



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 8FTD / pdb_00008ftd
EMDB ID : EMD-29423
Title : Structure of Escherichia coli CedA in complex with transcription initiation complex
Authors : Liu, M.; Vassyliev, N.; Nudler, E.
Deposited on : 2023-01-11
Resolution : 2.76 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:

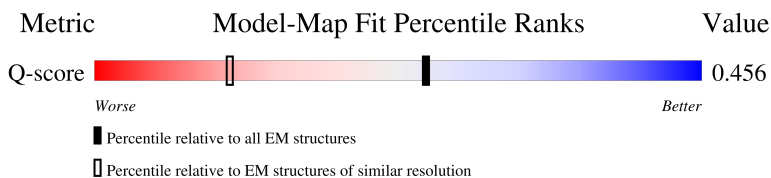
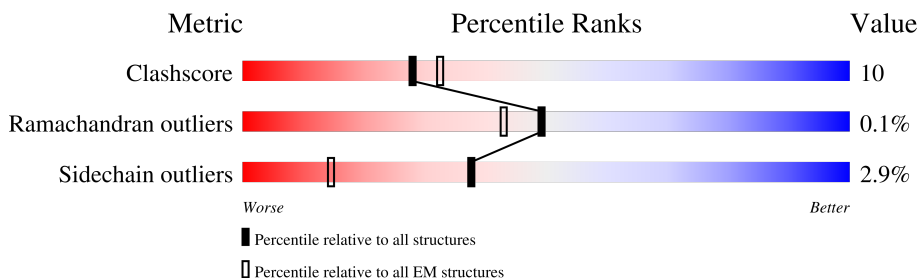
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.76 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10642 (2.26 - 3.26)

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

Mol	Chain	Length	Quality of chain
1	G	329	
1	H	329	
1	R	329	
2	I	1342	

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Mol	Chain	Length	Quality of chain
3	J	1407	79% 15% 5%
4	K	91	74% 13% 13%
5	L	608	7% 66% 12% 23%
6	P	85	18% 42% 29% 28%
7	Q	85	18% 36% 29% 34%
8	Z	80	19% 64% 26% 9%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 32529 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	231	Total 1789	C 1114	N 318	O 351	S 6	0	0
1	H	219	Total 1681	C 1050	N 295	O 330	S 6	0	0
1	R	73	Total 572	C 362	N 100	O 108	S 2	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	1341	Total 10575	C 6634	N 1842	O 2056	S 43	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	1337	Total 10386	C 6525	N 1851	O 1961	S 49	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	79	Total 627	C 382	N 118	O 126	S 1	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	470	Total 3812	C 2391	N 679	O 719	S 23	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	ALA	deletion	UNP Q0P6L9
L	?	-	LYS	deletion	UNP Q0P6L9
L	?	-	GLY	deletion	UNP Q0P6L9
L	?	-	ARG	deletion	UNP Q0P6L9
L	?	-	SER	deletion	UNP Q0P6L9

- Molecule 6 is a DNA chain called Transcription Unit *ssrA* Promoter Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	P	61	1252	597	222	372	61	0	0

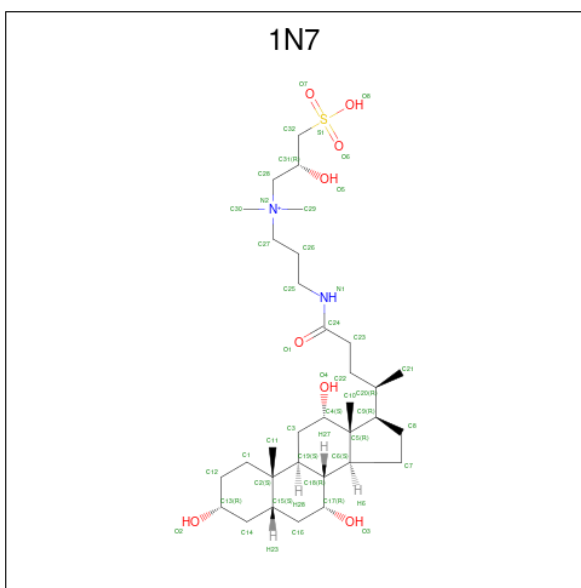
- Molecule 7 is a DNA chain called Transcription Unit *ssrA* Promoter Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	Q	56	1142	544	212	330	56	0	0

- Molecule 8 is a protein called Cell division activator CedaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	73	603	383	111	106	3	0	0

- Molecule 9 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				AltConf
9	I	1	Total	C	N	O	0
			29	24	1	4	
9	J	1	Total	C	N	O	0
			29	24	1	4	
9	L	1	Total	C	N	O	0
			29	24	1	4	

