Full wwPDB EM Validation Report ⓘ

Feb 8, 2022 – 06:13 am GMT

PDB ID	:	7OPL
EMDB ID	:	EMD-13020
Title	:	CryoEM structure of DNA Polymerase alpha - primase bound to SARS CoV nsp1
Authors	:	Kilkenny, M.L.; Pellegrini, L.
Deposited on	:	2021-06-01
Resolution	:	4.12 Å(reported)
Based on initial models	:	7K3N, 5EXR, 2HSX

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

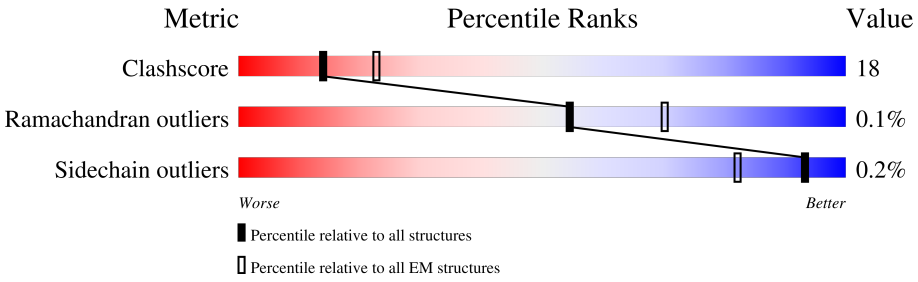
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.12 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1170	57% 34% 9%
2	B	452	65% 33% .
3	C	441	51% 38% 12%
4	D	509	. 53% 32% 15%
5	E	119	18% 55% 33% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19743 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 alpha catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1070	8641	5540	1452	1593	56	0	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	MET	-	initiating methionine	UNP P09884
A	294	SER	-	expression tag	UNP P09884
A	295	ALA	-	expression tag	UNP P09884
A	296	TRP	-	expression tag	UNP P09884
A	297	SER	-	expression tag	UNP P09884
A	298	HIS	-	expression tag	UNP P09884
A	299	PRO	-	expression tag	UNP P09884
A	300	GLN	-	expression tag	UNP P09884
A	301	PHE	-	expression tag	UNP P09884
A	302	GLU	-	expression tag	UNP P09884
A	303	LYS	-	expression tag	UNP P09884
A	304	GLY	-	expression tag	UNP P09884
A	305	GLY	-	expression tag	UNP P09884
A	306	GLY	-	expression tag	UNP P09884
A	307	SER	-	expression tag	UNP P09884
A	308	GLY	-	expression tag	UNP P09884
A	309	GLY	-	expression tag	UNP P09884
A	310	GLY	-	expression tag	UNP P09884
A	311	SER	-	expression tag	UNP P09884
A	312	GLY	-	expression tag	UNP P09884
A	313	GLY	-	expression tag	UNP P09884
A	314	GLY	-	expression tag	UNP P09884
A	315	SER	-	expression tag	UNP P09884
A	316	TRP	-	expression tag	UNP P09884
A	317	SER	-	expression tag	UNP P09884
A	318	HIS	-	expression tag	UNP P09884
A	319	PRO	-	expression tag	UNP P09884
A	320	GLN	-	expression tag	UNP P09884

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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	PHE	-	expression tag	UNP P09884
A	322	GLU	-	expression tag	UNP P09884
A	323	LYS	-	expression tag	UNP P09884
A	324	LEU	-	expression tag	UNP P09884
A	325	GLU	-	expression tag	UNP P09884
A	326	VAL	-	expression tag	UNP P09884
A	327	LEU	-	expression tag	UNP P09884
A	328	PHE	-	expression tag	UNP P09884
A	329	GLN	-	expression tag	UNP P09884
A	330	GLY	-	expression tag	UNP P09884
A	331	PRO	-	expression tag	UNP P09884
A	332	GLU	-	expression tag	UNP P09884
A	333	PHE	-	expression tag	UNP P09884

- Molecule 2 is a protein called DNA polymerase alpha subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	444	Total	C	N	O	S	0	0
			3451	2194	576	666	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	MET	-	initiating methionine	UNP Q14181
B	148	GLY	-	expression tag	UNP Q14181

- Molecule 3 is a protein called DNA primase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	389	Total	C	N	O	S	0	0
			3261	2099	564	583	15		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP P49642
C	-19	HIS	-	expression tag	UNP P49642
C	-18	HIS	-	expression tag	UNP P49642
C	-17	HIS	-	expression tag	UNP P49642
C	-16	HIS	-	expression tag	UNP P49642
C	-15	HIS	-	expression tag	UNP P49642
C	-14	HIS	-	expression tag	UNP P49642

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP P49642
C	-12	HIS	-	expression tag	UNP P49642
C	-11	HIS	-	expression tag	UNP P49642
C	-10	HIS	-	expression tag	UNP P49642
C	-9	GLY	-	expression tag	UNP P49642
C	-8	GLU	-	expression tag	UNP P49642
C	-7	ASN	-	expression tag	UNP P49642
C	-6	LEU	-	expression tag	UNP P49642
C	-5	TYR	-	expression tag	UNP P49642
C	-4	PHE	-	expression tag	UNP P49642
C	-3	GLN	-	expression tag	UNP P49642
C	-2	GLY	-	expression tag	UNP P49642
C	-1	THR	-	expression tag	UNP P49642
C	0	SER	-	expression tag	UNP P49642

- Molecule 4 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	434	Total	C	N	O	S	0	0
			3562	2280	616	653	13		

- Molecule 5 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	105	Total	C	N	O	S	0	0
			817	520	144	151	2		

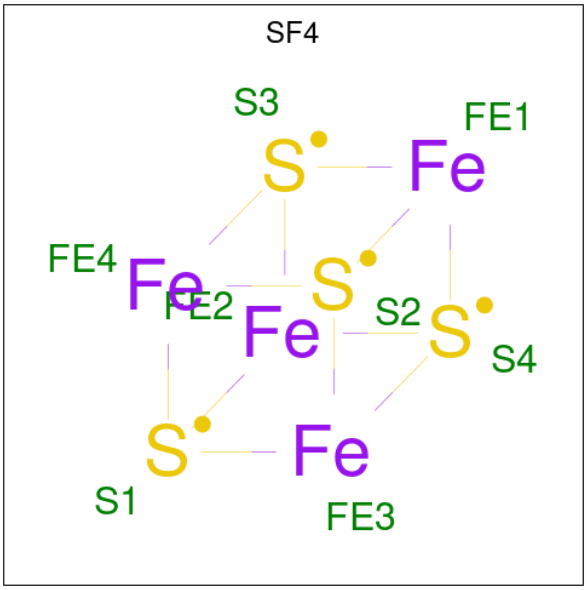
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	GLY	-	expression tag	UNP P0C6U8
E	10	SER	-	expression tag	UNP P0C6U8
E	11	MET	-	expression tag	UNP P0C6U8
E	12	GLY	-	expression tag	UNP P0C6U8

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Zn	0
			2	2	
6	C	1	Total	Zn	0
			1	1	

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



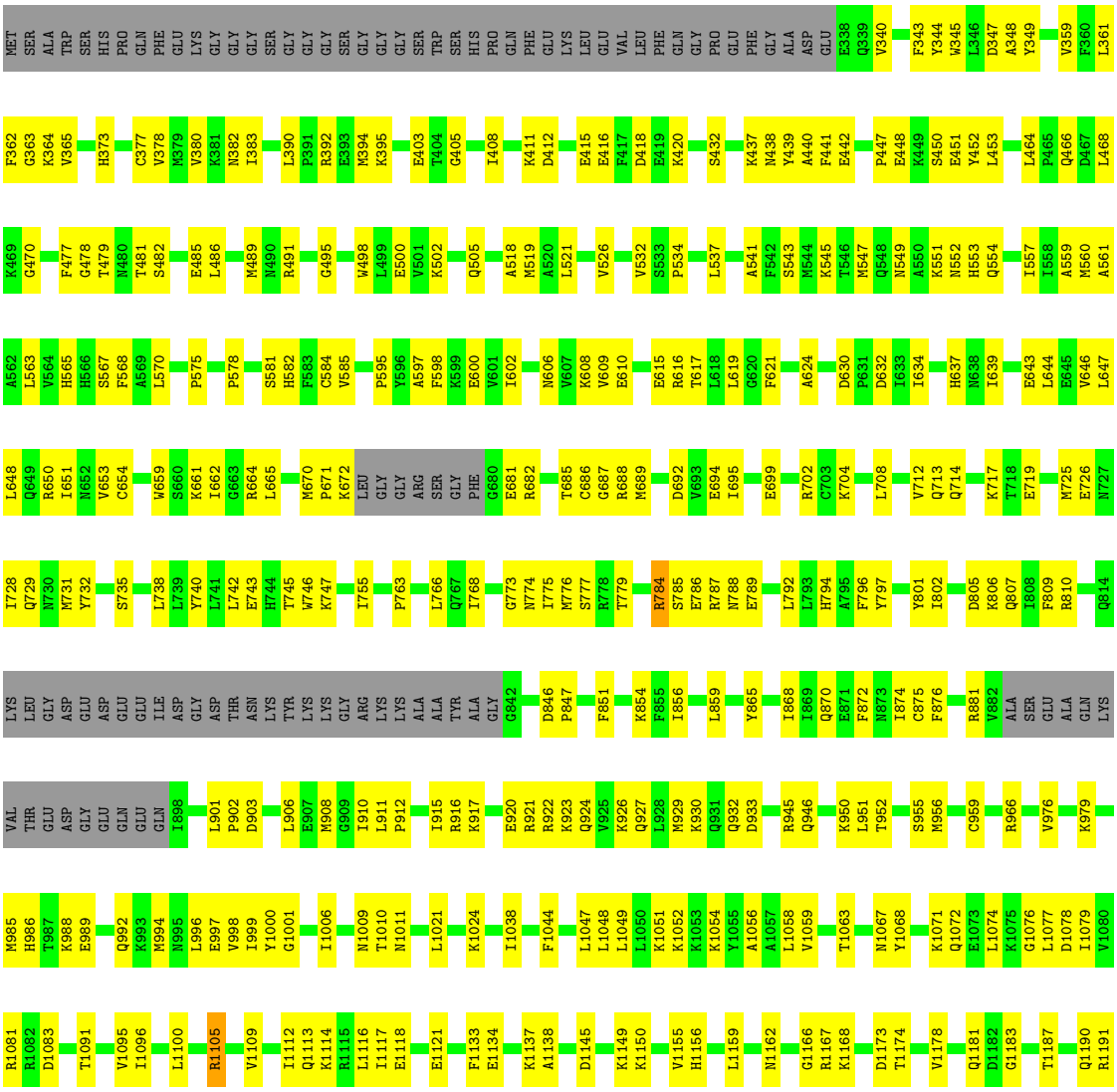
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	D	1	8	4	4	0

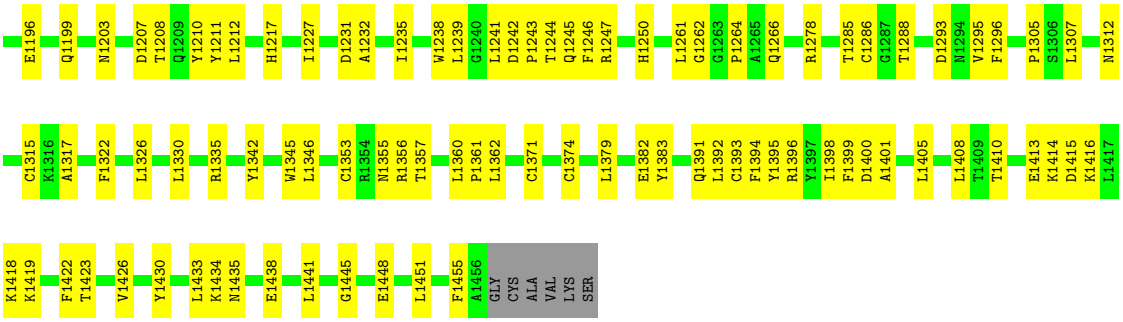
3 Residue-property plots (i)

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: DNA polymerase alpha catalytic subunit

Chain A:



