEU:HB2	1.86	0.75
1:A:861:VAL:HG12	1:A:985:ARG:HD3	1.63	0.74
6:H:254:LYS:HD2	6:H:254:LYS:N	2.01	0.74
5:E:232:ASP:OD1	6:H:343:PHE:HZ	1.70	0.74
6:H:26:TYR:CE2	6:H:204:ILE:HG12	2.23	0.74
5:E:234:PRO:CG	6:H:344:PHE:CE2	2.62	0.73
1:A:861:VAL:HG13	1:A:985:ARG:HD2	1.66	0.73
6:H:284:LEU:O	6:H:286:PRO:HD3	1.87	0.73
6:H:177:THR:HG22	6:H:178:GLU:H	1.52	0.73
1:A:1011:CYS:O	1:A:1098:ARG:NH1	2.22	0.72
5:E:125:GLN:O	6:H:347:THR:CA	2.37	0.72
1:A:164:LEU:HB3	1:A:190:VAL:HG21	1.72	0.72
1:A:188:LEU:N	1:A:188:LEU:HD23	2.04	0.71
6:H:221:GLU:HG2	6:H:284:LEU:HD11	1.71	0.71
5:E:128:ILE:HD11	6:H:344:PHE:CZ	2.25	0.71
5:F:166:GLY:HA3	5:F:182:LEU:O	1.90	0.71
6:H:272:GLU:HG3	6:H:273:ASN:H	1.56	0.71
6:H:67:MET:HE1	6:H:83:TYR:CD2	2.26	0.70
6:H:27:PHE:CD2	6:H:77:ASN:C	2.70	0.69
6:H:28:GLY:CA	6:H:335:SER:CA	2.69	0.69
5:E:120:ASP:C	6:H:352:SER:OG	2.36	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:GLY:CA	1:A:691:LEU:HD23	2.13	0.69
5:E:103:PHE:HB2	5:E:112:SER:HB2	1.75	0.69
6:H:321:ILE:O	6:H:325:VAL:HG22	1.93	0.69
5:E:234:PRO:HA	5:E:251:LEU:O	1.94	0.68
6:H:242:GLY:H	6:H:245:ARG:HB3	1.58	0.68
6:H:282:LEU:O	6:H:286:PRO:HG3	1.94	0.68
6:H:134:THR:HG22	6:H:135:LYS:H	1.58	0.68
5:E:126:LEU:HD13	6:H:344:PHE:HB2	1.76	0.68
6:H:264:ASP:N	6:H:265:PRO:HD2	2.09	0.68
6:H:27:PHE:CG	6:H:78:GLY:HA3	2.29	0.67
6:H:219:ASN:H	6:H:222:GLN:NE2	1.92	0.67
5:E:127:GLY:O	6:H:344:PHE:HB3	1.93	0.67
6:H:11:ALA:O	6:H:15:PRO:HG3	1.93	0.67
5:E:29:ASP:OD1	6:H:350:LEU:HD21	1.94	0.67
1:A:1091:ASP:OD1	1:A:1092:GLN:N	2.28	0.67
6:H:63:HIS:O	6:H:64:LEU:HD23	1.94	0.67
5:E:125:GLN:C	6:H:347:THR:HB	2.20	0.66
6:H:3:ILE:HG22	6:H:6:LEU:HB2	1.77	0.66
6:H:336:THR:HG22	6:H:337:GLN:H	1.61	0.66
6:H:78:GLY:O	6:H:334:GLY:HA3	1.96	0.66
1:A:1024:ALA:HB2	1:A:1098:ARG:HB3	1.76	0.66
5:G:27:CYS:HB3	5:G:121:LEU:HD21	1.78	0.66
6:H:264:ASP:H	6:H:265:PRO:CD	2.09	0.66
6:H:260:VAL:HG23	6:H:261:ARG:H	1.59	0.65
1:A:1026:CYS:O	1:A:1030:GLN:CG	2.43	0.65
5:F:166:GLY:HA2	5:F:197:ILE:HD13	1.77	0.65
6:H:141:CYS:C	6:H:143:HIS:H	2.02	0.65
1:A:525:ARG:O	1:A:682:ARG:NH2	2.29	0.65
5:E:120:ASP:CA	6:H:352:SER:OG	2.43	0.65
6:H:289:LEU:HD12	6:H:289:LEU:O	1.97	0.65
5:E:252:ALA:N	6:H:340:LEU:HD21	2.12	0.65
6:H:264:ASP:H	6:H:265:PRO:HD2	1.62	0.65
6:H:137:HIS:H	6:H:137:HIS:CD2	2.13	0.64
6:H:200:LYS:HB3	6:H:202:LEU:HD13	1.79	0.64
6:H:340:LEU:HD22	6:H:344:PHE:HE2	1.62	0.64
1:A:1027:GLU:HA	1:A:1030:GLN:CD	2.23	0.64
5:E:238:GLU:HG3	5:E:248:LYS:HG2	1.80	0.64
1:A:1002:LEU:HD21	5:F:47:LEU:HB2	1.79	0.64
5:G:47:LEU:HB3	5:G:250:TYR:HB2	1.80	0.64
6:H:340:LEU:HD22	6:H:344:PHE:CE2	2.34	0.63
6:H:263:LEU:HD12	6:H:263:LEU:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:27:PHE:CD1	6:H:334:GLY:HA2	2.33	0.62
6:H:28:GLY:HA2	6:H:335:SER:CA	2.28	0.62
6:H:64:LEU:HD11	6:H:140:GLU:HG2	1.80	0.62
5:E:128:ILE:CD1	6:H:344:PHE:CZ	2.82	0.62
5:E:129:PRO:HD3	6:H:344:PHE:CG	2.30	0.62
1:A:995:LEU:HB2	5:F:123:VAL:HA	1.80	0.62
6:H:26:TYR:OH	6:H:206:GLU:HG3	1.98	0.62
1:A:188:LEU:HD23	1:A:188:LEU:H	1.65	0.62
2:B:73:TRP:NE1	2:B:175:ASP:OD2	2.33	0.62
1:A:674:LEU:HD13	1:A:686:LEU:HB2	1.82	0.61
6:H:135:LYS:HD2	6:H:135:LYS:C	2.25	0.61
5:E:128:ILE:CD1	6:H:344:PHE:CE2	2.84	0.61
6:H:162:SER:O	6:H:165:ALA:HB3	2.00	0.61
6:H:304:GLU:HA	6:H:307:ILE:HG22	1.81	0.61
6:H:159:ALA:O	6:H:162:SER:N	2.33	0.61
5:E:125:GLN:O	6:H:347:THR:C	2.44	0.61
6:H:9:LEU:O	6:H:13:VAL:HG13	2.00	0.61
6:H:300:GLU:CD	6:H:301:PRO:HD2	2.25	0.61
1:A:432:ARG:HH21	1:A:434:SER:HB2	1.66	0.61
6:H:265:PRO:C	6:H:267:LYS:H	2.07	0.61
4:D:42:GLU:OE2	4:D:96:ARG:NH2	2.34	0.60
4:D:53:ASP:OD2	4:D:66:ARG:NH2	2.31	0.60
5:E:87:ILE:HB	5:E:104:GLU:HB2	1.82	0.60
1:A:583:GLY:O	1:A:725:ARG:NH1	2.34	0.60
5:E:226:THR:HB	5:E:238:GLU:HB2	1.83	0.60
6:H:311:CYS:SG	6:H:318:GLU:HA	2.42	0.60
1:A:1013:ILE:HD12	1:A:1024:ALA:HB1	1.84	0.60
1:A:525:ARG:HG2	1:A:682:ARG:HH22	1.67	0.60
5:F:5:ARG:HB3	5:F:59:THR:HB	1.84	0.60
1:A:995:LEU:HD22	5:F:124:GLU:H	1.67	0.60
6:H:218:LEU:HB2	6:H:222:GLN:HB2	1.83	0.60
4:D:61:CYS:SG	4:D:72:ARG:NH2	2.75	0.59
6:H:28:GLY:HA3	6:H:335:SER:CA	2.28	0.59
6:H:134:THR:HG22	6:H:135:LYS:N	2.17	0.59
1:A:186:ALA:HB3	1:A:188:LEU:CD2	2.33	0.59
1:A:187:VAL:HG22	1:A:187:VAL:O	2.02	0.59
1:A:1088:ASP:HA	1:A:1091:ASP:OD2	2.02	0.59
1:A:688:GLY:C	1:A:691:LEU:HG	2.24	0.59
1:A:986:GLY:O	1:A:990:ARG:N	2.36	0.59
5:E:234:PRO:CB	6:H:344:PHE:HZ	2.15	0.59
6:H:71:THR:HA	6:H:74:MET:HE3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:137:HIS:H	6:H:137:HIS:HD2	1.51	0.59
6:H:14:ALA:N	6:H:15:PRO:HD3	2.18	0.59
6:H:27:PHE:CE1	6:H:78:GLY:HA3	2.38	0.59
6:H:241:ILE:HG21	6:H:249:LEU:HD22	1.85	0.58
6:H:270:VAL:HG13	6:H:271:PRO:HD2	1.84	0.58
6:H:67:MET:HE1	6:H:145:LEU:HD11	1.84	0.58
5:G:238:GLU:HG3	5:G:248:LYS:HG2	1.85	0.58
5:E:133:TYR:HA	5:E:230:SER:HB2	1.85	0.58
1:A:1062:GLN:NE2	1:A:1068:ASP:O	2.37	0.58
2:B:184:GLN:HB2	2:B:398:CYS:HB3	1.85	0.58
1:A:186:ALA:HB3	1:A:188:LEU:HD21	1.86	0.58
5:E:125:GLN:O	6:H:347:THR:HB	2.03	0.58
5:F:7:VAL:HA	5:F:87:ILE:HG23	1.86	0.58
5:G:104:GLU:HB3	5:G:108:GLN:HE22	1.69	0.58
5:F:152:SER:HA	5:F:209:LEU:HD13	1.86	0.57
6:H:264:ASP:N	6:H:265:PRO:CD	2.66	0.57
1:A:539:THR:HA	1:A:558:GLN:HE21	1.69	0.57
5:E:121:LEU:HB2	6:H:352:SER:N	2.16	0.57
6:H:194:LEU:HG	6:H:194:LEU:O	2.04	0.57
1:A:357:LEU:HD11	1:A:374:GLU:HG2	1.85	0.57
1:A:688:GLY:O	1:A:691:LEU:CG	2.41	0.57
1:A:1056:THR:HG23	1:A:1060:ARG:HH21	1.70	0.57
6:H:308:LYS:NZ	6:H:308:LYS:HB3	2.19	0.57
1:A:161:MET:O	1:A:165:GLN:NE2	2.37	0.57
1:A:628:GLN:HB3	1:A:629:LYS:HD3	1.86	0.57
1:A:1039:LYS:O	1:A:1040:GLU:HG2	2.04	0.57
5:E:254:LYS:HA	6:H:337:GLN:HA	1.87	0.57
1:A:983:LEU:O	1:A:990:ARG:NH1	2.38	0.57
6:H:134:THR:C	6:H:136:GLN:H	2.11	0.57
2:B:1:MET:HG2	2:B:441:ASN:HD22	1.69	0.57
5:E:126:LEU:HB2	6:H:345:LYS:O	2.04	0.56
5:E:126:LEU:HB2	6:H:346:VAL:HA	1.82	0.56
6:H:27:PHE:CE2	6:H:77:ASN:C	2.83	0.56
1:A:981:ALA:O	1:A:985:ARG:HG3	2.05	0.56
6:H:29:ARG:HD3	6:H:173:TYR:CE2	2.41	0.56
5:F:5:ARG:NH2	5:F:104:GLU:OE1	2.38	0.56
6:H:37:MET:SD	6:H:177:THR:HG22	2.46	0.56
6:H:268:TYR:N	6:H:269:PRO:HD3	2.20	0.56
6:H:275:LEU:HD22	6:H:275:LEU:N	2.21	0.56
6:H:302:ASN:HD22	6:H:302:ASN:C	2.14	0.56
5:E:237:VAL:HG22	5:E:249:TYR:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:234:PRO:HA	5:G:253:PRO:HD3	1.87	0.56
5:E:29:ASP:OD1	6:H:350:LEU:CD2	2.53	0.56
5:G:89:THR:HB	5:G:102:VAL:HB	1.87	0.56
6:H:199:ALA:O	6:H:201:LYS:N	2.38	0.56
6:H:260:VAL:HG23	6:H:261:ARG:N	2.20	0.56
6:H:218:LEU:HB2	6:H:222:GLN:CB	2.36	0.56
6:H:307:ILE:HD11	6:H:311:CYS:SG	2.46	0.56
1:A:587:ILE:HD13	1:A:732:LYS:HD3	1.88	0.56
2:B:134:VAL:HG11	2:B:141:ARG:HH11	1.70	0.56
5:E:40:MET:HE2	5:E:126:LEU:CD2	2.28	0.56
6:H:6:LEU:HD22	6:H:10:ILE:HD11	1.87	0.56
1:A:142:HIS:NE2	1:A:289:ASP:OD1	2.38	0.56
6:H:26:TYR:OH	6:H:204:ILE:HD11	2.05	0.56
6:H:225:ASP:O	6:H:229:LEU:HG	2.06	0.56
1:A:1030:GLN:H	1:A:1031:PRO:CD	2.19	0.55
2:B:307:PRO:O	2:B:309:GLN:NE2	2.37	0.55
5:E:129:PRO:HD3	6:H:344:PHE:HD1	1.27	0.55
6:H:26:TYR:HH	6:H:206:GLU:HG3	1.70	0.55
1:A:1030:GLN:N	1:A:1031:PRO:CD	2.69	0.55
6:H:322:ARG:O	6:H:325:VAL:HG23	2.06	0.55
6:H:27:PHE:CG	6:H:77:ASN:O	2.60	0.55
6:H:71:THR:O	6:H:75:MET:HG2	2.06	0.55
5:E:47:LEU:HB3	5:E:250:TYR:HD2	1.72	0.55
1:A:981:ALA:CB	1:A:985:ARG:NH1	2.44	0.55
3:C:35:ASN:HA	3:C:38:LYS:HD2	1.88	0.55
6:H:14:ALA:HB1	6:H:215:GLU:HG3	1.89	0.54
1:A:153:PRO:HD2	1:A:158:PRO:HG2	1.88	0.54
6:H:258:GLU:OE1	6:H:262:ARG:NH2	2.41	0.54
6:H:74:MET:O	6:H:79:ILE:HB	2.08	0.54
5:E:139:MET:HE3	5:E:140:PRO:HD2	1.88	0.54
5:E:89:THR:HB	5:E:102:VAL:HB	1.90	0.54
5:E:232:ASP:OD1	6:H:343:PHE:CZ	2.56	0.54
2:B:295:MET:HG3	2:B:328:VAL:HG23	1.89	0.54
5:G:51:THR:O	5:G:245:GLY:HA3	2.08	0.54
6:H:33:ILE:HG22	6:H:34:ASP:N	2.22	0.54
2:B:32:TYR:HH	2:B:332:TYR:HH	1.52	0.54
4:D:66:ARG:NH1	4:D:97:PHE:O	2.41	0.54
6:H:330:LYS:HE2	6:H:330:LYS:CA	2.27	0.54
5:E:161:SER:HB3	5:E:168:LYS:HB2	1.90	0.54
6:H:263:LEU:HD12	6:H:263:LEU:C	2.33	0.54
6:H:332:ARG:O	6:H:333:GLN:CB	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:HIS:C	1:A:1021:HIS:CD2	2.86	0.53
2:B:298:GLU:HG3	2:B:347:GLN:HE21	1.73	0.53
4:D:47:GLU:OE1	4:D:50:ARG:NH1	2.41	0.53
6:H:69:TYR:O	6:H:72:ILE:HB	2.08	0.53
6:H:27:PHE:HD1	6:H:334:GLY:O	1.91	0.53
6:H:141:CYS:C	6:H:143:HIS:N	2.63	0.53
6:H:275:LEU:C	6:H:277:LYS:H	2.14	0.53
2:B:356:SER:OG	2:B:357:SER:N	2.40	0.53
5:E:252:ALA:HB2	6:H:340:LEU:HA	1.90	0.53
5:E:44:HIS:NE2	6:H:339:ARG:HD3	2.23	0.53
1:A:687:ASP:O	1:A:691:LEU:HD23	2.09	0.53
5:G:162:CYS:O	5:G:202:PRO:HA	2.08	0.53
6:H:65:MET:O	6:H:68:PHE:HB3	2.09	0.53
5:G:137:VAL:HA	5:G:196:THR:O	2.08	0.53
2:B:404:CYS:SG	2:B:405:GLY:N	2.79	0.53
5:E:234:PRO:CD	6:H:344:PHE:CZ	2.91	0.53
2:B:330:ASN:HB3	2:B:331:PRO:HD3	1.90	0.53
5:E:113:ASP:OD1	5:E:113:ASP:N	2.40	0.53
1:A:164:LEU:CB	1:A:190:VAL:HG21	2.38	0.53
5:F:91:ARG:HB3	5:F:100:ALA:HB3	1.90	0.53
1:A:617:CYS:HB3	1:A:620:THR:HG22	1.91	0.52
5:E:2:PHE:HB3	5:E:92:ALA:HB3	1.91	0.52
3:C:110:ASP:OD1	3:C:110:ASP:N	2.42	0.52
5:E:44:HIS:HD2	6:H:339:ARG:HD3	1.68	0.52
5:G:103:PHE:HB2	5:G:112:SER:HB2	1.92	0.52
6:H:220:GLN:O	6:H:223:PHE:HB3	2.09	0.52
5:F:113:ASP:OD1	5:F:113:ASP:N	2.40	0.52
6:H:273:ASN:O	6:H:275:LEU:HD22	2.09	0.52
3:C:59:VAL:HG12	3:C:103:ILE:HG22	1.92	0.52
5:G:7:VAL:HA	5:G:87:ILE:HG23	1.92	0.52
6:H:275:LEU:C	6:H:277:LYS:N	2.66	0.52
2:B:308:GLN:OE1	2:B:330:ASN:ND2	2.42	0.52
1:A:171:ALA:H	1:A:180:ARG:HG3	1.75	0.52
1:A:232:ARG:HH12	1:A:242:ALA:HB3	1.75	0.52
1:A:1027:GLU:HA	1:A:1030:GLN:NE2	2.25	0.51
5:E:124:GLU:HA	6:H:348:GLY:O	2.10	0.51
6:H:181:ALA:O	6:H:184:THR:N	2.42	0.51
6:H:321:ILE:O	6:H:321:ILE:HG22	2.11	0.51
1:A:394:THR:HG22	1:A:457:MET:HB2	1.91	0.51
6:H:88:LYS:HG3	6:H:88:LYS:O	2.10	0.51
6:H:303:GLU:O	6:H:307:ILE:HG22	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HB3	1:A:190:VAL:CG1	2.37	0.51
5:E:125:GLN:O	6:H:347:THR:CB	2.58	0.51
1:A:102:ASP:HB3	1:A:126:ARG:HB2	1.93	0.51
5:F:184:GLN:NE2	5:F:197:ILE:O	2.43	0.51
6:H:199:ALA:O	6:H:200:LYS:C	2.54	0.50
6:H:209:LEU:HD21	6:H:220:GLN:OE1	2.11	0.50
1:A:688:GLY:HA2	1:A:691:LEU:CG	2.34	0.50
6:H:3:ILE:HD12	6:H:3:ILE:N	2.25	0.50
6:H:61:THR:HG22	6:H:61:THR:O	2.12	0.50
1:A:191:GLU:HB3	1:A:211:ARG:HB3	1.93	0.50
5:E:128:ILE:HD12	6:H:344:PHE:CD2	2.46	0.50
6:H:275:LEU:HD22	6:H:275:LEU:H	1.76	0.50
6:H:336:THR:HG22	6:H:337:GLN:N	2.24	0.50
5:E:44:HIS:CD2	6:H:339:ARG:CD	2.87	0.50
5:E:128:ILE:HD12	6:H:344:PHE:CG	2.46	0.50
2:B:301:PRO:HG2	2:B:315:MET:HE1	1.93	0.50
5:F:16:LEU:HD22	5:F:79:LEU:HD12	1.93	0.50
1:A:984:LEU:HA	1:A:987:ASP:HB2	1.94	0.50
5:G:38:GLN:HG2	5:G:49:GLN:HG2	1.92	0.50
6:H:215:GLU:C	6:H:217:GLY:H	2.19	0.50
2:B:99:LYS:H	2:B:155:THR:HB	1.77	0.49
5:E:184:GLN:HG3	5:E:197:ILE:HD12	1.93	0.49
5:E:206:THR:HG23	5:E:254:LYS:HB2	1.92	0.49
1:A:974:LEU:HD22	1:A:978:ARG:HD3	1.95	0.49
5:G:161:SER:HB3	5:G:204:GLN:HE21	1.78	0.49
6:H:177:THR:HG22	6:H:178:GLU:N	2.23	0.49
5:E:16:LEU:HA	5:E:19:LEU:HB2	1.94	0.49
6:H:71:THR:HG21	6:H:150:ILE:CD1	2.36	0.49
1:A:587:ILE:HD12	1:A:754:GLY:HA3	1.94	0.49
5:E:126:LEU:HD12	5:E:126:LEU:C	2.38	0.49
5:G:105:ALA:O	5:G:108:GLN:NE2	2.45	0.49
5:G:138:LYS:O	5:G:195:VAL:HA	2.12	0.49
6:H:26:TYR:HD1	6:H:29:ARG:HD2	1.77	0.49
6:H:134:THR:C	6:H:136:GLN:N	2.70	0.49
6:H:316:PHE:HD1	6:H:317:SER:H	1.61	0.49
5:E:75:MET:HE1	5:E:101:LEU:HD11	1.94	0.49
1:A:248:VAL:HG11	1:A:560:LEU:HD11	1.95	0.49
2:B:18:SER:OG	2:B:19:ALA:N	2.45	0.49
1:A:421:LEU:H	1:A:421:LEU:HD22	1.78	0.48