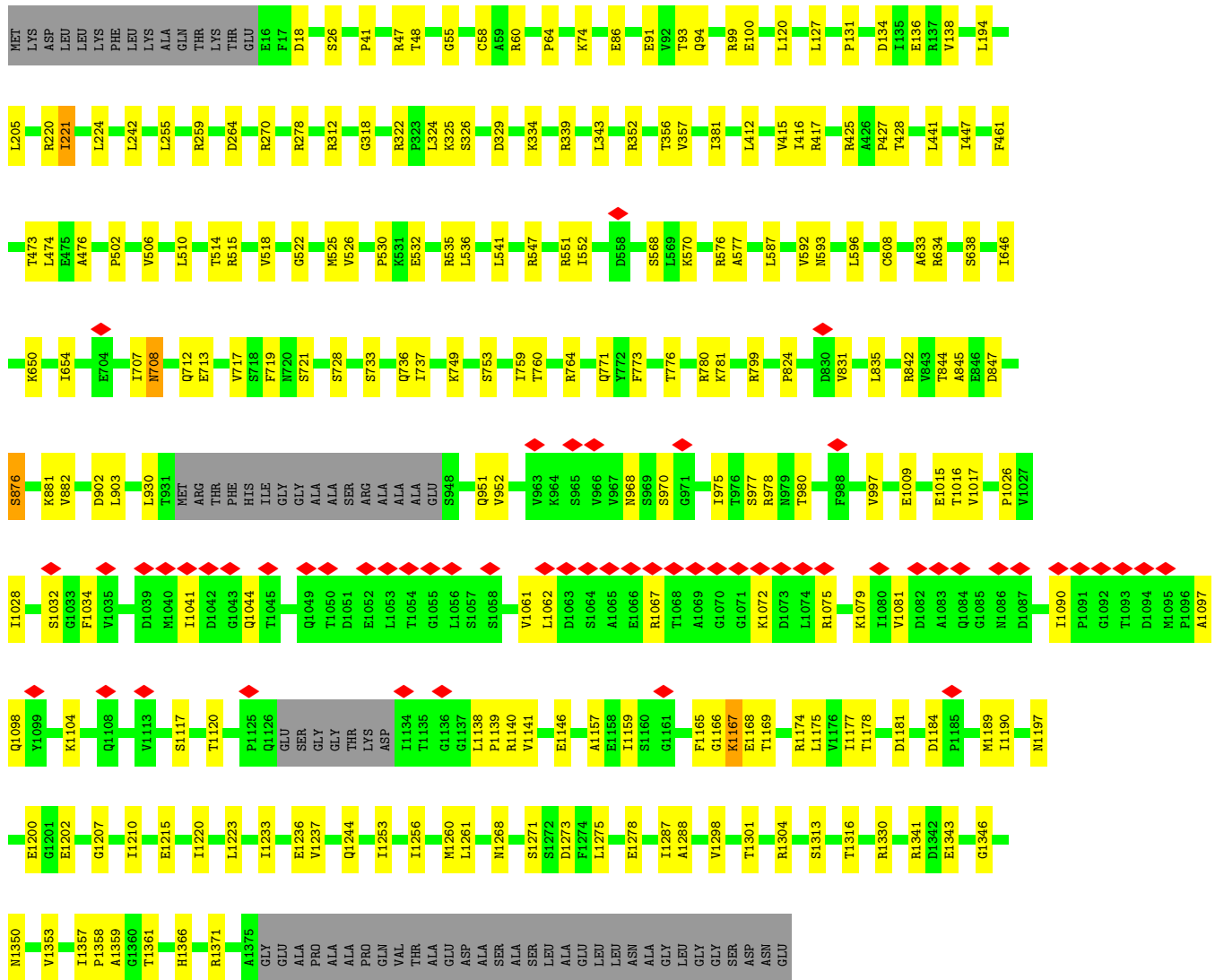
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	J	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	J	2	Total	Zn	0
			2	2	

Chain J: 79% 15% 5%



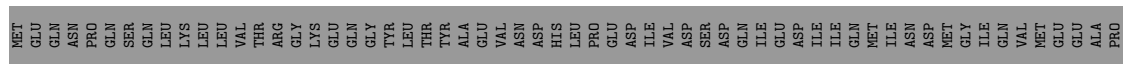
• Molecule 4: DNA-directed RNA polymerase subunit omega