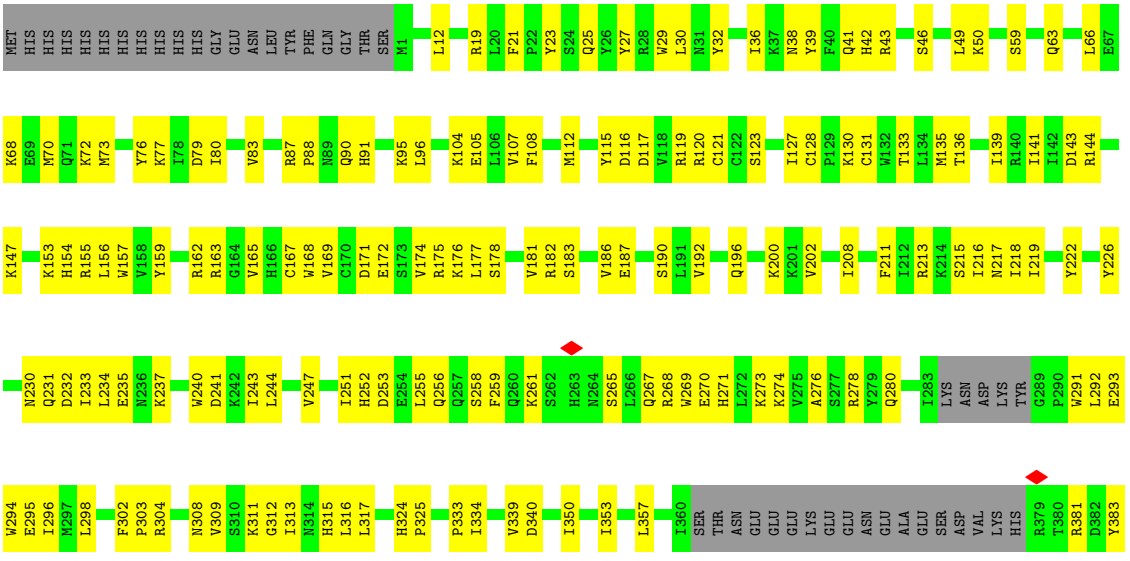


• Molecule 2: DNA polymerase alpha subunit B

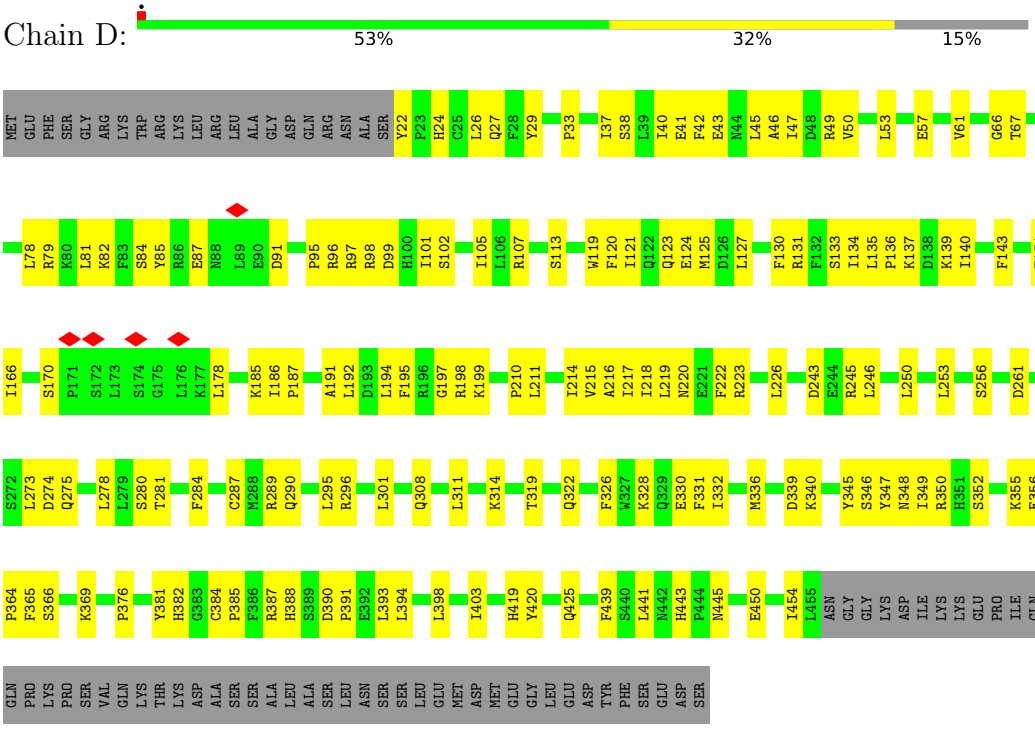
Chain B:

• Molecule 3: DNA primase small subunit

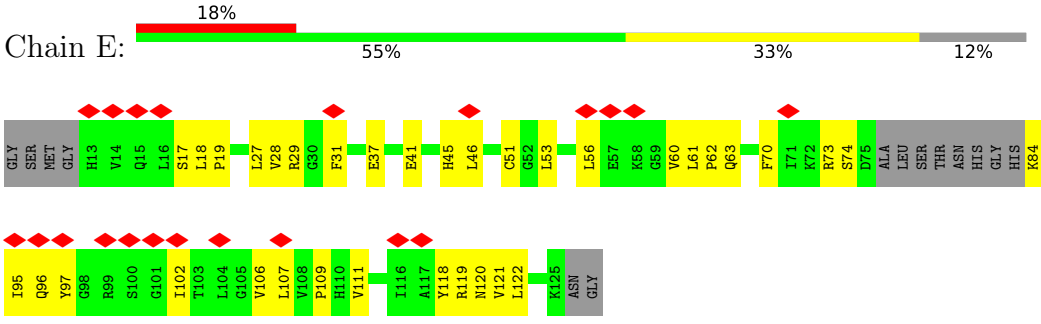
Chain C:



• Molecule 4: DNA primase large subunit



• Molecule 5: Non-structural protein 1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233476	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 ($e^-/Å^2$)	46.91	Depositor
Minimum defocus (nm)	-2.5	Depositor
Maximum defocus (nm)	-0.7	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	210.24, 210.24, 210.24	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.314, 1.314, 1.314	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.26	0/8825	0.52	0/11926
2	B	0.27	0/3529	0.55	0/4795
3	C	0.28	0/3343	0.55	1/4508 (0.0%)
4	D	0.28	0/3646	0.55	0/4908
5	E	0.24	0/828	0.56	0/1119
All	All	0.27	0/20171	0.54	1/27256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	333	PRO	CA-N-CD	-5.11	104.35	111.50

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	8641	0	8732	323	0
2	B	3451	0	3425	112	0
3	C	3261	0	3247	142	0
4	D	3562	0	3540	122	0
5	E	817	0	846	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	C	1	0	0	0	0
7	D	8	0	0	1	0
All	All	19743	0	19790	695	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 18.

