Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID	:	9IKZ / pdb_00009ikz
EMDB ID	:	EMD-60663
Title	:	SARS-CoV-2 E-RTC bound to pRNA-nsp9 and GDP-BeF3-
Authors	:	Yan, L.M.; Huang, Y.C.; Liu, Y.X.; Rao, Z.H.; Lou, Z.Y.
Deposited on	:	2024-06-29
Resolution	:	3.14 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:

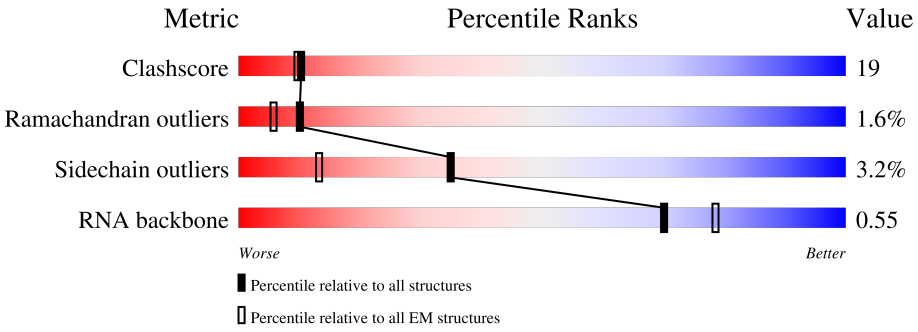
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

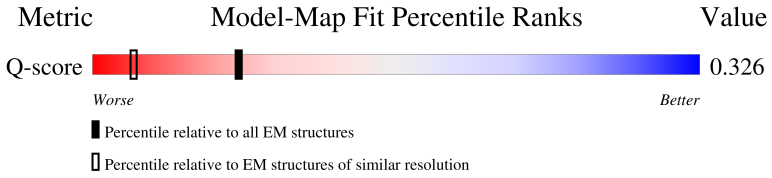
1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	931	82% 16%
2	B	187	76% 20%
2	D	187	63% 35%

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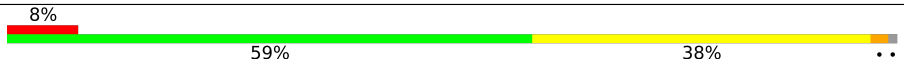
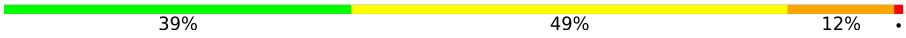
Mol	Chain	Length	Quality of chain
3	C	78	
4	E	593	
4	F	593	
5	G	113	
6	I	25	
7	J	27	

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	BEF	A	1004	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21944 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 RNA-directed RNA polymerase nsp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	931	Total	C	N	O	S	0	0
			7492	4784	1256	1398	54		

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1396	872	240	273	11		
2	D	187	Total	C	N	O	S	0	0
			1422	893	244	274	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	78	Total	C	N	O	S	0	0
			600	376	98	119	7		

- Molecule 4 is a protein called Helicase nsp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	586	Total	C	N	O	S	1	0
			4513	2878	751	849	35		
4	F	585	Total	C	N	O	S	1	0
			4502	2872	747	848	35		

- Molecule 5 is a protein called Viral protein genome-linked nsp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

- Molecule 6 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

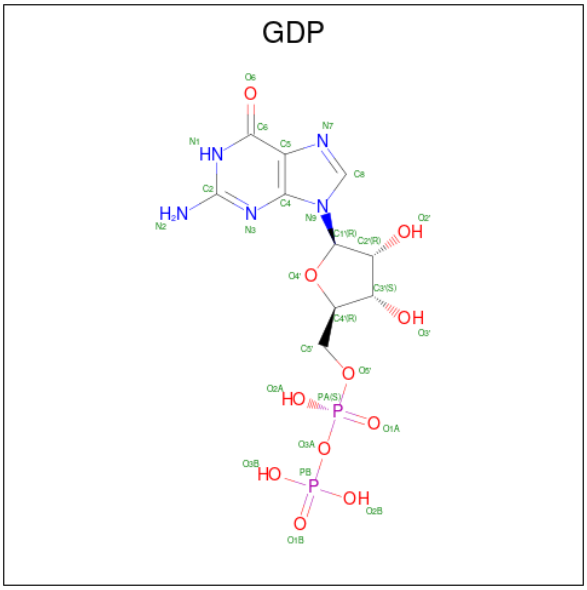
- Molecule 7 is a RNA chain called RNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	27	Total	C	N	O	P	0	0
			565	253	94	191	27		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	E	3	Total	Zn	0
			3	3	
8	F	3	Total	Zn	0
			3	3	

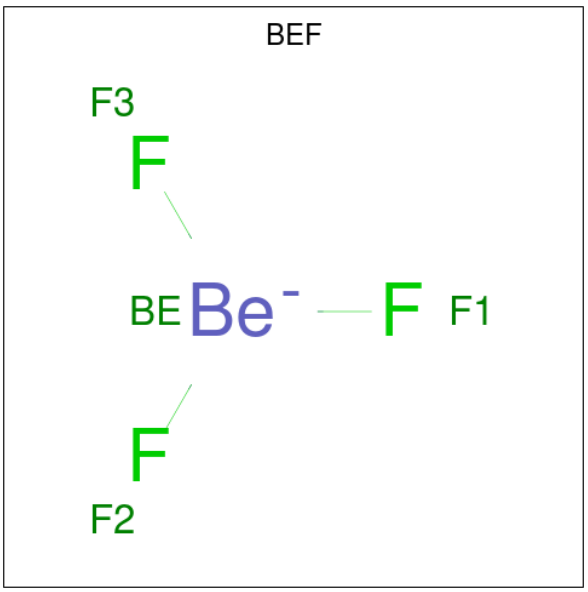
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	Be	F	0
			4	1	3	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

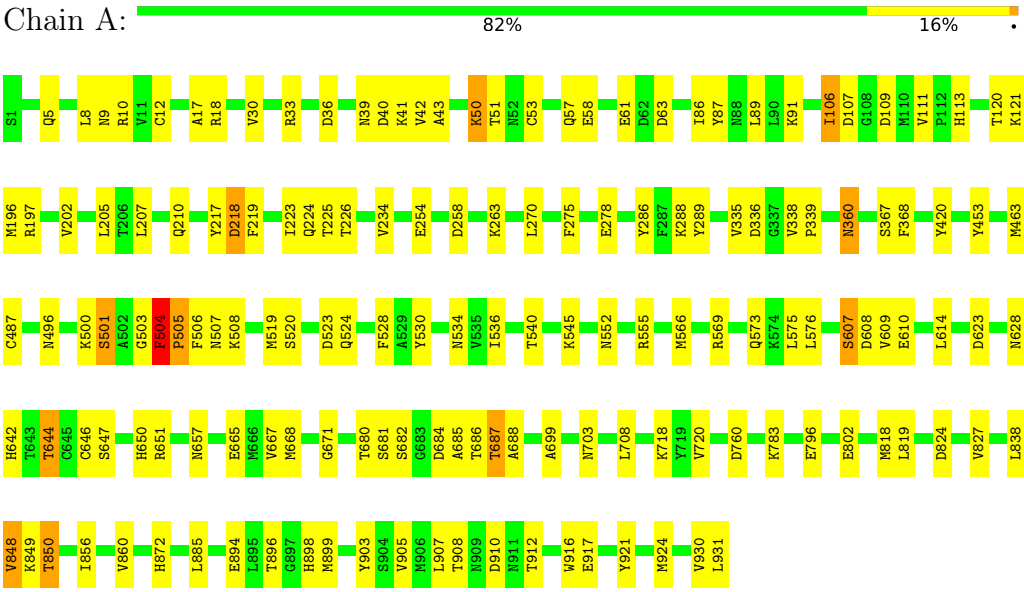
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

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.

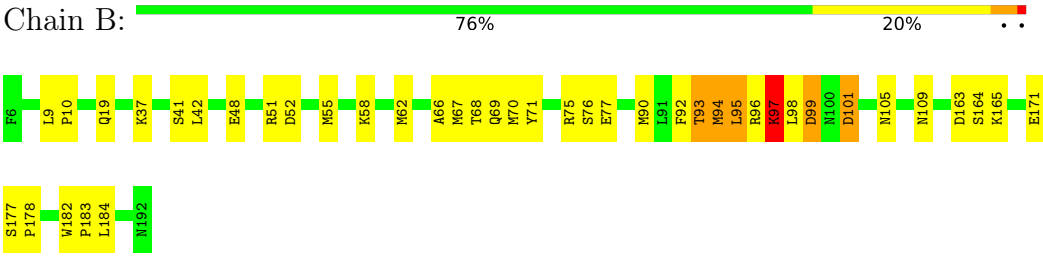
• Molecule 1: RNA-directed RNA polymerase nsp12

Chain A:



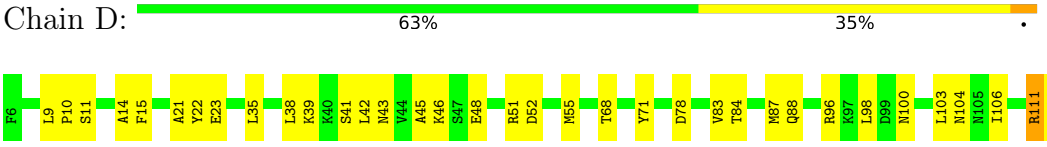
• Molecule 2: Non-structural protein 8

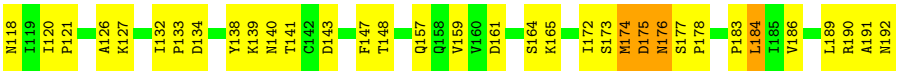
Chain B:



• Molecule 2: Non-structural protein 8

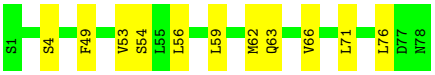
Chain D:





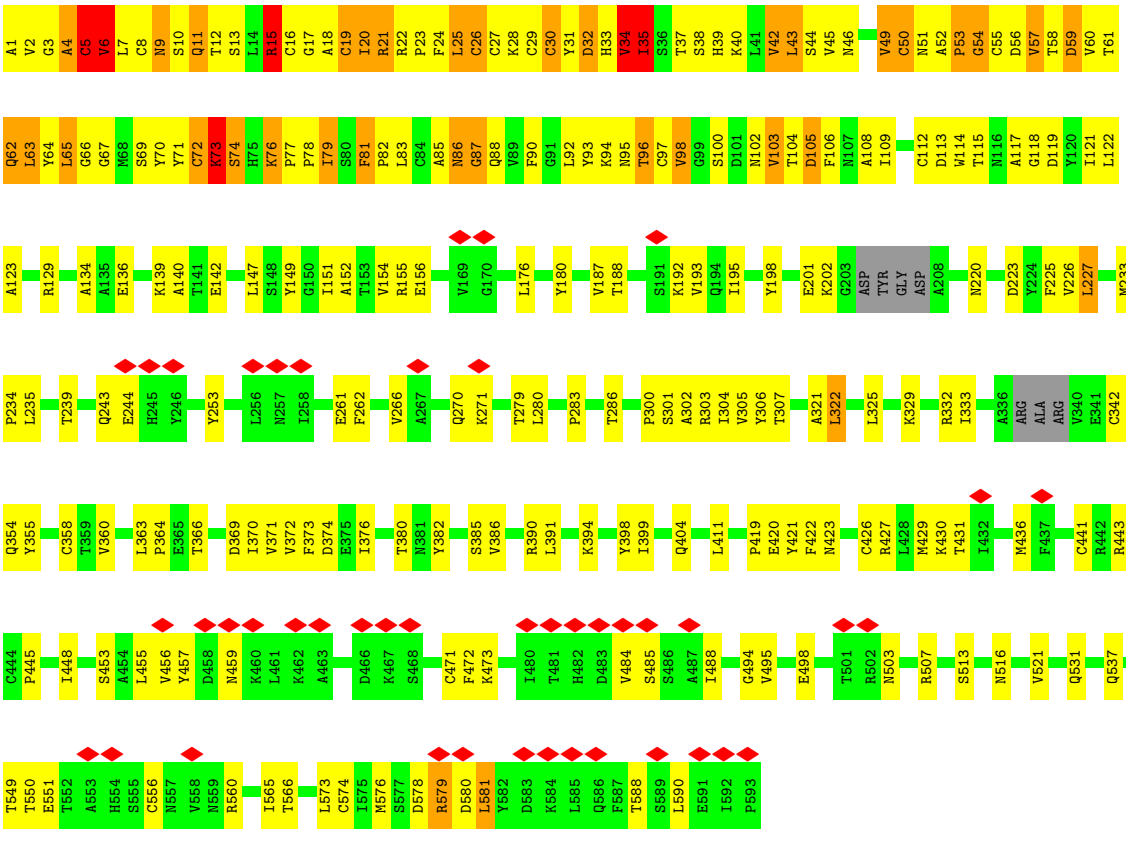
• Molecule 3: Non-structural protein 7

Chain C:



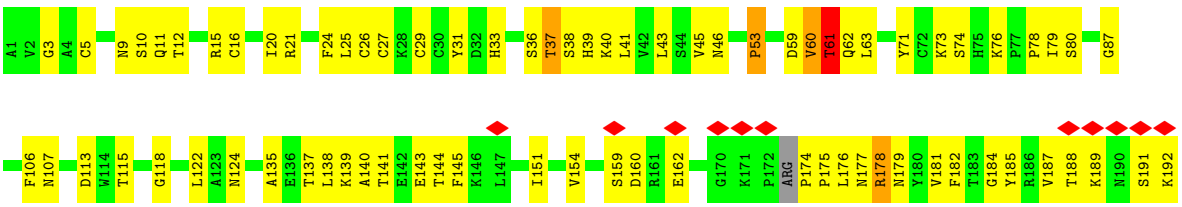
• Molecule 4: Helicase nsp13

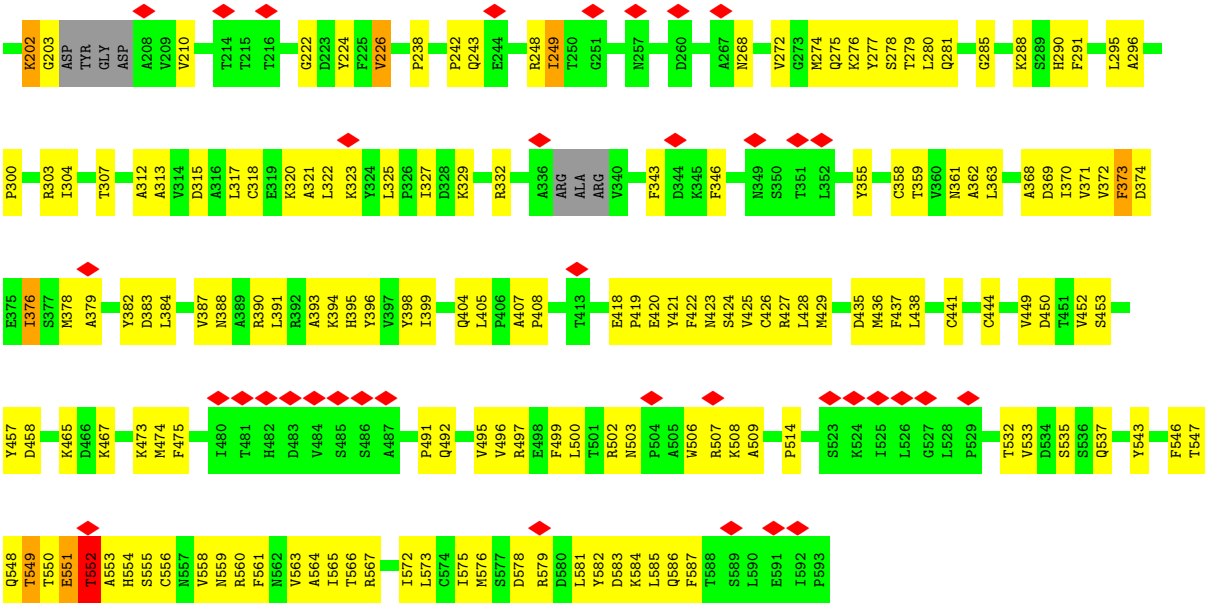
Chain E:



• Molecule 4: Helicase nsp13

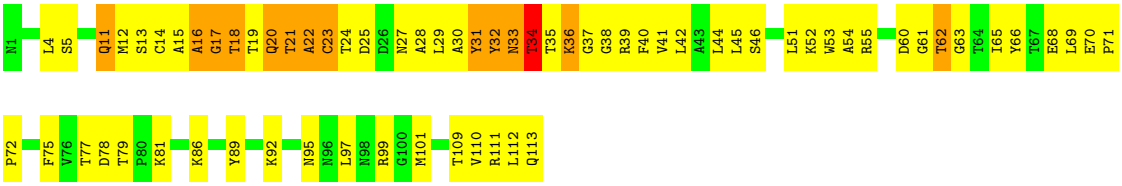
Chain F:





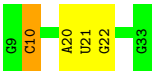
• Molecule 5: Viral protein genome-linked nsp9

Chain G:



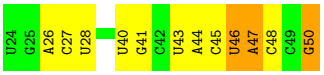
• Molecule 6: RNA (25-MER)

Chain I:



• Molecule 7: RNA (27-MER)