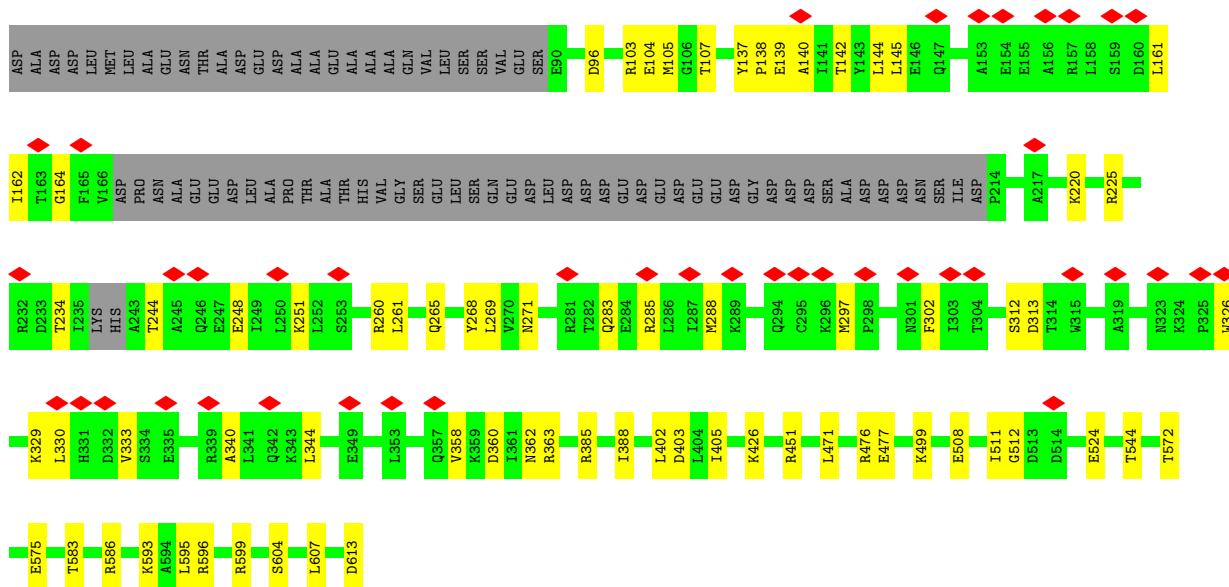
Chain K: 74% 13% 13%



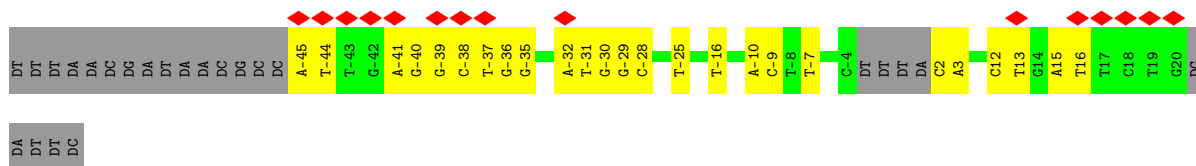
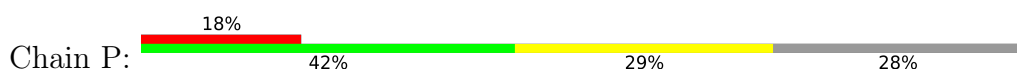
• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 7% 66% 12% 23%

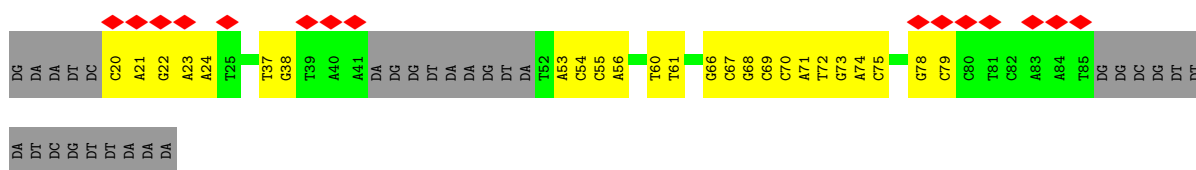




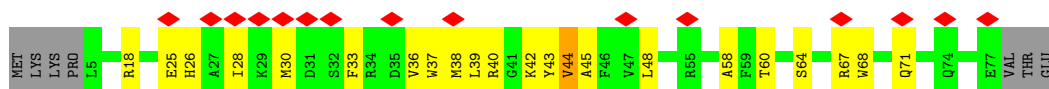
• Molecule 6: Transcription Unit *ssrA* Promoter Non-template DNA



• Molecule 7: Transcription Unit *ssrA* Promoter Template DNA



• Molecule 8: Cell division activator *CedA*



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Normal CTF correction in Relion or CryoSPARC	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.416	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	3.144	Depositor
Minimum map value	-1.937	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.22	Depositor
Map size (\AA)	306.72, 306.72, 306.72	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.852, 0.852, 0.852	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, ZN

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	G	0.44	0/1811	0.62	7/2454 (0.3%)
1	H	0.67	0/1700	0.73	3/2305 (0.1%)
1	R	0.08	0/579	0.24	0/784
2	I	0.18	0/10744	0.33	5/14496 (0.0%)
3	J	0.10	0/10543	0.27	0/14239
4	K	0.09	0/629	0.25	0/847
5	L	0.10	0/3863	0.26	0/5193
6	P	0.15	0/1401	0.37	0/2159
7	Q	0.16	0/1280	0.35	0/1968
8	Z	0.12	0/619	0.41	0/837
All	All	0.23	0/33169	0.36	15/45282 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	228	LEU	CA-C-N	-7.22	110.49	120.38
1	G	228	LEU	C-N-CA	-7.22	110.49	120.38
2	I	1004	ASP	N-CA-C	-7.16	103.50	113.37
2	I	50	GLU	N-CA-C	-6.87	103.79	111.28
2	I	234	ASP	N-CA-C	-6.84	100.60	110.24
1	G	232	VAL	N-CA-C	-6.40	100.49	110.09
2	I	1011	LEU	N-CA-C	-6.22	105.37	114.39
1	H	10	LYS	N-CA-C	-6.03	102.55	110.39
1	H	199	ASP	N-CA-C	5.74	117.90	109.24
2	I	1006	GLU	N-CA-C	-5.69	106.39	113.55
1	G	224	LEU	N-CA-C	5.68	117.16	110.97
1	G	230	ALA	CA-C-N	-5.65	110.92	120.58
1	G	230	ALA	C-N-CA	-5.65	110.92	120.58
1	H	215	GLU	N-CA-C	-5.43	105.47	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	THR	N-CA-C	5.09	117.69	108.69

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	G	1789	0	1810	66	0
1	H	1681	0	1708	109	0
1	R	572	0	602	9	0
2	I	10575	0	10584	210	0
3	J	10386	0	10594	146	0
4	K	627	0	634	9	0
5	L	3812	0	3878	50	0
6	P	1252	0	692	25	0
7	Q	1142	0	630	21	0
8	Z	603	0	594	21	0
9	I	29	0	39	6	0
9	J	29	0	39	5	0
9	L	29	0	39	6	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
All	All	32529	0	31843	612	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 10.