All (695) 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:500:GLU:OE2	1:A:502:LYS:HG3	1.76	0.85
3:C:291:TRP:HB3	3:C:294:TRP:CD1	2.13	0.83
1:A:1264:PRO:HG3	4:D:359:ARG:HD2	1.62	0.82
4:D:387:ARG:HD3	4:D:420:TYR:CZ	2.16	0.80
4:D:273:LEU:HD11	4:D:326:PHE:HB2	1.64	0.80
3:C:36:ILE:HB	3:C:39:TYR:HB2	1.65	0.79
2:B:211:GLN:NE2	2:B:521:ASP:OD1	2.16	0.78
1:A:489:MET:HE3	1:A:797:TYR:HB2	1.64	0.78
4:D:425:GLN:NE2	4:D:439:PHE:O	2.17	0.78
4:D:57:GLU:OE1	4:D:119:TRP:NE1	2.16	0.78
1:A:1246:PHE:O	1:A:1250:HIS:HB2	1.83	0.77
1:A:784:ARG:HG3	1:A:787:ARG:HH11	1.50	0.77
4:D:287:CYS:HB3	4:D:385:PRO:HD3	1.67	0.77
1:A:788:ASN:HB2	1:A:959:CYS:HB3	1.65	0.76
4:D:384:CYS:HB2	7:D:601:SF4:S3	2.25	0.76
1:A:796:PHE:HD1	1:A:801:TYR:HD2	1.34	0.76
3:C:177:LEU:HD22	3:C:181:VAL:HG11	1.68	0.75
1:A:927:GLN:HA	1:A:930:LYS:HE2	1.69	0.75
4:D:22:TYR:HB3	4:D:96:ARG:HD2	1.68	0.75
1:A:347:ASP:HB3	1:A:362:PHE:HB2	1.68	0.74
1:A:856:ILE:HB	1:A:1044:PHE:HB2	1.68	0.74
1:A:1400:ASP:HA	1:A:1434:LYS:HE2	1.70	0.74
2:B:579:PRO:HG2	2:B:587:GLN:HB3	1.70	0.74
1:A:1095:VAL:HG22	1:A:1112:ILE:HD11	1.70	0.74
1:A:1356:ARG:NH1	1:A:1382:GLU:OE1	2.21	0.73
3:C:213:ARG:NH1	3:C:217:ASN:OD1	2.21	0.73
1:A:901:LEU:HD12	1:A:902:PRO:HD2	1.71	0.72
1:A:1247:ARG:HD3	4:D:355:LYS:HD3	1.72	0.71
3:C:182:ARG:HH22	3:C:313:ILE:HB	1.53	0.71
4:D:387:ARG:HD3	4:D:420:TYR:CE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:LEU:HD12	4:D:136:PRO:HD2	1.73	0.71
3:C:216:ILE:HD13	3:C:294:TRP:HE3	1.56	0.71
1:A:549:ASN:ND2	1:A:554:GLN:OE1	2.24	0.70
1:A:553:HIS:CD2	2:B:315:VAL:HG11	2.27	0.70
1:A:1054:LYS:HG3	1:A:1076:GLY:HA3	1.74	0.69
1:A:1448:GLU:HA	4:D:38:SER:HA	1.73	0.68
1:A:713:GLN:HE21	1:A:719:GLU:HA	1.58	0.68
1:A:1335:ARG:NH2	2:B:426:LEU:O	2.26	0.68
4:D:314:LYS:NZ	4:D:352:SER:O	2.26	0.68
3:C:190:SER:O	4:D:198:ARG:NH2	2.27	0.68
2:B:503:LEU:HD12	2:B:534:THR:HG23	1.76	0.68
1:A:1207:ASP:OD1	1:A:1210:TYR:N	2.26	0.68
1:A:1383:TYR:OH	1:A:1391:GLN:OE1	2.12	0.67
3:C:105:GLU:HG2	3:C:168:TRP:CE3	2.28	0.67
2:B:164:ARG:NH2	2:B:362:ASP:OD2	2.27	0.67
5:E:85:VAL:HG22	5:E:122:LEU:HD22	1.76	0.67
2:B:341:MET:HB3	2:B:575:TYR:HD1	1.58	0.67
5:E:46:LEU:HD23	5:E:51:CYS:SG	2.34	0.67
4:D:81:LEU:O	4:D:98:ARG:NH2	2.28	0.66
2:B:414:ARG:NH2	2:B:448:GLU:OE2	2.29	0.66
1:A:682:ARG:NH1	1:A:686:CYS:SG	2.69	0.66
1:A:859:LEU:HB2	1:A:1006:ILE:HB	1.78	0.65
2:B:160:LYS:HD3	2:B:566:GLN:HB3	1.78	0.65
2:B:161:TYR:HE1	2:B:568:GLY:HA2	1.61	0.65
4:D:67:THR:HG23	4:D:70:TYR:H	1.61	0.65
2:B:248:GLN:HA	2:B:309:THR:HG22	1.77	0.65
4:D:87:GLU:HG2	4:D:96:ARG:HH22	1.60	0.65
1:A:584:CYS:HB2	1:A:609:VAL:HG23	1.78	0.65
3:C:25:GLN:HE21	3:C:399:LEU:HD12	1.60	0.65
5:E:29:ARG:NH1	5:E:63:GLN:O	2.30	0.65
2:B:185:ARG:NH1	2:B:339:GLN:O	2.24	0.64
1:A:1408:LEU:HB2	1:A:1414:LYS:HD3	1.78	0.64
3:C:29:TRP:HD1	3:C:399:LEU:HD21	1.63	0.64
3:C:144:ARG:HH21	3:C:215:SER:HB3	1.61	0.64
4:D:290:GLN:NE2	4:D:381:TYR:O	2.24	0.64
3:C:112:MET:HG3	3:C:127:ILE:HG22	1.78	0.64
3:C:162:ARG:HD2	3:C:163:ARG:HD3	1.77	0.64
4:D:295:LEU:HD11	4:D:330:GLU:HG2	1.80	0.63
1:A:1081:ARG:NH2	1:A:1083:ASP:OD2	2.31	0.63
4:D:243:ASP:OD1	4:D:245:ARG:NH1	2.31	0.63
1:A:442:GLU:OE2	1:A:881:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PRO:HG3	2:B:307:ILE:HD12	1.81	0.63
4:D:311:LEU:HD13	4:D:364:PRO:HA	1.81	0.62
2:B:426:LEU:HD21	2:B:435:TYR:HB2	1.80	0.62
1:A:390:LEU:HD21	1:A:447:PRO:HD2	1.82	0.62
1:A:570:LEU:HB3	1:A:766:LEU:HD11	1.81	0.62
5:E:84:LYS:HB2	5:E:121:VAL:HA	1.81	0.62
1:A:1261:LEU:O	4:D:369:LYS:HA	2.00	0.62
1:A:789:GLU:OE2	1:A:966:ARG:HB2	2.00	0.62
1:A:1266:GLN:HG3	4:D:43:GLU:OE1	1.99	0.62
4:D:308:GLN:OE1	4:D:382:HIS:HB2	1.99	0.62
2:B:364:ILE:HD12	2:B:412:GLY:HA3	1.82	0.62
3:C:41:GLN:O	3:C:59:SER:OG	2.17	0.62
3:C:144:ARG:NH2	3:C:211:PHE:O	2.33	0.62
1:A:875:CYS:HA	1:A:911:LEU:HD12	1.81	0.61
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.82	0.61
1:A:712:VAL:HG22	1:A:755:ILE:HD11	1.81	0.61
4:D:78:LEU:O	4:D:82:LYS:N	2.32	0.61
1:A:481:THR:OG1	1:A:805:ASP:OD1	2.19	0.61
1:A:466:GLN:HA	1:A:479:THR:HG21	1.83	0.61
2:B:476:LEU:HD22	2:B:502:ILE:HD12	1.83	0.60
3:C:120:ARG:HH12	3:C:235:GLU:HG2	1.66	0.60
3:C:139:ILE:HD11	3:C:165:VAL:HG21	1.82	0.60
1:A:505:GLN:HB2	1:A:519:MET:HB3	1.82	0.60
4:D:53:LEU:HD22	4:D:123:GLN:HB3	1.83	0.60
1:A:1410:THR:HG23	1:A:1413:GLU:HB3	1.84	0.60
3:C:309:VAL:HG12	3:C:315:HIS:CE1	2.37	0.60
1:A:997:GLU:N	1:A:997:GLU:OE1	2.34	0.60
1:A:1346:LEU:HD12	1:A:1379:LEU:HB3	1.83	0.60
3:C:104:LYS:HG2	3:C:105:GLU:H	1.66	0.60
1:A:1360:LEU:HD12	1:A:1361:PRO:HD2	1.82	0.60
4:D:295:LEU:HB2	4:D:301:LEU:HD11	1.82	0.60
3:C:87:ARG:HB2	3:C:90:GLN:HG3	1.82	0.60
1:A:378:VAL:HG12	1:A:518:ALA:HB3	1.83	0.60
1:A:1393:CYS:HA	1:A:1396:ARG:HG2	1.83	0.60
1:A:1074:LEU:HG	1:A:1077:LEU:HD22	1.84	0.59
1:A:1181:GLN:OE1	1:A:1191:ARG:NH1	2.34	0.59
2:B:389:VAL:HG12	2:B:394:LEU:HD11	1.84	0.59
1:A:1137:LYS:NZ	1:A:1138:ALA:O	2.32	0.59
2:B:220:LEU:O	2:B:224:ILE:HG12	2.03	0.59
3:C:208:ILE:HD12	3:C:213:ARG:HD3	1.83	0.59
1:A:1231:ASP:OD1	1:A:1232:ALA:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1246:PHE:O	1:A:1250:HIS:CB	2.51	0.59
3:C:226:TYR:HA	3:C:230:ASN:HB2	1.85	0.58
3:C:308:ASN:OD1	3:C:311:LYS:NZ	2.36	0.58
3:C:77:LYS:HE2	3:C:325:PRO:HG2	1.85	0.58
1:A:500:GLU:OE2	1:A:502:LYS:CG	2.51	0.58
1:A:1342:TYR:CD2	2:B:519:ALA:HB1	2.37	0.58
2:B:252:THR:HA	2:B:305:GLU:HA	1.85	0.58
3:C:172:GLU:HA	3:C:175:ARG:HE	1.68	0.58
1:A:1395:TYR:HA	1:A:1398:ILE:HD12	1.86	0.58
3:C:88:PRO:O	3:C:91:HIS:ND1	2.28	0.58
3:C:156:LEU:O	3:C:168:TRP:N	2.36	0.58
2:B:185:ARG:NH2	2:B:340:SER:OG	2.35	0.58
4:D:398:LEU:HD13	4:D:403:ILE:HD13	1.85	0.58
1:A:1242:ASP:HB3	1:A:1246:PHE:HB2	1.85	0.58
1:A:1285:THR:HG21	1:A:1317:ALA:HB3	1.85	0.58
1:A:1415:ASP:HA	1:A:1418:LYS:HE3	1.85	0.58
1:A:1001:GLY:HA3	1:A:1006:ILE:HD13	1.85	0.58
3:C:120:ARG:HH11	3:C:233:ILE:HA	1.68	0.58
3:C:259:PHE:HA	3:C:268:ARG:HG2	1.85	0.58
1:A:403:GLU:HG3	1:A:405:GLY:H	1.69	0.57
1:A:994:MET:SD	1:A:996:LEU:HD23	2.44	0.57
2:B:295:SER:OG	2:B:501:HIS:NE2	2.20	0.57
1:A:784:ARG:HG3	1:A:787:ARG:NH1	2.20	0.57
1:A:932:GLN:HG3	1:A:933:ASP:H	1.69	0.57
3:C:50:LYS:HA	3:C:76:TYR:HE2	1.68	0.57
1:A:1286:CYS:SG	1:A:1315:CYS:HB2	2.43	0.57
1:A:1296:PHE:HA	1:A:1305:PRO:HA	1.87	0.57
2:B:405:CYS:O	2:B:409:ILE:HD12	2.04	0.57
1:A:380:VAL:HG13	1:A:383:ILE:HD11	1.85	0.57
4:D:152:GLU:O	4:D:185:LYS:N	2.30	0.57
1:A:1392:LEU:HD22	1:A:1441:LEU:HD13	1.86	0.57
2:B:173:SER:HB2	2:B:594:GLN:HE22	1.70	0.57
1:A:438:ASN:HB2	1:A:801:TYR:CD1	2.40	0.57
3:C:12:LEU:HD23	3:C:350:ILE:HG23	1.86	0.57
1:A:988:LYS:HG2	1:A:998:VAL:HG11	1.85	0.57
1:A:906:LEU:HD21	3:C:96:LEU:HD21	1.86	0.57
5:E:17:SER:HA	5:E:120:ASN:HA	1.86	0.57
1:A:549:ASN:OD1	1:A:554:GLN:N	2.35	0.56
3:C:381:ARG:HE	3:C:383:TYR:HE1	1.53	0.56
1:A:585:VAL:HA	1:A:610:GLU:O	2.06	0.56
1:A:661:LYS:O	1:A:688:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:LEU:HB3	2:B:375:CYS:HA	1.87	0.56
3:C:50:LYS:NZ	3:C:73:MET:O	2.28	0.56
1:A:416:GLU:O	1:A:420:LYS:HG2	2.04	0.56
1:A:662:ILE:HG22	1:A:685:THR:HG23	1.87	0.56
1:A:999:ILE:HD12	1:A:1049:LEU:HD22	1.88	0.56
1:A:785:SER:O	1:A:789:GLU:HB2	2.06	0.56
1:A:876:PHE:HD1	1:A:881:ARG:HH22	1.53	0.56
2:B:205:SER:O	2:B:438:PRO:HB3	2.05	0.56
4:D:49:ARG:HB2	4:D:102:SER:HB2	1.87	0.56
1:A:1413:GLU:HA	1:A:1416:LYS:HE2	1.88	0.56
3:C:104:LYS:HD3	3:C:313:ILE:O	2.06	0.56
3:C:108:PHE:N	3:C:167:CYS:SG	2.78	0.56
4:D:75:GLU:HG3	4:D:130:PHE:HZ	1.70	0.56
1:A:581:SER:HA	1:A:608:LYS:NZ	2.20	0.56
1:A:784:ARG:HB3	1:A:955:SER:HB2	1.87	0.56
1:A:854:LYS:HG3	1:A:1011:ASN:HA	1.89	0.56
1:A:1162:ASN:O	1:A:1168:LYS:NZ	2.34	0.56
3:C:192:VAL:HG11	3:C:304:ARG:HG2	1.88	0.56
2:B:374:VAL:HG23	2:B:419:HIS:HB3	1.87	0.55
2:B:578:ARG:HD3	2:B:579:PRO:HD2	1.88	0.55
2:B:170:VAL:HA	2:B:596:VAL:HA	1.88	0.55
1:A:1278:ARG:HD2	1:A:1293:ASP:HB3	1.89	0.55
3:C:115:TYR:HB2	3:C:119:ARG:HH11	1.71	0.55
4:D:215:VAL:HA	4:D:218:ILE:HG12	1.89	0.55
1:A:664:ARG:H	1:A:687:GLY:HA3	1.71	0.55
3:C:119:ARG:NH2	3:C:123:SER:O	2.37	0.55
4:D:331:PHE:HB3	4:D:336:MET:SD	2.47	0.55
3:C:159:TYR:HA	3:C:165:VAL:HG12	1.89	0.55
1:A:908:MET:SD	1:A:912:PRO:HB2	2.46	0.55
3:C:25:GLN:NE2	3:C:399:LEU:HD12	2.21	0.55
1:A:439:TYR:CZ	1:A:441:PHE:HB2	2.41	0.55
1:A:1445:GLY:HA2	2:B:209:MET:H	1.72	0.55
2:B:341:MET:HB3	2:B:575:TYR:CD1	2.39	0.55
2:B:342:VAL:HG13	2:B:374:VAL:HG13	1.89	0.55
1:A:1371:CYS:SG	1:A:1374:CYS:N	2.70	0.54
2:B:404:GLN:HE22	2:B:407:ARG:HE	1.56	0.54
3:C:291:TRP:O	3:C:294:TRP:HB2	2.06	0.54
4:D:79:ARG:NH1	4:D:84:SER:O	2.41	0.54
3:C:38:ASN:HB3	3:C:41:GLN:HB2	1.88	0.54
1:A:1243:PRO:HB2	4:D:355:LYS:HZ1	1.72	0.54
3:C:187:GLU:O	4:D:198:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HD21	1:A:1239:LEU:HB3	1.89	0.54
1:A:985:MET:HE1	4:D:113:SER:HA	1.88	0.54
1:A:1113:GLN:HG3	1:A:1238:TRP:CD2	2.42	0.54
1:A:1145:ASP:O	2:B:266:ASN:ND2	2.39	0.54
1:A:1244:THR:HG22	1:A:1247:ARG:HH12	1.73	0.54
2:B:551:VAL:HG22	2:B:552:LEU:HG	1.90	0.54
3:C:42:HIS:HB2	3:C:83:VAL:HG13	1.89	0.54
2:B:476:LEU:HD11	2:B:510:PRO:HD2	1.88	0.54
3:C:68:LYS:HE3	3:C:72:LYS:HD3	1.89	0.54
3:C:258:SER:HA	3:C:261:LYS:HE3	1.89	0.54
4:D:356:GLU:HA	4:D:358:LYS:HG3	1.90	0.54
1:A:547:MET:HG3	1:A:728:ILE:HD11	1.88	0.54
1:A:1212:LEU:HB3	1:A:1239:LEU:HD13	1.90	0.54
1:A:1342:TYR:HD2	2:B:519:ALA:HB1	1.73	0.54
2:B:577:ARG:HB3	2:B:591:ILE:HD11	1.90	0.54
4:D:79:ARG:HH12	4:D:85:TYR:HB2	1.72	0.54
4:D:135:LEU:HD11	4:D:139:LYS:HB2	1.89	0.53
2:B:231:LEU:HD11	2:B:322:GLY:HA2	1.91	0.53
2:B:547:PHE:H	2:B:558:ASN:HB3	1.73	0.53
4:D:439:PHE:CE2	4:D:450:GLU:HG3	2.43	0.53
3:C:63:GLN:HE22	3:C:66:LEU:HD23	1.74	0.53
1:A:732:TYR:HA	1:A:738:LEU:HD12	1.90	0.53
3:C:155:ARG:HD3	3:C:157:TRP:CD1	2.44	0.53
4:D:387:ARG:CD	4:D:420:TYR:CZ	2.90	0.53
1:A:807:GLN:HE22	1:A:809:PHE:HB3	1.74	0.53
2:B:386:HIS:HB3	2:B:389:VAL:HG22	1.91	0.53
1:A:1156:HIS:HA	1:A:1159:LEU:HD12	1.89	0.53
5:E:19:PRO:HA	5:E:118:TYR:HA	1.91	0.53
4:D:267:ASN:OD1	4:D:268:VAL:N	2.37	0.53
1:A:1430:TYR:O	1:A:1434:LYS:HG3	2.08	0.53
3:C:144:ARG:HA	3:C:147:LYS:HE3	1.91	0.53
3:C:215:SER:O	3:C:219:ILE:HG13	2.09	0.53
4:D:281:THR:OG1	4:D:289:ARG:NH2	2.42	0.53
1:A:547:MET:HA	1:A:725:MET:SD	2.49	0.53
3:C:292:LEU:O	3:C:296:ILE:HG12	2.09	0.53
1:A:619:LEU:HD23	1:A:651:ILE:HG22	1.91	0.52
1:A:659:TRP:CH2	1:A:671:PRO:HD3	2.45	0.52
1:A:851:PHE:HB2	1:A:1227:ILE:HG13	1.91	0.52
1:A:1133:PHE:HD2	1:A:1211:TYR:CE2	2.27	0.52