2:B:276:VAL:HG11	2:B:315:MET:HB3	1.95	0.48
6:H:245:ARG:HG2	6:H:245:ARG:HH11	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:122:ASP:HA	6:H:351:SER:OG	2.13	0.48
6:H:63:HIS:C	6:H:64:LEU:HD23	2.38	0.48
6:H:221:GLU:HA	6:H:224:VAL:HG23	1.95	0.48
6:H:238:ILE:HG23	6:H:241:ILE:CD1	2.35	0.48
1:A:188:LEU:H	1:A:188:LEU:CD2	2.24	0.48
6:H:26:TYR:CZ	6:H:204:ILE:HG12	2.48	0.48
6:H:330:LYS:HA	6:H:330:LYS:CE	2.31	0.48
1:A:736:GLU:HG3	1:A:751:VAL:HG23	1.94	0.48
5:F:160:ILE:O	5:F:204:GLN:HA	2.13	0.48
6:H:30:LYS:C	6:H:172:VAL:HG22	2.38	0.48
1:A:1047:LEU:HB3	1:A:1089:LEU:HD13	1.96	0.48
2:B:49:GLN:NE2	4:D:62:THR:OG1	2.46	0.48
5:G:160:ILE:HD11	5:G:229:MET:HE3	1.96	0.48
5:E:162:CYS:O	5:E:202:PRO:HA	2.14	0.48
5:F:169:PHE:O	5:F:179:ASN:HA	2.14	0.48
6:H:80:LYS:HB3	6:H:298:TRP:CE2	2.49	0.48
5:E:44:HIS:HD2	6:H:339:ARG:CD	2.25	0.48
6:H:167:VAL:HG12	6:H:188:PRO:CG	2.43	0.48
1:A:1039:LYS:O	1:A:1040:GLU:CG	2.61	0.47
6:H:175:ALA:O	6:H:190:LEU:HD12	2.14	0.47
1:A:964:LYS:HG3	1:A:965:PRO:HD3	1.95	0.47
5:E:69:GLY:HA2	5:E:121:LEU:CD1	2.38	0.47
6:H:10:ILE:HG22	6:H:18:ILE:HD11	1.95	0.47
6:H:336:THR:O	6:H:337:GLN:O	2.32	0.47
5:E:128:ILE:HD12	6:H:344:PHE:CD1	2.49	0.47
6:H:67:MET:CE	6:H:145:LEU:HD21	2.44	0.47
5:G:68:MET:HB3	5:G:118:LEU:HD11	1.94	0.47
6:H:24:LYS:HA	6:H:77:ASN:HD22	1.79	0.47
1:A:467:TYR:O	1:A:472:TYR:OH	2.32	0.47
5:E:129:PRO:CG	6:H:344:PHE:CD1	2.78	0.47
5:E:69:GLY:HA2	5:E:121:LEU:HD11	1.93	0.47
5:G:205:LEU:HD13	5:G:253:PRO:HG3	1.95	0.47
3:C:6:TYR:OH	3:C:43:ASP:OD2	2.32	0.47
5:E:218:ALA:HA	5:E:221:LEU:HD23	1.96	0.47
6:H:30:LYS:HA	6:H:80:LYS:O	2.14	0.47
6:H:202:LEU:N	6:H:202:LEU:HD12	2.29	0.47
5:E:12:LEU:HD23	5:E:88:ILE:HG21	1.96	0.47
5:E:138:LYS:O	5:E:195:VAL:HA	2.15	0.47
6:H:251:GLN:O	6:H:254:LYS:NZ	2.43	0.47
1:A:240:SER:HA	1:A:241:PHE:HA	1.62	0.47
1:A:810:ALA:HA	1:A:825:ASP:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:LEU:HD23	2:B:107:ILE:HD13	1.96	0.47
1:A:1039:LYS:O	1:A:1040:GLU:CB	2.62	0.46
6:H:27:PHE:CE1	6:H:78:GLY:CA	2.97	0.46
6:H:167:VAL:HG12	6:H:188:PRO:HG2	1.96	0.46
5:E:240:LYS:HD3	5:E:246:HIS:HB3	1.96	0.46
6:H:63:HIS:CD2	6:H:137:HIS:HB2	2.50	0.46
5:E:252:ALA:CA	6:H:340:LEU:CD2	2.93	0.46
1:A:1088:ASP:O	1:A:1091:ASP:OD1	2.32	0.46
1:A:360:CYS:SG	1:A:361:ALA:N	2.84	0.46
1:A:611:MET:HE2	1:A:611:MET:HB3	1.85	0.46
5:E:252:ALA:CA	6:H:340:LEU:HD23	2.43	0.46
5:G:50:LEU:HD13	5:G:247:LEU:HD13	1.97	0.46
6:H:135:LYS:HA	6:H:138:ASN:HB3	1.97	0.46
2:B:240:ARG:NH2	2:B:293:ASP:OD2	2.37	0.46
6:H:3:ILE:N	6:H:3:ILE:CD1	2.79	0.46
1:A:163:ASP:HA	1:A:166:ARG:HB2	1.98	0.46
5:F:51:THR:O	5:F:245:GLY:HA3	2.16	0.46
1:A:618:TYR:OH	1:A:711:LEU:O	2.31	0.46
4:D:50:ARG:HG3	4:D:101:LEU:HD21	1.96	0.46
5:E:137:VAL:HA	5:E:196:THR:O	2.16	0.46
6:H:64:LEU:HA	6:H:67:MET:HB2	1.97	0.46
6:H:239:ARG:HG3	6:H:239:ARG:HH11	1.80	0.46
2:B:83:CYS:HB3	2:B:140:GLN:HE22	1.80	0.46
5:E:134:SER:HA	5:E:200:ASN:HD21	1.81	0.46
5:F:159:VAL:HA	5:F:205:LEU:O	2.16	0.46
6:H:265:PRO:C	6:H:267:LYS:N	2.73	0.46
1:A:1098:ARG:HG2	1:A:1098:ARG:NH2	2.31	0.46
5:E:121:LEU:C	6:H:351:SER:HA	2.38	0.46
2:B:439:LEU:HG	2:B:450:ILE:HD11	1.98	0.45
3:C:104:GLN:NE2	3:C:106:ALA:O	2.49	0.45
4:D:79:GLU:OE1	4:D:79:GLU:HA	2.13	0.45
5:F:13:LYS:NZ	5:F:82:ALA:O	2.43	0.45
6:H:302:ASN:C	6:H:302:ASN:ND2	2.74	0.45
1:A:186:ALA:C	1:A:188:LEU:HD23	2.41	0.45
5:G:5:ARG:HB3	5:G:59:THR:HB	1.99	0.45
6:H:62:SER:C	6:H:64:LEU:N	2.75	0.45
6:H:167:VAL:HG12	6:H:188:PRO:HD2	1.98	0.45
5:E:140:PRO:HG3	5:E:193:GLU:HA	1.98	0.45
6:H:3:ILE:HG12	6:H:227:CYS:HB3	1.98	0.45
6:H:6:LEU:HD22	6:H:10:ILE:CD1	2.47	0.45
6:H:74:MET:HE1	6:H:83:TYR:OH	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:219:ASN:CB	6:H:222:GLN:HE21	2.29	0.45
2:B:246:ASN:H	2:B:297:GLY:HA3	1.82	0.45
5:E:128:ILE:HD12	6:H:344:PHE:CE2	2.51	0.45
6:H:284:LEU:C	6:H:286:PRO:HD3	2.42	0.45
2:B:366:GLU:HG3	2:B:415:ILE:HD13	1.99	0.45
6:H:180:MET:O	6:H:181:ALA:C	2.59	0.45
1:A:843:LEU:HD22	1:A:867:VAL:HG11	1.99	0.45
2:B:70:GLN:HG2	2:B:77:VAL:HG11	1.99	0.45
6:H:35:ALA:HB3	6:H:84:VAL:O	2.17	0.45
6:H:139:ASP:C	6:H:141:CYS:H	2.24	0.45
6:H:143:HIS:C	6:H:145:LEU:N	2.75	0.45
6:H:200:LYS:C	6:H:202:LEU:H	2.24	0.45
6:H:204:ILE:HD11	6:H:206:GLU:HG3	1.99	0.45
6:H:238:ILE:O	6:H:240:GLY:N	2.50	0.45
1:A:834:ARG:HH21	1:A:921:ARG:HH11	1.65	0.45
1:A:1030:GLN:H	1:A:1031:PRO:HD2	1.82	0.45
6:H:298:TRP:HE3	6:H:298:TRP:H	1.64	0.45
6:H:37:MET:HE1	6:H:179:ASP:OD1	2.17	0.45
6:H:202:LEU:HA	6:H:203:PRO:HD3	1.84	0.45
6:H:135:LYS:HD2	6:H:135:LYS:O	2.17	0.44
1:A:736:GLU:OE2	1:A:751:VAL:N	2.39	0.44
6:H:289:LEU:HD12	6:H:289:LEU:C	2.43	0.44
6:H:316:PHE:O	6:H:317:SER:C	2.61	0.44
1:A:1107:TRP:CD1	1:A:1107:TRP:H	2.35	0.44
5:G:26:ALA:HB3	5:G:72:LEU:HD21	1.99	0.44
5:G:94:ASP:OD1	5:G:94:ASP:N	2.50	0.44
6:H:134:THR:O	6:H:137:HIS:CD2	2.71	0.44
6:H:244:LYS:HE3	6:H:244:LYS:HB2	1.86	0.44
5:F:151:LEU:HD22	5:F:171:ALA:HB3	1.99	0.44
1:A:164:LEU:CB	1:A:190:VAL:HG11	2.41	0.44
1:A:187:VAL:O	1:A:187:VAL:HG13	2.18	0.44
1:A:981:ALA:C	1:A:985:ARG:HH11	2.25	0.44
2:B:161:VAL:HG23	2:B:176:TYR:HB3	2.00	0.44
5:G:212:LEU:O	5:G:216:THR:OG1	2.29	0.44
5:E:252:ALA:HB2	6:H:340:LEU:HG	1.99	0.44
5:G:79:LEU:HA	5:G:103:PHE:HZ	1.82	0.44
6:H:166:LEU:O	6:H:169:ALA:N	2.50	0.44
6:H:91:GLN:HA	6:H:91:GLN:OE1	2.17	0.44
6:H:139:ASP:C	6:H:141:CYS:N	2.73	0.44
2:B:193:ASP:N	2:B:193:ASP:OD1	2.49	0.44
5:E:128:ILE:HD11	6:H:344:PHE:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:10:ILE:HD13	6:H:212:ILE:HD11	1.99	0.44
6:H:200:LYS:CB	6:H:202:LEU:HD13	2.47	0.44
5:E:56:GLY:HA3	5:E:244:MET:HA	1.99	0.44
6:H:220:GLN:O	6:H:224:VAL:HG23	2.18	0.44
1:A:1078:ILE:CG1	10:A:1202:SF4:S1	2.99	0.43
6:H:279:ALA:C	6:H:281:GLN:N	2.75	0.43
6:H:236:GLU:HG3	6:H:271:PRO:HB3	2.00	0.43
1:A:594:TYR:HB2	1:A:801:TYR:HB3	2.00	0.43
1:A:815:SER:OG	1:A:819:ASP:OD2	2.35	0.43
4:D:66:ARG:HG2	4:D:88:LEU:HD11	2.01	0.43
5:F:238:GLU:HG3	5:F:248:LYS:HG2	2.00	0.43
1:A:682:ARG:HA	1:A:685:VAL:HG22	2.00	0.43
5:F:133:TYR:HA	5:F:230:SER:HB2	1.99	0.43
5:G:12:LEU:HA	5:G:15:VAL:HB	2.00	0.43
6:H:204:ILE:HD12	6:H:205:GLN:N	2.33	0.43
5:E:25:GLU:OE2	5:E:121:LEU:HD22	2.19	0.43
5:E:124:GLU:HA	6:H:349:SER:OG	2.19	0.43
5:E:128:ILE:HD12	6:H:344:PHE:CE1	2.54	0.43
5:E:254:LYS:HA	6:H:338:GLY:H	1.83	0.43
6:H:67:MET:HE1	6:H:145:LEU:HD21	2.01	0.43
6:H:254:LYS:O	6:H:255:SER:HB3	2.18	0.43
1:A:687:ASP:OD1	1:A:690:GLN:NE2	2.50	0.43
5:F:141:SER:HB3	5:F:225:VAL:HG13	2.01	0.43
6:H:218:LEU:HD12	6:H:218:LEU:O	2.19	0.43
6:H:239:ARG:HG3	6:H:239:ARG:NH1	2.33	0.43
1:A:1030:GLN:N	1:A:1031:PRO:HD2	2.34	0.43
6:H:198:GLU:CD	6:H:198:GLU:H	2.26	0.43
1:A:617:CYS:SG	1:A:618:TYR:N	2.92	0.43
5:E:254:LYS:HD2	6:H:337:GLN:CB	2.49	0.43
5:G:83:GLY:N	5:G:86:ASP:OD2	2.52	0.43
1:A:1098:ARG:CG	1:A:1098:ARG:HH21	2.32	0.43
6:H:10:ILE:CG2	6:H:18:ILE:HD11	2.49	0.43
6:H:236:GLU:CD	6:H:236:GLU:H	2.27	0.43
6:H:304:GLU:O	6:H:305:GLU:C	2.61	0.43
1:A:594:TYR:HE2	1:A:762:ARG:HH11	1.67	0.42
1:A:830:GLU:HG3	1:A:965:PRO:HB3	1.99	0.42
6:H:225:ASP:HB3	6:H:250:ILE:HD11	2.01	0.42
1:A:188:LEU:CA	1:A:213:THR:O	2.62	0.42
2:B:378:ALA:HA	2:B:379:PRO:HA	1.81	0.42
2:B:137:ASP:OD1	2:B:138:GLU:N	2.45	0.42
5:E:234:PRO:CB	6:H:344:PHE:CZ	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:215:GLU:C	6:H:217:GLY:N	2.78	0.42
6:H:275:LEU:O	6:H:277:LYS:N	2.52	0.42
2:B:131:ASP:OD1	2:B:131:ASP:N	2.52	0.42
6:H:311:CYS:SG	6:H:321:ILE:HB	2.60	0.42
1:A:137:VAL:HG22	1:A:286:LEU:HB2	2.00	0.42
1:A:740:THR:HA	1:A:748:SER:HA	2.01	0.42
2:B:168:ASP:OD1	2:B:168:ASP:N	2.47	0.42
2:B:407:THR:HG21	2:B:427:THR:HB	2.01	0.42
3:C:108:LEU:H	3:C:108:LEU:HG	1.73	0.42
5:E:44:HIS:HD2	6:H:339:ARG:CG	2.32	0.42
5:E:223:SER:OG	5:E:224:THR:N	2.53	0.42
6:H:318:GLU:O	6:H:319:GLU:C	2.61	0.42
1:A:421:LEU:HD22	1:A:421:LEU:N	2.33	0.42
1:A:687:ASP:C	1:A:691:LEU:HD23	2.44	0.42
5:G:95:ASN:OD1	5:G:95:ASN:N	2.52	0.42
6:H:29:ARG:NH1	6:H:173:TYR:CE2	2.87	0.42
6:H:139:ASP:HA	6:H:142:LYS:HD3	2.01	0.42
6:H:181:ALA:O	6:H:182:CYS:C	2.60	0.42
4:D:61:CYS:HB2	4:D:69:ARG:HH21	1.85	0.42
6:H:190:LEU:HD12	6:H:191:MET:N	2.34	0.42
6:H:192:ARG:O	6:H:193:HIS:HB2	2.20	0.42
6:H:197:SER:HB3	6:H:200:LYS:HG2	2.01	0.42
6:H:272:GLU:HG3	6:H:273:ASN:N	2.31	0.42
3:C:62:LEU:HD12	3:C:79:VAL:HG22	2.01	0.42
5:F:7:VAL:HG23	5:F:8:GLN:HG3	2.02	0.42
1:A:385:ILE:HG21	1:A:421:LEU:HD12	2.02	0.42
6:H:194:LEU:O	6:H:194:LEU:CG	2.67	0.42
5:E:162:CYS:HB3	5:E:199:MET:HE1	2.02	0.41
6:H:26:TYR:CD1	6:H:29:ARG:HD2	2.55	0.41
6:H:62:SER:C	6:H:64:LEU:H	2.26	0.41
6:H:63:HIS:HD2	6:H:137:HIS:O	2.03	0.41
6:H:238:ILE:O	6:H:238:ILE:HG12	2.19	0.41
6:H:252:LYS:HD3	6:H:252:LYS:HA	1.92	0.41
6:H:253:HIS:C	6:H:255:SER:H	2.26	0.41
1:A:260:ILE:HG22	1:A:297:SER:HB2	2.01	0.41
1:A:682:ARG:O	1:A:686:LEU:HG	2.20	0.41
6:H:134:THR:CG2	6:H:135:LYS:H	2.21	0.41
6:H:192:ARG:O	6:H:193:HIS:CB	2.68	0.41
6:H:202:LEU:N	6:H:202:LEU:CD1	2.84	0.41
1:A:523:LEU:HD12	1:A:528:VAL:HB	2.02	0.41
6:H:248:ASP:O	6:H:251:GLN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:263:LEU:HD13	6:H:268:TYR:CB	2.50	0.41
6:H:308:LYS:HB3	6:H:308:LYS:HZ3	1.83	0.41
1:A:579:GLU:O	1:A:707:GLN:NE2	2.51	0.41
5:E:252:ALA:H	6:H:340:LEU:HD21	1.85	0.41
5:G:209:LEU:HD23	5:G:212:LEU:HD12	2.03	0.41
6:H:245:ARG:HD2	6:H:245:ARG:HA	1.90	0.41
6:H:302:ASN:CG	6:H:305:GLU:HB3	2.46	0.41
1:A:597:PRO:HD2	1:A:766:SER:HA	2.02	0.41
1:A:981:ALA:C	1:A:985:ARG:NH1	2.79	0.41
6:H:79:ILE:O	6:H:81:PRO:HD3	2.21	0.41
6:H:212:ILE:HG22	6:H:213:LEU:N	2.35	0.41
6:H:258:GLU:O	6:H:262:ARG:HG2	2.20	0.41
6:H:320:ARG:C	6:H:322:ARG:H	2.28	0.41
2:B:295:MET:HE3	2:B:330:ASN:O	2.20	0.41
5:E:38:GLN:HE21	5:E:125:GLN:NE2	2.19	0.41
1:A:400:ASN:HD21	1:A:446:THR:HG23	1.85	0.41
1:A:1039:LYS:N	1:A:1039:LYS:HD3	2.33	0.41
4:D:105:TYR:O	4:D:107:LEU:N	2.54	0.41
5:G:162:CYS:SG	5:G:163:ALA:N	2.94	0.41
6:H:166:LEU:O	6:H:167:VAL:C	2.64	0.41
6:H:316:PHE:CD1	6:H:317:SER:N	2.88	0.41
5:F:182:LEU:HD12	5:F:182:LEU:HA	1.95	0.41
5:G:63:ASP:OD1	5:G:63:ASP:N	2.43	0.41
6:H:9:LEU:HD11	6:H:247:VAL:HG21	2.02	0.41
6:H:336:THR:O	6:H:337:GLN:C	2.64	0.41
1:A:367:LYS:HE3	1:A:369:GLN:HE21	1.85	0.40
1:A:1030:GLN:O	1:A:1033:GLU:HB2	2.21	0.40
5:E:151:LEU:HA	5:E:154:ILE:HD12	2.03	0.40
6:H:17:ALA:HB2	6:H:211:ARG:CG	2.52	0.40
6:H:135:LYS:HA	6:H:138:ASN:CB	2.51	0.40
1:A:323:LYS:HE3	1:A:323:LYS:HB3	1.92	0.40
5:G:14:LYS:HA	5:G:17:GLU:HB2	2.02	0.40
5:G:138:LYS:HB3	5:G:196:THR:HG22	2.02	0.40
6:H:3:ILE:CG2	6:H:6:LEU:HB2	2.48	0.40
6:H:159:ALA:O	6:H:160:GLU:C	2.63	0.40
6:H:308:LYS:NZ	6:H:308:LYS:CB	2.83	0.40
2:B:35:SER:O	2:B:333:GLN:NE2	2.54	0.40
5:E:159:VAL:HG13	5:E:170:SER:HB3	2.03	0.40
5:G:1:MET:HE3	5:G:91:ARG:HD2	2.03	0.40
6:H:39:ILE:HA	6:H:42:PHE:HD2	1.86	0.40
6:H:238:ILE:C	6:H:240:GLY:N	2.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:320:ARG:C	6:H:322:ARG:N	2.80	0.40
5:E:234:PRO:HB2	6:H:344:PHE:HZ	1.84	0.40
6:H:26:TYR:HH	6:H:206:GLU:CG	2.34	0.40
5:E:179:ASN:OD1	5:E:179:ASN:N	2.54	0.40
6:H:300:GLU:OE2	6:H:301:PRO:HD2	2.22	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	1003/1107 (91%)	933 (93%)	66 (7%)	4 (0%)	30	65
2	B	425/469 (91%)	398 (94%)	27 (6%)	0	100	100
3	C	141/474 (30%)	131 (93%)	10 (7%)	0	100	100
4	D	64/137 (47%)	49 (77%)	12 (19%)	3 (5%)	2	19
5	E	247/264 (94%)	239 (97%)	8 (3%)	0	100	100
5	F	243/264 (92%)	236 (97%)	7 (3%)	0	100	100
5	G	245/264 (93%)	229 (94%)	16 (6%)	0	100	100
6	H	300/380 (79%)	215 (72%)	63 (21%)	22 (7%)	1	13
All	All	2668/3359 (79%)	2430 (91%)	209 (8%)	29 (1%)	14	44