All (612) 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:H:152:TYR:CD2	3:J:541:LEU:HD13	1.83	1.14
1:H:152:TYR:HD2	3:J:541:LEU:CD1	1.60	1.12
2:I:1009:ASN:HA	2:I:1012:GLU:HB3	1.31	1.10
1:H:29:GLU:HB3	1:H:30:PRO:HD2	1.13	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:TYR:HD2	3:J:541:LEU:HD13	1.11	1.07
3:J:1166:GLY:HA3	3:J:1174:ARG:HB2	1.35	1.02
1:H:152:TYR:CE2	3:J:536:LEU:HD11	1.94	1.02
2:I:1007:LYS:HB3	2:I:1010:GLN:HB2	1.35	1.01
2:I:1009:ASN:HB2	2:I:1013:GLN:HB2	1.48	0.94
1:H:232:VAL:HG13	1:H:233:ASP:H	1.34	0.92
1:H:37:HIS:NE2	1:H:187:VAL:HG11	1.83	0.92
1:H:47:LEU:HD23	1:H:51:MET:HE1	1.52	0.92
1:H:58:GLU:HG3	1:H:145:LYS:HD3	1.51	0.90
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.02	0.88
1:G:107:ILE:HG22	1:G:107:ILE:O	1.74	0.88
1:H:37:HIS:CD2	1:H:187:VAL:HG11	2.08	0.87
1:H:107:ILE:O	1:H:107:ILE:HG22	1.74	0.87
2:I:1000:LEU:HD12	2:I:1002:LEU:HB2	1.57	0.87
1:H:228:LEU:O	1:H:232:VAL:HG12	1.76	0.85
2:I:1004:ASP:OD1	2:I:1010:GLN:HB3	1.78	0.83
1:H:58:GLU:HG3	1:H:145:LYS:CD	2.08	0.82
2:I:1000:LEU:HG	2:I:1001:GLY:N	1.94	0.82
1:H:152:TYR:CD2	3:J:541:LEU:CD1	2.51	0.81
1:H:44:ARG:NH2	1:H:185:TYR:HE1	1.80	0.80
1:G:194:GLN:N	1:G:194:GLN:OE1	2.14	0.80
2:I:232:ILE:HD12	2:I:331:LYS:HA	1.65	0.79
2:I:1000:LEU:HG	2:I:1001:GLY:H	1.48	0.77
1:H:29:GLU:CB	1:H:30:PRO:HD2	2.05	0.76
1:H:37:HIS:NE2	1:H:187:VAL:CG1	2.48	0.76
2:I:1010:GLN:HG3	2:I:1011:LEU:HD22	1.67	0.76
1:H:57:THR:C	1:H:58:GLU:HG2	2.10	0.76
1:H:58:GLU:CG	1:H:145:LYS:HD3	2.15	0.75
2:I:996:ARG:HH21	2:I:999:GLU:HG3	1.50	0.75
1:H:152:TYR:CE2	3:J:536:LEU:CD1	2.70	0.75
1:G:205:MET:HE1	1:G:217:ILE:CG1	2.17	0.74
2:I:1003:THR:C	2:I:1005:GLU:H	1.94	0.73
1:G:107:ILE:O	1:G:107:ILE:CG2	2.36	0.73
1:H:107:ILE:O	1:H:107:ILE:CG2	2.36	0.72
2:I:966:ILE:HD11	9:I:1401:1N7:H8	1.71	0.72
2:I:234:ASP:O	2:I:235:ASN:HB3	1.90	0.72
3:J:1165:PHE:HE1	3:J:1200:GLU:HA	1.53	0.72
9:J:1504:1N7:H26	9:L:701:1N7:H26	1.71	0.71
2:I:808:ASN:H	3:J:633:ALA:HB2	1.54	0.71
2:I:979:LEU:HD12	2:I:1010:GLN:CD	2.16	0.71
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:38:MET:HA	8:Z:43:TYR:HB3	1.72	0.71
1:G:13:LEU:HD13	1:G:27:THR:O	1.90	0.71
2:I:966:ILE:CD1	9:I:1401:1N7:H8	2.20	0.70
1:H:58:GLU:HG3	1:H:145:LYS:HB3	1.74	0.70
3:J:425:ARG:HG2	3:J:427:PRO:HD2	1.73	0.70
2:I:983:GLY:HA3	2:I:1003:THR:HB	1.73	0.70
6:P:-37:DT:H2'	6:P:-36:DG:H8	1.56	0.70
2:I:263:VAL:HG21	2:I:269:ILE:HG13	1.74	0.69
7:Q:72:DT:H2''	7:Q:73:DG:C8	2.28	0.69
3:J:749:LYS:HD2	3:J:753:SER:HB2	1.75	0.69
1:H:211:ILE:HD11	1:H:216:ALA:HB2	1.75	0.69
6:P:12:DC:H2''	6:P:13:DT:H5'	1.73	0.68
1:H:215:GLU:HA	1:H:218:ARG:HH11	1.59	0.68
1:G:222:THR:HA	1:H:232:VAL:HG23	1.76	0.67
3:J:1165:PHE:CE1	3:J:1200:GLU:HA	2.28	0.67