2:B:371:ARG:NH1	2:B:415:SER:O	2.35	0.52
1:A:616:ARG:NH1	1:A:654:CYS:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:TYR:HB3	3:C:406:ARG:CZ	2.39	0.52
4:D:439:PHE:HE1	4:D:441:LEU:HB3	1.75	0.52
1:A:362:PHE:CD2	1:A:687:GLY:HA2	2.44	0.52
4:D:29:TYR:O	4:D:107:ARG:NH2	2.42	0.52
1:A:557:ILE:HD11	1:A:646:VAL:HG13	1.91	0.52
1:A:725:MET:O	1:A:729:GLN:NE2	2.43	0.52
3:C:29:TRP:HB2	3:C:399:LEU:HD11	1.91	0.52
3:C:222:TYR:OH	3:C:340:ASP:OD1	2.27	0.52
3:C:159:TYR:HB2	3:C:334:ILE:HD11	1.91	0.52
1:A:617:THR:HG23	5:E:28:VAL:HG21	1.92	0.52
1:A:1400:ASP:OD1	1:A:1434:LYS:NZ	2.34	0.52
1:A:1235:ILE:HG22	1:A:1239:LEU:HD23	1.92	0.51
1:A:541:ALA:HB3	1:A:563:LEU:HB2	1.92	0.51
2:B:404:GLN:NE2	2:B:407:ARG:HE	2.08	0.51
1:A:639:ILE:HG22	1:A:644:LEU:HB2	1.93	0.51
2:B:343:LEU:HD13	2:B:367:ILE:HD11	1.92	0.51
3:C:30:LEU:HD13	3:C:43:ARG:HD3	1.93	0.51
1:A:704:LYS:NZ	1:A:1076:GLY:H	2.08	0.51
1:A:1231:ASP:O	1:A:1235:ILE:HD12	2.10	0.51
1:A:1418:LYS:HA	1:A:1422:PHE:HB2	1.91	0.51
4:D:33:PRO:HG3	4:D:101:ILE:HG13	1.91	0.51
5:E:73:ARG:HB3	5:E:102:ILE:HG23	1.93	0.51
2:B:477:LEU:HG	2:B:540:ILE:HG21	1.92	0.51
4:D:366:SER:HA	4:D:443:HIS:CD2	2.45	0.51
2:B:346:CYS:HA	2:B:378:PHE:HB2	1.93	0.51
3:C:244:LEU:O	3:C:252:HIS:NE2	2.44	0.51
2:B:230:GLU:O	2:B:233:GLU:HG3	2.11	0.51
2:B:377:LEU:HB2	2:B:422:PHE:HD1	1.74	0.51
3:C:105:GLU:OE2	3:C:169:VAL:N	2.43	0.51
3:C:237:LYS:HA	3:C:240:TRP:CE2	2.46	0.51
4:D:137:LYS:O	4:D:140:ILE:HG12	2.10	0.51
5:E:53:LEU:HD21	5:E:119:ARG:HB2	1.92	0.51
1:A:1330:LEU:HD22	1:A:1399:PHE:HE2	1.76	0.51
3:C:70:MET:HE3	3:C:70:MET:HA	1.92	0.51
1:A:650:ARG:HA	1:A:653:VAL:HG12	1.93	0.51
1:A:921:ARG:HH12	1:A:945:ARG:HH22	1.58	0.51
3:C:79:ASP:OD1	3:C:80:ILE:N	2.44	0.51
3:C:251:ILE:HG22	3:C:255:LEU:HG	1.92	0.51
4:D:41:GLU:OE2	4:D:97:ARG:NH1	2.42	0.51
1:A:491:ARG:NH2	1:A:526:VAL:O	2.37	0.50
1:A:1410:THR:O	1:A:1414:LYS:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:ILE:HA	3:C:353:ILE:HG12	1.93	0.50
1:A:637:HIS:CE1	1:A:708:LEU:HB2	2.46	0.50
3:C:271:HIS:HA	3:C:274:LYS:HD3	1.92	0.50
1:A:1241:LEU:HD23	1:A:1241:LEU:H	1.77	0.50
2:B:431:HIS:ND1	2:B:437:GLN:OE1	2.44	0.50
1:A:450:SER:OG	1:A:451:GLU:N	2.45	0.50
3:C:389:ALA:HB1	3:C:393:LYS:NZ	2.27	0.50
1:A:344:TYR:O	1:A:364:LYS:N	2.44	0.50
3:C:216:ILE:HG21	3:C:294:TRP:CZ3	2.46	0.50
1:A:349:TYR:HB2	1:A:682:ARG:HH12	1.76	0.50
1:A:1116:LEU:HD11	1:A:1235:ILE:HG23	1.93	0.50
1:A:786:GLU:N	1:A:786:GLU:OE1	2.43	0.50
2:B:363:LEU:HD21	2:B:562:LEU:HD11	1.94	0.50
2:B:545:ARG:NH1	2:B:546:TYR:O	2.45	0.50
3:C:274:LYS:O	3:C:278:ARG:HG2	2.12	0.50
4:D:197:GLY:HA3	4:D:199:LYS:HZ2	1.77	0.50
1:A:1362:LEU:HD23	2:B:273:GLU:HG3	1.93	0.49
4:D:91:ASP:OD2	4:D:96:ARG:NH2	2.45	0.49
1:A:865:TYR:HD1	1:A:976:VAL:HG12	1.77	0.49
1:A:1262:GLY:N	4:D:256:SER:HB2	2.27	0.49
3:C:19:ARG:HD2	3:C:357:LEU:HD21	1.94	0.49
1:A:630:ASP:HA	1:A:688:ARG:HH21	1.76	0.49
1:A:1072:GLN:OE1	1:A:1100:LEU:HD13	2.11	0.49
4:D:37:ILE:HD11	4:D:42:PHE:HD1	1.77	0.49
1:A:699:GLU:OE2	1:A:784:ARG:NH1	2.45	0.49
1:A:774:ASN:ND2	1:A:779:THR:OG1	2.45	0.49
1:A:926:LYS:HG3	1:A:930:LYS:HZ3	1.77	0.49
2:B:218:GLU:HA	2:B:221:THR:HG22	1.93	0.49
2:B:405:CYS:O	2:B:408:THR:OG1	2.20	0.49
1:A:495:GLY:N	1:A:773:GLY:HA2	2.27	0.49
1:A:1063:THR:N	1:A:1067:ASN:O	2.44	0.49
4:D:192:LEU:HA	4:D:195:PHE:CE1	2.47	0.49
1:A:411:LYS:HG3	1:A:415:GLU:OE1	2.12	0.49
4:D:75:GLU:O	4:D:79:ARG:HG2	2.12	0.49
4:D:356:GLU:HG2	4:D:358:LYS:HE2	1.94	0.49
1:A:615:GLU:OE1	1:A:650:ARG:NH2	2.40	0.49
1:A:872:PHE:HB3	1:A:901:LEU:HD11	1.93	0.49
1:A:1133:PHE:HD2	1:A:1211:TYR:HE2	1.59	0.49
2:B:296:LEU:HA	2:B:300:GLN:NE2	2.27	0.49
3:C:23:TYR:HE1	3:C:70:MET:HG3	1.77	0.49
4:D:296:ARG:NH1	4:D:330:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ILE:HG12	1:A:951:LEU:HD11	1.93	0.49
1:A:340:VAL:HG11	1:A:502:LYS:HG2	1.94	0.49
4:D:364:PRO:HB2	4:D:443:HIS:CE1	2.47	0.49
5:E:56:LEU:HD12	5:E:60:VAL:CG1	2.43	0.49
1:A:582:HIS:CE1	1:A:608:LYS:HE3	2.48	0.48
3:C:174:VAL:HA	3:C:177:LEU:HG	1.95	0.48
3:C:141:ILE:O	3:C:144:ARG:HG3	2.13	0.48
5:E:74:SER:HB3	5:E:87:GLU:HG3	1.95	0.48
1:A:773:GLY:HA3	1:A:794:HIS:CD2	2.48	0.48
1:A:1451:LEU:HD12	1:A:1455:PHE:CE2	2.48	0.48
5:E:37:GLU:O	5:E:41:GLU:HG2	2.13	0.48
1:A:1149:LYS:HA	1:A:1155:VAL:HG21	1.95	0.48
1:A:1394:PHE:CZ	1:A:1398:ILE:HD11	2.48	0.48
4:D:50:VAL:HG21	4:D:253:LEU:HB3	1.94	0.48
1:A:634:ILE:HG22	1:A:689:MET:O	2.14	0.48
1:A:1048:LEU:HB3	1:A:1056:ALA:HB3	1.95	0.48
1:A:1288:THR:HG21	1:A:1312:ASN:HB2	1.95	0.48
2:B:431:HIS:CE1	2:B:438:PRO:HG2	2.49	0.48
2:B:494:ARG:H	2:B:494:ARG:HD2	1.78	0.48
1:A:570:LEU:HD12	1:A:766:LEU:HD11	1.96	0.48
1:A:1322:PHE:O	1:A:1326:LEU:HD23	2.13	0.48
4:D:339:ASP:OD1	4:D:340:LYS:N	2.47	0.48
1:A:728:ILE:HA	1:A:731:MET:HB2	1.95	0.48
1:A:922:ARG:HH21	1:A:946:GLN:HE21	1.61	0.48
1:A:1353:CYS:HB2	1:A:1374:CYS:SG	2.52	0.48
1:A:952:THR:HG22	1:A:956:MET:HE3	1.95	0.48
2:B:364:ILE:HD11	2:B:409:ILE:HA	1.96	0.48
2:B:517:ASP:OD1	2:B:517:ASP:N	2.46	0.48
1:A:916:ARG:O	1:A:920:GLU:HG2	2.14	0.48
2:B:509:TYR:CE1	2:B:511:LEU:HB3	2.48	0.48
2:B:255:GLY:HA2	2:B:274:GLY:HA2	1.96	0.47
3:C:107:VAL:HG21	3:C:317:LEU:HD23	1.95	0.47
3:C:154:HIS:O	3:C:169:VAL:HA	2.14	0.47
1:A:545:LYS:HB2	1:A:559:ALA:HB3	1.96	0.47
3:C:267:GLN:O	3:C:270:GLU:HG3	2.13	0.47
4:D:376:PRO:HD2	4:D:388:HIS:CG	2.49	0.47
1:A:581:SER:HA	1:A:608:LYS:HZ2	1.80	0.47
1:A:1167:ARG:HD2	1:A:1168:LYS:O	2.14	0.47
1:A:1196:GLU:O	1:A:1199:GLN:HG2	2.14	0.47
1:A:1307:LEU:HD12	1:A:1430:TYR:CZ	2.49	0.47
1:A:1396:ARG:NE	1:A:1438:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:LYS:HG2	3:C:105:GLU:N	2.29	0.47
3:C:144:ARG:HG2	3:C:218:ILE:CD1	2.45	0.47
4:D:49:ARG:NH1	4:D:99:ASP:OD1	2.47	0.47
5:E:84:LYS:O	5:E:122:LEU:N	2.38	0.47
1:A:632:ASP:O	1:A:689:MET:HB3	2.14	0.47
1:A:1295:VAL:HG11	1:A:1401:ALA:HA	1.95	0.47
2:B:343:LEU:HD22	2:B:367:ILE:HD11	1.96	0.47
3:C:178:SER:O	3:C:182:ARG:HG3	2.14	0.47
1:A:432:SER:HB2	1:A:453:LEU:HD11	1.97	0.47
1:A:689:MET:HE3	1:A:776:MET:HG2	1.97	0.47
1:A:846:ASP:OD1	1:A:846:ASP:N	2.48	0.47
2:B:383:ASP:O	2:B:389:VAL:HG21	2.15	0.47
3:C:133:THR:HG21	3:C:226:TYR:HB2	1.97	0.47
4:D:250:LEU:HA	4:D:253:LEU:HD23	1.97	0.47
3:C:121:CYS:HB3	3:C:231:GLN:HE22	1.80	0.47
3:C:276:ALA:O	3:C:280:GLN:HG2	2.15	0.47
4:D:390:ASP:O	4:D:394:LEU:HG	2.15	0.47
1:A:448:GLU:HG3	3:C:95:LYS:HA	1.96	0.47
1:A:1396:ARG:O	1:A:1400:ASP:HB2	2.14	0.47
4:D:222:PHE:O	4:D:226:LEU:HD23	2.15	0.47
1:A:1056:ALA:HA	1:A:1074:LEU:HB2	1.95	0.47
3:C:183:SER:O	3:C:186:VAL:HG22	2.15	0.47
3:C:308:ASN:HA	3:C:311:LYS:HG2	1.95	0.47
4:D:130:PHE:CE2	4:D:134:ILE:HD11	2.50	0.47
1:A:415:GLU:HA	1:A:418:ASP:OD2	2.15	0.46
1:A:1114:LYS:O	1:A:1118:GLU:OE1	2.33	0.46
1:A:1405:LEU:HD23	1:A:1414:LYS:HZ1	1.79	0.46
1:A:364:LYS:HD2	1:A:373:HIS:HB3	1.97	0.46
1:A:792:LEU:HD11	1:A:911:LEU:HD23	1.97	0.46
3:C:144:ARG:HA	3:C:147:LYS:HG2	1.97	0.46
3:C:232:ASP:OD2	3:C:235:GLU:HB3	2.14	0.46
1:A:340:VAL:CG1	1:A:502:LYS:HG2	2.45	0.46
1:A:876:PHE:HA	1:A:881:ARG:HH21	1.80	0.46
1:A:1117:ILE:O	1:A:1121:GLU:HG2	2.15	0.46
1:A:1434:LYS:O	1:A:1438:GLU:HG2	2.15	0.46
2:B:431:HIS:HE1	2:B:438:PRO:HG2	1.80	0.46
3:C:216:ILE:HD13	3:C:294:TRP:CE3	2.44	0.46
5:E:18:LEU:N	5:E:119:ARG:O	2.46	0.46
1:A:1227:ILE:H	1:A:1227:ILE:HD12	1.81	0.46
3:C:399:LEU:HA	3:C:399:LEU:HD23	1.74	0.46
1:A:477:PHE:HD1	1:A:802:ILE:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:LEU:O	1:A:1024:LYS:HG2	2.16	0.46
1:A:1051:LYS:HE3	1:A:1054:LYS:HD3	1.97	0.46
1:A:1353:CYS:SG	1:A:1355:ASN:HB2	2.56	0.46
2:B:341:MET:HA	2:B:574:LEU:O	2.14	0.46
3:C:120:ARG:NH2	3:C:235:GLU:OE2	2.46	0.46
4:D:151:PHE:HD1	4:D:186:ILE:HG13	1.80	0.46
4:D:280:SER:HA	4:D:284:PHE:CG	2.50	0.46
1:A:1243:PRO:HB2	4:D:355:LYS:NZ	2.30	0.46
2:B:339:GLN:HA	2:B:577:ARG:HB2	1.98	0.46
1:A:359:VAL:HG12	1:A:361:LEU:HD22	1.96	0.46
1:A:870:GLN:NE2	1:A:916:ARG:HG3	2.30	0.46
2:B:228:GLY:HA3	2:B:254:LEU:HD11	1.98	0.46
1:A:464:LEU:HD23	1:A:468:LEU:HD22	1.98	0.46
1:A:551:LYS:HG3	1:A:552:ASN:H	1.80	0.46
1:A:624:ALA:HB3	5:E:27:LEU:HD23	1.97	0.46
3:C:39:TYR:CE1	3:C:83:VAL:HG21	2.50	0.46
3:C:43:ARG:HA	3:C:83:VAL:HG22	1.98	0.46
3:C:128:CYS:SG	3:C:131:CYS:N	2.89	0.46
4:D:346:SER:OG	4:D:350:ARG:NH2	2.49	0.46
1:A:923:LYS:O	1:A:927:GLN:HG2	2.16	0.46
1:A:1116:LEU:HD22	1:A:1238:TRP:HB3	1.98	0.46
3:C:269:TRP:NE1	3:C:273:LYS:HD2	2.31	0.46
4:D:159:LYS:HE2	4:D:178:LEU:HD23	1.98	0.46
4:D:194:LEU:HD13	4:D:217:ILE:HD11	1.98	0.46
1:A:1051:LYS:HB3	1:A:1054:LYS:HB3	1.98	0.45
1:A:1286:CYS:SG	1:A:1288:THR:OG1	2.64	0.45
4:D:42:PHE:CZ	4:D:105:ILE:HD13	2.51	0.45
1:A:786:GLU:O	1:A:789:GLU:HB3	2.16	0.45
1:A:345:TRP:HA	1:A:363:GLY:HA3	1.99	0.45
1:A:598:PHE:CZ	1:A:738:LEU:HD22	2.52	0.45
3:C:135:MET:O	3:C:139:ILE:HG12	2.17	0.45
4:D:166:ILE:O	4:D:170:SER:OG	2.16	0.45
1:A:637:HIS:NE2	1:A:694:GLU:OE1	2.49	0.45
3:C:388:LEU:O	3:C:392:VAL:HG23	2.17	0.45
4:D:26:LEU:HD11	4:D:135:LEU:HD22	1.97	0.45
1:A:482:SER:O	1:A:486:LEU:HD23	2.17	0.45
3:C:243:ILE:O	3:C:247:VAL:HG23	2.16	0.45
1:A:582:HIS:CG	1:A:746:TRP:HE1	2.34	0.45
1:A:911:LEU:O	1:A:915:ILE:HG12	2.16	0.45
1:A:1149:LYS:HE2	1:A:1159:LEU:HD11	1.98	0.45
2:B:435:TYR:CE1	2:B:459:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASP:HA	1:A:688:ARG:HE	1.82	0.45
1:A:664:ARG:HB2	1:A:687:GLY:HA3	1.98	0.45
1:A:872:PHE:HB2	1:A:874:ILE:HD11	1.98	0.45
1:A:1074:LEU:HD21	1:A:1077:LEU:HD13	1.98	0.45
2:B:215:ASP:O	2:B:219:VAL:HG23	2.15	0.45
3:C:131:CYS:HA	3:C:226:TYR:HE1	1.82	0.45
5:E:91:GLU:OE1	5:E:97:TYR:HB2	2.16	0.45
5:E:91:GLU:OE1	5:E:94:GLY:HA2	2.16	0.45
5:E:95:ILE:HG22	5:E:96:GLN:HG2	1.97	0.45
1:A:395:LYS:HB2	1:A:408:ILE:HD11	1.99	0.45
1:A:742:LEU:O	1:A:745:THR:OG1	2.25	0.45
3:C:27:TYR:HB2	3:C:63:GLN:HE21	1.82	0.45
3:C:104:LYS:HE2	3:C:312:GLY:O	2.16	0.45
4:D:192:LEU:HD23	4:D:195:PHE:HE1	1.81	0.45
4:D:328:LYS:O	4:D:332:ILE:HG12	2.17	0.45
1:A:364:LYS:CD	1:A:373:HIS:HB3	2.47	0.45
1:A:482:SER:O	1:A:485:GLU:HG2	2.17	0.45
1:A:1009:ASN:OD1	1:A:1010:THR:N	2.49	0.45
2:B:160:LYS:NZ	2:B:566:GLN:OE1	2.49	0.45
2:B:161:TYR:CE1	2:B:568:GLY:HA2	2.46	0.45
2:B:527:VAL:HG13	2:B:528:TYR:CD2	2.51	0.45
4:D:105:ILE:HD11	4:D:250:LEU:HD21	1.99	0.45
1:A:903:ASP:OD2	1:A:906:LEU:N	2.50	0.45
1:A:1063:THR:HG23	1:A:1068:TYR:HA	1.99	0.45
3:C:240:TRP:NE1	3:C:256:GLN:OE1	2.50	0.45
1:A:537:LEU:HG	1:A:570:LEU:HD21	1.98	0.44
3:C:182:ARG:O	3:C:186:VAL:HG13	2.16	0.44
3:C:216:ILE:HG21	3:C:294:TRP:CE3	2.52	0.44