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	79	GLU
6	H	93	LYS
6	H	271	PRO
6	H	272	GLU
6	H	315	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	337	GLN
6	H	157	SER
6	H	200	LYS
6	H	239	ARG
6	H	254	LYS
6	H	333	GLN
6	H	201	LYS
6	H	264	ASP
1	A	85	PRO
6	H	36	SER
6	H	199	ALA
6	H	240	GLY
6	H	262	ARG
6	H	305	GLU
6	H	317	SER
6	H	334	GLY
1	A	756	THR
1	A	1021	HIS
1	A	1040	GLU
4	D	106	PRO
6	H	216	LEU
4	D	105	TYR
6	H	90	PRO
6	H	231	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	857/944 (91%)	848 (99%)	9 (1%)	65	74
2	B	367/403 (91%)	365 (100%)	2 (0%)	81	82
3	C	125/413 (30%)	125 (100%)	0	100	100
4	D	59/120 (49%)	58 (98%)	1 (2%)	53	68
5	E	217/230 (94%)	213 (98%)	4 (2%)	51	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	216/230 (94%)	215 (100%)	1 (0%)	81	82
5	G	217/230 (94%)	217 (100%)	0	100	100
6	H	232/321 (72%)	213 (92%)	19 (8%)	10	33
All	All	2290/2891 (79%)	2254 (98%)	36 (2%)	54	70