1:G:158:ARG:NH2	1:G:173:VAL:O	2.27	0.67
1:H:100:LEU:HD23	1:H:115:ILE:HG21	1.76	0.67
7:Q:69:DC:H2''	7:Q:70:DC:C5	2.29	0.67
2:I:965:GLN:HE22	9:I:1401:1N7:H26	1.61	0.66
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.76	0.66
1:H:232:VAL:HG13	1:H:233:ASP:N	2.06	0.66
1:G:166:ARG:HD2	1:G:170:ARG:HD2	1.77	0.66
1:G:10:LYS:HD2	1:H:227:GLN:HA	1.76	0.66
2:I:1219:GLU:OE2	3:J:634:ARG:NH1	2.25	0.66
1:G:205:MET:HE1	1:G:217:ILE:HG12	1.78	0.66
3:J:1174:ARG:NH2	3:J:1189:MET:SD	2.69	0.65
1:H:152:TYR:HE2	3:J:536:LEU:HD11	1.55	0.65
1:G:13:LEU:HD22	1:G:28:LEU:CD1	2.26	0.65
8:Z:42:LYS:HG2	8:Z:58:ALA:HB1	1.79	0.65
3:J:1175:LEU:HB2	3:J:1190:ILE:HD11	1.80	0.64
1:G:57:THR:HG22	1:G:58:GLU:HG3	1.78	0.64
1:H:58:GLU:CD	1:H:145:LYS:HD3	2.23	0.64
1:H:232:VAL:O	1:H:233:ASP:C	2.40	0.64
2:I:161:LYS:HA	2:I:170:VAL:HG12	1.80	0.63
1:H:205:MET:HG3	1:H:206:GLU:N	2.13	0.63
1:H:51:MET:C	1:H:150:ARG:HG2	2.24	0.63
2:I:240:GLU:HB2	2:I:283:LYS:HE3	1.80	0.63
5:L:145:LEU:HD22	5:L:225:ARG:HE	1.63	0.63
1:H:58:GLU:HG3	1:H:145:LYS:CB	2.28	0.63
5:L:144:LEU:HD12	5:L:261:LEU:HD21	1.79	0.63
2:I:979:LEU:HD12	2:I:1010:GLN:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:235:ASN:C	2:I:237:LEU:H	2.06	0.63
2:I:898:GLU:HG2	5:L:544:THR:HG21	1.81	0.63
2:I:992:LEU:HD23	2:I:997:TRP:HA	1.80	0.63
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.81	0.63
6:P:12:DC:H2'	6:P:13:DT:H72	1.79	0.62
1:H:152:TYR:HD2	3:J:541:LEU:HD12	1.58	0.62
2:I:236:LYS:HD3	8:Z:48:LEU:HD21	1.81	0.62
7:Q:70:DC:H2''	7:Q:71:DA:C8	2.35	0.61
2:I:103:VAL:HG12	2:I:117:ILE:HG22	1.82	0.61
2:I:1000:LEU:HD12	2:I:1002:LEU:H	1.64	0.61
9:J:1504:1N7:H26	9:L:701:1N7:C17	2.30	0.61
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.33	0.61
2:I:20:GLN:NE2	2:I:23:ASP:OD1	2.31	0.61
5:L:512:GLY:N	9:L:701:1N7:O1	2.33	0.61
1:H:219:ARG:O	1:H:223:ILE:HG12	2.01	0.61
2:I:996:ARG:HA	2:I:999:GLU:HB2	1.81	0.61
3:J:473:THR:HG23	3:J:476:ALA:H	1.66	0.61
5:L:105:MET:HE2	5:L:388:ILE:HD12	1.83	0.61
1:H:107:ILE:HD11	1:H:136:GLU:OE1	2.01	0.60
1:H:84:ASN:OD1	3:J:551:ARG:NH2	2.33	0.60
1:H:86:LYS:NZ	3:J:532:GLU:OE1	2.25	0.60
1:H:58:GLU:CG	1:H:145:LYS:HB3	2.31	0.60
2:I:233:ARG:NH1	2:I:233:ARG:HA	2.16	0.60
2:I:354:ASP:O	8:Z:18:ARG:NH1	2.35	0.60
3:J:1275:LEU:HB2	3:J:1278:GLU:HB2	1.84	0.60
5:L:402:LEU:HD23	5:L:405:ILE:HD11	1.83	0.60
1:G:222:THR:CA	1:H:232:VAL:HG23	2.32	0.60
3:J:1028:ILE:HG22	3:J:1120:THR:HA	1.84	0.60
1:G:228:LEU:O	1:G:229:GLU:C	2.40	0.60
1:G:107:ILE:HD11	1:G:136:GLU:OE1	2.01	0.60
3:J:264:ASP:HB3	3:J:324:LEU:HD22	1.83	0.60
2:I:528:ARG:NH2	2:I:576:SER:O	2.35	0.59
1:G:86:LYS:HE3	1:G:174:ASP:HB2	1.84	0.59
1:G:222:THR:HA	1:H:232:VAL:CG2	2.32	0.59
2:I:238:GLN:HB2	2:I:284:LEU:HG	1.84	0.59