4:D:278:LEU:HA	4:D:281:THR:HG22	1.99	0.44
1:A:912:PRO:HA	1:A:915:ILE:HG12	1.98	0.44
1:A:1345:TRP:HZ3	2:B:262:ASN:HD21	1.63	0.44
3:C:46:SER:HB3	3:C:79:ASP:HB3	2.00	0.44
1:A:1445:GLY:CA	2:B:209:MET:H	2.29	0.44
2:B:436:PRO:HB3	2:B:459:PRO:HD2	2.00	0.44
3:C:79:ASP:OD1	3:C:317:LEU:N	2.50	0.44
4:D:66:GLY:O	4:D:71:GLN:NE2	2.50	0.44
1:A:344:TYR:CE2	1:A:534:PRO:HB3	2.52	0.44
1:A:362:PHE:HE1	1:A:377:CYS:HG	1.65	0.44
1:A:1134:GLU:HA	1:A:1178:VAL:HG12	1.99	0.44
4:D:61:VAL:HG11	4:D:419:HIS:CG	2.53	0.44
1:A:926:LYS:HA	1:A:929:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:ASN:HA	1:A:1438:GLU:HB2	2.00	0.44
1:A:568:PHE:CE1	1:A:575:PRO:HD2	2.52	0.44
1:A:1105:ARG:CZ	1:A:1109:VAL:HG21	2.48	0.44
2:B:240:PHE:HA	2:B:252:THR:HG23	1.99	0.44
2:B:383:ASP:OD1	2:B:384:ALA:N	2.50	0.44
3:C:143:ASP:OD2	3:C:155:ARG:NH2	2.50	0.44
4:D:243:ASP:OD2	4:D:246:LEU:N	2.50	0.44
4:D:364:PRO:HB2	4:D:443:HIS:HE1	1.81	0.44
4:D:443:HIS:ND1	4:D:445:ASN:HB2	2.33	0.44
5:E:45:HIS:HB3	5:E:51:CYS:HB3	2.00	0.44
1:A:807:GLN:HE22	1:A:809:PHE:CB	2.30	0.44
1:A:1074:LEU:HD11	1:A:1096:ILE:HD11	2.00	0.44
3:C:202:VAL:HG12	3:C:295:GLU:HB2	2.00	0.44
1:A:343:PHE:CE2	1:A:378:VAL:HG11	2.53	0.44
1:A:343:PHE:HB3	1:A:365:VAL:HG23	2.00	0.44
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.85	0.44
3:C:172:GLU:HG2	3:C:175:ARG:HH21	1.82	0.44
1:A:491:ARG:HA	1:A:491:ARG:NH1	2.31	0.43
1:A:1150:LYS:O	1:A:1190:GLN:NE2	2.47	0.43
2:B:449:ASP:O	2:B:453:VAL:HG12	2.17	0.43
3:C:202:VAL:HG11	3:C:298:LEU:HB2	2.00	0.43
4:D:120:PHE:O	4:D:124:GLU:HG3	2.18	0.43
5:E:51:CYS:HB2	5:E:107:LEU:HD21	2.00	0.43
1:A:670:MET:HG2	1:A:671:PRO:HD2	1.99	0.43
3:C:253:ASP:N	3:C:253:ASP:OD1	2.50	0.43
4:D:45:LEU:HD12	4:D:102:SER:HB3	2.00	0.43
4:D:450:GLU:O	4:D:454:ILE:HG12	2.18	0.43
1:A:347:ASP:OD2	1:A:682:ARG:NH2	2.51	0.43
1:A:412:ASP:HA	1:A:415:GLU:OE2	2.18	0.43
1:A:437:LYS:HB2	1:A:452:TYR:CD2	2.52	0.43
4:D:125:MET:HE3	4:D:223:ARG:HB3	1.99	0.43
4:D:387:ARG:CD	4:D:420:TYR:OH	2.66	0.43
5:E:53:LEU:HD11	5:E:119:ARG:HD2	2.00	0.43
1:A:847:PRO:HB3	1:A:1052:LYS:HZ3	1.83	0.43
3:C:175:ARG:NH2	3:C:406:ARG:HH22	2.17	0.43
3:C:240:TRP:CD2	3:C:259:PHE:HD2	2.36	0.43
4:D:211:LEU:HA	4:D:214:ILE:HD12	1.99	0.43
1:A:911:LEU:HB2	1:A:912:PRO:HD3	2.00	0.43
1:A:921:ARG:HH12	1:A:945:ARG:NH2	2.16	0.43
1:A:992:GLN:OE1	1:A:997:GLU:HA	2.18	0.43
1:A:1166:GLY:O	1:A:1168:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ARG:HH12	3:C:324:HIS:HE2	1.66	0.43
1:A:1113:GLN:O	1:A:1117:ILE:HG13	2.19	0.43
3:C:21:PHE:HB3	3:C:23:TYR:CE2	2.54	0.43
1:A:717:LYS:HE3	1:A:717:LYS:HB2	1.92	0.43
1:A:1415:ASP:C	1:A:1419:LYS:HZ2	2.22	0.43
2:B:179:GLY:O	2:B:182:TRP:NE1	2.51	0.43
2:B:357:TYR:HB3	2:B:360:LEU:HB3	2.00	0.43
3:C:49:LEU:HD22	3:C:73:MET:HG2	2.01	0.43
3:C:162:ARG:HB3	3:C:163:ARG:HH11	1.83	0.43
4:D:191:ALA:HB1	4:D:194:LEU:HB3	2.00	0.43
4:D:210:PRO:O	4:D:214:ILE:HG13	2.19	0.43
4:D:345:TYR:O	4:D:349:ILE:HD12	2.18	0.43
1:A:565:HIS:CD2	1:A:567:SER:O	2.71	0.43
1:A:1208:THR:O	1:A:1212:LEU:HG	2.18	0.43
3:C:136:THR:HG23	3:C:339:VAL:HG12	2.01	0.43
4:D:387:ARG:HD3	4:D:420:TYR:OH	2.19	0.43
1:A:796:PHE:HB3	1:A:801:TYR:HB2	2.00	0.43
2:B:406:LEU:O	2:B:410:ILE:HG12	2.18	0.43
3:C:130:LYS:HG2	3:C:130:LYS:O	2.18	0.43
3:C:309:VAL:HG12	3:C:315:HIS:HE1	1.81	0.43
1:A:746:TRP:CE3	1:A:747:LYS:HE3	2.54	0.43
1:A:1396:ARG:HD2	1:A:1441:LEU:HD22	2.00	0.43
2:B:344:VAL:HA	2:B:376:ILE:HB	2.00	0.43
2:B:524:SER:HA	2:B:527:VAL:HG12	2.01	0.43
3:C:176:LYS:HD2	3:C:176:LYS:HA	1.87	0.43
4:D:130:PHE:O	4:D:134:ILE:HG13	2.18	0.43
4:D:347:TYR:HD2	4:D:350:ARG:HH12	1.67	0.43
1:A:543:SER:N	1:A:561:ALA:O	2.41	0.42
1:A:597:ALA:HB1	1:A:600:GLU:HB2	2.01	0.42
1:A:692:ASP:HB3	1:A:695:ILE:HG12	2.01	0.42
2:B:219:VAL:HG13	2:B:526:TYR:HB2	2.02	0.42
3:C:155:ARG:HH11	3:C:157:TRP:HD1	1.65	0.42
4:D:79:ARG:NH1	4:D:85:TYR:HB2	2.33	0.42
1:A:382:ASN:HB2	1:A:521:LEU:O	2.19	0.42
1:A:856:ILE:HD13	1:A:1009:ASN:HA	2.00	0.42
1:A:876:PHE:HA	1:A:881:ARG:NH2	2.34	0.42
1:A:1078:ASP:OD1	1:A:1079:ILE:N	2.52	0.42
2:B:574:LEU:HB3	2:B:593:VAL:HG22	2.01	0.42
3:C:68:LYS:O	3:C:72:LYS:HB2	2.19	0.42
3:C:79:ASP:OD2	3:C:316:LEU:HB3	2.18	0.42
3:C:293:GLU:HA	3:C:296:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:PHE:O	4:D:133:SER:OG	2.28	0.42
1:A:647:LEU:HD21	1:A:662:ILE:HD13	2.01	0.42
1:A:784:ARG:HA	1:A:787:ARG:HG2	2.00	0.42
1:A:979:LYS:HA	1:A:979:LYS:HD2	1.80	0.42
1:A:505:GLN:HB2	1:A:505:GLN:HE21	1.59	0.42
1:A:1413:GLU:HA	1:A:1416:LYS:CE	2.49	0.42
2:B:182:TRP:CZ2	2:B:594:GLN:HG2	2.54	0.42
2:B:206:TYR:HE2	2:B:208:SER:O	2.03	0.42
5:E:61:LEU:HG	5:E:62:PRO:HD3	2.00	0.42
1:A:643:GLU:HA	1:A:646:VAL:HG12	2.01	0.42
1:A:746:TRP:HE3	1:A:747:LYS:HE3	1.84	0.42
1:A:868:ILE:HG23	1:A:872:PHE:HD2	1.84	0.42
3:C:162:ARG:HE	3:C:324:HIS:CE1	2.37	0.42
4:D:37:ILE:HG22	4:D:97:ARG:HH22	1.84	0.42
5:E:31:PHE:CE1	5:E:109:PRO:HG3	2.55	0.42
1:A:681:GLU:OE1	1:A:681:GLU:N	2.42	0.42
2:B:158:SER:H	2:B:566:GLN:HE21	1.66	0.42
4:D:26:LEU:HB2	4:D:143:PHE:CE1	2.54	0.42
1:A:763:PRO:HA	1:A:766:LEU:HD12	2.01	0.42
1:A:921:ARG:O	1:A:924:GLN:HG2	2.19	0.42
1:A:1203:ASN:OD1	1:A:1203:ASN:N	2.51	0.42
2:B:296:LEU:HA	2:B:300:GLN:HE22	1.84	0.42
3:C:234:LEU:HB2	3:C:265:SER:HA	2.01	0.42
1:A:708:LEU:O	1:A:712:VAL:HG23	2.20	0.42
1:A:986:HIS:HA	1:A:989:GLU:CD	2.40	0.42
2:B:173:SER:HB2	2:B:594:GLN:NE2	2.33	0.42
1:A:598:PHE:CZ	1:A:602:ILE:HD11	2.54	0.42
1:A:648:LEU:O	1:A:651:ILE:HG12	2.20	0.42
1:A:740:TYR:O	1:A:743:GLU:HG2	2.20	0.42
1:A:775:ILE:HG22	1:A:777:SER:H	1.85	0.42
3:C:233:ILE:HD12	3:C:243:ILE:HD11	2.02	0.42
3:C:241:ASP:HA	3:C:244:LEU:HD12	2.00	0.42
4:D:319:THR:HG23	4:D:322:GLN:H	1.85	0.42
1:A:702:ARG:O	1:A:714:GLN:NE2	2.43	0.42
1:A:792:LEU:HD12	1:A:796:PHE:CE2	2.55	0.42
1:A:1173:ASP:OD1	1:A:1174:THR:N	2.53	0.42
1:A:1357:THR:HA	2:B:262:ASN:ND2	2.35	0.42
1:A:1399:PHE:CE2	1:A:1433:LEU:HD12	2.54	0.42
2:B:402:PHE:CZ	2:B:406:LEU:HD11	2.54	0.42
3:C:181:VAL:HG22	4:D:192:LEU:HD21	2.01	0.42
4:D:91:ASP:O	4:D:95:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:70:PHE:CE1	5:E:106:VAL:HG22	2.55	0.42
1:A:602:ILE:O	1:A:606:ASN:N	2.52	0.41
1:A:859:LEU:HD13	1:A:1038:ILE:HD11	2.02	0.41
1:A:950:LYS:HE2	1:A:950:LYS:HB3	1.89	0.41
2:B:265:LEU:HD23	2:B:266:ASN:N	2.35	0.41
2:B:447:ARG:H	2:B:447:ARG:HG2	1.68	0.41
1:A:672:LYS:HA	1:A:672:LYS:HD2	1.75	0.41
1:A:856:ILE:HG21	1:A:1047:LEU:HD13	2.01	0.41
1:A:1091:THR:O	1:A:1095:VAL:HG23	2.21	0.41
1:A:1187:THR:O	1:A:1191:ARG:HG3	2.20	0.41
1:A:1241:LEU:C	1:A:1243:PRO:HD2	2.41	0.41
2:B:350:THR:HB	2:B:357:TYR:CD1	2.55	0.41
3:C:159:TYR:HD1	3:C:165:VAL:HG12	1.85	0.41
4:D:186:ILE:HG22	4:D:187:PRO:O	2.20	0.41
5:E:27:LEU:HD13	5:E:111:VAL:HG21	2.02	0.41
1:A:498:TRP:CD1	1:A:532:VAL:HB	2.55	0.41
1:A:921:ARG:HH22	1:A:945:ARG:NH2	2.18	0.41
1:A:1212:LEU:HB3	1:A:1239:LEU:CD1	2.50	0.41
2:B:328:TYR:HB2	2:B:533:VAL:HG21	2.02	0.41
3:C:107:VAL:HG23	3:C:167:CYS:O	2.21	0.41
1:A:552:ASN:HB2	1:A:553:HIS:NE2	2.35	0.41
1:A:1059:VAL:HB	1:A:1071:LYS:HB3	2.03	0.41
1:A:362:PHE:HZ	1:A:665:LEU:HD13	1.86	0.41
1:A:726:GLU:OE1	1:A:726:GLU:N	2.46	0.41
1:A:1000:TYR:CE1	1:A:1052:LYS:HD2	2.55	0.41
4:D:46:ALA:HB1	4:D:253:LEU:HD11	2.02	0.41
1:A:408:ILE:HD13	1:A:408:ILE:HA	1.91	0.41
1:A:875:CYS:SG	1:A:910:ILE:HB	2.61	0.41
2:B:494:ARG:O	2:B:497:ARG:HG2	2.20	0.41
2:B:574:LEU:O	2:B:574:LEU:HD12	2.20	0.41
4:D:135:LEU:HD23	4:D:140:ILE:HG22	2.02	0.41
4:D:345:TYR:O	4:D:348:ASN:N	2.54	0.41
1:A:438:ASN:O	1:A:802:ILE:N	2.53	0.41
1:A:478:GLY:HA2	1:A:481:THR:OG1	2.21	0.41
2:B:207:LYS:HA	2:B:207:LYS:HD2	1.96	0.41
3:C:27:TYR:CD2	3:C:63:GLN:HB2	2.56	0.41
3:C:157:TRP:HA	3:C:167:CYS:HA	2.02	0.41
3:C:169:VAL:HG13	3:C:169:VAL:O	2.21	0.41
4:D:121:ILE:HA	4:D:124:GLU:HG3	2.01	0.41
1:A:565:HIS:HB2	1:A:578:PRO:O	2.21	0.41
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:ASP:OD1	3:C:117:ASP:N	2.53	0.41
3:C:144:ARG:NH2	3:C:215:SER:HB3	2.33	0.41
3:C:392:VAL:O	3:C:396:GLU:OE1	2.39	0.41
1:A:392:ARG:NH1	1:A:470:GLY:O	2.44	0.41
1:A:1181:GLN:NE2	1:A:1183:GLY:H	2.19	0.41
1:A:1217:HIS:NE2	1:A:1232:ALA:HB1	2.36	0.41
3:C:302:PHE:CD1	3:C:303:PRO:HD2	2.55	0.41
4:D:127:LEU:HD21	4:D:131:ARG:NH2	2.36	0.41
4:D:261:ASP:OD1	4:D:261:ASP:N	2.54	0.41
4:D:274:ASP:OD1	4:D:275:GLN:N	2.54	0.41
4:D:311:LEU:CD1	4:D:365:PHE:H	2.34	0.41
1:A:1423:THR:O	1:A:1426:VAL:HG12	2.21	0.41
2:B:196:LEU:O	2:B:461:SER:HB2	2.21	0.41
2:B:396:SER:HB2	2:B:401:ILE:HD11	2.03	0.41
3:C:171:ASP:O	3:C:175:ARG:HG3	2.21	0.41
4:D:40:ILE:O	4:D:43:GLU:HG3	2.21	0.41
4:D:216:ALA:O	4:D:219:LEU:HG	2.21	0.41
1:A:394:MET:HG3	1:A:403:GLU:CD	2.41	0.40
1:A:1244:THR:OG1	1:A:1245:GLN:OE1	2.37	0.40
2:B:515:GLN:HG2	2:B:516:GLU:H	1.85	0.40
2:B:548:VAL:HG13	2:B:557:VAL:HG12	2.02	0.40
2:B:598:ILE:HD12	2:B:598:ILE:HA	1.95	0.40
4:D:47:ILE:HD13	4:D:47:ILE:HA	1.95	0.40
4:D:214:ILE:O	4:D:218:ILE:HG23	2.21	0.40
4:D:390:ASP:OD1	4:D:393:LEU:HD13	2.21	0.40
1:A:347:ASP:OD1	1:A:348:ALA:N	2.54	0.40
1:A:438:ASN:HB2	1:A:801:TYR:HD1	1.81	0.40
1:A:495:GLY:H	1:A:773:GLY:HA2	1.84	0.40
1:A:806:LYS:HD3	1:A:810:ARG:HD3	2.04	0.40
4:D:45:LEU:HA	4:D:45:LEU:HD13	1.88	0.40
4:D:220:ASN:O	4:D:223:ARG:HG2	2.20	0.40
1:A:440:ALA:HA	3:C:95:LYS:HE2	2.03	0.40
1:A:1345:TRP:HZ3	2:B:262:ASN:ND2	2.18	0.40
2:B:227:LEU:HB3	2:B:301:VAL:HG21	2.03	0.40
2:B:297:PHE:CZ	2:B:300:GLN:HB3	2.56	0.40
2:B:363:LEU:CD2	2:B:562:LEU:HD21	2.52	0.40
2:B:499:LEU:O	2:B:503:LEU:HD23	2.22	0.40
3:C:115:TYR:OH	3:C:303:PRO:HA	2.21	0.40
1:A:560:MET:HA	1:A:560:MET:HE3	2.03	0.40
1:A:1145:ASP:CG	2:B:268:LYS:HD2	2.42	0.40
3:C:153:LYS:HG3	3:C:154:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:LYS:O	4:D:271:ILE:HD13	2.22	0.40
1:A:595:PRO:HB2	1:A:735:SER:OG	2.22	0.40
1:A:621:PHE:CD1	5:E:27:LEU:HD22	2.57	0.40
1:A:650:ARG:NH1	1:A:653:VAL:HG11	2.37	0.40
1:A:1056:ALA:HB1	1:A:1100:LEU:HD21	2.03	0.40
1:A:1405:LEU:HD21	1:A:1422:PHE:HE2	1.87	0.40
2:B:385:LYS:HD3	2:B:427:ARG:NH2	2.37	0.40
3:C:196:GLN:O	3:C:196:GLN:HG2	2.22	0.40
4:D:391:PRO:HA	4:D:394:LEU:HG	2.04	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	1062/1170 (91%)	1004 (94%)	58 (6%)	0	100	100
2	B	442/452 (98%)	417 (94%)	24 (5%)	1 (0%)	47	80
3	C	383/441 (87%)	375 (98%)	8 (2%)	0	100	100
4	D	432/509 (85%)	414 (96%)	17 (4%)	1 (0%)	47	80
5	E	101/119 (85%)	100 (99%)	1 (1%)	0	100	100
All	All	2420/2691 (90%)	2310 (96%)	108 (4%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	PRO
4	D	27	GLN