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	190	VAL
1	A	993	THR
1	A	1019	LEU
1	A	1021	HIS
1	A	1032	ARG
1	A	1038	GLN
1	A	1039	LYS
1	A	1098	ARG
2	B	180	ASP
2	B	220	ASP
4	D	79	GLU
5	E	11	ILE
5	E	45	VAL
5	E	48	VAL
5	E	247	LEU
5	F	153	HIS
6	H	6	LEU
6	H	13	VAL
6	H	41	GLN
6	H	67	MET
6	H	137	HIS
6	H	172	VAL
6	H	204	ILE
6	H	230	LEU
6	H	238	ILE
6	H	241	ILE
6	H	271	PRO
6	H	275	LEU
6	H	276	HIS
6	H	287	GLU
6	H	308	LYS
6	H	325	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	330	LYS
6	H	331	SER
6	H	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	369	GLN
1	A	400	ASN
1	A	430	ASN
1	A	558	GLN
1	A	614	HIS
1	A	842	ASN
1	A	865	GLN
1	A	880	GLN
1	A	961	GLN
1	A	1021	HIS
1	A	1038	GLN
1	A	1043	HIS
1	A	1045	ASN
1	A	1092	GLN
2	B	21	ASN
2	B	70	GLN
2	B	140	GLN
2	B	184	GLN
3	C	116	ASN
5	E	44	HIS
5	E	84	ASN
5	F	65	ASN
5	F	71	ASN
5	F	125	GLN
5	F	179	ASN
5	G	36	ASN
5	G	38	GLN
5	G	44	HIS
5	G	71	ASN
5	G	108	GLN
5	G	125	GLN
5	G	204	GLN
5	G	213	ASN
6	H	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	21	ASN
6	H	77	ASN
6	H	137	HIS
6	H	138	ASN
6	H	193	HIS
6	H	222	GLN
6	H	253	HIS
6	H	273	ASN
6	H	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	DOC	P	25	7,8	16,19,20	4.86	12 (75%)	20,26,29	1.90	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DOC	P	25	7,8	-	2/7/18/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	25	DOC	O4'-C4'	-8.58	1.28	1.44
7	P	25	DOC	C3'-C2'	-8.43	1.31	1.54
7	P	25	DOC	C2-N3	6.19	1.48	1.36
7	P	25	DOC	O4'-C1'	5.90	1.55	1.42
7	P	25	DOC	C6-C5	5.90	1.48	1.35
7	P	25	DOC	C1'-N1	-5.57	1.34	1.48
7	P	25	DOC	C4-N4	5.25	1.46	1.33
7	P	25	DOC	C4-N3	5.03	1.44	1.34
7	P	25	DOC	C2-N1	3.91	1.48	1.40
7	P	25	DOC	O2-C2	-3.06	1.18	1.23
7	P	25	DOC	C6-N1	2.62	1.44	1.38
7	P	25	DOC	C5-C4	2.26	1.48	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	25	DOC	C4'-O4'-C1'	-6.07	104.08	109.81
7	P	25	DOC	C3'-C2'-C1'	3.02	106.35	102.87
7	P	25	DOC	C2'-C3'-C4'	2.22	106.88	102.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	25	DOC	C3'-C4'-C5'-O5'
7	P	25	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SF4	A	1202	1	0,12,12	-	-	-		
11	TTP	A	1203	-	29,30,30	4.50	18 (62%)	43,47,47	1.96	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SF4	A	1202	1	-	-	0/6/5/5
11	TTP	A	1203	-	-	4/22/34/34	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1203	TTP	C2'-C3'	-12.11	1.22	1.52
11	A	1203	TTP	C6-C5	8.28	1.48	1.34
11	A	1203	TTP	O4'-C4'	-7.90	1.27	1.45
11	A	1203	TTP	C2-N3	6.50	1.49	1.38
11	A	1203	TTP	C2-N1	6.27	1.48	1.38
11	A	1203	TTP	PA-O3A	6.11	1.66	1.59
11	A	1203	TTP	PB-O3A	5.98	1.66	1.59
11	A	1203	TTP	C1'-N1	-5.42	1.34	1.48
11	A	1203	TTP	PB-O3B	5.01	1.64	1.59
11	A	1203	TTP	C3'-C4'	4.62	1.65	1.53
11	A	1203	TTP	C6-N1	3.76	1.44	1.38
11	A	1203	TTP	O4'-C1'	3.46	1.50	1.42
11	A	1203	TTP	C4-N3	3.28	1.45	1.38
11	A	1203	TTP	O3'-C3'	2.96	1.49	1.43
11	A	1203	TTP	O4-C4	-2.86	1.18	1.23
11	A	1203	TTP	O2-C2	-2.80	1.18	1.23
11	A	1203	TTP	C4-C5	2.37	1.48	1.44
11	A	1203	TTP	C2'-C1'	2.04	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1203	TTP	C4-N3-C2	-6.01	119.46	127.34
11	A	1203	TTP	C5-C4-N3	4.86	119.55	115.32
11	A	1203	TTP	N3-C2-N1	4.72	121.04	114.89
11	A	1203	TTP	O4-C4-C5	-3.85	120.51	124.92
11	A	1203	TTP	C6-C5-C4	2.80	120.32	118.02
11	A	1203	TTP	C5M-C5-C6	-2.60	119.33	122.85
11	A	1203	TTP	O2-C2-N1	-2.56	119.46	122.80
11	A	1203	TTP	C6-N1-C2	-2.45	118.86	121.30
11	A	1203	TTP	C5-C6-N1	-2.35	120.76	123.31
11	A	1203	TTP	O4'-C1'-N1	2.19	111.75	107.86
11	A	1203	TTP	C3'-C2'-C1'	2.15	107.86	102.60
11	A	1203	TTP	C2'-C1'-N1	-2.12	108.52	113.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