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.222	Depositor
Minimum map value	-1.208	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	360.8, 360.8, 360.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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, MG, GDP, BEF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.45	7/7681 (0.1%)	0.65	20/10426 (0.2%)
2	B	0.42	0/1414	0.87	8/1922 (0.4%)
2	D	0.51	1/1441 (0.1%)	0.83	6/1955 (0.3%)
3	C	0.27	0/603	0.69	1/812 (0.1%)
4	E	0.51	1/4615 (0.0%)	0.66	7/6290 (0.1%)
4	F	0.41	2/4603 (0.0%)	0.63	4/6272 (0.1%)
5	G	0.51	0/884	0.99	8/1200 (0.7%)
6	I	0.25	0/611	0.30	0/953
7	J	0.26	0/628	0.45	0/974
All	All	0.45	11/22480 (0.0%)	0.68	54/30804 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	848	VAL	CA-C	-8.29	1.42	1.52
4	F	226	VAL	CB-CG1	-7.49	1.27	1.52
1	A	210	GLN	CA-C	-6.47	1.45	1.52
2	D	191	ALA	CA-C	-6.45	1.50	1.53
1	A	845	ASP	CA-C	5.82	1.59	1.53
1	A	846	ASP	N-CA	5.65	1.53	1.46
1	A	642	HIS	CA-C	-5.63	1.47	1.53
1	A	849	LYS	CA-C	-5.56	1.46	1.53
4	F	202	LYS	CE-NZ	-5.54	1.32	1.49
1	A	850	THR	N-CA	-5.38	1.39	1.46
4	E	4	ALA	CA-C	-5.21	1.46	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	76	SER	N-CA-CB	-11.97	90.88	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	850	THR	N-CA-C	-11.72	95.55	113.02
5	G	34	THR	N-CA-C	-11.21	98.82	111.71
1	A	106	ILE	CB-CA-C	10.16	124.98	111.87
1	A	217	TYR	N-CA-C	9.49	131.02	110.80
4	E	73	LYS	N-CA-C	-9.39	102.19	114.31
5	G	16	ALA	N-CA-C	-8.96	95.73	107.73
2	B	75	ARG	CB-CA-C	8.83	128.00	110.42
1	A	682	SER	N-CA-C	-8.76	94.45	108.73
4	F	179	ASN	N-CA-C	-8.73	92.20	110.80
1	A	219	PHE	N-CA-C	-8.07	100.75	110.44
5	G	62	THR	N-CA-C	-7.62	94.58	107.99
4	E	96	THR	N-CA-C	-7.49	104.24	113.15
5	G	32	TYR	N-CA-C	7.48	126.73	110.80
1	A	681	SER	N-CA-C	-7.42	96.86	109.24
5	G	31	TYR	N-CA-C	7.40	120.98	108.02
2	B	94	MET	N-CA-C	-7.35	103.88	112.92
2	B	183	PRO	N-CA-C	-7.31	97.41	112.47
2	D	176	ASN	N-CA-C	-7.22	104.20	112.87
2	B	77	GLU	N-CA-C	-7.16	101.74	112.04
1	A	848	VAL	CA-C-N	-6.98	112.41	122.67
1	A	848	VAL	C-N-CA	-6.98	112.41	122.67
4	F	178	ARG	N-CA-C	-6.70	100.72	110.64
3	C	63	GLN	CB-CA-C	-6.38	109.20	116.54
2	D	183	PRO	N-CA-C	-6.20	99.69	112.47
4	F	249	ILE	N-CA-C	-6.17	106.42	111.91
1	A	107	ASP	N-CA-CB	-6.09	100.20	110.49
5	G	63	GLY	N-CA-C	-6.06	98.82	113.18
1	A	504	PHE	C-N-CD	-6.05	100.21	125.00
2	D	111	ARG	N-CA-C	-5.95	106.66	114.04
1	A	681	SER	CB-CA-C	5.83	120.90	109.35
1	A	218	ASP	N-CA-C	-5.67	99.03	108.34
4	F	61	THR	N-CA-C	-5.54	99.01	110.80
2	D	41	SER	N-CA-C	-5.53	107.19	114.04
5	G	18	THR	N-CA-C	-5.50	106.51	113.43
1	A	720	VAL	N-CA-C	-5.46	107.05	111.91
1	A	53	CYS	N-CA-C	5.45	117.97	108.76
1	A	503	GLY	N-CA-C	5.42	120.85	112.45
4	E	81	PHE	CA-C-N	-5.33	114.07	119.83
4	E	81	PHE	C-N-CA	-5.33	114.07	119.83
2	D	184	LEU	N-CA-C	-5.33	102.58	110.46
2	B	93	THR	N-CA-C	-5.32	106.67	114.39
5	G	17	GLY	N-CA-C	5.24	119.25	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	846	ASP	N-CA-C	5.23	121.95	110.80
2	B	76	SER	CB-CA-C	5.23	120.92	109.99
1	A	912	THR	N-CA-C	-5.19	107.97	114.56
1	A	86	ILE	N-CA-C	-5.18	107.78	112.96
4	E	5	CYS	N-CA-C	-5.16	102.27	109.96
4	E	83	LEU	N-CA-C	-5.14	105.75	111.36
1	A	217	TYR	CB-CA-C	-5.14	100.19	110.42
4	E	35	ILE	N-CA-C	-5.10	106.17	111.58
2	B	184	LEU	N-CA-C	-5.09	101.40	109.59
2	D	191	ALA	CB-CA-C	-5.04	109.81	117.07
1	A	644	THR	N-CA-C	-5.04	106.48	113.18

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	7492	0	7231	122	0
2	B	1396	0	1365	30	0
2	D	1422	0	1422	69	0
3	C	600	0	629	13	0
4	E	4513	0	4439	243	0
4	F	4502	0	4422	279	0
5	G	868	0	880	69	0
6	I	545	0	272	4	0
7	J	565	0	291	20	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	28	0	12	1	0
10	A	4	0	0	4	0
11	A	1	0	0	0	0
All	All	21944	0	20963	819	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 19.