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.85	0.59
5:L:330:LEU:HB3	5:L:333:VAL:HG12	1.84	0.59
8:Z:44:VAL:HG13	8:Z:45:ALA:H	1.68	0.59
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.32	0.59
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.69	0.58
2:I:1273:MET:HB3	3:J:428:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:60:DT:H2''	7:Q:61:DT:C5	2.38	0.58
3:J:587:LEU:HD11	3:J:608:CYS:HB2	1.85	0.58
1:G:205:MET:CE	1:G:217:ILE:HD11	2.33	0.58
1:H:19:VAL:HG22	1:H:23:HIS:HB3	1.87	0.57
2:I:744:GLY:HA3	2:I:1013:GLN:HG3	1.87	0.57
2:I:633:LEU:HD13	2:I:644:LEU:HD13	1.86	0.57
6:P:-45:DA:H2''	6:P:-44:DT:H71	1.87	0.57
7:Q:22:DG:H2'	7:Q:23:DA:C8	2.39	0.57
2:I:979:LEU:HD11	2:I:1000:LEU:HD21	1.84	0.57
2:I:320:ASP:OD1	2:I:320:ASP:N	2.37	0.57
5:L:326:TRP:O	5:L:329:LYS:NZ	2.35	0.57
2:I:1009:ASN:O	2:I:1010:GLN:C	2.48	0.57
5:L:96:ASP:OD1	5:L:96:ASP:N	2.38	0.57
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.87	0.56
5:L:511:ILE:HG22	9:L:701:1N7:H9	1.86	0.56
2:I:69:GLN:OE1	2:I:101:ARG:HD2	2.04	0.56
2:I:236:LYS:CD	8:Z:48:LEU:HD11	2.34	0.56
2:I:890:LYS:HE3	2:I:914:LYS:HB2	1.88	0.56
3:J:903:LEU:HD23	3:J:903:LEU:H	1.70	0.56
9:J:1504:1N7:H24	9:L:701:1N7:H24	1.88	0.56
5:L:140:ALA:HA	5:L:269:LEU:HD22	1.88	0.56
2:I:239:MET:HE2	2:I:287:VAL:HG21	1.88	0.56
2:I:979:LEU:O	2:I:984:VAL:HB	2.04	0.56
2:I:1011:LEU:HA	2:I:1014:LEU:HD23	1.87	0.56
3:J:773:PHE:O	3:J:776:THR:OG1	2.23	0.56
2:I:57:PHE:HE1	2:I:468:LEU:HD11	1.69	0.56
2:I:233:ARG:O	2:I:236:LYS:N	2.38	0.56
3:J:514:THR:HG21	3:J:596:LEU:HD12	1.88	0.56
1:G:12:ARG:HH22	1:H:230:ALA:HB2	1.71	0.56
1:G:155:ALA:O	1:G:159:ILE:HG13	2.06	0.56
5:L:297:MET:SD	5:L:302:PHE:HB2	2.47	0.56
1:G:205:MET:HE1	1:G:217:ILE:HD11	1.87	0.55
2:I:1142:ARG:NH2	2:I:1164:PHE:O	2.39	0.55
1:H:56:VAL:HA	1:H:146:VAL:HG22	1.88	0.55
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.89	0.55
3:J:708:ASN:OD1	3:J:708:ASN:N	2.38	0.55
2:I:1003:THR:C	2:I:1005:GLU:N	2.57	0.55
6:P:-37:DT:H2'	6:P:-36:DG:C8	2.41	0.55
7:Q:37:DT:H2'	7:Q:38:DG:C8	2.41	0.55
1:G:193:GLU:HG2	1:G:194:GLN:OE1	2.06	0.55
2:I:813:GLU:HB2	3:J:461:PHE:HD2	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:965:GLN:HE22	9:I:1401:1N7:C17	2.19	0.55
2:I:978:VAL:HG12	2:I:1010:GLN:OE1	2.07	0.55
1:G:13:LEU:HD11	1:G:26:VAL:HG12	1.89	0.54
2:I:993:PRO:O	2:I:997:TRP:N	2.40	0.54
3:J:930:LEU:HB2	3:J:1138:LEU:HD22	1.88	0.54
5:L:105:MET:SD	5:L:385:ARG:HG3	2.47	0.54
3:J:417:ARG:NH1	4:K:43:ASN:O	2.39	0.54
3:J:1079:LYS:HD3	3:J:1098:GLN:HB3	1.88	0.54
5:L:164:GLY:HA3	5:L:260:ARG:HH21	1.71	0.54
8:Z:30:MET:HE1	8:Z:36:VAL:H	1.72	0.54
5:L:572:THR:HG23	5:L:575:GLU:H	1.72	0.54
2:I:48:GLY:O	2:I:51:ALA:HB3	2.08	0.54
2:I:515:MET:HE3	2:I:517:GLN:HB3	1.89	0.54