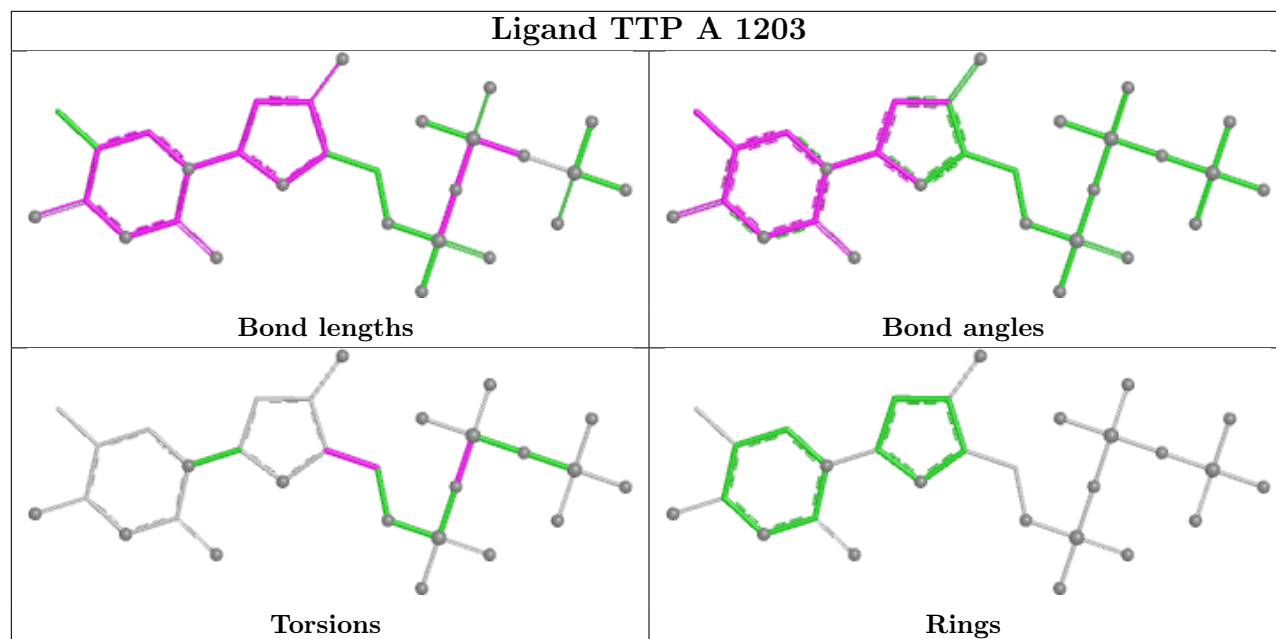
Mol	Chain	Res	Type	Atoms
11	A	1203	TTP	O4'-C4'-C5'-O5'
11	A	1203	TTP	C3'-C4'-C5'-O5'
11	A	1203	TTP	PA-O3A-PB-O1B
11	A	1203	TTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1202	SF4	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