All (819) 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)
4:F:290:HIS:CE1	4:F:320:LYS:NZ	1.68	1.60
4:F:421:TYR:CB	4:F:427:ARG:HH21	1.23	1.51
4:F:421:TYR:CA	4:F:427:ARG:HH21	1.30	1.42
4:F:421:TYR:CB	4:F:427:ARG:NH2	1.76	1.41
4:F:421:TYR:HB3	4:F:427:ARG:NH2	1.01	1.31
4:F:362:ALA:O	4:F:363:LEU:HD23	1.33	1.26
4:F:290:HIS:HE1	4:F:320:LYS:NZ	0.76	1.26
4:F:33:HIS:CE1	4:F:106:PHE:HB3	1.79	1.18
4:F:358:CYS:SG	4:F:390:ARG:NH2	2.18	1.16
4:F:435:ASP:HB3	4:F:436:MET:HE2	1.17	1.12
4:E:32:ASP:HB2	4:E:103:VAL:HG11	1.29	1.09
4:F:358:CYS:HA	4:F:363:LEU:CD1	1.83	1.07
4:F:202:LYS:HD2	4:F:203:GLY:N	1.73	1.03
4:F:551:GLU:HA	4:F:555:SER:HB2	1.39	1.02
4:E:473:LYS:HD2	4:E:576:MET:HE3	1.36	1.02
4:F:362:ALA:O	4:F:363:LEU:CD2	2.08	1.02
4:F:370:ILE:HD13	4:F:395:HIS:HB3	1.42	1.02
1:A:218:ASP:OD2	10:A:1004:BEF:F3	1.68	1.01
4:F:322:LEU:HB2	4:F:327:ILE:HD13	1.41	1.00
4:F:16:CYS:SG	4:F:25:LEU:HD13	2.02	0.99
4:E:63:LEU:HA	4:E:72:CYS:HA	1.40	0.99
3:C:76:LEU:HA	2:D:96:ARG:HH21	1.27	0.98
4:E:376:ILE:CG2	4:E:398:TYR:HB3	1.92	0.98
4:E:373:PHE:CD2	4:E:376:ILE:HG22	1.99	0.97
4:E:376:ILE:HG21	4:E:398:TYR:HB3	0.99	0.97
4:F:421:TYR:CA	4:F:427:ARG:NH2	2.15	0.97
4:F:325:LEU:HD12	4:F:329:LYS:HE2	1.45	0.96
4:F:475:PHE:HZ	4:F:582:TYR:CE2	1.85	0.93
4:F:435:ASP:CB	4:F:436:MET:HE2	1.97	0.92
4:F:202:LYS:HZ2	4:F:210:VAL:HB	1.33	0.92
4:F:278:SER:O	4:F:398:TYR:HD1	1.53	0.91
4:F:290:HIS:CE1	4:F:320:LYS:HZ3	1.69	0.91
1:A:899:MET:HE1	2:D:68:THR:CG2	1.99	0.91
4:E:386:VAL:HG22	4:E:390:ARG:HD2	1.53	0.91
4:E:63:LEU:HA	4:E:72:CYS:CA	2.02	0.90
4:F:202:LYS:HZ2	4:F:210:VAL:CB	1.84	0.90
4:E:376:ILE:HG21	4:E:398:TYR:CB	1.96	0.89
4:F:135:ALA:HA	4:F:138:LEU:HG	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:33:HIS:CE1	4:F:106:PHE:CB	2.56	0.88
4:E:419:PRO:HA	4:E:422:PHE:CE2	2.08	0.88
4:F:421:TYR:HA	4:F:427:ARG:HH21	1.34	0.88
1:A:569:ARG:NH1	7:J:28:U:OP1	2.07	0.88
4:E:546:PHE:HD2	4:E:574:CYS:HG	1.12	0.88
4:E:305:VAL:HB	4:E:371:VAL:HG22	1.56	0.87
1:A:576:LEU:HD11	1:A:686:THR:HG22	1.57	0.87
4:F:159:SER:HB2	4:F:162:GLU:OE2	1.74	0.86
4:F:396:TYR:HD2	4:F:398:TYR:OH	1.58	0.86
1:A:668:MET:HE3	1:A:671:GLY:HA2	1.57	0.86
2:D:15:PHE:HE2	2:D:46:LYS:HG3	1.40	0.85
1:A:500:LYS:HD3	7:J:27:C:OP2	1.76	0.85
5:G:12:MET:HE1	5:G:29:LEU:HD13	1.58	0.85
4:F:370:ILE:CD1	4:F:395:HIS:HB3	2.06	0.85
2:D:15:PHE:HE2	2:D:46:LYS:CG	1.89	0.84
4:E:495:VAL:HA	4:E:498:GLU:OE2	1.77	0.84
4:E:30:CYS:O	4:E:34:VAL:HB	1.79	0.83
7:J:47:A:H2'	7:J:48:C:C6	2.13	0.83
4:F:358:CYS:HA	4:F:363:LEU:HD11	1.58	0.83
4:F:278:SER:O	4:F:398:TYR:CD1	2.31	0.83
4:E:147:LEU:O	4:E:147:LEU:HD23	1.80	0.82
4:F:551:GLU:HB3	4:F:556:CYS:HB2	1.60	0.82
1:A:18:ARG:HH12	1:A:61:GLU:HA	1.44	0.82
4:E:546:PHE:CD2	4:E:574:CYS:SG	2.72	0.81
2:B:9:LEU:HD21	2:B:52:ASP:HB3	1.63	0.81
4:F:435:ASP:HB3	4:F:436:MET:CE	2.07	0.81
1:A:899:MET:HE1	2:D:68:THR:HG23	1.62	0.81
5:G:12:MET:CE	5:G:29:LEU:HD13	2.11	0.81
4:F:396:TYR:HD2	4:F:398:TYR:HH	0.82	0.80
4:F:281:GLN:HE21	4:F:429:MET:CE	1.95	0.80
1:A:575:LEU:HD13	1:A:641:LYS:HD2	1.61	0.80
4:F:325:LEU:HD12	4:F:329:LYS:CE	2.11	0.80
1:A:218:ASP:OD2	10:A:1004:BEF:F1	1.90	0.80
2:B:19:GLN:HA	2:B:42:LEU:HD12	1.63	0.79
5:G:45:LEU:HD11	5:G:86:LYS:HB3	1.62	0.79
4:E:453:SER:HA	4:E:457:TYR:HB2	1.65	0.78
4:E:4:ALA:HB1	4:E:9:ASN:HA	1.65	0.78
4:E:19:CYS:SG	4:E:23:PRO:HD2	2.23	0.78
2:B:165:LYS:HB3	2:B:165:LYS:HZ2	1.48	0.78
4:F:31:TYR:CE2	4:F:87:GLY:HA2	2.18	0.78
4:F:279:THR:O	4:F:280:LEU:HD22	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:52:ALA:HB3	4:E:55:CYS:SG	2.25	0.77
6:I:10:C:H42	7:J:50:G:H1	1.29	0.77
4:F:421:TYR:HB3	4:F:427:ARG:HH22	0.94	0.77
4:E:419:PRO:HA	4:E:422:PHE:CD2	2.20	0.77
4:E:495:VAL:HA	4:E:498:GLU:CG	2.14	0.77
4:F:37:THR:HB	4:F:39:HIS:CD2	2.20	0.76
1:A:646:CYS:SG	1:A:650:HIS:CB	2.74	0.76
4:E:152:ALA:HB3	4:E:225:PHE:HB2	1.66	0.76
4:F:281:GLN:HE21	4:F:429:MET:HE2	1.50	0.76
4:F:371:VAL:HG23	4:F:393:ALA:HB3	1.66	0.76
1:A:899:MET:HE1	2:D:68:THR:OG1	1.85	0.76
4:F:162:GLU:O	4:F:162:GLU:HG2	1.86	0.76
4:F:248:ARG:HD2	4:F:249:ILE:H	1.49	0.75
1:A:225:THR:HG22	1:A:226:THR:H	1.51	0.75
2:D:22:TYR:HA	2:D:38:LEU:HD23	1.67	0.75
4:F:332:ARG:NH2	4:F:343:PHE:O	2.19	0.75
4:E:16:CYS:HB2	4:E:19:CYS:SG	2.27	0.75
4:F:138:LEU:HD12	4:F:139:LYS:N	2.01	0.75
4:F:358:CYS:CA	4:F:363:LEU:CD1	2.63	0.75
4:E:149:TYR:HB2	4:E:227:LEU:HD21	1.69	0.75
1:A:569:ARG:NH1	7:J:28:U:P	2.60	0.74
2:D:126:ALA:HB3	2:D:190:ARG:HB2	1.68	0.74
4:E:5:CYS:HB3	4:E:26:CYS:HB2	1.67	0.74
4:E:239:THR:HG22	4:E:385:SER:HB3	1.67	0.74
4:E:495:VAL:HA	4:E:498:GLU:CD	2.13	0.74
1:A:899:MET:CE	2:D:68:THR:HG23	2.17	0.74
4:E:304:ILE:HD11	4:E:355:TYR:CD1	2.21	0.74
2:D:175:ASP:O	2:D:178:PRO:HD2	1.88	0.74
1:A:12:CYS:SG	1:A:17:ALA:HB3	2.27	0.74
4:E:122:LEU:HD12	4:E:123:ALA:N	2.02	0.74
4:F:396:TYR:HB3	4:F:398:TYR:CE1	2.23	0.74
3:C:76:LEU:HA	2:D:96:ARG:NH2	2.00	0.74
4:F:33:HIS:HE1	4:F:106:PHE:HB3	1.49	0.73
4:F:421:TYR:HA	4:F:427:ARG:HE	1.53	0.73
4:E:5:CYS:SG	4:E:8:CYS:HB2	2.29	0.73
7:J:40:U:H2'	7:J:41:G:H8	1.53	0.73
1:A:646:CYS:SG	1:A:651:ARG:HG3	2.29	0.73
1:A:420:TYR:OH	3:C:4:SER:OG	2.04	0.73
4:F:33:HIS:NE2	4:F:39:HIS:CD2	2.56	0.73
4:F:202:LYS:HZ2	4:F:210:VAL:CG2	2.01	0.73
1:A:646:CYS:SG	1:A:650:HIS:HB3	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:268:ASN:O	4:F:272:VAL:HG22	1.88	0.72
1:A:668:MET:CE	1:A:671:GLY:HA2	2.19	0.72
4:E:65:LEU:HB3	4:E:81:PHE:HB3	1.71	0.72
1:A:218:ASP:CG	10:A:1004:BEF:F1	2.23	0.72
4:E:494:GLY:O	4:E:498:GLU:HG2	1.89	0.72
1:A:930:VAL:HG13	1:A:931:LEU:HD12	1.72	0.72
4:E:34:VAL:HG12	4:E:35:ILE:HG12	1.69	0.72
4:E:423:ASN:ND2	4:E:426:CYS:SG	2.63	0.72
5:G:97:LEU:HG	5:G:101:MET:HE3	1.72	0.72
4:F:290:HIS:CE1	4:F:320:LYS:CE	2.71	0.72
6:I:10:C:N4	7:J:50:G:H1	1.88	0.72
2:B:165:LYS:HB3	2:B:165:LYS:NZ	2.04	0.72
1:A:504:PHE:O	1:A:506:PHE:N	2.23	0.71
4:F:16:CYS:SG	4:F:25:LEU:CD1	2.79	0.71
1:A:500:LYS:HE3	7:J:26:A:OP2	1.90	0.71
2:B:67:MET:HG2	4:E:90:PHE:CZ	2.26	0.71
2:D:48:GLU:HG3	2:D:51:ARG:NH2	2.06	0.71
1:A:18:ARG:NH2	1:A:63:ASP:OD1	2.24	0.71
5:G:30:ALA:HB1	5:G:41:VAL:HG21	1.71	0.71
4:F:202:LYS:NZ	4:F:210:VAL:HB	2.06	0.71
4:E:63:LEU:CA	4:E:72:CYS:HA	2.19	0.70
4:F:138:LEU:HD12	4:F:139:LYS:H	1.56	0.70
1:A:540:THR:OG1	1:A:665:GLU:OE1	2.08	0.70
4:E:376:ILE:HD13	4:E:398:TYR:HB2	1.72	0.70
2:D:15:PHE:CE2	2:D:46:LYS:CG	2.74	0.70
5:G:34:THR:O	5:G:39:ARG:HA	1.92	0.70
5:G:62:THR:HG23	5:G:62:THR:O	1.90	0.70
4:E:546:PHE:HD2	4:E:574:CYS:SG	2.13	0.70
4:F:358:CYS:SG	4:F:359:THR:N	2.65	0.69
4:F:12:THR:HG21	4:F:26:CYS:HA	1.73	0.69
4:F:359:THR:N	4:F:363:LEU:HD11	2.07	0.69
4:F:202:LYS:NZ	4:F:210:VAL:H	1.90	0.69
4:E:73:LYS:HA	4:E:76:LYS:HD2	1.74	0.69
1:A:5:GLN:OE1	1:A:9:ASN:ND2	2.24	0.69
2:D:39:LYS:HG2	2:D:43:ASN:HD21	1.58	0.69
4:E:113:ASP:OD1	4:E:115:THR:OG1	2.09	0.69
4:E:548:GLN:HE22	4:E:551:GLU:HG2	1.56	0.69
5:G:33:ASN:HD22	5:G:42:LEU:HD21	1.57	0.69
4:F:358:CYS:SG	4:F:390:ARG:CZ	2.81	0.68
4:F:371:VAL:HG21	4:F:396:TYR:CE1	2.28	0.68
1:A:569:ARG:HH11	7:J:28:U:P	2.15	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5:CYS:SG	4:E:9:ASN:N	2.66	0.68
4:F:187:VAL:HG23	4:F:224:TYR:HE2	1.58	0.68
3:C:71:LEU:HD11	2:D:88:GLN:HB3	1.76	0.68
4:F:565:ILE:HA	4:F:567:ARG:HH21	1.59	0.68
4:F:396:TYR:CD2	4:F:398:TYR:OH	2.39	0.68
4:F:187:VAL:HG23	4:F:224:TYR:CE2	2.29	0.68
4:F:551:GLU:C	4:F:556:CYS:H	2.02	0.68
5:G:11:GLN:NE2	5:G:39:ARG:HH22	1.92	0.67
5:G:18:THR:HG22	5:G:51:LEU:HG	1.75	0.67
4:E:373:PHE:CE2	4:E:376:ILE:HG22	2.30	0.67
4:F:322:LEU:HB2	4:F:327:ILE:CD1	2.21	0.67
4:F:551:GLU:CA	4:F:555:SER:HB2	2.19	0.67
2:D:15:PHE:CE2	2:D:46:LYS:HG2	2.29	0.67
4:F:387:VAL:HA	4:F:390:ARG:HD3	1.77	0.66
4:F:551:GLU:HA	4:F:555:SER:CB	2.20	0.66
5:G:75:PHE:HB2	5:G:77:THR:HG23	1.77	0.66
4:E:366:THR:CG2	4:E:391:LEU:HD11	2.25	0.66
5:G:35:THR:HG21	5:G:40:PHE:HB3	1.78	0.66
4:E:3:GLY:O	4:E:11:GLN:HA	1.95	0.66
4:E:118:GLY:O	4:E:122:LEU:HG	1.95	0.66
4:F:296:ALA:O	4:F:355:TYR:OH	2.14	0.66
1:A:668:MET:HE3	1:A:671:GLY:CA	2.26	0.66
4:E:63:LEU:HA	4:E:72:CYS:CB	2.25	0.66
4:F:497:ARG:HA	4:F:500:LEU:HD12	1.77	0.66
4:F:421:TYR:HA	4:F:427:ARG:NH2	1.99	0.65
1:A:89:LEU:HD11	1:A:224:GLN:OE1	1.97	0.65
1:A:646:CYS:SG	1:A:650:HIS:HB2	2.36	0.65
4:F:9:ASN:OD1	4:F:9:ASN:O	2.13	0.65
2:D:48:GLU:HG3	2:D:51:ARG:HH21	1.60	0.65
4:F:202:LYS:HD2	4:F:203:GLY:H	1.59	0.65
4:F:404:GLN:C	4:F:405:LEU:HD12	2.21	0.65
4:E:147:LEU:HA	4:E:227:LEU:HD11	1.79	0.65
4:F:359:THR:HG22	4:F:361:ASN:H	1.59	0.65
4:F:503:ASN:HB2	4:F:506:TRP:HD1	1.61	0.65
4:F:313:ALA:HB2	4:F:537:GLN:HB3	1.79	0.65
4:E:21:ARG:HD3	4:E:136:GLU:HG2	1.78	0.65
4:F:135:ALA:O	4:F:138:LEU:HD12	1.96	0.65
5:G:19:THR:HB	5:G:22:ALA:HB3	1.79	0.65
2:D:161:ASP:HB2	2:D:165:LYS:HB2	1.78	0.65
4:F:141:THR:O	4:F:145:PHE:HD2	1.80	0.65
4:F:371:VAL:HB	4:F:396:TYR:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:549:THR:HA	4:F:551:GLU:N	2.11	0.65
4:F:124:ASN:HB2	4:F:427:ARG:NH1	2.12	0.65
5:G:18:THR:HG23	5:G:27:ASN:HB3	1.79	0.65
1:A:218:ASP:OD1	10:A:1004:BEF:F1	2.05	0.64
4:E:5:CYS:O	4:E:6:VAL:C	2.40	0.64
4:E:58:THR:O	4:E:59:ASP:C	2.40	0.64
4:F:238:PRO:O	4:F:388:ASN:ND2	2.25	0.64
4:F:371:VAL:HG13	4:F:373:PHE:CZ	2.32	0.64
4:F:535:SER:HB2	4:F:537:GLN:HE21	1.62	0.64
4:F:317:LEU:O	4:F:321:ALA:HB2	1.97	0.64
4:F:404:GLN:O	4:F:405:LEU:HD12	1.98	0.64
4:E:495:VAL:HA	4:E:498:GLU:HG2	1.78	0.64
4:F:492:GLN:OE1	4:F:496:VAL:HG23	1.99	0.63
4:F:475:PHE:CZ	4:F:582:TYR:CE2	2.77	0.63
4:F:428:LEU:HD23	4:F:429:MET:H	1.64	0.63
4:F:359:THR:H	4:F:363:LEU:CD1	2.12	0.63
5:G:16:ALA:HB1	5:G:54:ALA:HB1	1.81	0.63
4:E:556:CYS:SG	4:E:560:ARG:NE	2.71	0.62
4:F:21:ARG:HG3	4:F:137:THR:HG22	1.80	0.62
4:F:358:CYS:HA	4:F:363:LEU:HD12	1.77	0.62
4:E:546:PHE:HB3	4:E:574:CYS:HA	1.81	0.62
4:F:358:CYS:CA	4:F:363:LEU:HD11	2.27	0.62
4:E:1:ALA:O	4:E:13:SER:HA	1.99	0.62
4:E:471:CYS:O	4:E:588:THR:OG1	2.15	0.62
4:F:421:TYR:HA	4:F:427:ARG:NE	2.14	0.62
4:E:566:THR:HG22	4:E:566:THR:O	2.00	0.62
2:D:121:PRO:HG2	2:D:126:ALA:HB1	1.82	0.61
4:E:180:TYR:O	4:E:180:TYR:CD1	2.53	0.61
1:A:818:MET:HE1	1:A:872:HIS:HA	1.83	0.61
4:E:580:ASP:O	4:E:581:LEU:C	2.44	0.61
4:F:387:VAL:HA	4:F:390:ARG:CD	2.31	0.61
4:E:63:LEU:HA	4:E:72:CYS:HB3	1.83	0.61
2:B:177:SER:OG	2:B:178:PRO:HD3	2.00	0.61
4:E:453:SER:HB3	4:E:459:ASN:HA	1.82	0.61
4:F:135:ALA:O	4:F:138:LEU:CD1	2.48	0.61
4:F:36:SER:OG	4:F:107:ASN:ND2	2.33	0.61
4:E:109:ILE:HD13	4:E:134:ALA:HB2	1.82	0.61
4:F:78:PRO:O	4:F:80:SER:N	2.33	0.61
4:F:363:LEU:HB2	4:F:390:ARG:NH2	2.16	0.61
5:G:19:THR:HB	5:G:22:ALA:CB	2.31	0.61
4:E:40:LYS:HB3	4:E:59:ASP:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:303:ARG:O	4:E:370:ILE:HG22	2.01	0.60
4:E:376:ILE:HD13	4:E:398:TYR:CB	2.31	0.60
5:G:22:ALA:O	5:G:23:CYS:C	2.42	0.60
4:E:64:TYR:N	4:E:72:CYS:HA	2.16	0.60
5:G:62:THR:O	5:G:62:THR:CG2	2.47	0.60
4:E:114:TRP:HB3	4:E:411:LEU:HD21	1.83	0.60
1:A:360:ASN:HD22	1:A:360:ASN:C	2.08	0.60
4:E:366:THR:HG23	4:E:391:LEU:HD11	1.82	0.60
4:F:177:ASN:O	4:F:178:ARG:C	2.44	0.60
4:F:369:ASP:HA	4:F:394:LYS:HE3	1.84	0.60
7:J:47:A:H2'	7:J:48:C:H6	1.65	0.60
1:A:33:ARG:NH2	1:A:121:LYS:O	2.35	0.60
4:E:53:PRO:O	4:E:54:GLY:C	2.45	0.59
7:J:43:U:H2'	7:J:44:A:C8	2.37	0.59
1:A:519:MET:HE2	1:A:523:ASP:HB3	1.84	0.59
4:F:59:ASP:C	4:F:61:THR:H	2.10	0.59
5:G:12:MET:SD	5:G:29:LEU:HD22	2.43	0.59
4:F:135:ALA:HA	4:F:138:LEU:CG	2.28	0.59
5:G:19:THR:O	5:G:20:GLN:C	2.46	0.59
4:E:261:GLU:OE2	4:E:262:PHE:CE2	2.55	0.59
4:F:281:GLN:NE2	4:F:429:MET:SD	2.76	0.59
1:A:908:THR:HG22	1:A:910:ASP:H	1.68	0.59
4:E:495:VAL:HG22	4:E:498:GLU:OE2	2.03	0.59
1:A:846:ASP:C	1:A:848:VAL:H	2.11	0.59
4:F:59:ASP:O	4:F:61:THR:N	2.32	0.59
4:F:140:ALA:HA	4:F:143:GLU:HG2	1.84	0.59
4:F:421:TYR:C	4:F:427:ARG:HH21	2.03	0.59
3:C:53:VAL:HG13	2:D:106:ILE:HD13	1.85	0.59
4:E:472:PHE:CD2	4:E:590:LEU:HD23	2.38	0.59
4:F:38:SER:HA	4:F:40:LYS:HZ3	1.67	0.59
4:F:363:LEU:HB2	4:F:390:ARG:HH22	1.68	0.59