2:I:979:LEU:HD21	2:I:1000:LEU:CD2	2.37	0.54
3:J:532:GLU:HA	3:J:535:ARG:HB2	1.89	0.54
6:P:-32:DA:C8	6:P:-31:DT:H72	2.42	0.54
2:I:235:ASN:O	2:I:237:LEU:N	2.40	0.54
3:J:1268:ASN:OD1	3:J:1301:THR:OG1	2.24	0.54
1:H:154:PRO:O	1:H:158:ARG:HG3	2.08	0.54
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.42	0.54
7:Q:71:DA:H2"	7:Q:72:DT:H71	1.90	0.54
1:G:13:LEU:HD22	1:G:28:LEU:HD13	1.90	0.54
1:H:58:GLU:OE1	1:H:145:LYS:HD3	2.08	0.54
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.90	0.54
2:I:65:ASN:CG	2:I:105:TYR:HB2	2.33	0.53
1:G:162:GLU:HG2	1:G:163:GLU:H	1.73	0.53
1:H:44:ARG:NH2	1:H:185:TYR:CE1	2.69	0.53
2:I:104:ILE:O	2:I:115:LYS:N	2.38	0.53
2:I:1019:ASP:O	2:I:1023:HIS:ND1	2.41	0.53
3:J:518:VAL:O	3:J:547:ARG:NH2	2.41	0.53
8:Z:40:ARG:H	8:Z:43:TYR:HA	1.72	0.53
1:G:205:MET:HE1	1:G:217:ILE:CD1	2.37	0.53
2:I:232:ILE:HG23	2:I:236:LYS:HE2	1.90	0.53
3:J:1271:SER:OG	3:J:1298:VAL:O	2.22	0.53
1:H:58:GLU:HG3	1:H:145:LYS:CG	2.38	0.53
2:I:101:ARG:HG3	2:I:119:GLU:HG2	1.91	0.53
1:H:205:MET:HG2	1:H:213:PRO:HB3	1.90	0.53
2:I:197:ARG:HE	2:I:203:LYS:HB3	1.74	0.53
2:I:1136:GLN:HG3	2:I:1140:LYS:HD2	1.91	0.53
3:J:194:LEU:HD22	3:J:224:LEU:HD11	1.90	0.53
3:J:1215:GLU:HB3	3:J:1220:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:LYS:HZ3	3:J:532:GLU:CD	2.16	0.52
2:I:236:LYS:HA	2:I:238:GLN:HE22	1.75	0.52
3:J:518:VAL:HB	3:J:707:ILE:HD11	1.91	0.52
1:H:215:GLU:HG2	1:H:218:ARG:HH12	1.75	0.52
2:I:802:VAL:HG12	2:I:1096:ILE:HB	1.91	0.52
3:J:1167:LYS:HD3	3:J:1167:LYS:O	2.10	0.52
5:L:613:ASP:OD1	5:L:613:ASP:N	2.43	0.52
2:I:705:GLU:HB3	2:I:794:LEU:H	1.75	0.52
3:J:278:ARG:NH1	5:L:403:ASP:OD1	2.41	0.52
3:J:356:THR:N	3:J:447:ILE:O	2.36	0.52
1:G:150:ARG:HG3	1:H:5:VAL:CG2	2.40	0.52
3:J:1174:ARG:HH21	3:J:1189:MET:HA	1.74	0.52
8:Z:28:ILE:HG22	8:Z:38:MET:H	1.75	0.52
3:J:127:LEU:O	3:J:220:ARG:NH2	2.42	0.52
3:J:134:ASP:O	3:J:138:VAL:HG23	2.11	0.51
1:G:8:PHE:N	1:G:8:PHE:CD1	2.78	0.51
2:I:232:ILE:HG22	2:I:232:ILE:O	2.09	0.51
2:I:424:ASP:O	2:I:428:VAL:HG23	2.11	0.51
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.34	0.51
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.39	0.51
3:J:522:GLY:HA3	3:J:525:MET:HE2	1.92	0.51
7:Q:74:DA:H2''	7:Q:75:DC:O5'	2.10	0.51
2:I:46:GLN:O	2:I:51:ALA:HB2	2.11	0.51
6:P:-30:DG:H2''	6:P:-29:DG:N7	2.26	0.51
1:G:235:ARG:HD2	1:G:235:ARG:C	2.36	0.51
2:I:375:PRO:HD3	5:L:103:ARG:HD3	1.93	0.51
2:I:593:LYS:O	2:I:600:THR:OG1	2.27	0.51
2:I:232:ILE:HG23	2:I:236:LYS:CE	2.41	0.51
3:J:712:GLN:HG2	3:J:713:GLU:H	1.76	0.51
1:R:289:LEU:HD23	1:R:300:LEU:HD13	1.93	0.51
2:I:232:ILE:HD11	2:I:333:ILE:CD1	2.41	0.51
3:J:515:ARG:HH22	3:J:717:VAL:HB	1.75	0.51
1:G:45:ARG:HH21	1:H:37:HIS:HB2	1.75	0.50