5.3.2 Protein sidechains (i)

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	971/1044 (93%)	968 (100%)	3 (0%)	92 95
2	B	390/397 (98%)	390 (100%)	0	100 100
3	C	363/412 (88%)	362 (100%)	1 (0%)	92 95
4	D	394/459 (86%)	393 (100%)	1 (0%)	92 95
5	E	91/100 (91%)	91 (100%)	0	100 100
All	All	2209/2412 (92%)	2204 (100%)	5 (0%)	93 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	784	ARG
1	A	917	LYS
1	A	1105	ARG
3	C	200	LYS
4	D	24	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
7	SF4	D	601	4	0,12,12	-	-	-		

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	SF4	D	601	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	601	SF4	1	0

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.

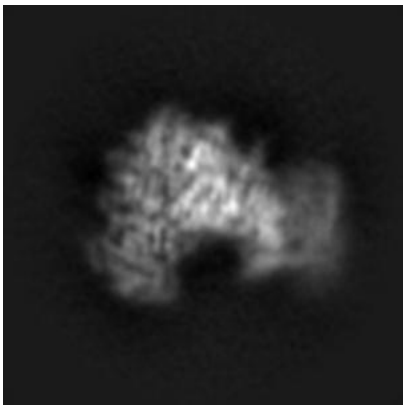
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13020. These allow visual inspection of the internal detail of the map and identification of artifacts.

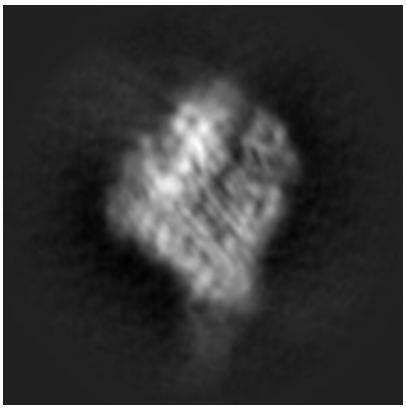
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

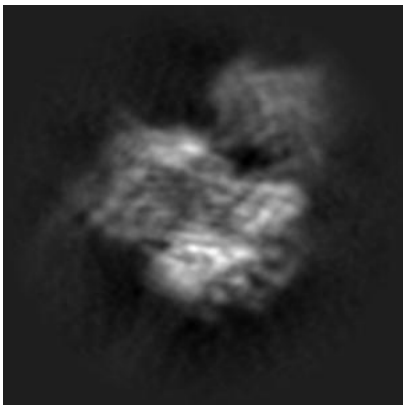
6.1.1 Primary map



X

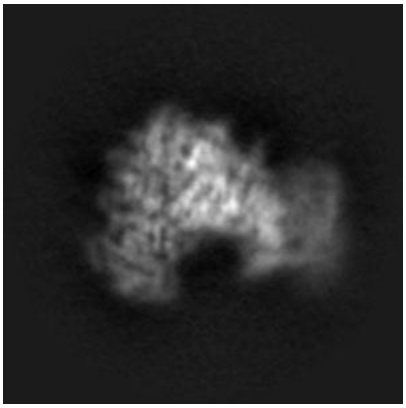


Y

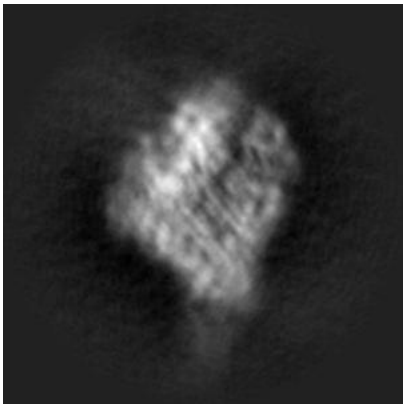


Z

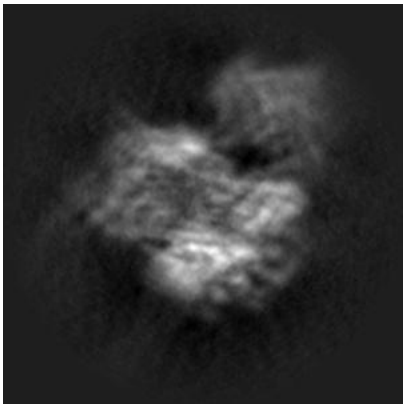
6.1.2 Raw map



X



Y

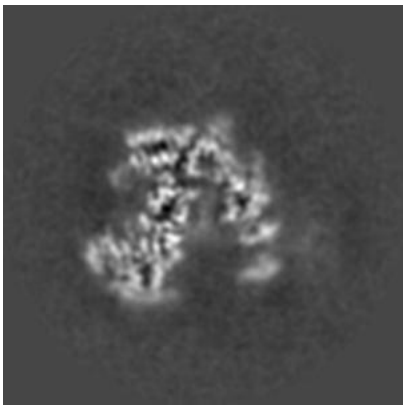


Z

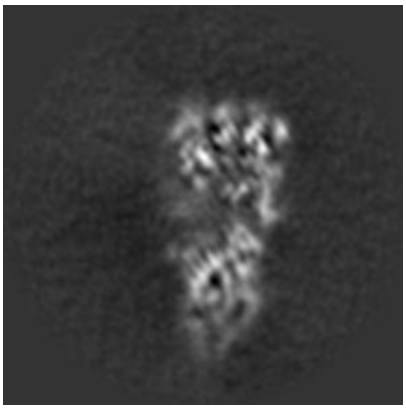
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