2:D:9:LEU:HD23	2:D:10:PRO:HD2	1.84	0.58
1:A:899:MET:HE1	2:D:68:THR:CB	2.32	0.58
4:F:369:ASP:OD1	4:F:394:LYS:NZ	2.30	0.58
4:F:124:ASN:CB	4:F:427:ARG:NH1	2.66	0.58
4:F:280:LEU:HD11	4:F:436:MET:O	2.03	0.58
4:E:5:CYS:HA	4:E:24:PHE:O	2.02	0.58
4:F:38:SER:HA	4:F:40:LYS:NZ	2.19	0.58
2:B:71:TYR:CE2	4:E:92:LEU:HD22	2.38	0.58
2:D:161:ASP:OD1	2:D:184:LEU:HD22	2.04	0.58
4:F:368:ALA:HB2	4:F:391:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:304:ILE:HD12	4:F:355:TYR:CE1	2.39	0.58
4:F:554:HIS:O	4:F:560:ARG:NH1	2.36	0.58
5:G:77:THR:HA	5:G:112:LEU:HG	1.86	0.58
2:D:11:SER:O	2:D:11:SER:OG	2.22	0.58
4:E:139:LYS:HE2	4:E:382:TYR:CZ	2.39	0.58
1:A:5:GLN:OE1	1:A:5:GLN:O	2.21	0.57
1:A:197:ARG:NH1	1:A:289:TYR:OH	2.37	0.57
4:E:25:LEU:HD21	4:E:106:PHE:CE2	2.40	0.57
4:E:484:VAL:HG22	4:E:485:SER:H	1.70	0.57
4:F:369:ASP:CG	4:F:394:LYS:HZ1	2.13	0.57
2:B:55:MET:HE1	4:E:79:ILE:HG22	1.86	0.57
4:E:253:TYR:HB2	4:E:301:SER:OG	2.05	0.57
4:F:33:HIS:ND1	4:F:106:PHE:HB2	2.19	0.57
4:F:322:LEU:HD12	4:F:323:LYS:HD2	1.86	0.57
4:F:514:PRO:HG2	4:F:548:GLN:O	2.04	0.57
4:F:33:HIS:ND1	4:F:106:PHE:CB	2.67	0.57
2:D:39:LYS:O	2:D:43:ASN:ND2	2.38	0.56
4:F:383:ASP:OD1	4:F:384:LEU:N	2.38	0.56
4:E:239:THR:HG22	4:E:385:SER:CB	2.35	0.56
4:F:33:HIS:CE1	4:F:39:HIS:CD2	2.92	0.56
1:A:40:ASP:OD1	1:A:40:ASP:O	2.23	0.56
4:E:26:CYS:N	4:E:29:CYS:SG	2.78	0.56
4:E:73:LYS:O	4:E:74:SER:C	2.48	0.56
4:E:286:THR:HA	4:E:441:CYS:HA	1.87	0.56
5:G:109:THR:HG22	5:G:109:THR:O	2.05	0.56
2:D:78:ASP:OD1	2:D:78:ASP:O	2.22	0.56
4:F:140:ALA:O	4:F:144:THR:OG1	2.22	0.56
4:F:555:SER:HA	4:F:560:ARG:HH12	1.71	0.56
2:D:133:PRO:O	2:D:134:ASP:OD1	2.24	0.56
4:F:26:CYS:SG	4:F:27:CYS:N	2.76	0.56
4:E:37:THR:HG23	4:E:39:HIS:HB2	1.88	0.56
4:E:342:CYS:SG	4:E:343:PHE:N	2.79	0.56
4:F:551:GLU:O	4:F:552:THR:C	2.48	0.56
1:A:504:PHE:HB3	1:A:505:PRO:HD2	1.86	0.56
4:E:121:ILE:HG23	4:E:421:TYR:CE2	2.40	0.56
4:E:239:THR:CG2	4:E:385:SER:HB3	2.33	0.55
4:F:492:GLN:NE2	4:F:575:ILE:HG21	2.22	0.55
3:C:54:SER:OG	2:D:120:ILE:O	2.22	0.55
4:E:64:TYR:H	4:E:72:CYS:HA	1.70	0.55
4:F:25:LEU:HD23	4:F:29:CYS:HB3	1.87	0.55
4:E:38:SER:O	4:E:40:LYS:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:578:ASP:C	4:E:580:ASP:H	2.14	0.55
5:G:52:LYS:HB3	5:G:53:TRP:CE3	2.42	0.55
4:E:81:PHE:HD1	4:E:82:PRO:HD2	1.71	0.55
4:E:280:LEU:HD23	4:E:436:MET:SD	2.46	0.55
4:E:443:ARG:HH12	4:E:445:PRO:HD3	1.72	0.55
4:F:359:THR:N	4:F:363:LEU:CD1	2.69	0.55
4:F:404:GLN:HA	4:F:563:VAL:HG21	1.87	0.55
2:B:48:GLU:CD	2:B:51:ARG:HE	2.15	0.55
7:J:46:U:H3'	7:J:47:A:H8	1.71	0.55
2:B:98:LEU:O	2:B:99:ASP:C	2.48	0.55
4:F:378:MET:SD	4:F:407:ALA:HA	2.47	0.55
5:G:109:THR:O	5:G:109:THR:CG2	2.54	0.55
1:A:225:THR:HG22	1:A:226:THR:N	2.20	0.55
4:E:180:TYR:O	4:E:180:TYR:CG	2.59	0.55
2:D:175:ASP:C	2:D:177:SER:N	2.64	0.55
4:E:302:ALA:O	4:E:304:ILE:HG23	2.07	0.54
1:A:487:CYS:SG	1:A:528:PHE:HE2	2.28	0.54
4:F:363:LEU:HD12	4:F:390:ARG:NH2	2.22	0.54
4:F:450:ASP:OD1	4:F:584:LYS:NZ	2.39	0.54
2:D:175:ASP:C	2:D:177:SER:H	2.15	0.54
5:G:17:GLY:H	5:G:54:ALA:HB1	1.71	0.54
1:A:684:ASP:OD1	1:A:687:THR:OG1	2.13	0.54
4:E:31:TYR:O	4:E:35:ILE:HG13	2.08	0.54
2:D:21:ALA:O	2:D:22:TYR:C	2.49	0.54
4:F:159:SER:CB	4:F:162:GLU:OE2	2.54	0.54
2:D:9:LEU:HD11	2:D:52:ASP:O	2.08	0.54
4:E:373:PHE:HD2	4:E:376:ILE:HG22	1.64	0.54
4:E:566:THR:O	4:E:566:THR:CG2	2.56	0.54
4:F:138:LEU:CD1	4:F:139:LYS:HD3	2.38	0.54
4:F:138:LEU:O	4:F:141:THR:HG22	2.08	0.54
4:F:159:SER:HB2	4:F:162:GLU:CD	2.31	0.54
4:F:362:ALA:O	4:F:363:LEU:CG	2.55	0.54
4:F:492:GLN:OE1	4:F:492:GLN:O	2.25	0.54
5:G:19:THR:HB	5:G:22:ALA:H	1.72	0.54
4:E:17:GLY:O	4:E:18:ALA:C	2.51	0.54
4:F:576:MET:HE1	4:F:582:TYR:N	2.22	0.54
4:F:358:CYS:SG	4:F:363:LEU:HD12	2.48	0.54
4:F:358:CYS:CA	4:F:363:LEU:HD12	2.34	0.54
5:G:17:GLY:HA3	5:G:23:CYS:HB3	1.89	0.54
4:E:304:ILE:HD11	4:E:355:TYR:CE1	2.43	0.53
4:F:242:PRO:O	4:F:276:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:22:ALA:C	5:G:24:THR:N	2.63	0.53
2:B:69:GLN:O	2:B:69:GLN:NE2	2.42	0.53
2:D:164:SER:H	2:D:165:LYS:HD2	1.73	0.53
4:E:25:LEU:HD21	4:E:106:PHE:CZ	2.43	0.53
4:F:421:TYR:HA	4:F:427:ARG:CZ	2.38	0.53
5:G:60:ASP:OD1	5:G:61:GLY:N	2.41	0.53
2:D:22:TYR:HA	2:D:38:LEU:CD2	2.36	0.53
4:E:44:SER:O	4:E:45:VAL:C	2.48	0.53
4:E:117:ALA:O	4:E:121:ILE:HG13	2.09	0.53
5:G:31:TYR:CE1	5:G:45:LEU:HB3	2.43	0.53
5:G:36:LYS:O	5:G:37:GLY:C	2.51	0.53
4:E:66:GLY:O	4:E:67:GLY:C	2.51	0.53
4:E:86:ASN:O	4:E:87:GLY:C	2.49	0.53
4:F:59:ASP:C	4:F:61:THR:N	2.65	0.53
4:F:369:ASP:CG	4:F:394:LYS:NZ	2.67	0.53
1:A:504:PHE:CB	1:A:505:PRO:HD2	2.38	0.53
4:E:85:ALA:O	4:E:86:ASN:C	2.51	0.53
5:G:35:THR:CB	5:G:40:PHE:HB3	2.38	0.53
1:A:506:PHE:C	1:A:508:LYS:H	2.17	0.53
1:A:685:ALA:HA	7:J:27:C:O2'	2.09	0.53
1:A:202:VAL:HB	1:A:223:ILE:HG12	1.90	0.52
1:A:569:ARG:O	1:A:573:GLN:HB2	2.10	0.52
4:E:9:ASN:HB2	4:E:129:ARG:HH22	1.74	0.52
4:E:235:LEU:HD13	4:E:385:SER:OG	2.10	0.52
4:E:360:VAL:HA	4:E:363:LEU:HD11	1.92	0.52
4:F:549:THR:HA	4:F:550:THR:C	2.34	0.52
1:A:360:ASN:O	1:A:360:ASN:ND2	2.32	0.52
2:B:68:THR:HG23	4:F:53:PRO:HG2	1.91	0.52
4:F:202:LYS:HD2	4:F:202:LYS:C	2.30	0.52
5:G:79:THR:HG22	5:G:81:LYS:H	1.73	0.52
4:E:59:ASP:O	4:E:60:VAL:C	2.53	0.52
4:F:396:TYR:HB3	4:F:398:TYR:CZ	2.44	0.52
4:F:76:LYS:O	4:F:76:LYS:HG3	2.10	0.52
1:A:120:THR:O	9:A:1003:GDP:N1	2.40	0.52
5:G:12:MET:HE1	5:G:29:LEU:CD1	2.35	0.52
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.91	0.52
4:F:202:LYS:HZ2	4:F:210:VAL:HG23	1.71	0.52
1:A:506:PHE:C	1:A:508:LYS:N	2.68	0.52
1:A:699:ALA:O	1:A:703:ASN:ND2	2.42	0.52
2:D:21:ALA:C	2:D:23:GLU:N	2.65	0.51
4:E:578:ASP:N	4:E:578:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:CYS:SG	1:A:528:PHE:CE2	3.03	0.51
4:F:424:SER:O	4:F:428:LEU:HD22	2.09	0.51
1:A:254:GLU:OE2	1:A:286:TYR:OH	2.23	0.51
4:E:52:ALA:O	4:E:53:PRO:C	2.52	0.51
4:E:57:VAL:HG12	4:E:62:GLN:NE2	2.26	0.51
4:E:306:TYR:HA	4:E:372:VAL:HG12	1.91	0.51
4:F:45:VAL:O	4:F:46:ASN:ND2	2.44	0.51
1:A:628:ASN:O	1:A:632:ILE:HG13	2.11	0.51
4:E:95:ASN:C	4:E:97:CYS:H	2.18	0.51
4:F:358:CYS:CB	4:F:363:LEU:HD12	2.41	0.51
4:F:555:SER:HA	4:F:560:ARG:NH1	2.25	0.51
5:G:35:THR:O	5:G:36:LYS:C	2.51	0.51
4:F:181:VAL:HG12	4:F:182:PHE:H	1.75	0.51
4:E:151:ILE:HG23	4:E:226:VAL:HG12	1.93	0.51
4:E:266:VAL:O	4:E:270:GLN:HG2	2.11	0.51
1:A:30:VAL:HG22	1:A:51:THR:HG22	1.93	0.51
4:E:103:VAL:HA	4:E:106:PHE:HB3	1.93	0.51
5:G:17:GLY:HA2	5:G:27:ASN:HB2	1.92	0.51
4:F:358:CYS:C	4:F:363:LEU:HD11	2.35	0.51
4:F:363:LEU:CG	4:F:390:ARG:HH22	2.24	0.51
4:F:422:PHE:HB3	4:F:426:CYS:HB3	1.93	0.51
4:E:32:ASP:CB	4:E:103:VAL:HG11	2.20	0.50
4:E:112:CYS:HB2	4:E:119:ASP:OD1	2.12	0.50
2:D:139:LYS:NZ	2:D:140:ASN:OD1	2.44	0.50
4:E:21:ARG:HD2	4:E:140:ALA:HB2	1.93	0.50
4:E:366:THR:HG22	4:E:391:LEU:HD11	1.92	0.50
5:G:35:THR:CG2	5:G:40:PHE:HB3	2.41	0.50
1:A:504:PHE:C	1:A:506:PHE:H	2.20	0.50
2:B:174:MET:O	2:B:174:MET:SD	2.69	0.50
4:E:9:ASN:HB2	4:E:129:ARG:NH2	2.26	0.50
4:E:455:LEU:HG	4:E:456:VAL:HG23	1.94	0.50
4:F:437:PHE:C	4:F:438:LEU:HD12	2.36	0.50
1:A:846:ASP:C	1:A:848:VAL:N	2.68	0.50
4:E:380:THR:HG22	4:E:382:TYR:H	1.76	0.50
1:A:609:VAL:HG12	1:A:610:GLU:H	1.77	0.50
2:D:15:PHE:CE2	2:D:46:LYS:HG3	2.32	0.50
4:F:507:ARG:O	4:F:508:LYS:HD3	2.11	0.50
1:A:569:ARG:HD3	7:J:28:U:OP1	2.11	0.50
4:F:20:ILE:HG23	4:F:21:ARG:H	1.76	0.50
4:F:202:LYS:CG	4:F:210:VAL:HB	2.42	0.50
4:F:394:LYS:HD3	4:F:394:LYS:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:O	1:A:10:ARG:NH1	2.45	0.50
4:F:63:LEU:HD22	4:F:71:TYR:O	2.12	0.50
6:I:21:U:H2'	6:I:22:G:C8	2.46	0.50
4:E:20:ILE:HD13	4:E:21:ARG:HG2	1.94	0.49
4:E:548:GLN:NE2	4:E:551:GLU:HG2	2.27	0.49
4:F:325:LEU:CD1	4:F:329:LYS:HE2	2.31	0.49
4:E:105:ASP:O	4:E:106:PHE:C	2.55	0.49
4:F:372:VAL:HG13	4:F:399:ILE:HD13	1.94	0.49
4:F:118:GLY:O	4:F:122:LEU:HG	2.12	0.49
2:D:14:ALA:HB1	2:D:45:ALA:HB1	1.94	0.49
4:F:202:LYS:NZ	4:F:210:VAL:HG23	2.28	0.49
4:F:275:GLN:HE21	4:F:436:MET:CE	2.24	0.49
4:F:382:TYR:CD1	4:F:382:TYR:C	2.90	0.49
5:G:33:ASN:HB2	5:G:42:LEU:HG	1.94	0.49
1:A:484:ASP:OD1	1:A:484:ASP:C	2.55	0.49
1:A:783:LYS:HE2	1:A:796:GLU:OE2	2.12	0.49
2:D:127:LYS:HA	2:D:189:LEU:HD23	1.94	0.49
4:E:495:VAL:CA	4:E:498:GLU:HG2	2.40	0.49
4:F:322:LEU:CB	4:F:327:ILE:HD13	2.29	0.49
4:F:551:GLU:O	4:F:553:ALA:N	2.46	0.49
5:G:44:LEU:HD13	5:G:69:LEU:HD11	1.94	0.49
4:F:3:GLY:O	4:F:11:GLN:NE2	2.45	0.49
4:F:162:GLU:O	4:F:162:GLU:CG	2.59	0.49
5:G:33:ASN:C	5:G:35:THR:N	2.65	0.49
1:A:336:ASP:OD1	1:A:336:ASP:O	2.29	0.49
4:E:2:VAL:HA	4:E:12:THR:O	2.13	0.49
4:E:429:MET:SD	4:E:430:LYS:HD2	2.53	0.49
2:D:173:SER:O	2:D:174:MET:C	2.54	0.49
4:F:37:THR:OG1	4:F:107:ASN:ND2	2.46	0.49
4:F:141:THR:O	4:F:145:PHE:CD2	2.63	0.49
4:F:174:PRO:N	4:F:175:PRO:HD3	2.28	0.49
4:F:421:TYR:C	4:F:427:ARG:NH2	2.67	0.49
5:G:16:ALA:O	5:G:27:ASN:HB2	2.13	0.49
2:D:22:TYR:CA	2:D:38:LEU:HD23	2.40	0.49
2:D:165:LYS:HD2	2:D:165:LYS:N	2.27	0.49
4:E:21:ARG:O	4:E:22:ARG:HB2	2.13	0.49
5:G:14:CYS:SG	5:G:15:ALA:N	2.85	0.49
5:G:34:THR:O	5:G:39:ARG:HD2	2.12	0.49
1:A:504:PHE:CD2	1:A:505:PRO:HD3	2.48	0.49
4:E:12:THR:HB	4:E:26:CYS:HA	1.94	0.49
4:E:50:CYS:SG	4:E:63:LEU:HD11	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ASN:HB3	2:D:103:LEU:HB2	1.94	0.48
4:E:495:VAL:CG2	4:E:498:GLU:OE2	2.60	0.48
4:F:285:GLY:H	4:F:288:LYS:HE2	1.78	0.48
5:G:36:LYS:HA	5:G:36:LYS:HD3	1.53	0.48
2:B:90:MET:C	2:B:92:PHE:H	2.20	0.48
2:B:90:MET:O	2:B:93:THR:HG22	2.12	0.48
4:F:583:ASP:OD1	4:F:583:ASP:N	2.46	0.48
5:G:35:THR:OG1	5:G:40:PHE:HB3	2.13	0.48
4:E:155:ARG:HB2	4:E:156:GLU:OE1	2.13	0.48
4:F:154:VAL:O	4:F:222:GLY:CA	2.61	0.48
4:F:441:CYS:O	4:F:465:LYS:NZ	2.46	0.48
4:F:551:GLU:CA	4:F:556:CYS:H	2.25	0.48
4:E:118:GLY:HA2	4:E:121:ILE:HD12	1.95	0.48
3:C:76:LEU:CA	2:D:96:ARG:HH21	2.14	0.48
4:E:42:VAL:HB	4:E:60:VAL:HG21	1.95	0.48
4:E:79:ILE:HD13	4:E:79:ILE:H	1.78	0.48
4:E:119:ASP:O	4:E:122:LEU:HD12	2.14	0.48
4:F:31:TYR:CZ	4:F:87:GLY:HA2	2.49	0.48
4:F:449:VAL:HA	4:F:452:VAL:HG12	1.96	0.48
4:E:19:CYS:CB	4:E:23:PRO:HD2	2.44	0.48
4:E:73:LYS:HD2	4:E:76:LYS:HD2	1.94	0.48
4:F:15:ARG:HG3	4:F:43:LEU:HB2	1.95	0.48
4:E:5:CYS:SG	4:E:10:SER:N	2.86	0.48
5:G:53:TRP:HD1	5:G:66:TYR:HB3	1.79	0.48
4:E:329:LYS:HE2	4:E:355:TYR:HE2	1.78	0.48
4:E:545:ILE:HD12	4:E:573:LEU:HD22	1.96	0.48
4:F:398:TYR:CD1	4:F:398:TYR:N	2.82	0.48
4:F:582:TYR:HA	4:F:585:LEU:HB3	1.96	0.48
4:E:427:ARG:O	4:E:431:THR:HG23	2.14	0.47
4:F:275:GLN:HE21	4:F:436:MET:HE3	1.78	0.47
4:F:371:VAL:HG13	4:F:373:PHE:CE2	2.49	0.47
5:G:17:GLY:H	5:G:54:ALA:CB	2.27	0.47
7:J:46:U:H3'	7:J:47:A:C8	2.49	0.47
2:B:182:TRP:HE3	2:B:182:TRP:O	1.97	0.47
4:E:6:VAL:CG2	4:E:23:PRO:HB2	2.44	0.47
4:E:304:ILE:HD11	4:E:355:TYR:HD1	1.75	0.47
4:E:386:VAL:O	4:E:390:ARG:HG3	2.14	0.47
3:C:59:LEU:HD11	3:C:66:VAL:HG21	1.95	0.47
4:E:187:VAL:HG12	4:E:192:LYS:HD3	1.97	0.47
4:E:261:GLU:OE2	4:E:262:PHE:CZ	2.68	0.47
4:F:560:ARG:HG3	4:F:561:PHE:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LYS:O	1:A:718:LYS:HG2	2.13	0.47
2:D:22:TYR:HE1	2:D:35:LEU:O	1.96	0.47
4:F:419:PRO:O	4:F:420:GLU:C	2.58	0.47
5:G:24:THR:OG1	5:G:25:ASP:N	2.48	0.47
1:A:57:GLN:HG2	1:A:58:GLU:H	1.80	0.47
1:A:552:ASN:OD1	1:A:552:ASN:O	2.32	0.47
2:B:105:ASN:O	2:B:109:ASN:ND2	2.47	0.47
4:E:271:LYS:HD2	4:E:271:LYS:O	2.14	0.47
1:A:903:TYR:O	1:A:905:VAL:N	2.45	0.47
2:B:9:LEU:HD12	2:B:10:PRO:HD3	1.96	0.47
2:B:66:ALA:O	2:B:70:MET:HB3	2.14	0.47
1:A:111:VAL:HG23	1:A:113:HIS:CE1	2.50	0.47
2:D:143:ASP:OD1	2:D:143:ASP:O	2.32	0.47
4:E:27:CYS:O	4:E:28:LYS:C	2.55	0.47
4:F:564:ALA:O	4:F:567:ARG:NH2	2.48	0.47
5:G:72:PRO:HB3	5:G:89:TYR:CD2	2.50	0.47
2:B:19:GLN:CA	2:B:42:LEU:HD12	2.42	0.46
4:E:322:LEU:C	4:E:322:LEU:HD12	2.40	0.46
4:F:425:VAL:HA	4:F:428:LEU:CD2	2.45	0.46
4:F:425:VAL:C	4:F:428:LEU:CD2	2.88	0.46
1:A:903:TYR:CE2	2:D:71:TYR:CD1	3.04	0.46
4:E:19:CYS:HB2	4:E:23:PRO:HD2	1.97	0.46
4:F:124:ASN:HB2	4:F:427:ARG:HH12	1.81	0.46