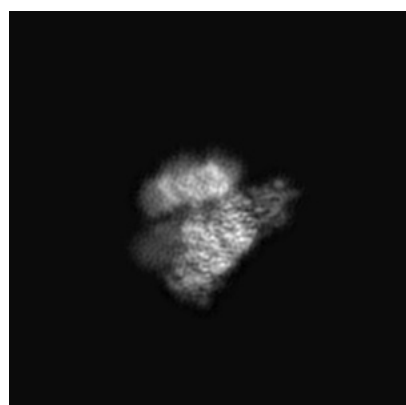
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10540. These allow visual inspection of the internal detail of the map and identification of artifacts.

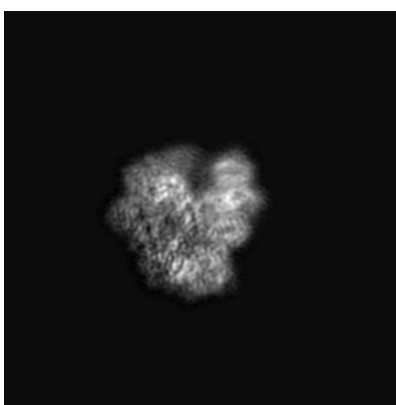
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

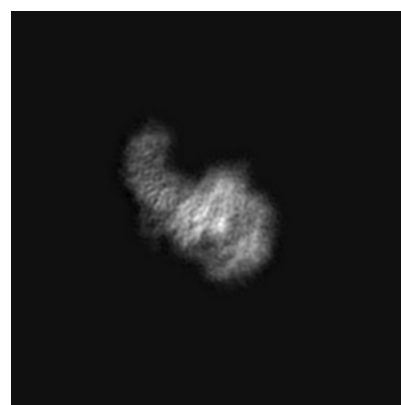
6.1.1 Primary map



X



Y

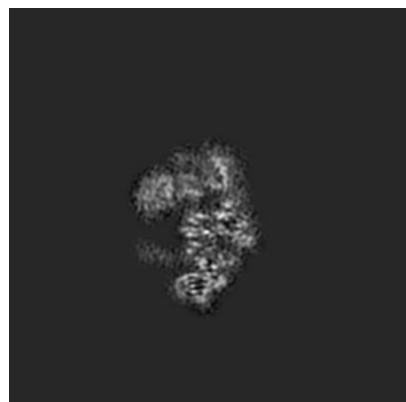


Z

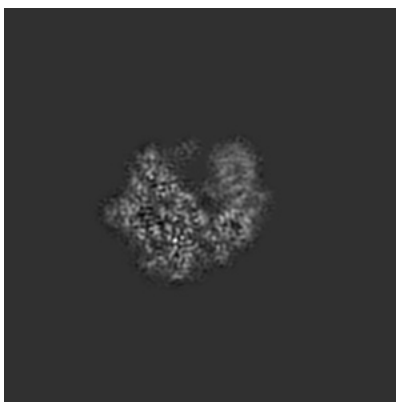
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

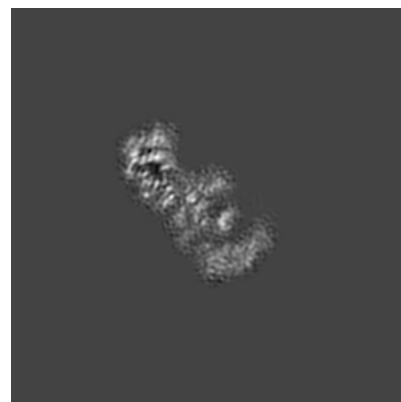
6.2.1 Primary map



X Index: 200



Y Index: 200

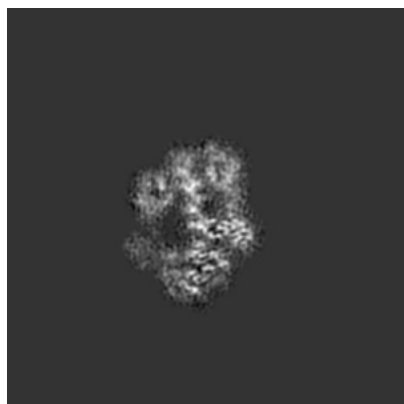


Z Index: 200

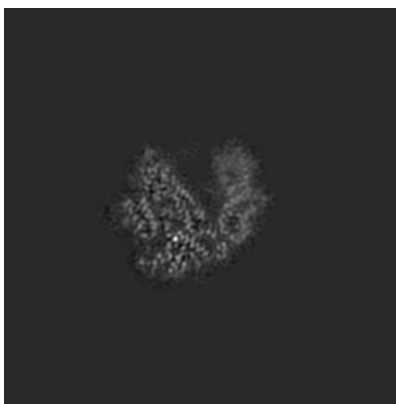
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

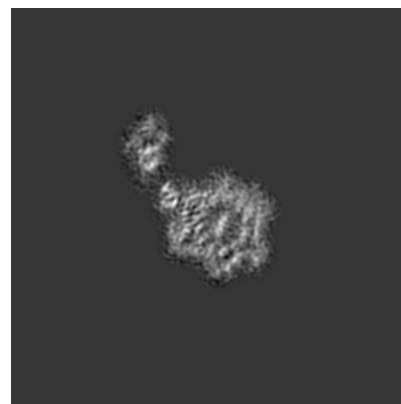
6.3.1 Primary map



X Index: 209



Y Index: 204

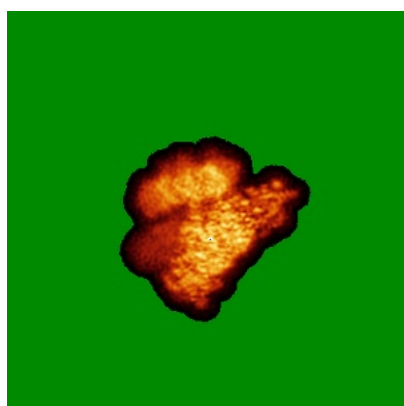


Z Index: 220

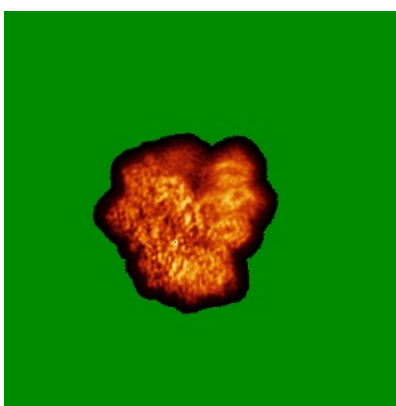
The images above show the largest variance slices of the map in three orthogonal directions.

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

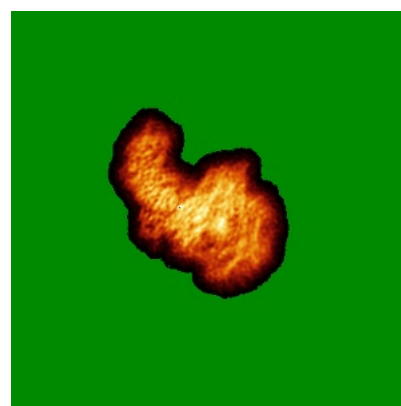
6.4.1 Primary map



X



Y



Z

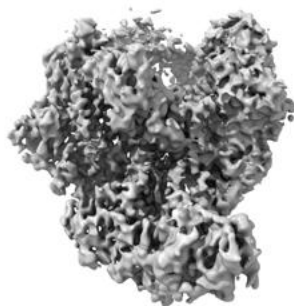
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0073. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

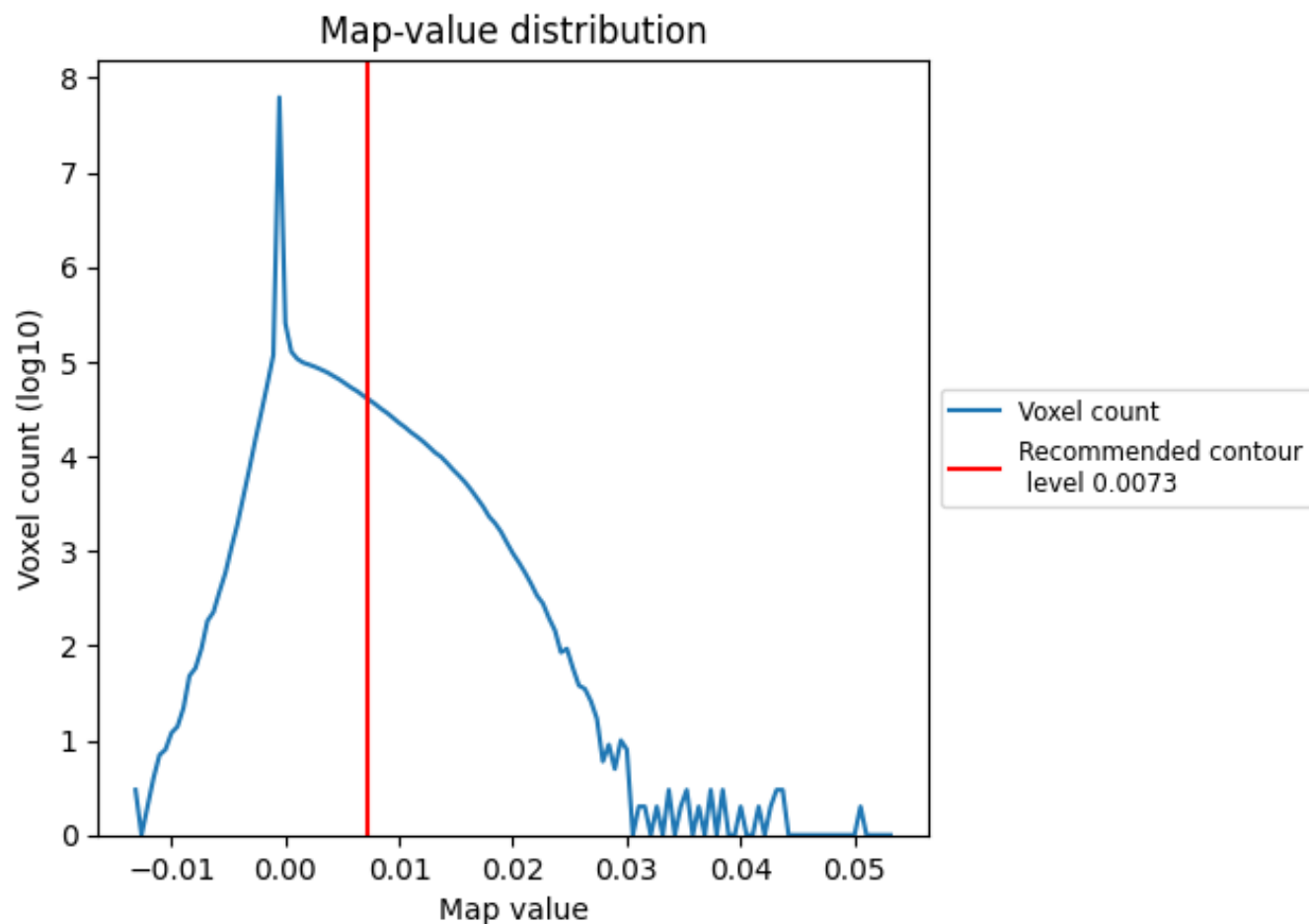
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