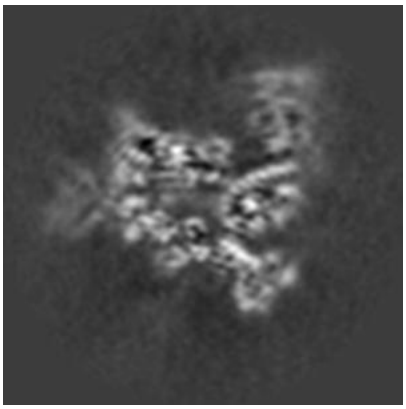
6.2.1 Primary map



X Index: 80

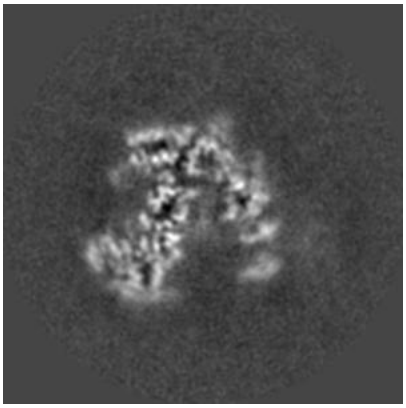


Y Index: 80

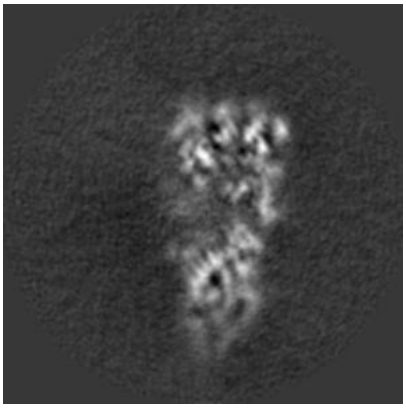


Z Index: 80

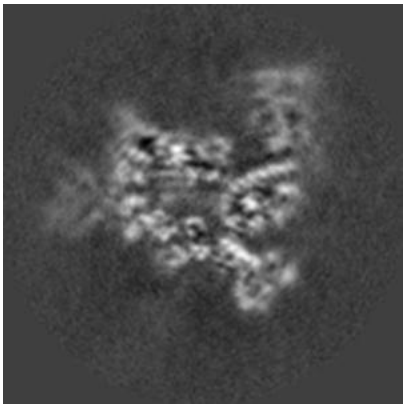
6.2.2 Raw map



X Index: 80



Y Index: 80

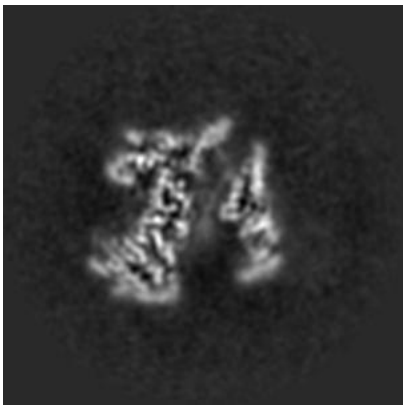


Z Index: 80

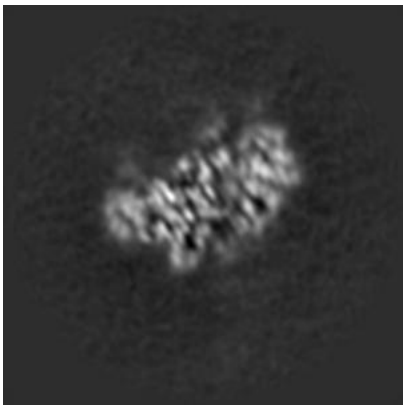
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

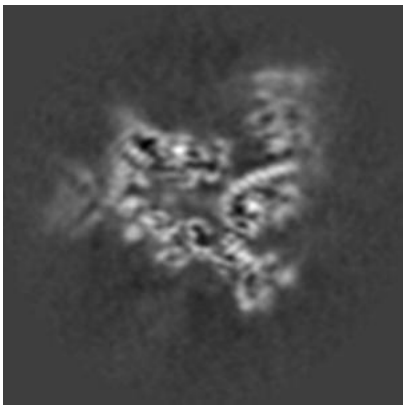
6.3.1 Primary map



X Index: 76

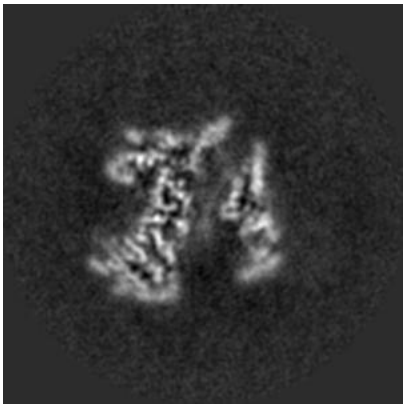


Y Index: 61

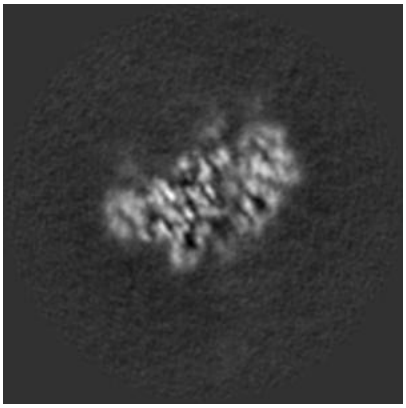


Z Index: 79

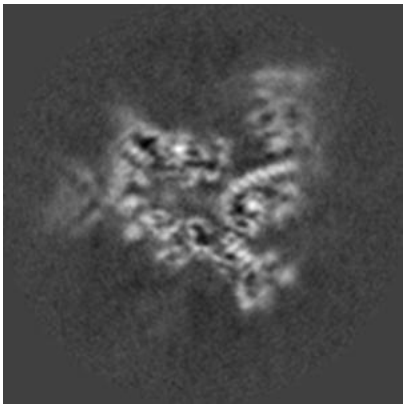
6.3.2 Raw map



X Index: 76



Y Index: 61

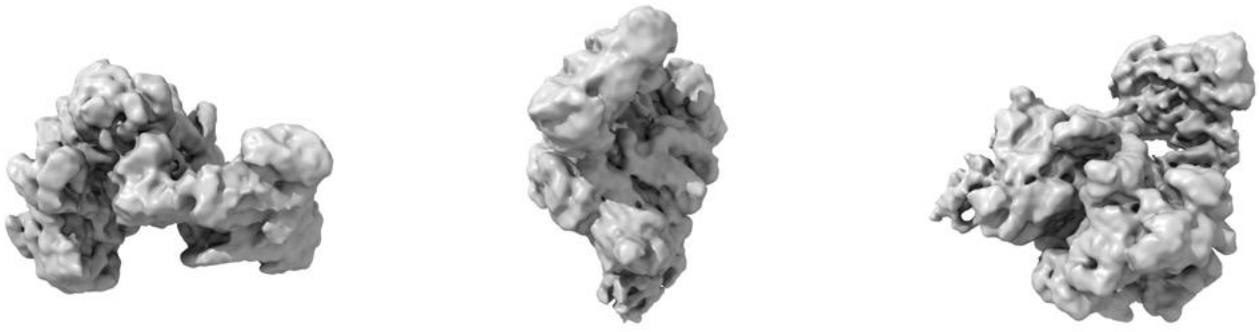


Z Index: 79

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

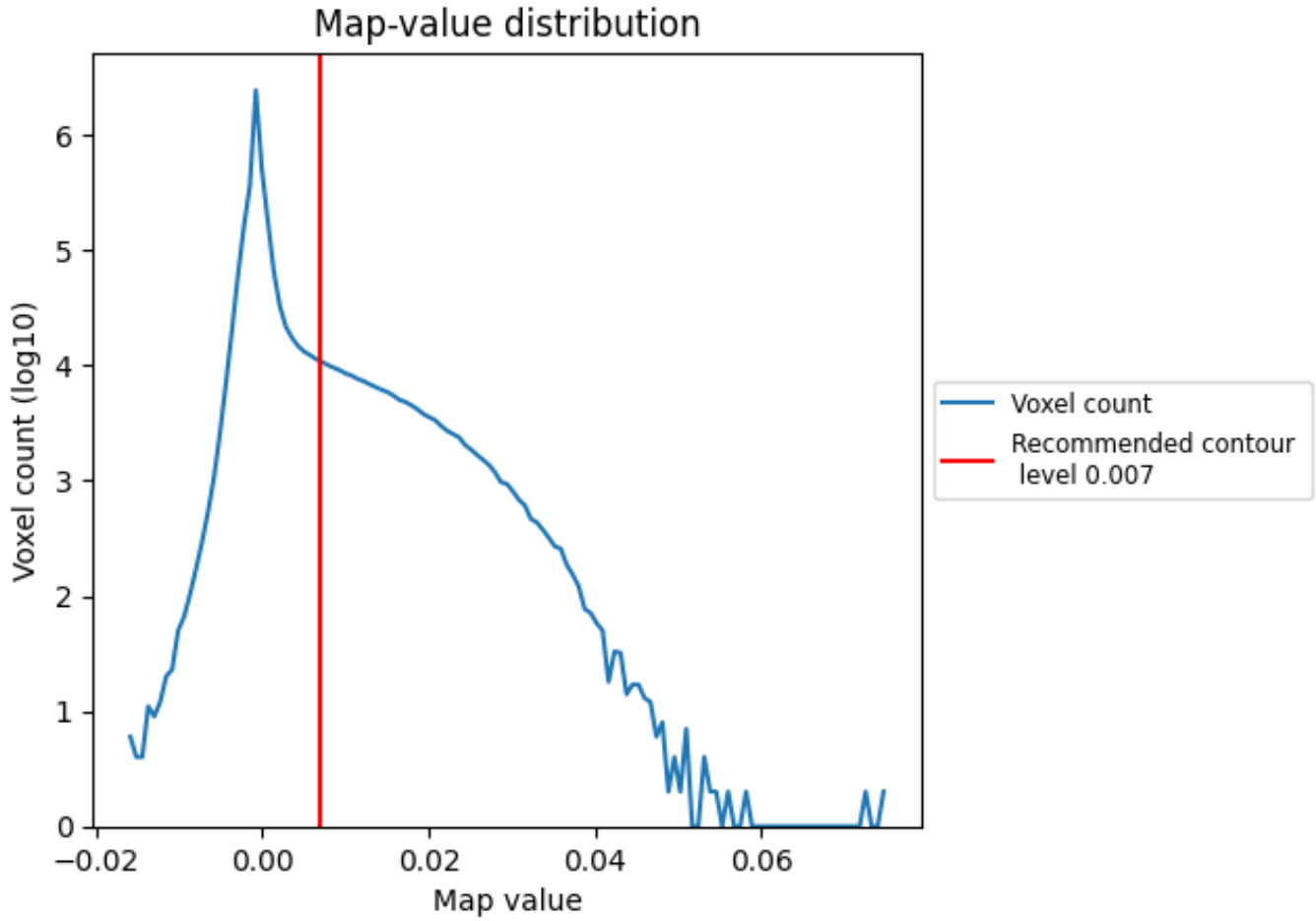
6.5 Mask visualisation (i)

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

7 Map analysis

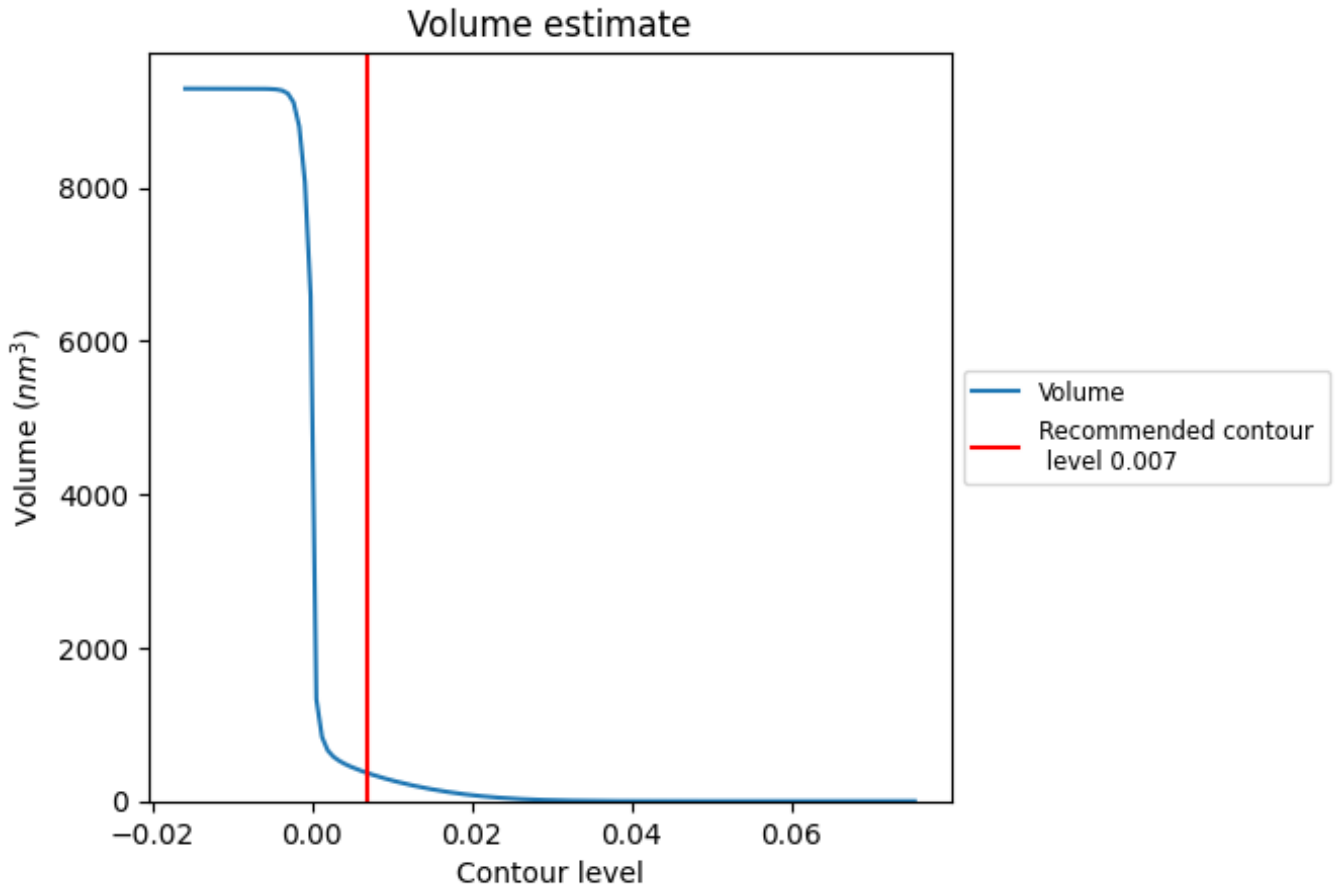
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