4:E:304:ILE:HA	4:E:370:ILE:HG23	1.97	0.46
4:E:12:THR:OG1	4:E:13:SER:N	2.48	0.46
4:F:276:LYS:O	4:F:395:HIS:ND1	2.42	0.46
1:A:504:PHE:CB	1:A:505:PRO:CD	2.93	0.46
1:A:687:THR:O	1:A:688:ALA:C	2.57	0.46
4:F:279:THR:O	4:F:280:LEU:CD2	2.61	0.46
4:F:291:PHE:CE2	4:F:295:LEU:HD11	2.50	0.46
4:F:425:VAL:HA	4:F:428:LEU:HD22	1.97	0.46
4:F:551:GLU:O	4:F:556:CYS:N	2.44	0.46
7:J:43:U:H2'	7:J:44:A:H8	1.79	0.46
1:A:885:LEU:HD22	1:A:916:TRP:HA	1.98	0.46
2:D:118:ASN:OD1	2:D:118:ASN:N	2.47	0.46
4:E:49:VAL:O	4:E:51:ASN:N	2.49	0.46
4:F:138:LEU:HD13	4:F:139:LYS:HD3	1.97	0.46
1:A:496:ASN:OD1	1:A:496:ASN:N	2.48	0.46
2:B:177:SER:HB2	2:B:182:TRP:HZ2	1.80	0.46
4:E:15:ARG:O	4:E:43:LEU:HD12	2.16	0.46
4:E:19:CYS:O	4:E:20:ILE:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:GLU:O	2:B:176:ASN:ND2	2.38	0.46
3:C:49:PHE:HZ	2:D:98:LEU:HD22	1.80	0.46
4:E:5:CYS:CB	4:E:26:CYS:HB2	2.41	0.46
7:J:45:C:H2'	7:J:46:U:C6	2.49	0.46
4:E:176:LEU:HD12	4:E:516:ASN:HB3	1.98	0.46
4:F:551:GLU:HA	4:F:556:CYS:H	1.79	0.46
1:A:109:ASP:N	1:A:109:ASP:OD1	2.46	0.46
1:A:234:VAL:HG23	1:A:234:VAL:O	2.16	0.46
5:G:28:ALA:HB2	5:G:51:LEU:HD21	1.98	0.46
4:E:57:VAL:HG12	4:E:62:GLN:HE22	1.80	0.45
4:F:3:GLY:HA3	4:F:24:PHE:CE2	2.52	0.45
4:F:535:SER:HB2	4:F:537:GLN:NE2	2.31	0.45
4:F:248:ARG:HD2	4:F:249:ILE:HD12	1.98	0.45
4:F:473:LYS:HB2	4:F:587:PHE:HB3	1.97	0.45
4:F:576:MET:HE2	4:F:582:TYR:HB2	1.98	0.45
1:A:623:ASP:OD1	1:A:623:ASP:N	2.39	0.45
2:B:101:ASP:C	2:B:101:ASP:OD1	2.60	0.45
2:D:22:TYR:CE1	2:D:39:LYS:HB2	2.51	0.45
4:E:69:SER:OG	4:E:70:TYR:N	2.47	0.45
4:E:548:GLN:NE2	4:E:550:THR:O	2.49	0.45
2:D:141:THR:O	2:D:148:THR:HG22	2.17	0.45
4:E:279:THR:O	4:E:436:MET:HE3	2.16	0.45
4:F:576:MET:CE	4:F:582:TYR:HB2	2.46	0.45
4:E:78:PRO:HG2	4:E:79:ILE:HD13	1.98	0.45
4:E:548:GLN:C	4:E:549:THR:OG1	2.60	0.45
2:D:100:ASN:O	2:D:104:ASN:HB2	2.16	0.45
4:F:188:THR:HG23	4:F:189:LYS:H	1.82	0.45
4:F:453:SER:HA	4:F:457:TYR:HB2	1.98	0.45
1:A:894:GLU:O	1:A:898:HIS:N	2.49	0.45
4:E:60:VAL:O	4:E:61:THR:C	2.58	0.45
4:E:261:GLU:HG2	4:E:262:PHE:CD2	2.51	0.45
4:F:191:SER:OG	4:F:192:LYS:N	2.49	0.45
1:A:288:LYS:HD3	1:A:289:TYR:CE1	2.52	0.45
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.85	0.45
4:F:368:ALA:O	4:F:369:ASP:OD1	2.35	0.45
4:E:59:ASP:OD2	4:E:62:GLN:HB3	2.17	0.45
2:D:159:VAL:HG13	2:D:186:VAL:HG22	1.98	0.45
4:E:95:ASN:C	4:E:97:CYS:N	2.74	0.45
4:F:184:GLY:HA2	4:F:226:VAL:O	2.17	0.45
2:B:58:LYS:O	2:B:62:MET:HG2	2.17	0.44
4:E:12:THR:HG21	4:E:24:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:32:ASP:OD1	4:E:32:ASP:N	2.50	0.44
4:E:65:LEU:HD13	4:E:70:TYR:HD2	1.82	0.44
4:E:72:CYS:SG	4:E:73:LYS:N	2.90	0.44
1:A:87:TYR:O	1:A:91:LYS:HB3	2.17	0.44
4:E:488:ILE:HD11	4:E:521:VAL:HG11	1.98	0.44
4:F:73:LYS:HG3	4:F:74:SER:H	1.83	0.44
1:A:614:LEU:HB2	1:A:802:GLU:HB3	2.00	0.44
4:E:64:TYR:H	4:E:71:TYR:C	2.26	0.44
5:G:52:LYS:HB3	5:G:53:TRP:HE3	1.82	0.44
2:B:99:ASP:O	2:B:101:ASP:N	2.45	0.44
7:J:50:G:H2'	7:J:50:G:N3	2.33	0.44
1:A:504:PHE:C	1:A:506:PHE:N	2.75	0.44
1:A:896:THR:HA	1:A:907:LEU:HD12	2.00	0.44
4:E:513:SER:OG	4:E:531:GLN:O	2.30	0.44
7:J:45:C:H2'	7:J:46:U:H6	1.83	0.44
4:E:37:THR:CG2	4:E:39:HIS:HB2	2.47	0.44
4:E:154:VAL:HB	4:E:223:ASP:HB3	1.98	0.44
5:G:31:TYR:O	5:G:32:TYR:HB2	2.18	0.44
4:E:29:CYS:HA	4:E:32:ASP:OD2	2.17	0.44
4:E:76:LYS:HB3	4:E:76:LYS:HE2	1.65	0.44
1:A:89:LEU:CD1	1:A:224:GLN:OE1	2.65	0.44
2:B:96:ARG:H	2:B:96:ARG:HG2	1.57	0.44
4:E:374:ASP:OD1	4:E:399:ILE:HB	2.18	0.44
4:E:448:ILE:HD12	4:E:448:ILE:HA	1.90	0.44
5:G:35:THR:HB	5:G:40:PHE:H	1.83	0.44
1:A:566:MET:HE3	1:A:566:MET:HB2	1.86	0.43
1:A:718:LYS:HE3	1:A:718:LYS:HB3	1.70	0.43
4:E:19:CYS:O	4:E:22:ARG:N	2.49	0.43
4:E:50:CYS:C	4:E:52:ALA:N	2.75	0.43
4:E:419:PRO:O	4:E:420:GLU:C	2.60	0.43
4:F:405:LEU:HD23	4:F:535:SER:HA	2.00	0.43
5:G:21:THR:OG1	5:G:22:ALA:N	2.51	0.43
1:A:36:ASP:C	1:A:36:ASP:OD1	2.61	0.43
2:D:48:GLU:CG	2:D:51:ARG:HH21	2.30	0.43
4:E:243:GLN:O	4:E:244:GLU:HG3	2.18	0.43
4:F:303:ARG:HE	4:F:369:ASP:CG	2.27	0.43
4:F:422:PHE:CG	4:F:423:ASN:N	2.84	0.43
1:A:8:LEU:HD23	1:A:8:LEU:O	2.18	0.43
4:F:243:GLN:HG2	4:F:277:TYR:HE2	1.83	0.43
5:G:34:THR:O	5:G:35:THR:HB	2.18	0.43
1:A:504:PHE:CG	1:A:505:PRO:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:CYS:C	4:E:52:ALA:H	2.25	0.43
4:F:318:CYS:HB2	4:F:346:PHE:CE2	2.53	0.43
1:A:609:VAL:HG12	1:A:610:GLU:N	2.33	0.43
1:A:367:SER:OG	1:A:368:PHE:N	2.51	0.43
4:E:358:CYS:SG	4:E:363:LEU:HG	2.59	0.43
4:F:39:HIS:O	4:F:41:LEU:N	2.41	0.43
5:G:55:ARG:HA	5:G:65:ILE:O	2.19	0.43
4:E:63:LEU:C	4:E:72:CYS:HA	2.44	0.43
4:E:321:ALA:HA	4:E:325:LEU:HD23	2.00	0.43
4:F:154:VAL:O	4:F:222:GLY:N	2.52	0.43
4:F:362:ALA:C	4:F:363:LEU:HD23	2.29	0.43
4:F:514:PRO:HG2	4:F:548:GLN:CA	2.49	0.43
6:I:20:A:H2'	6:I:21:U:C6	2.53	0.43
1:A:607:SER:HB3	1:A:608:ASP:H	1.51	0.43
4:E:24:PHE:O	4:E:25:LEU:C	2.62	0.43
4:E:100:SER:O	4:E:102:ASN:N	2.52	0.43
4:E:547:THR:HB	4:E:549:THR:HG23	2.00	0.43
4:F:378:MET:CE	4:F:408:PRO:HD3	2.48	0.43
1:A:466:ILE:HD12	1:A:466:ILE:HA	1.90	0.43
2:D:22:TYR:CD1	2:D:38:LEU:HD23	2.54	0.43
2:D:83:VAL:HG13	2:D:84:THR:N	2.34	0.43
5:G:78:ASP:HB2	5:G:113:GLN:HE22	1.83	0.43
5:G:110:VAL:HG12	5:G:111:ARG:N	2.33	0.43
1:A:258:ASP:OD2	1:A:263:LYS:NZ	2.52	0.43
4:E:108:ALA:HB1	4:E:122:LEU:HD22	2.01	0.43
4:E:579:ARG:H	4:E:579:ARG:HG2	1.43	0.43
4:F:315:ASP:HA	4:F:318:CYS:SG	2.59	0.43
5:G:45:LEU:HD12	5:G:46:SER:H	1.83	0.43
1:A:453:TYR:CE1	1:A:667:VAL:HG21	2.54	0.42
4:E:44:SER:C	4:E:46:ASN:N	2.74	0.42
4:E:300:PRO:O	4:E:354:GLN:NE2	2.42	0.42
4:E:578:ASP:C	4:E:580:ASP:N	2.73	0.42
4:F:312:ALA:HB3	4:F:537:GLN:OE1	2.19	0.42
4:F:444:CYS:SG	4:F:566:THR:HB	2.59	0.42
1:A:275:PHE:HA	1:A:278:GLU:OE1	2.18	0.42
1:A:504:PHE:CG	1:A:505:PRO:CD	3.02	0.42
2:B:163:ASP:O	2:B:164:SER:HB2	2.19	0.42
2:D:132:ILE:CD1	2:D:186:VAL:HG21	2.48	0.42
4:F:202:LYS:NZ	4:F:210:VAL:CB	2.68	0.42
4:F:363:LEU:CB	4:F:390:ARG:HH22	2.31	0.42
4:F:370:ILE:HD13	4:F:370:ILE:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:576:MET:HE1	4:F:581:LEU:C	2.43	0.42
1:A:335:VAL:O	1:A:335:VAL:HG13	2.20	0.42
2:D:141:THR:HB	2:D:147:PHE:HE1	1.84	0.42
4:F:274:MET:O	4:F:274:MET:CG	2.67	0.42
4:F:558:VAL:HG22	4:F:559:ASN:H	1.84	0.42
5:G:18:THR:HA	5:G:51:LEU:HG	2.00	0.42
1:A:192:PHE:O	1:A:196:MET:HB2	2.19	0.42
1:A:530:TYR:CD2	1:A:536:ILE:HD11	2.54	0.42
4:E:65:LEU:CB	4:E:81:PHE:HB3	2.46	0.42
4:E:304:ILE:HG12	4:E:354:GLN:O	2.19	0.42
4:E:565:ILE:HG22	4:E:574:CYS:SG	2.59	0.42
2:D:9:LEU:CD2	2:D:10:PRO:HD2	2.49	0.42
4:E:63:LEU:HD12	4:E:72:CYS:HB3	2.02	0.42
4:E:363:LEU:HD23	4:E:391:LEU:HD22	2.02	0.42
4:F:418:GLU:O	4:F:419:PRO:C	2.63	0.42
2:D:157:GLN:CD	2:D:189:LEU:HD12	2.45	0.42
4:E:44:SER:O	4:E:46:ASN:N	2.53	0.42
4:E:503:ASN:O	4:E:507:ARG:NE	2.41	0.42
4:F:307:THR:HG22	4:F:373:PHE:HD1	1.85	0.42
4:F:586:GLN:CD	4:F:586:GLN:O	2.63	0.42
5:G:33:ASN:O	5:G:34:THR:C	2.62	0.42
5:G:95:ASN:O	5:G:99:ARG:HG3	2.19	0.42
2:B:92:PHE:HA	2:B:95:LEU:HD23	2.02	0.42
2:D:121:PRO:O	2:D:190:ARG:NH1	2.52	0.42
4:E:15:ARG:HD3	4:E:22:ARG:HB3	2.02	0.42
4:E:304:ILE:HA	4:E:370:ILE:CG2	2.50	0.42
4:F:371:VAL:HG21	4:F:396:TYR:CD1	2.55	0.42
4:F:379:ALA:HB3	4:F:383:ASP:OD2	2.20	0.42
4:F:382:TYR:CD1	4:F:382:TYR:O	2.73	0.42
4:F:546:PHE:HB3	4:F:573:LEU:O	2.20	0.42
3:C:53:VAL:HG12	2:D:120:ILE:HD12	2.00	0.42
4:E:195:ILE:HG22	4:E:198:TYR:CE1	2.55	0.42
4:F:3:GLY:HA3	4:F:24:PHE:CZ	2.55	0.42
5:G:5:SER:HB2	5:G:101:MET:HG2	2.00	0.42
5:G:68:GLU:OE2	5:G:92:LYS:HG2	2.20	0.42
5:G:97:LEU:HG	5:G:101:MET:CE	2.46	0.42
1:A:824:ASP:OD1	1:A:824:ASP:C	2.63	0.42
4:E:6:VAL:HG23	4:E:25:LEU:HD23	2.02	0.42
4:E:20:ILE:HG23	4:E:21:ARG:HG2	2.02	0.42
4:E:63:LEU:HG	4:E:72:CYS:N	2.35	0.42
4:E:202:LYS:HA	4:E:202:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:332:ARG:HE	4:E:333:ILE:H	1.67	0.42
4:F:113:ASP:OD1	4:F:115:THR:HG22	2.19	0.42
4:F:453:SER:O	4:F:458:ASP:HA	2.20	0.42
4:E:176:LEU:HD21	4:E:201:GLU:O	2.20	0.42
4:F:62:GLN:NE2	4:F:73:LYS:HG2	2.35	0.42
1:A:856:ILE:O	1:A:860:VAL:HG23	2.20	0.41
4:E:34:VAL:HG12	4:E:35:ILE:N	2.35	0.41
4:E:76:LYS:HA	4:E:77:PRO:HD2	1.91	0.41
4:F:467:LYS:HE3	4:F:586:GLN:OE1	2.20	0.41
4:F:548:GLN:OE1	4:F:555:SER:HB3	2.20	0.41
1:A:534:ASN:O	1:A:657:ASN:ND2	2.54	0.41
1:A:819:LEU:HD12	1:A:827:VAL:O	2.19	0.41
4:E:307:THR:HG23	4:E:373:PHE:HD1	1.85	0.41
4:E:404:GLN:HE21	4:E:537:GLN:HE22	1.68	0.41
4:F:382:TYR:O	4:F:382:TYR:HD1	2.03	0.41
4:F:425:VAL:O	4:F:425:VAL:HG12	2.20	0.41
4:E:33:HIS:NE2	4:E:39:HIS:ND1	2.64	0.41
4:E:235:LEU:HD11	4:E:382:TYR:CD2	2.54	0.41
4:E:354:GLN:O	4:E:354:GLN:HG3	2.19	0.41
1:A:924:MET:HE3	1:A:924:MET:HB3	1.80	0.41
2:D:132:ILE:HG21	2:D:138:TYR:HB2	2.01	0.41
4:E:94:LYS:O	4:E:97:CYS:HB3	2.20	0.41
4:E:321:ALA:O	4:E:325:LEU:HB2	2.20	0.41
4:E:386:VAL:CG2	4:E:390:ARG:HH11	2.34	0.41
4:F:428:LEU:HD23	4:F:429:MET:N	2.33	0.41
4:F:491:PRO:O	4:F:495:VAL:HG12	2.20	0.41
1:A:42:VAL:HG12	1:A:43:ALA:N	2.36	0.41
1:A:885:LEU:HD21	1:A:921:TYR:CE2	2.56	0.41
4:F:187:VAL:HG23	4:F:224:TYR:CD2	2.54	0.41
1:A:629:MET:HE3	1:A:629:MET:HB3	1.83	0.41
4:F:387:VAL:HA	4:F:390:ARG:HG2	2.02	0.41
4:F:572:ILE:HG12	4:F:573:LEU:H	1.86	0.41
2:D:42:LEU:O	2:D:46:LYS:HB2	2.21	0.41
2:D:55:MET:HE2	2:D:55:MET:HB3	1.95	0.41
4:E:139:LYS:HA	4:E:142:GLU:HG2	2.03	0.41
4:F:135:ALA:CA	4:F:138:LEU:HG	2.36	0.41
1:A:50:LYS:HB2	1:A:50:LYS:HE2	1.32	0.41
1:A:520:SER:O	1:A:524:GLN:HG3	2.21	0.41
4:E:34:VAL:O	4:E:40:LYS:HD3	2.21	0.41
4:F:5:CYS:N	4:F:10:SER:O	2.48	0.41
4:F:160:ASP:O	4:F:162:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:39:ARG:HA	5:G:39:ARG:HD2	1.75	0.41
1:A:39:ASN:C	1:A:41:LYS:H	2.29	0.41
1:A:760:ASP:OD1	1:A:760:ASP:C	2.64	0.41
2:B:95:LEU:O	2:B:97:LYS:N	2.51	0.41
2:D:133:PRO:C	2:D:134:ASP:OD1	2.63	0.41
2:D:143:ASP:OD1	2:D:143:ASP:C	2.63	0.41
4:E:233:MET:SD	4:E:234:PRO:HD2	2.61	0.41
4:E:548:GLN:O	4:E:549:THR:OG1	2.37	0.41
4:F:46:ASN:HD22	4:F:46:ASN:HA	1.67	0.41
4:F:496:VAL:O	4:F:500:LEU:HG	2.21	0.41
4:F:578:ASP:O	4:F:579:ARG:NH2	2.54	0.41
3:C:62:MET:HE2	3:C:62:MET:HB3	1.96	0.41
4:E:15:ARG:CD	4:E:22:ARG:HB3	2.51	0.41
4:E:18:ALA:HB3	4:E:39:HIS:ND1	2.36	0.41
4:E:495:VAL:CA	4:E:498:GLU:OE2	2.60	0.41
7:J:40:U:H2'	7:J:41:G:C8	2.43	0.41
1:A:338:VAL:HA	1:A:339:PRO:HD3	1.92	0.40
3:C:49:PHE:CZ	2:D:98:LEU:HD22	2.54	0.40
4:E:283:PRO:HB2	4:E:286:THR:HG21	2.03	0.40
4:F:499:PHE:HA	4:F:502:ARG:HD3	2.02	0.40
4:F:374:ASP:O	4:F:376:ILE:HG23	2.21	0.40
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.92	0.40
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.89	0.40
4:E:18:ALA:CB	4:E:39:HIS:CG	3.04	0.40
4:E:261:GLU:HG2	4:E:262:PHE:CG	2.56	0.40
4:F:394:LYS:N	4:F:394:LYS:CD	2.84	0.40
4:F:514:PRO:HG2	4:F:548:GLN:C	2.47	0.40
4:F:532:THR:OG1	4:F:533:VAL:N	2.54	0.40
1:A:205:LEU:HB2	1:A:234:VAL:HG12	2.03	0.40
4:E:188:THR:HG23	4:E:193:VAL:HG21	2.02	0.40
4:E:369:ASP:HB3	4:E:394:LYS:HZ1	1.86	0.40
4:E:472:PHE:HB2	4:E:573:LEU:HD12	2.04	0.40
4:F:378:MET:SD	4:F:405:LEU:O	2.79	0.40
4:F:473:LYS:NZ	4:F:576:MET:HG2	2.36	0.40
5:G:11:GLN:CD	5:G:39:ARG:HH22	2.30	0.40
5:G:22:ALA:O	5:G:24:THR:N	2.55	0.40
1:A:545:LYS:HE3	1:A:555:ARG:HE	1.86	0.40
2:B:37:LYS:O	2:B:41:SER:HB3	2.22	0.40
4:E:354:GLN:HG2	4:E:355:TYR:CE2	2.56	0.40
4:E:364:PRO:O	4:E:391:LEU:HD13	2.22	0.40
4:F:151:ILE:HG12	4:F:226:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:509:ALA:HB2	4:F:543:TYR:HB3	2.03	0.40
5:G:70:GLU:HB2	5:G:71:PRO:HD2	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	929/931 (100%)	854 (92%)	67 (7%)	8 (1%)	14 41
2	B	185/187 (99%)	164 (89%)	19 (10%)	2 (1%)	11 36
2	D	185/187 (99%)	157 (85%)	27 (15%)	1 (0%)	24 54
3	C	76/78 (97%)	69 (91%)	7 (9%)	0	100 100
4	E	581/593 (98%)	491 (84%)	71 (12%)	19 (3%)	3 14
4	F	578/593 (98%)	512 (89%)	57 (10%)	9 (2%)	7 28
5	G	111/113 (98%)	89 (80%)	18 (16%)	4 (4%)	2 13
All	All	2645/2682 (99%)	2336 (88%)	266 (10%)	43 (2%)	10 28