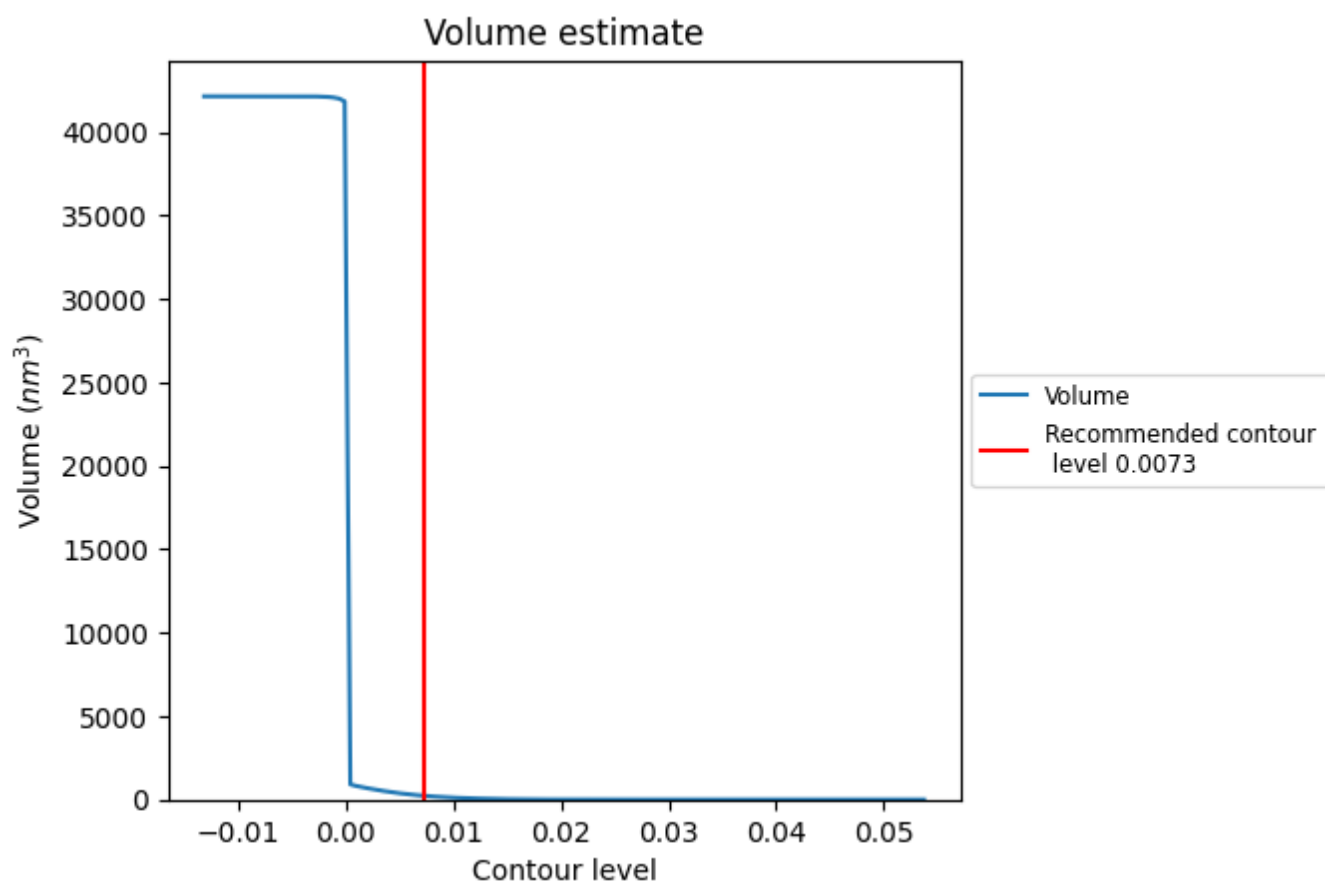
This section contains the results of statistical analysis of the map.

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.

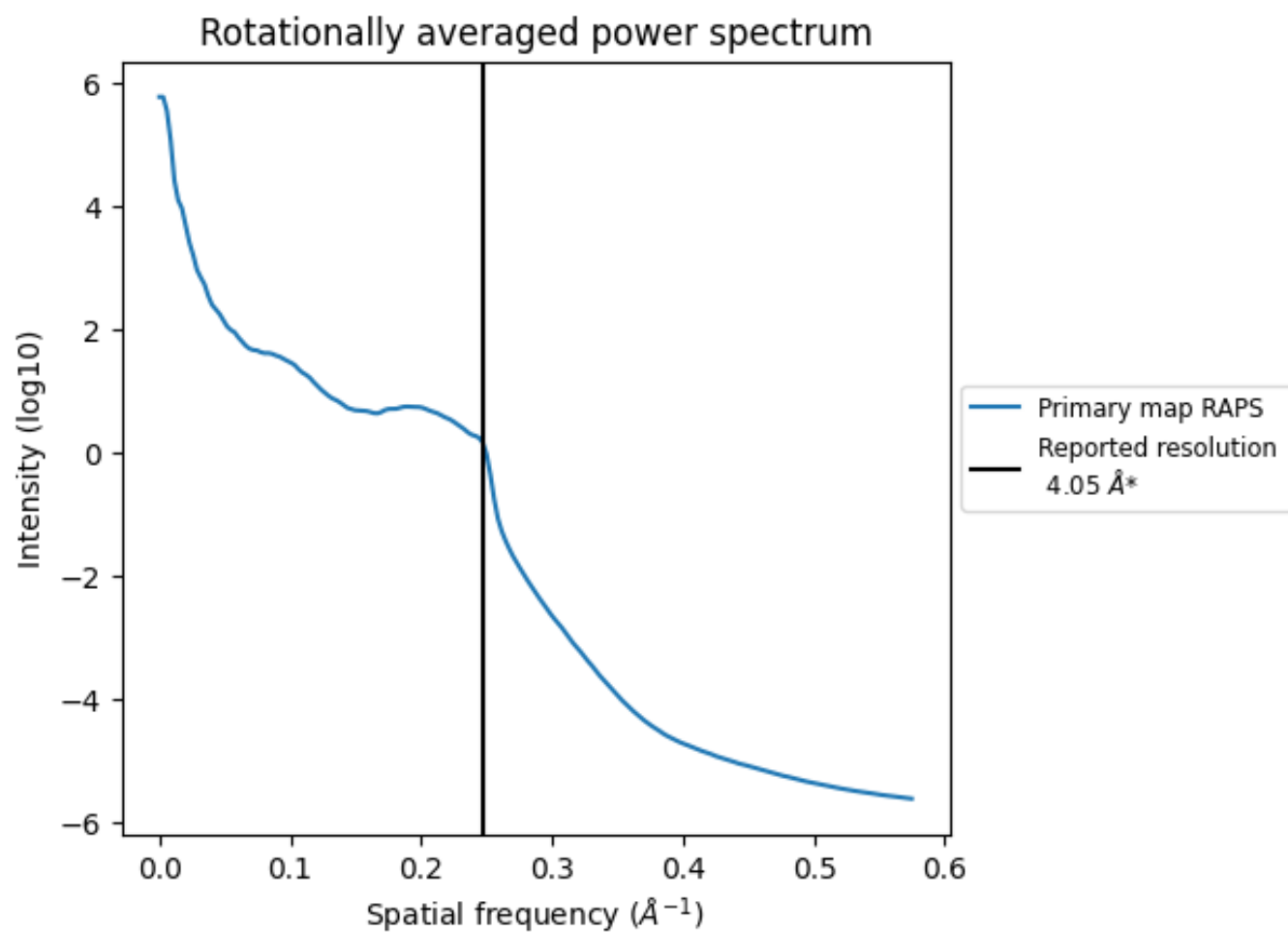
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm^3 ; this corresponds to an approximate mass of 204 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 ⓘ