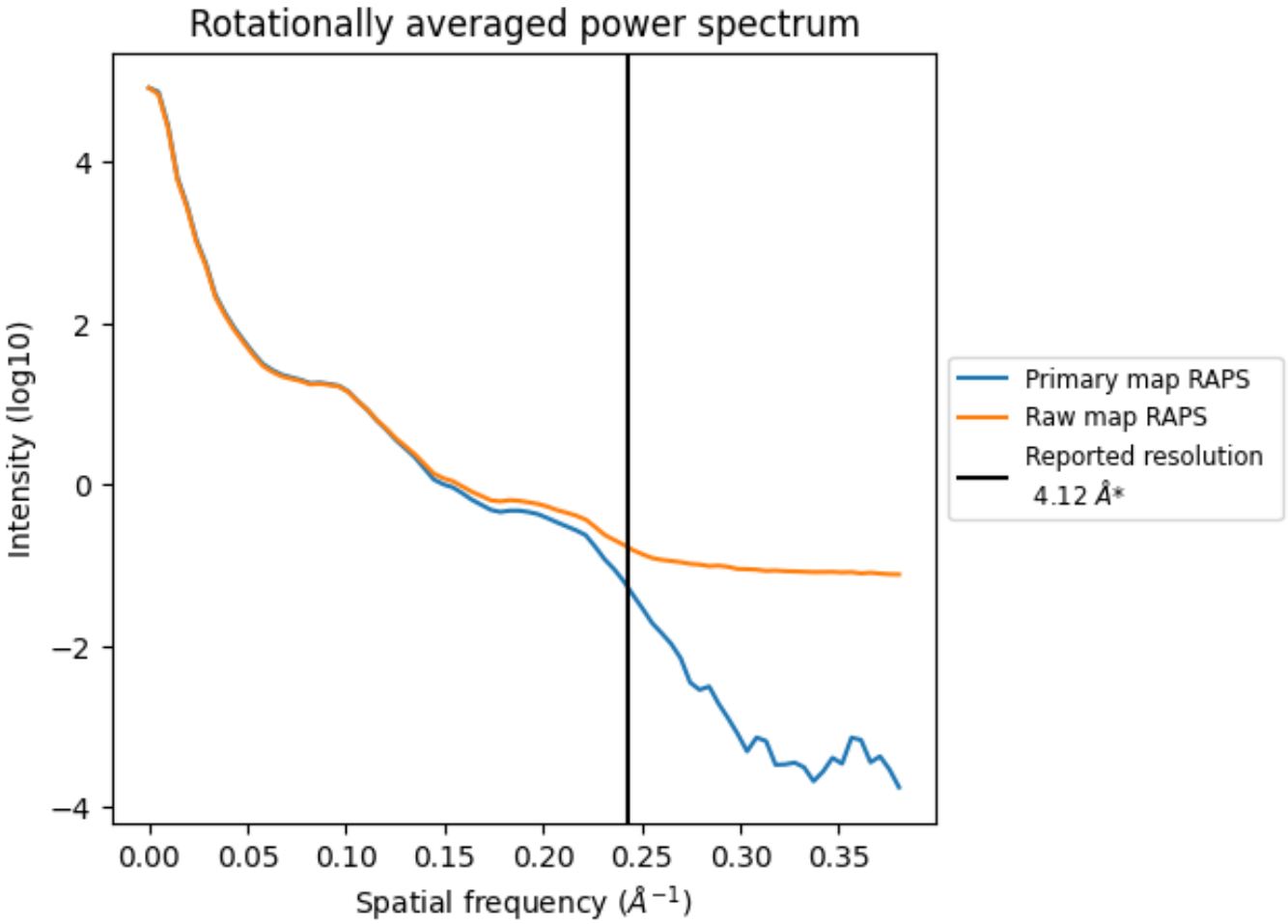
7.2 Volume estimate



The volume at the recommended contour level is 365 nm^3; this corresponds to an approximate mass of 330 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 (i)

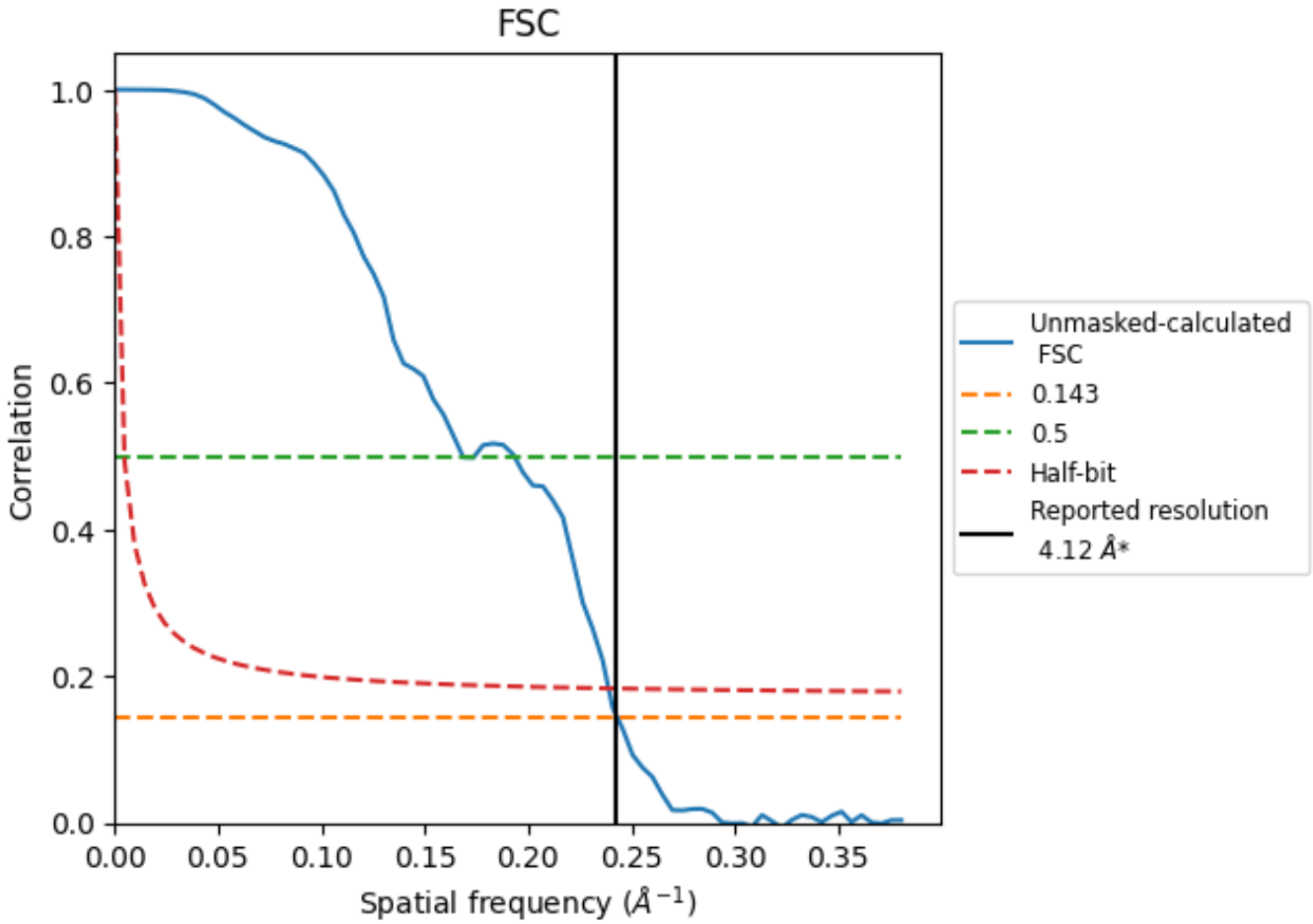


*Reported resolution corresponds to spatial frequency of 0.243 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.243 Å^{-1}

8.2 Resolution estimates (i)

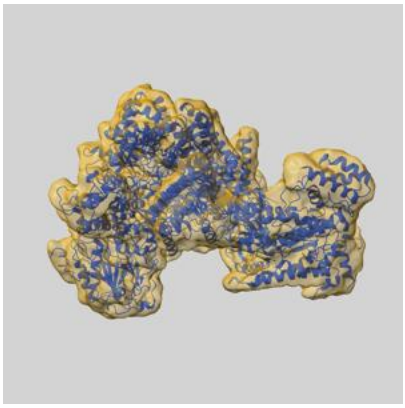
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.12	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	5.94	4.19

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

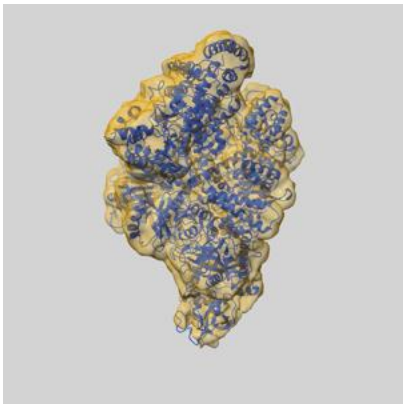
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13020 and PDB model 7OPL. Per-residue inclusion information can be found in section 3 on page 7.

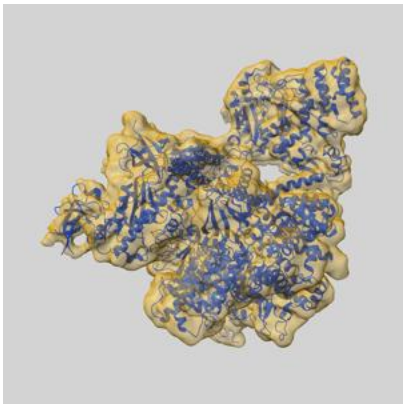
9.1 Map-model overlay



X



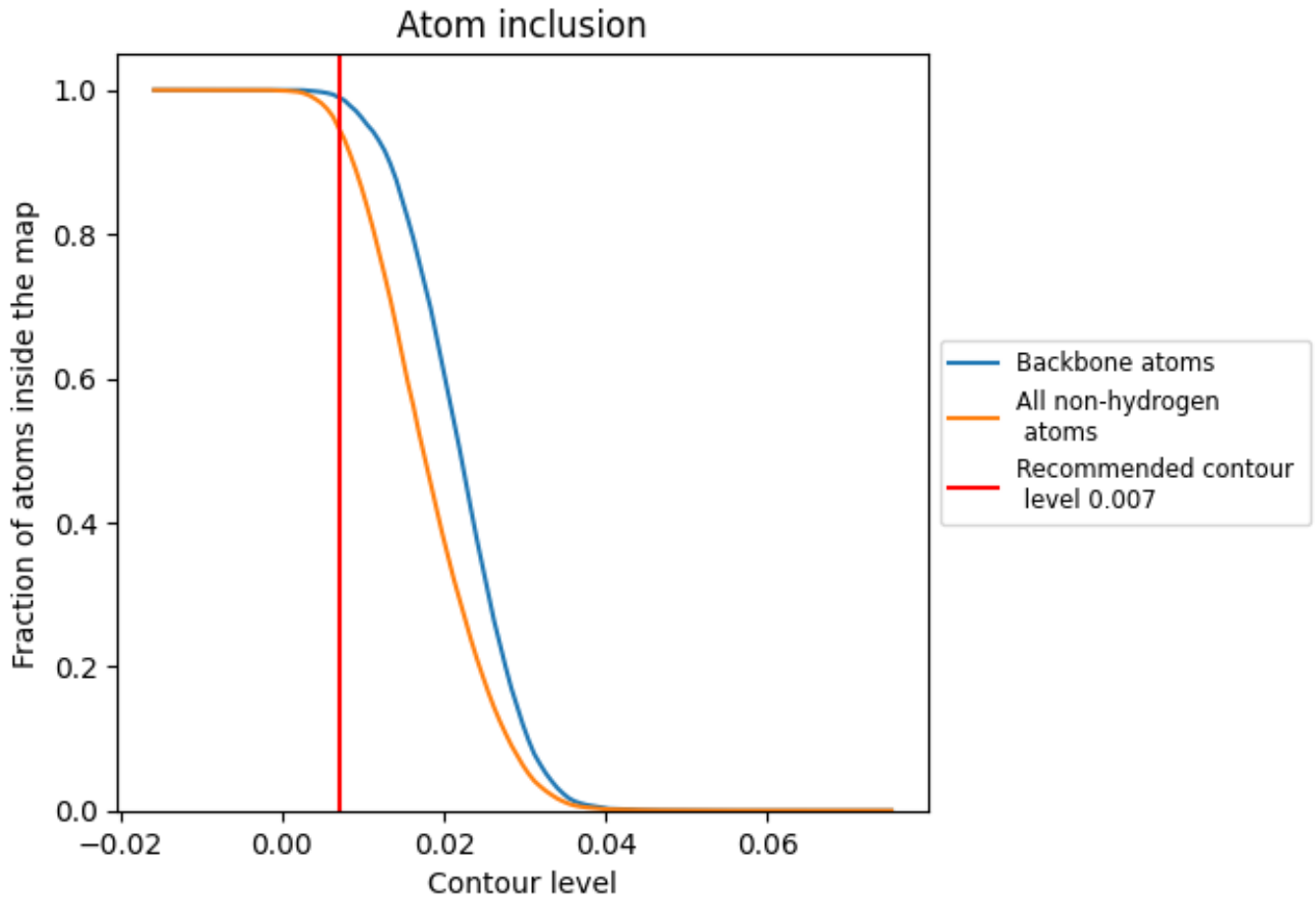
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.