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	PHE
1	A	505	PRO
1	A	607	SER
1	A	846	ASP
4	E	34	VAL
4	E	59	ASP
4	E	72	CYS
4	E	98	VAL
4	F	79	ILE

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Mol	Chain	Res	Type
4	F	185	TYR
4	F	552	THR
5	G	22	ALA
1	A	501	SER
1	A	847	ILE
2	B	97	LYS
4	E	50	CYS
4	E	54	GLY
4	E	56	ASP
4	E	86	ASN
4	E	87	GLY
4	E	220	ASN
4	F	60	VAL
4	F	551	GLU
5	G	33	ASN
1	A	507	ASN
1	A	844	VAL
4	E	15	ARG
4	E	19	CYS
4	E	26	CYS
4	E	104	THR
4	E	581	LEU
4	F	549	THR
2	D	175	ASP
4	E	53	PRO
4	E	74	SER
4	E	93	TYR
2	B	99	ASP
4	F	61	THR
5	G	11	GLN
4	F	300	PRO
4	F	53	PRO
4	E	6	VAL
5	G	38	GLY

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	821/822 (100%)	807 (98%)	14 (2%)	53 70
2	B	144/159 (91%)	140 (97%)	4 (3%)	38 62
2	D	150/159 (94%)	142 (95%)	8 (5%)	20 47
3	C	73/73 (100%)	73 (100%)	0	100 100
4	E	498/516 (96%)	467 (94%)	31 (6%)	16 42
4	F	497/516 (96%)	487 (98%)	10 (2%)	48 68
5	G	94/94 (100%)	87 (93%)	7 (7%)	13 36
All	All	2277/2339 (97%)	2203 (97%)	74 (3%)	35 59

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	106	ILE
1	A	155	ASP
1	A	207	LEU
1	A	360	ASN
1	A	463	MET
1	A	501	SER
1	A	644	THR
1	A	647	SER
1	A	680	THR
1	A	687	THR
1	A	847	ILE
1	A	850	THR
1	A	917	GLU
2	B	94	MET
2	B	95	LEU
2	B	97	LYS
2	B	101	ASP
2	D	87	MET
2	D	111	ARG
2	D	112	ASP
2	D	115	VAL
2	D	172	ILE
2	D	174	MET
2	D	176	ASN
2	D	192	ASN
4	E	5	CYS
4	E	6	VAL
4	E	7	LEU

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Mol	Chain	Res	Type
4	E	9	ASN
4	E	11	GLN
4	E	15	ARG
4	E	20	ILE
4	E	21	ARG
4	E	25	LEU
4	E	30	CYS
4	E	32	ASP
4	E	34	VAL
4	E	35	ILE
4	E	42	VAL
4	E	43	LEU
4	E	49	VAL
4	E	57	VAL
4	E	62	GLN
4	E	63	LEU
4	E	65	LEU
4	E	73	LYS
4	E	76	LYS
4	E	79	ILE
4	E	88	GLN
4	E	96	THR
4	E	98	VAL
4	E	103	VAL
4	E	105	ASP
4	E	227	LEU
4	E	322	LEU
4	E	579	ARG
4	F	37	THR
4	F	60	VAL
4	F	61	THR
4	F	176	LEU
4	F	373	PHE
4	F	376	ILE
4	F	474[A]	MET
4	F	474[B]	MET
4	F	547	THR
4	F	552	THR
5	G	4	LEU
5	G	13	SER
5	G	20	GLN
5	G	21	THR

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Mol	Chain	Res	Type
5	G	23	CYS
5	G	34	THR
5	G	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	79	ASN
1	A	133	HIS
1	A	297	ASN
1	A	468	GLN
1	A	611	ASN
1	A	642	HIS
1	A	705	ASN
1	A	722	ASN
1	A	810	HIS
1	A	886	GLN
2	B	69	GLN
2	B	100	ASN
2	B	109	ASN
3	C	36	HIS
2	D	43	ASN
2	D	73	GLN
2	D	168	GLN
4	E	179	ASN
4	E	404	GLN
4	E	482	HIS
4	E	519	ASN
4	F	33	HIS
4	F	39	HIS
4	F	46	ASN
4	F	107	ASN
4	F	245	HIS
4	F	275	GLN
4	F	281	GLN
4	F	290	HIS
4	F	311	HIS
4	F	537	GLN
5	G	11	GLN
5	G	33	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	24/25 (96%)	1 (4%)	0
7	J	26/27 (96%)	3 (11%)	0
All	All	50/52 (96%)	4 (8%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	10	C
7	J	46	U
7	J	47	A
7	J	50	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 9 are 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	BEF	A	1004	9,1	0,3,3	-	-	-		
9	GDP	A	1003	11,10	29,30,30	1.38	4 (13%)	45,47,47	1.96	7 (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
9	GDP	A	1003	11,10	-	5/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GDP	C6-N1	-4.08	1.31	1.38
9	A	1003	GDP	C5-N7	-2.79	1.33	1.39
9	A	1003	GDP	C5-C4	2.68	1.46	1.38
9	A	1003	GDP	C2-N1	-2.41	1.31	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1003	GDP	C5-C4-N3	-6.81	117.55	128.39
9	A	1003	GDP	C2-N3-C4	5.78	122.26	112.30
9	A	1003	GDP	N9-C4-N3	5.28	136.52	125.95
9	A	1003	GDP	C6-C5-N7	3.18	136.07	130.29
9	A	1003	GDP	O2A-PA-O3A	2.33	113.56	107.27
9	A	1003	GDP	C4-C5-N7	-2.14	107.28	110.67
9	A	1003	GDP	C3'-C2'-C1'	2.05	105.33	101.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	GDP	C5'-O5'-PA-O1A
9	A	1003	GDP	O4'-C4'-C5'-O5'
9	A	1003	GDP	C3'-C4'-C5'-O5'
9	A	1003	GDP	C2'-C1'-N9-C8
9	A	1003	GDP	C2'-C1'-N9-C4

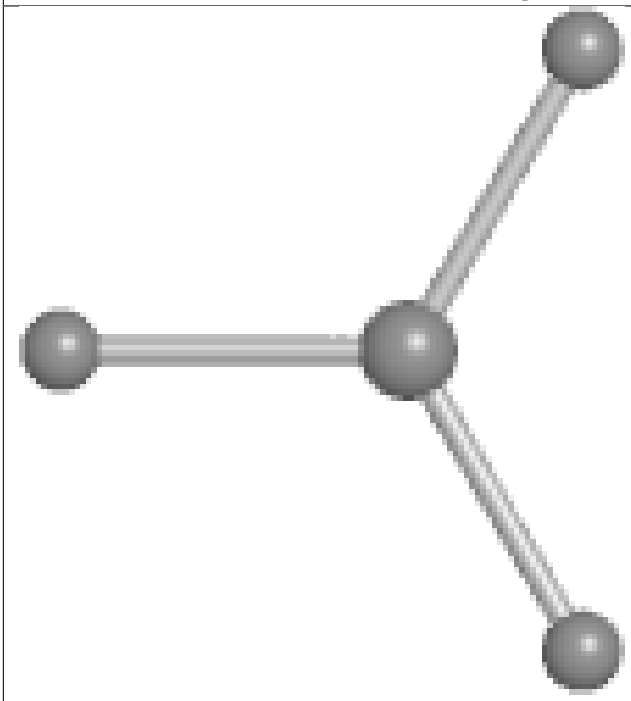
There are no ring outliers.

2 monomers are involved in 5 short contacts:

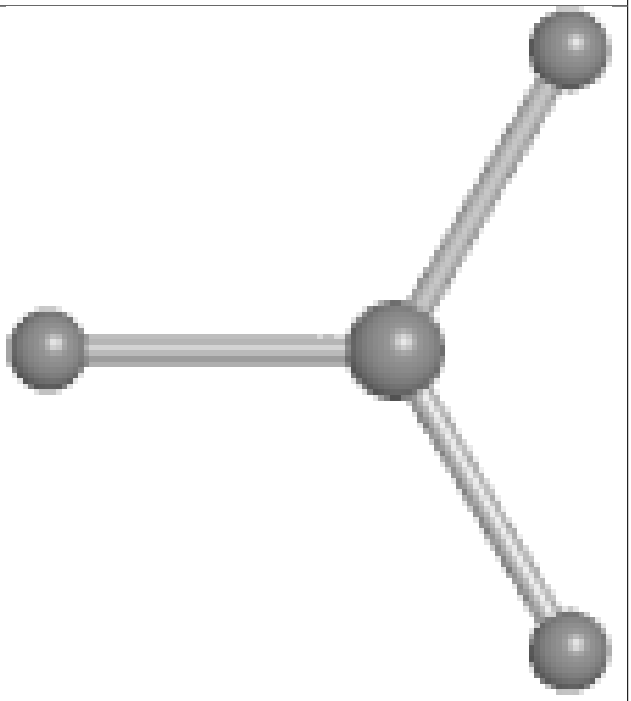
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1004	BEF	4	0
9	A	1003	GDP	1	0

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 then 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.

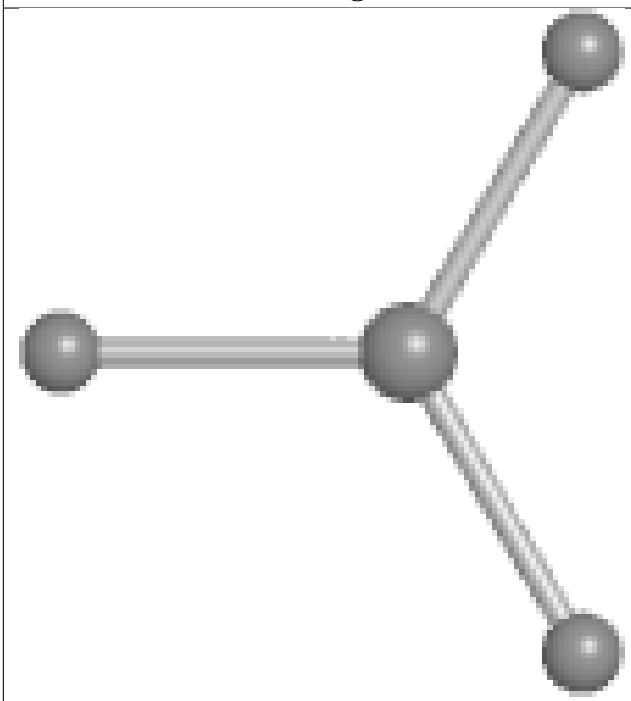
Ligand BEF A 1004



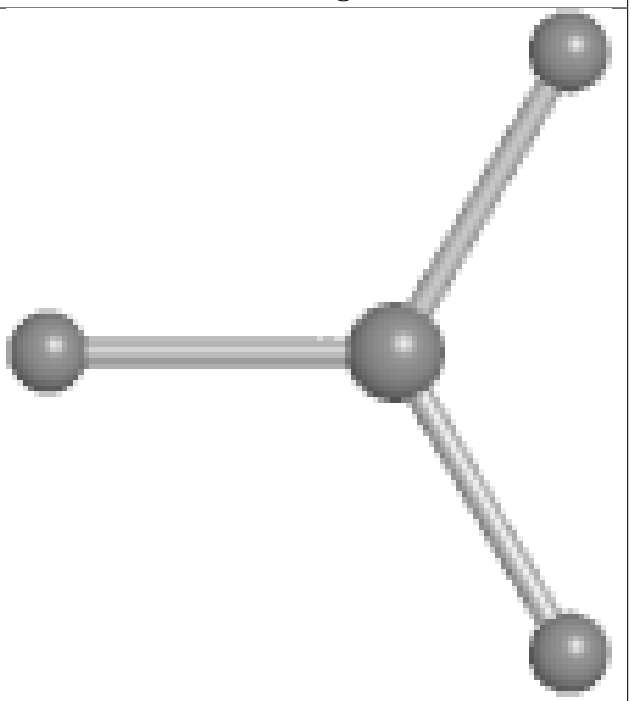
Bond lengths



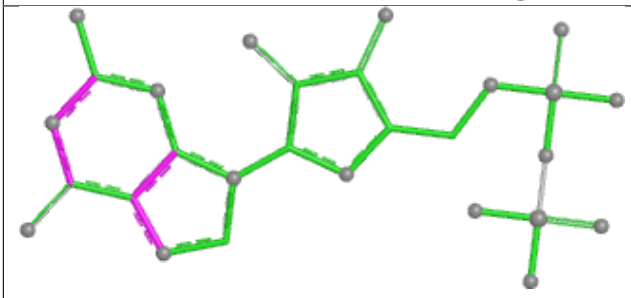
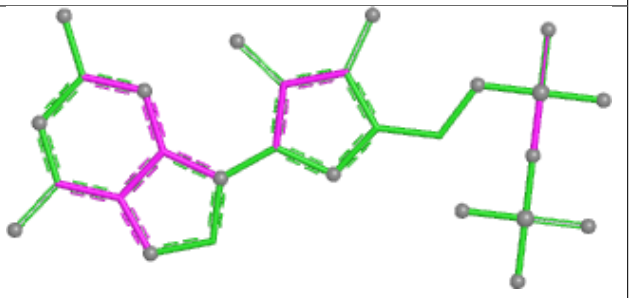
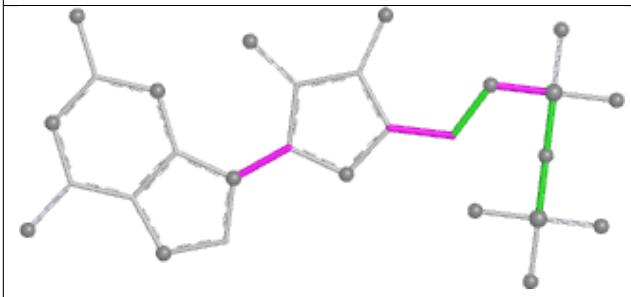
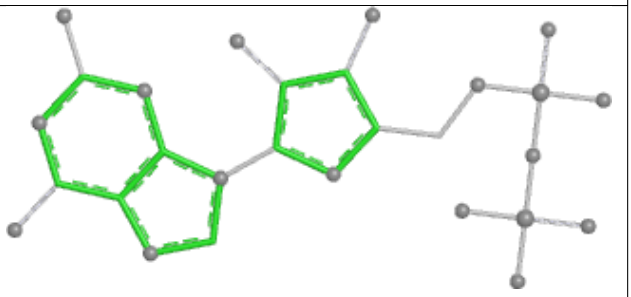
Bond angles



Torsions



Rings

Ligand GDP A 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

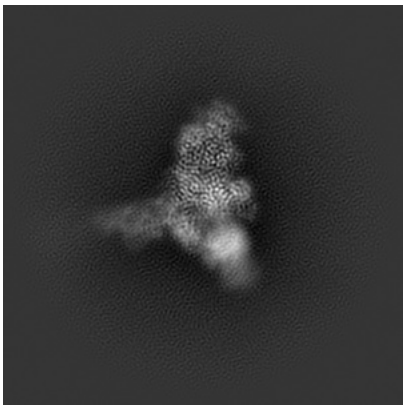
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60663. These allow visual inspection of the internal detail of the map and identification of artifacts.