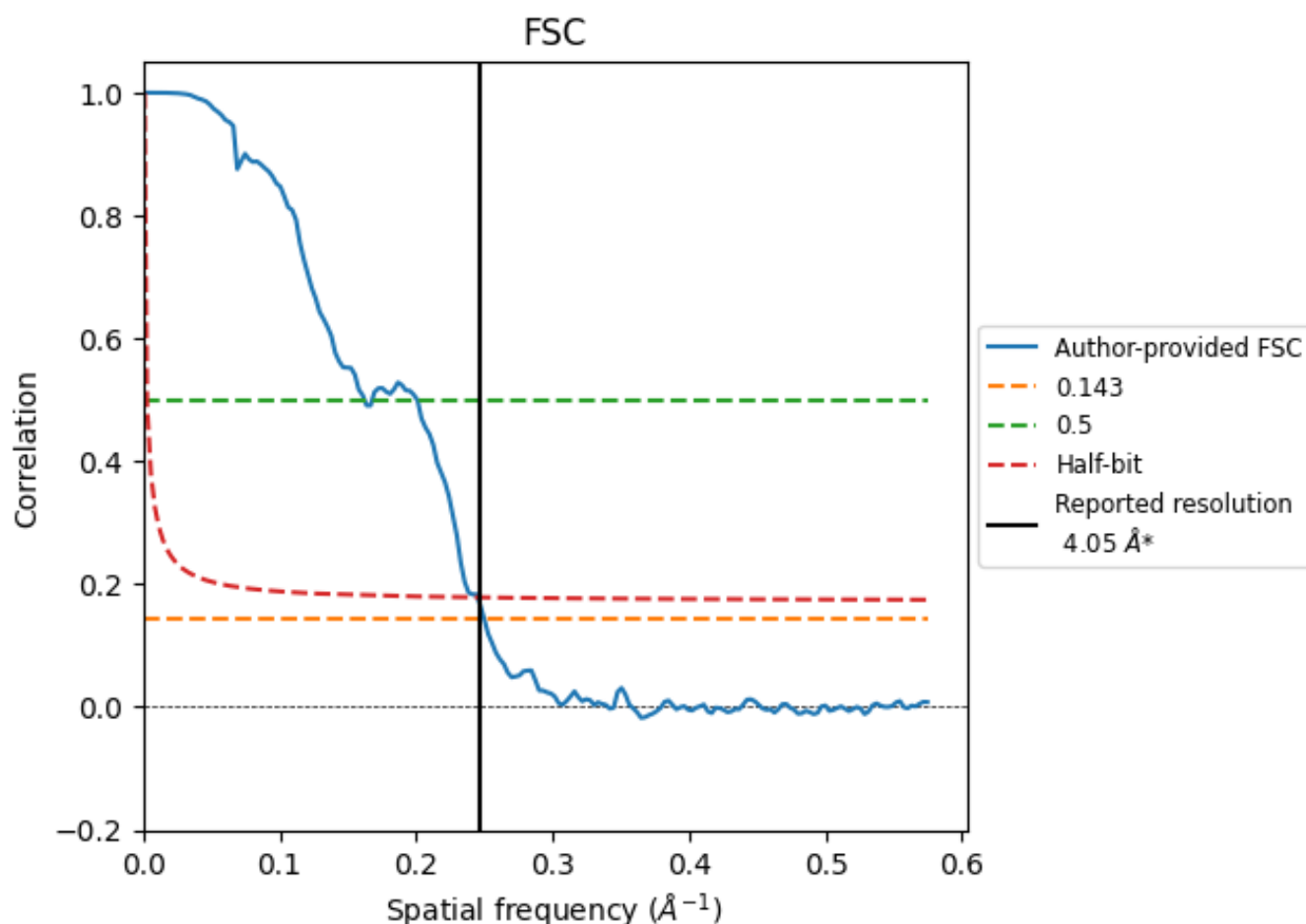


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

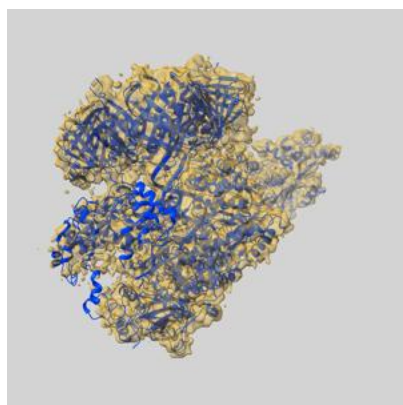
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.00	6.17	4.08
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

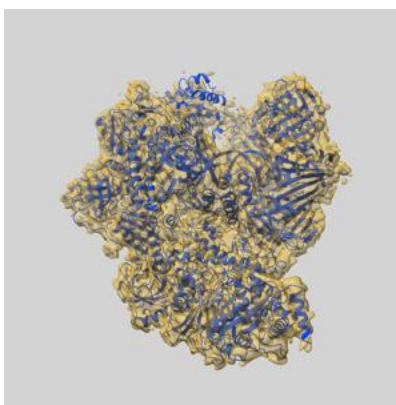
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10540 and PDB model 6TNZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

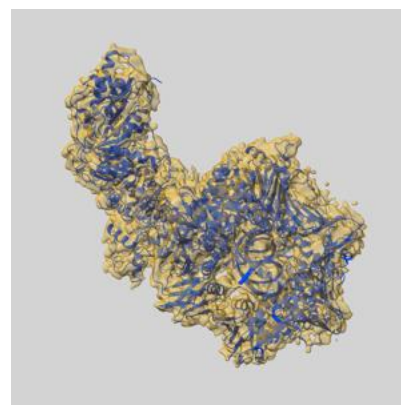
9.1 Map-model overlay [i](#)



X



Y



Z

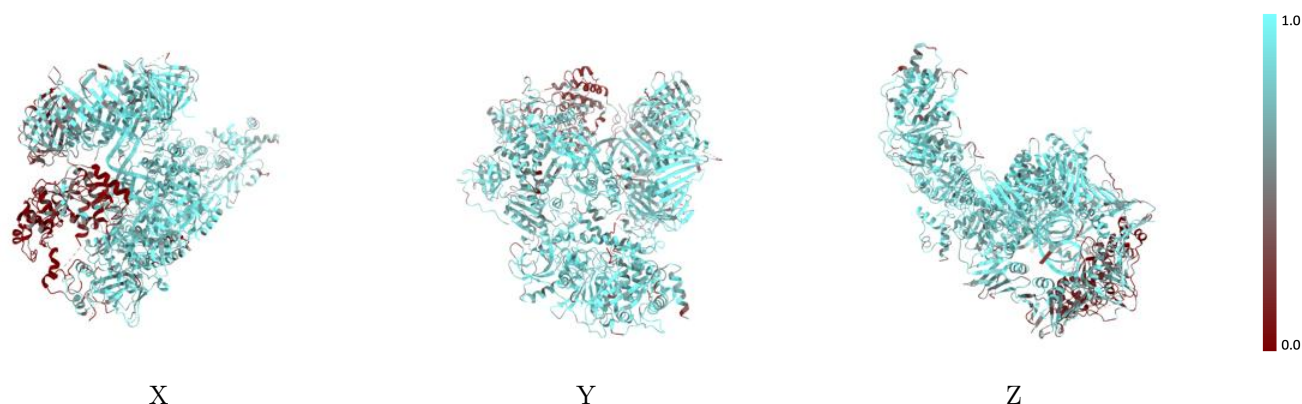
The images above show the 3D surface view of the map at the recommended contour level 0.0073 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



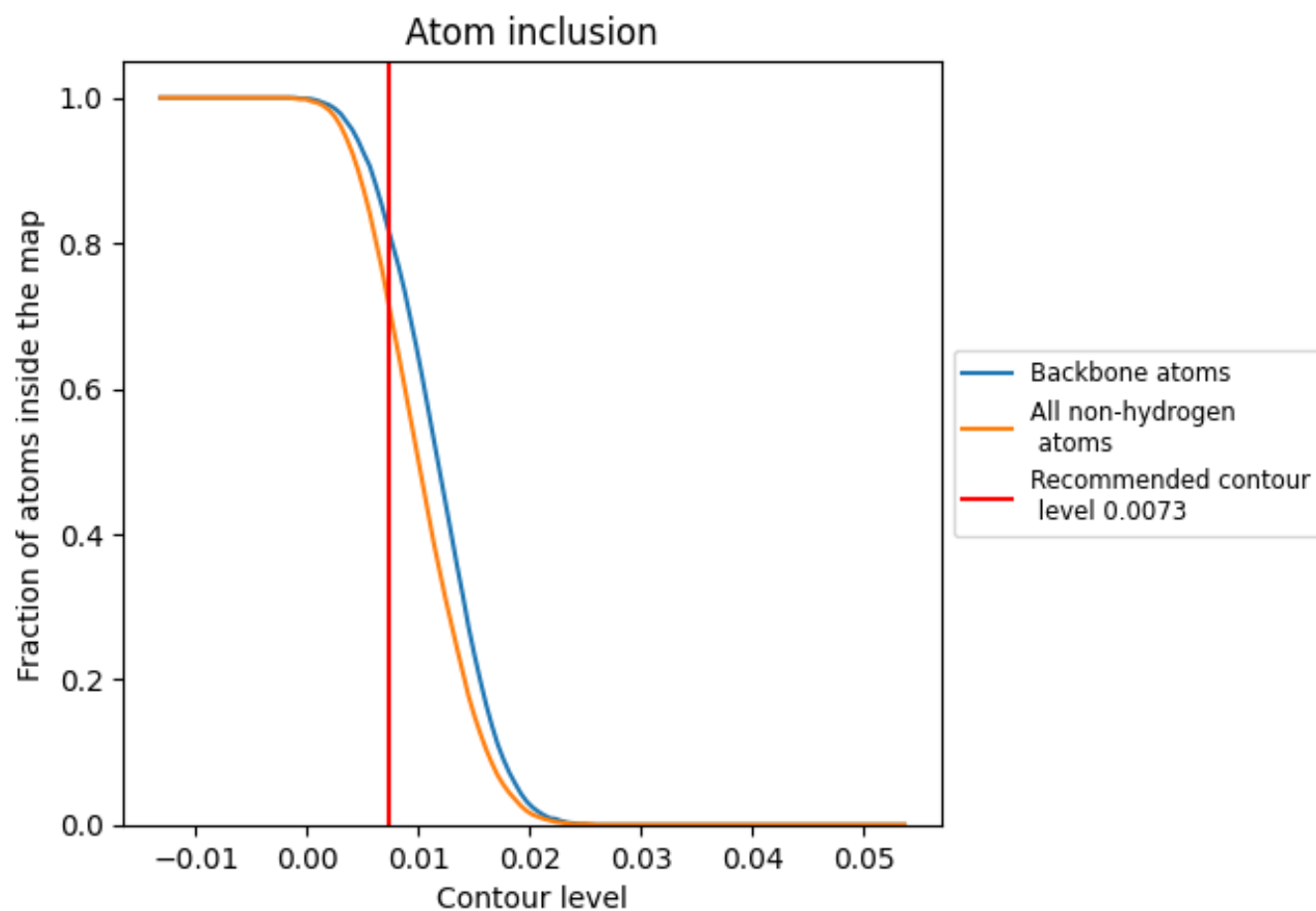
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0073).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.2830
A	0.7890	0.3420
B	0.8130	0.3860
C	0.7570	0.3090
D	0.7950	0.3810
E	0.6220	0.1430
F	0.8230	0.3340
G	0.7700	0.1720
H	0.1820	0.0570
P	0.8810	0.2780
T	0.9190	0.3140

1.0

0.0

<0.0