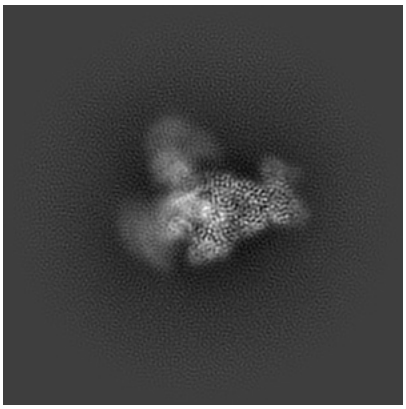
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

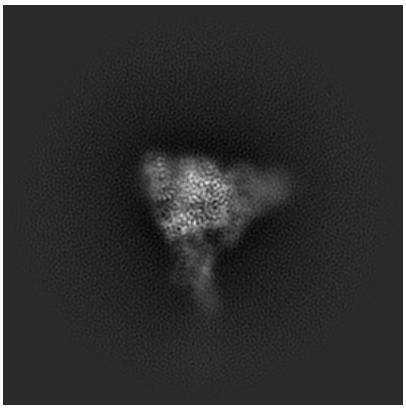
6.1.1 Primary map



X

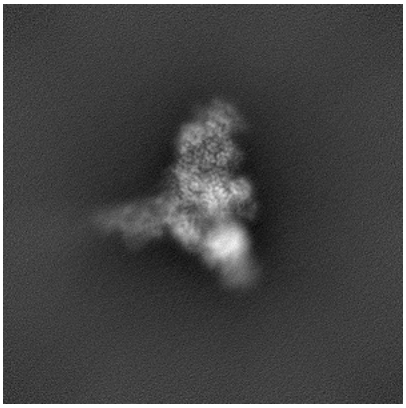


Y

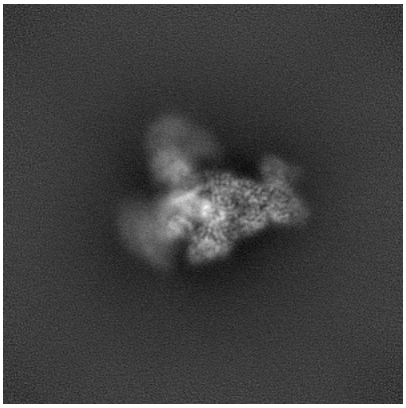


Z

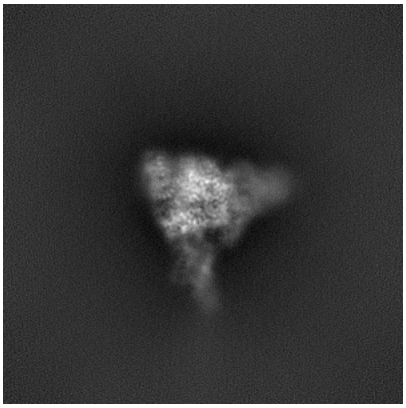
6.1.2 Raw map



X



Y

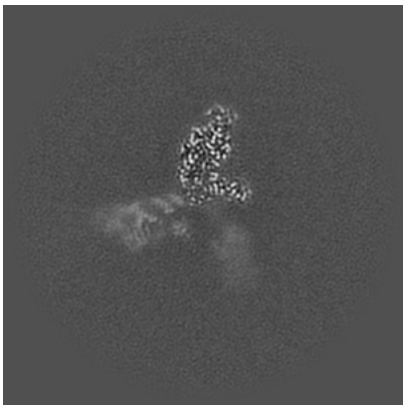


Z

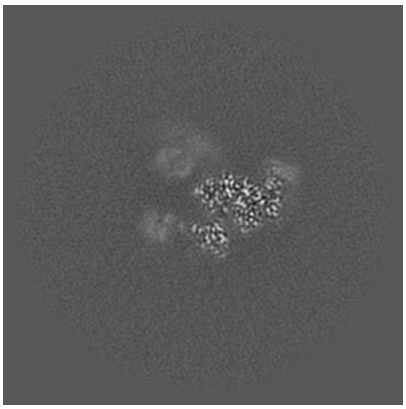
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

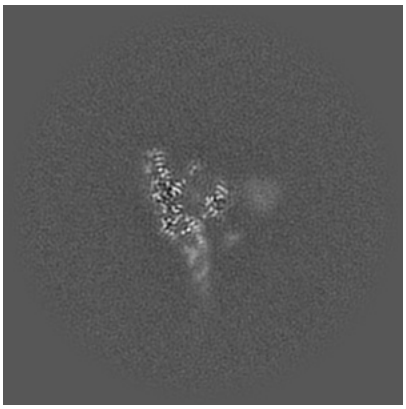
6.2.1 Primary map



X Index: 220

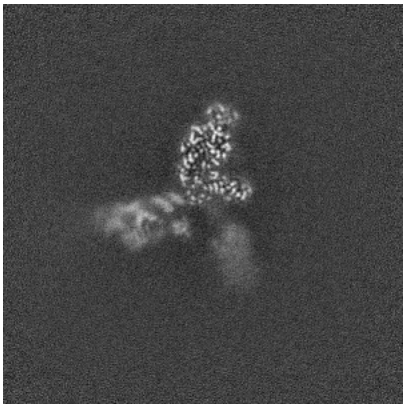


Y Index: 220



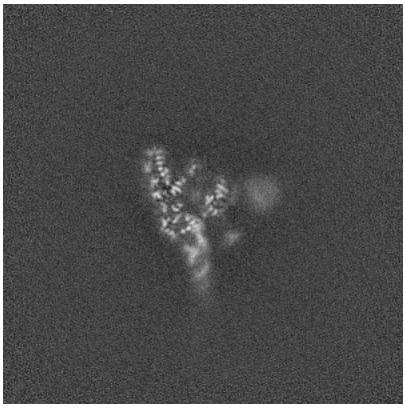
Z Index: 220

6.2.2 Raw map



X Index: 220

Y Index: 220

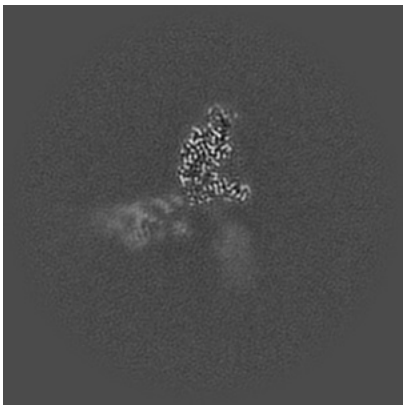


Z Index: 220

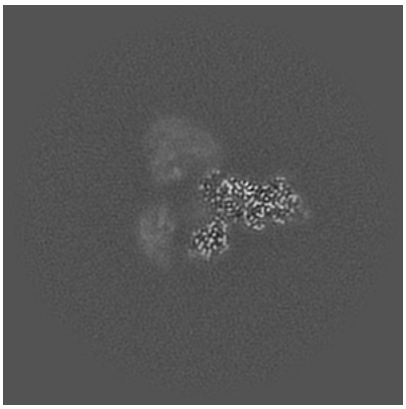
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

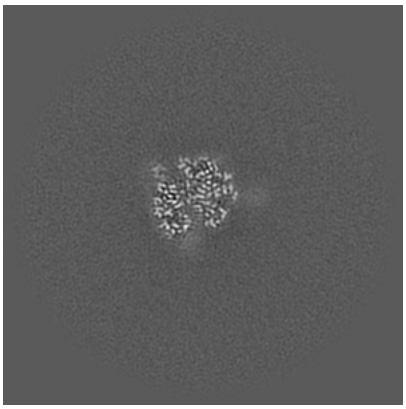
6.3.1 Primary map



X Index: 221

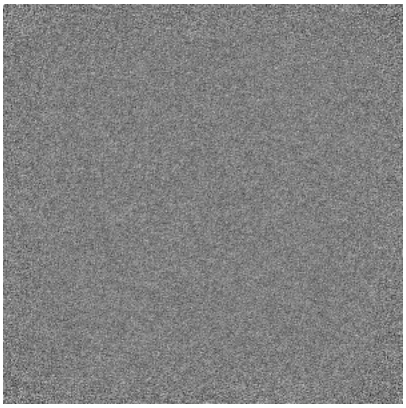


Y Index: 231

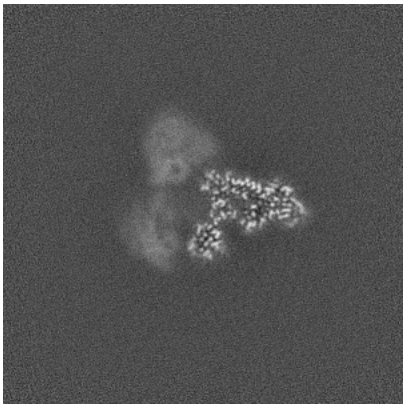


Z Index: 236

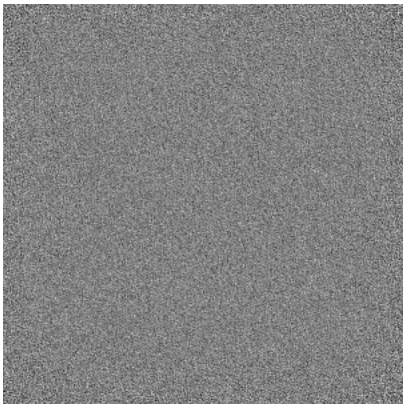
6.3.2 Raw map



X Index: 0



Y Index: 240

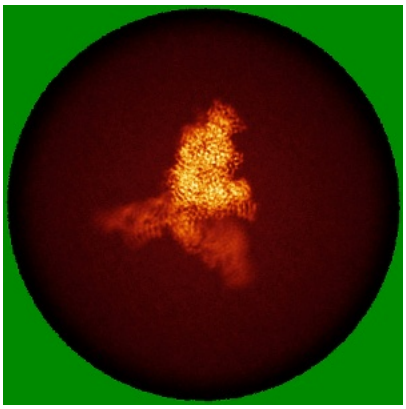


Z Index: 0

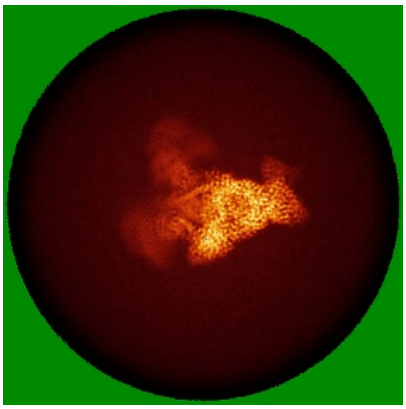
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

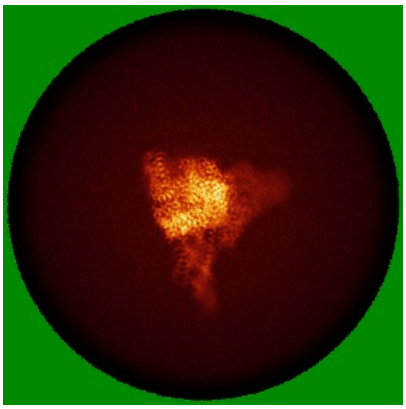
6.4.1 Primary map



X

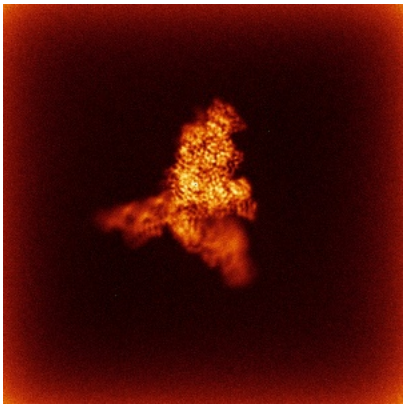


Y

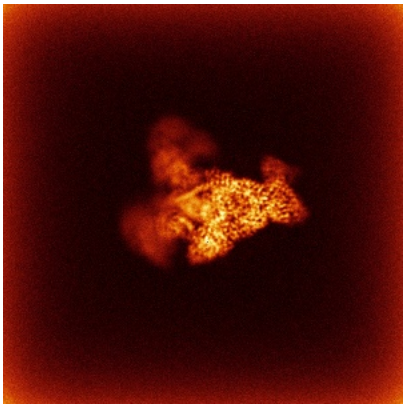


Z

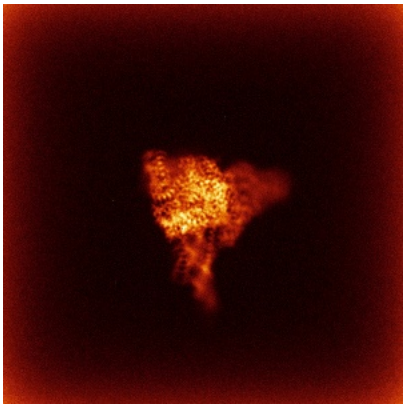
6.4.2 Raw map



X



Y

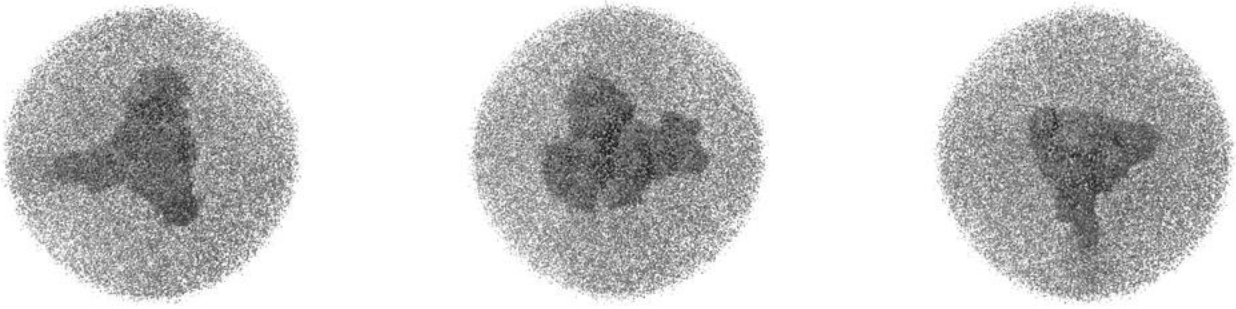


Z

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)

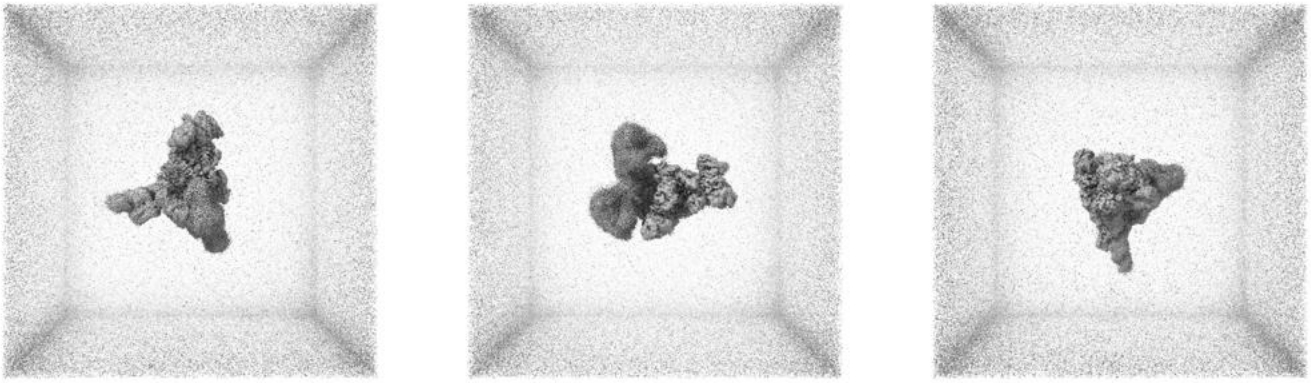
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

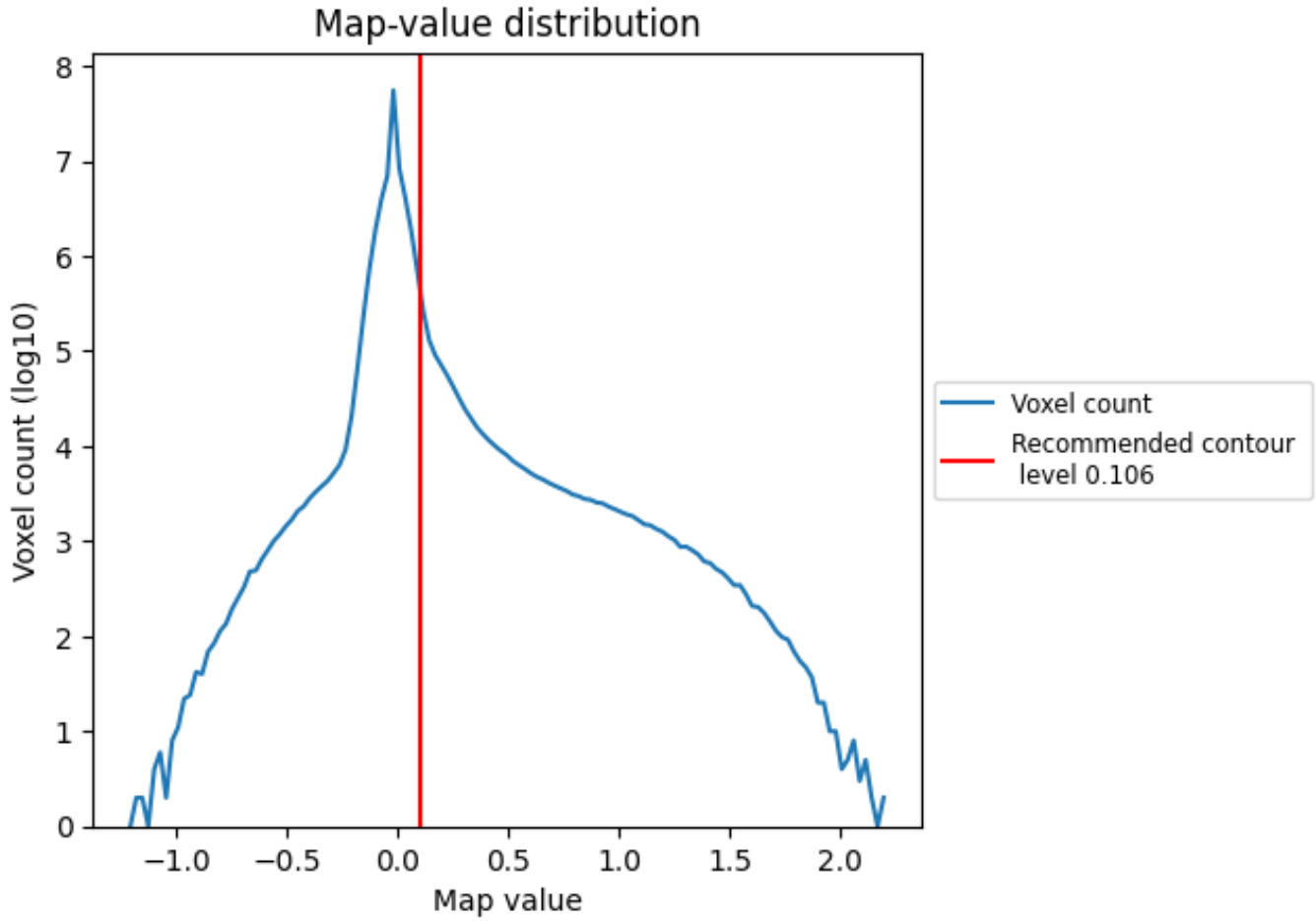
6.6 Mask visualisation (i)

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

7 Map analysis

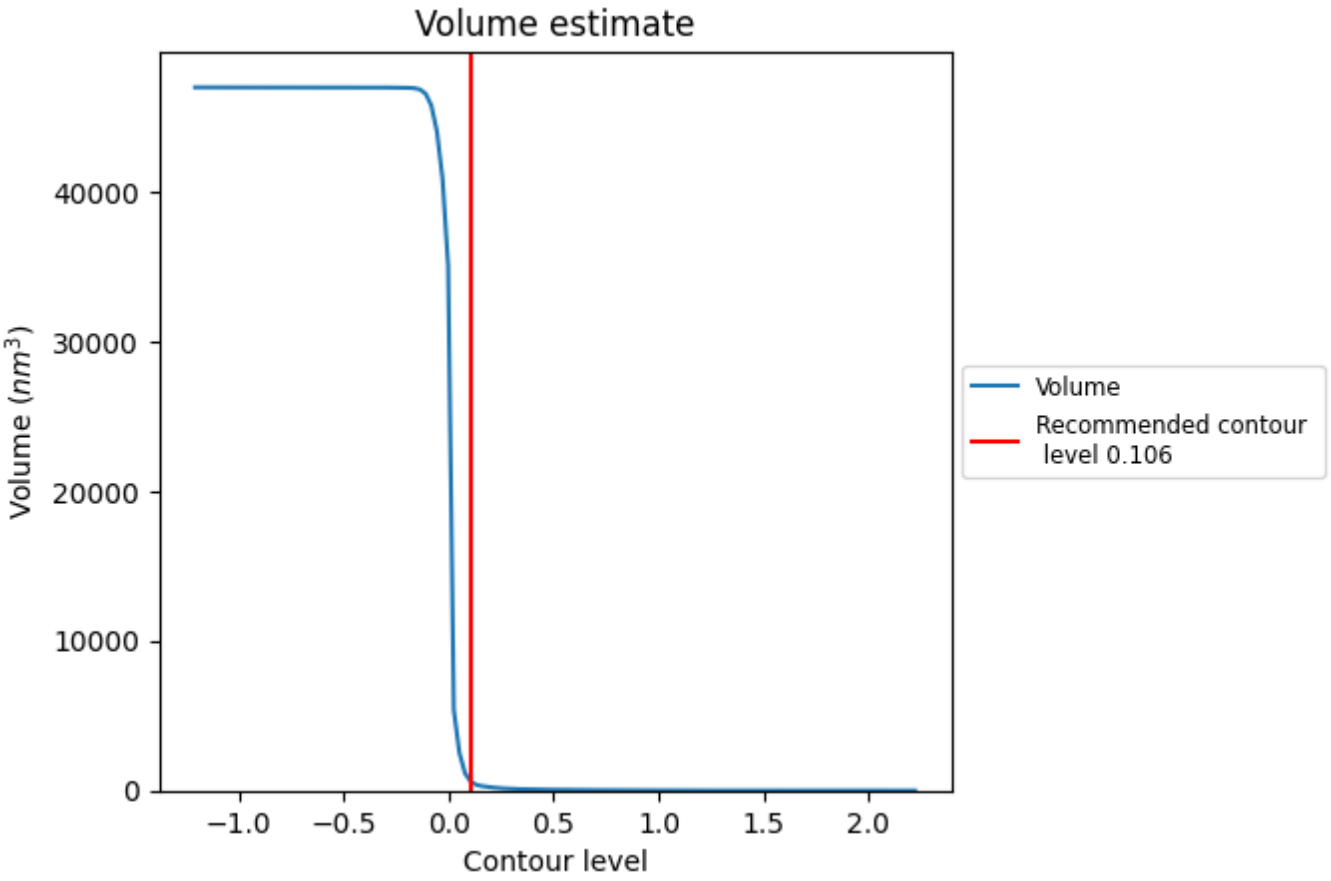
This section contains the results of statistical analysis of the map.

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.

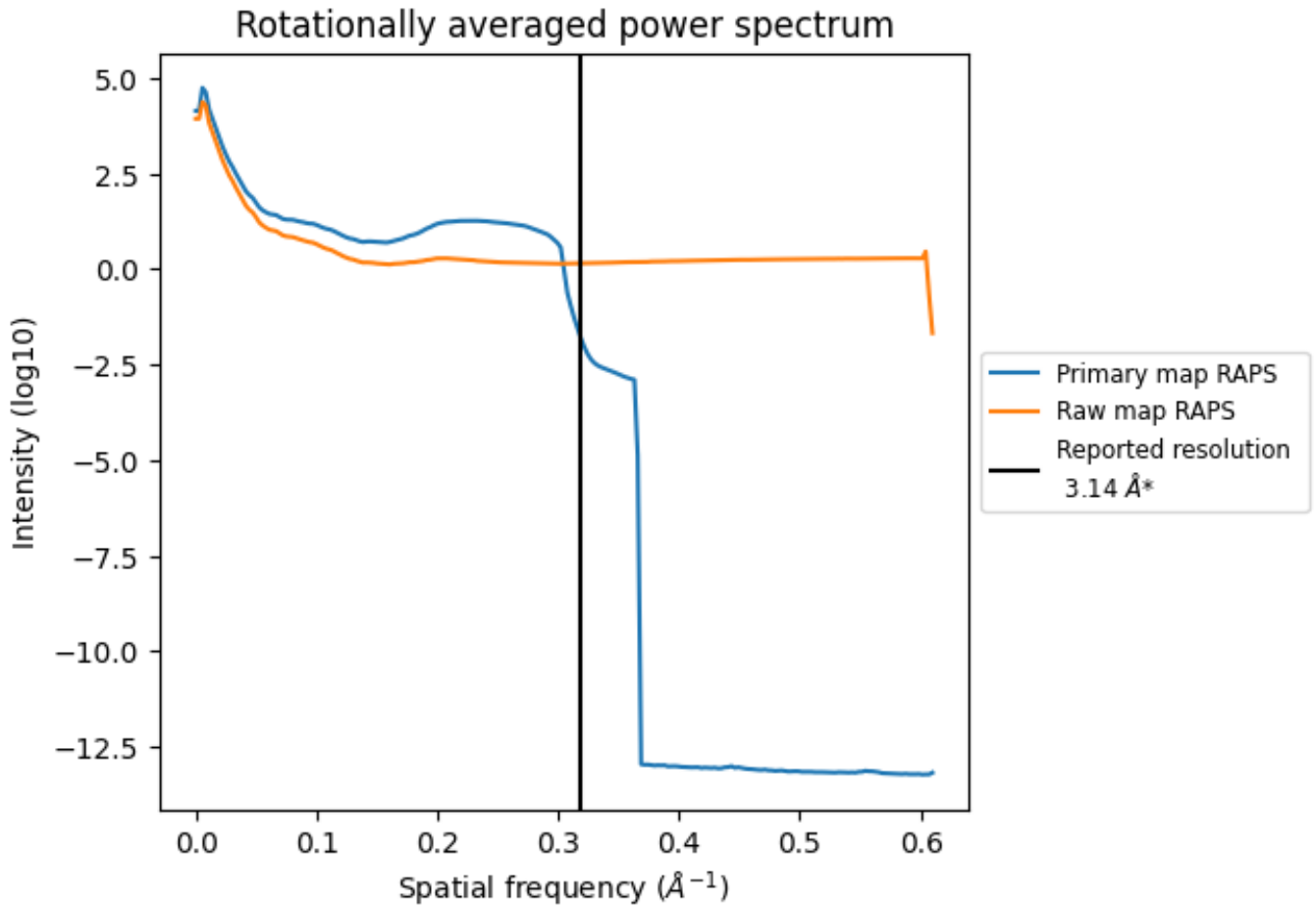
7.2 Volume estimate



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 531 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)

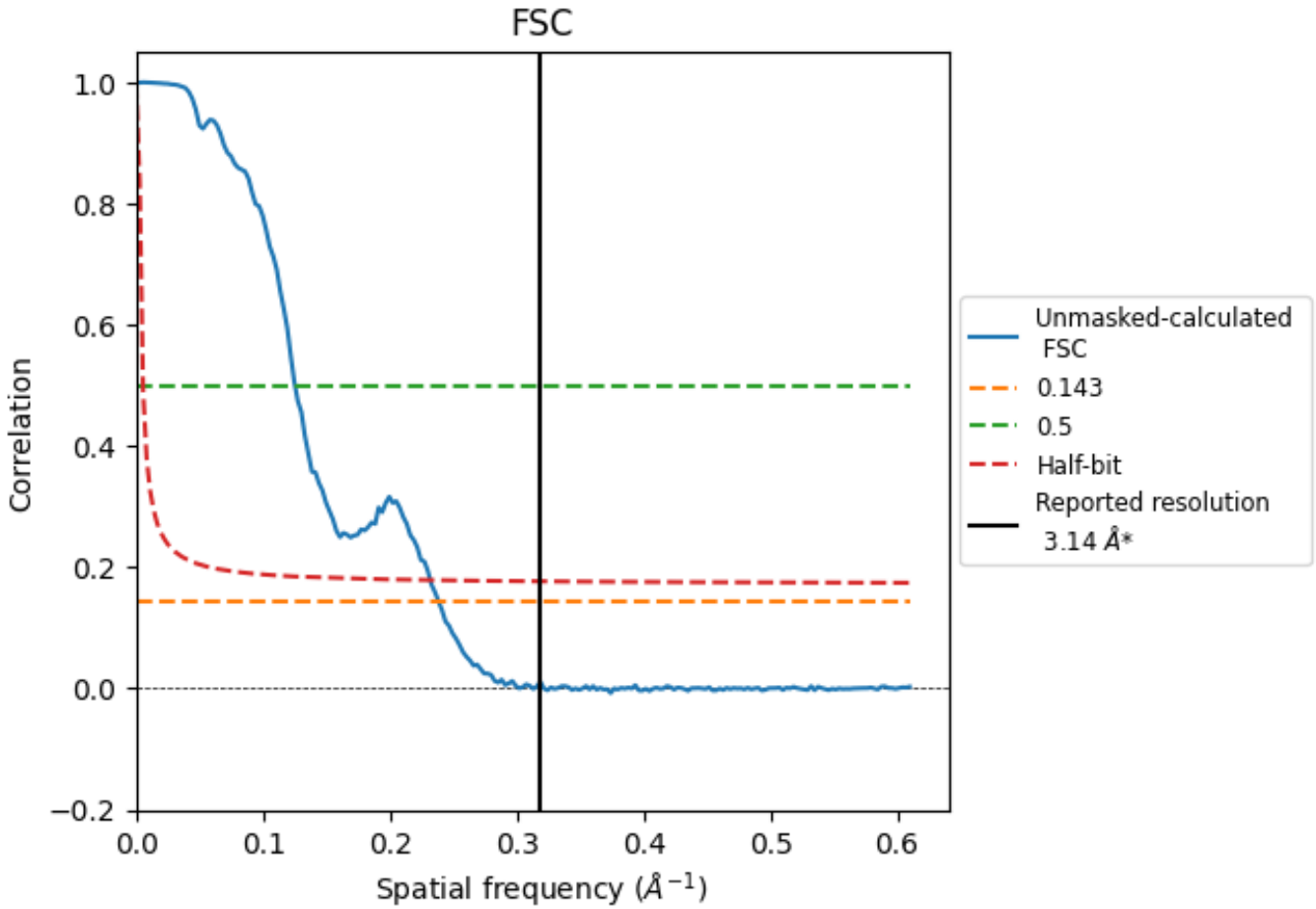


*Reported resolution corresponds to spatial frequency of 0.318 $Å^{-1}$

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 0.318 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.19	7.99	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.14 by more than 10 %

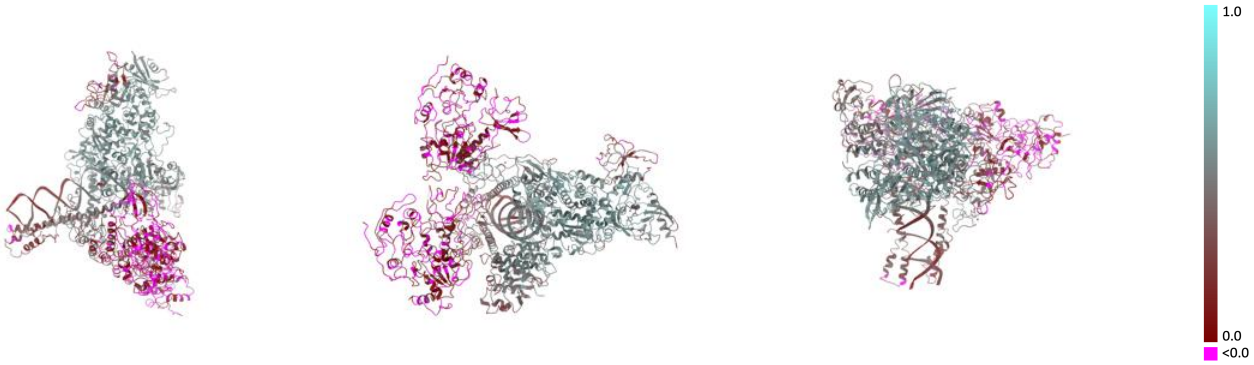
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60663 and PDB model 9IKZ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

This section was not generated.

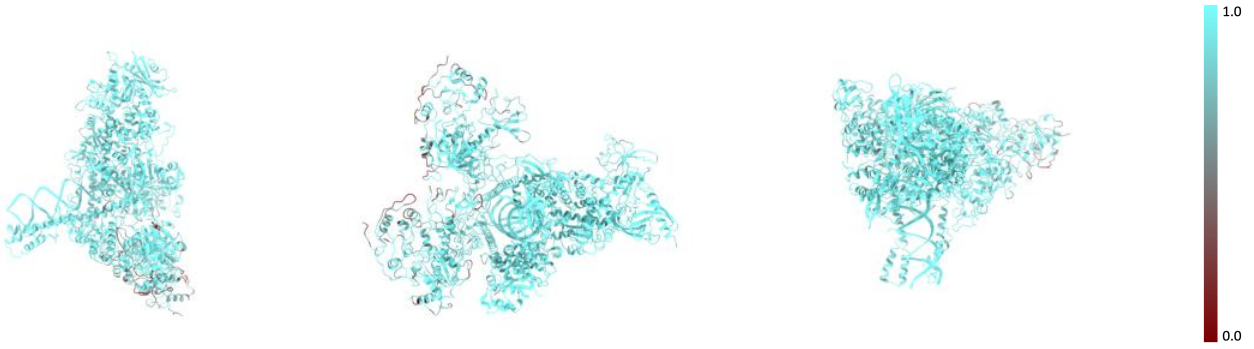
9.2 Q-score mapped to coordinate model



X Y Z

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

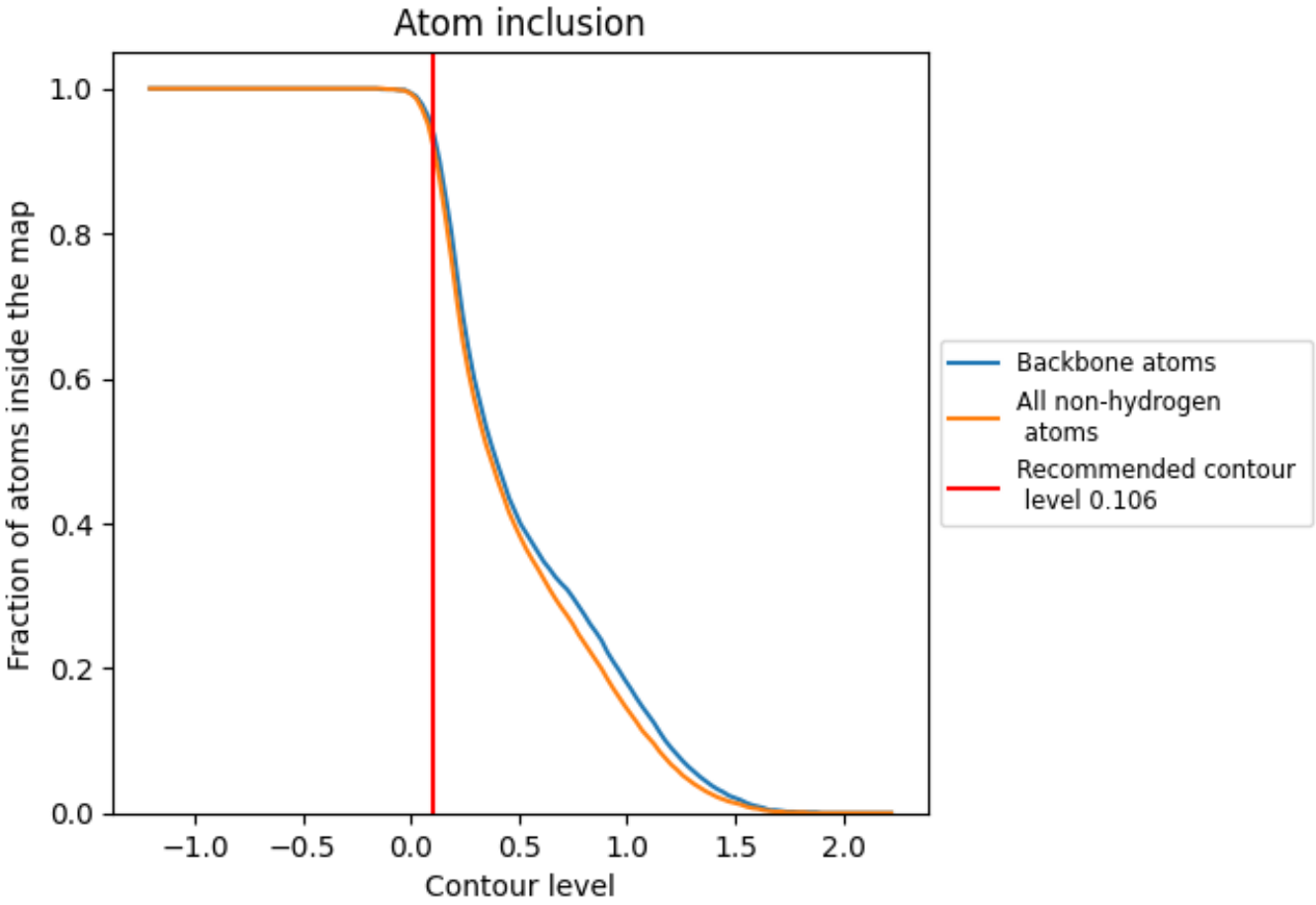
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9170	0.3260
A	0.9850	0.5520
B	0.9630	0.4250
C	0.9350	0.4730
D	0.9600	0.3820
E	0.8480	0.1280
F	0.8250	0.0820
G	0.9270	0.2720
I	0.9910	0.3450
J	0.9860	0.3660