1:H:194:GLN:CD	1:H:194:GLN:H	2.20	0.50
1:H:228:LEU:HA	1:H:231:PHE:CZ	2.46	0.50
1:H:86:LYS:HE3	1:H:174:ASP:HB2	1.92	0.50
1:H:228:LEU:HD13	1:H:232:VAL:HG11	1.92	0.50
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.94	0.50
3:J:74:LYS:NZ	3:J:86:GLU:OE2	2.37	0.50
1:R:265:ARG:HA	1:R:268:ASN:HD21	1.77	0.50
2:I:406:ASN:ND2	2:I:413:GLU:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.94	0.50
3:J:975:ILE:HD12	3:J:997:VAL:HG11	1.94	0.50
5:L:312:SER:OG	5:L:313:ASP:N	2.44	0.50
1:G:33:ARG:HH12	1:G:197:ASP:HB3	1.75	0.50
2:I:478:ARG:HG2	2:I:492:MET:HG2	1.92	0.50
1:R:260:LEU:HA	1:R:310:ARG:HH22	1.77	0.50
2:I:1136:GLN:HG2	2:I:1137:GLU:H	1.77	0.50
2:I:235:ASN:C	2:I:237:LEU:N	2.70	0.50
2:I:471:VAL:HG21	2:I:498:ILE:HD11	1.94	0.50
2:I:799:ASN:ND2	2:I:799:ASN:O	2.43	0.50
3:J:1167:LYS:HZ2	3:J:1169:THR:HG23	1.77	0.50
1:H:232:VAL:CG1	1:H:233:ASP:H	2.15	0.50
2:I:985:GLU:H	2:I:989:LEU:HD12	1.77	0.50
2:I:105:TYR:HA	2:I:114:VAL:HA	1.94	0.50
4:K:3:ARG:HH21	4:K:52:ARG:HG2	1.77	0.49
2:I:540:ARG:O	2:I:548:ARG:NH2	2.46	0.49
2:I:989:LEU:CD1	2:I:1000:LEU:HD13	2.42	0.49
3:J:1256:ILE:HG22	3:J:1260:MET:HE2	1.93	0.49
5:L:593:LYS:HG2	5:L:596:ARG:HH22	1.76	0.49
6:P:2:DC:H2'	6:P:3:DA:C8	2.48	0.49
2:I:233:ARG:O	2:I:234:ASP:C	2.53	0.49
1:G:192:VAL:HG11	1:G:195:ARG:HB3	1.95	0.49
2:I:844:LYS:HG3	2:I:845:LEU:HD12	1.93	0.49
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.95	0.49
1:H:104:LYS:HG2	1:H:110:VAL:HG22	1.95	0.49
3:J:1041:ILE:HB	3:J:1044:GLN:HB2	1.94	0.49
6:P:-28:DC:N3	7:Q:68:DG:N2	2.61	0.49
1:G:62:ASP:OD1	1:G:63:GLY:N	2.46	0.49
1:G:232:VAL:O	1:G:233:ASP:CG	2.56	0.49
1:H:57:THR:C	1:H:58:GLU:CG	2.85	0.49
1:H:86:LYS:NZ	3:J:532:GLU:CD	2.70	0.49
2:I:300:ASP:HB2	2:I:309:LEU:HD11	1.93	0.49
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.95	0.49
1:H:152:TYR:CZ	3:J:536:LEU:HD11	2.44	0.49
3:J:845:ALA:HB3	3:J:881:LYS:HE2	1.93	0.49
3:J:1138:LEU:HB2	3:J:1141:VAL:HB	1.93	0.49
6:P:-41:DA:H2''	6:P:-40:DG:C8	2.47	0.49
5:L:268:TYR:HA	5:L:271:ASN:ND2	2.27	0.49
1:G:12:ARG:HB3	1:G:12:ARG:CZ	2.41	0.48
1:H:44:ARG:HH21	1:H:185:TYR:HE1	1.57	0.48
2:I:232:ILE:CG2	2:I:236:LYS:HG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.46	0.48
2:I:966:ILE:HD13	9:I:1401:1N7:H8	1.94	0.48
3:J:568:SER:OG	3:J:570:LYS:NZ	2.46	0.48
2:I:232:ILE:HA	2:I:236:LYS:HA	1.96	0.48
3:J:952:VAL:HG12	3:J:1015:GLU:H	1.77	0.48
5:L:248:GLU:HA	5:L:251:LYS:HE2	1.96	0.48
8:Z:33:PHE:HB3	8:Z:36:VAL:HB	1.95	0.48
8:Z:42:LYS:HD2	8:Z:43:TYR:N	2.28	0.48
1:H:55:ALA:O	1:H:146:VAL:HG13	2.13	0.48
1:H:222:THR:O	1:H:226:GLU:HG2	2.13	0.48
8:Z:28:ILE:HB	8:Z:37:TRP:CD1	2.48	0.48
1:H:64:VAL:HG11	1:H:78:ILE:HG21	1.95	0.48
3:J:474:LEU:HD21	4:K:27:ALA:HB3	1.96	0.48
3:J:1273:ASP:OD1	3:J:1273:ASP:N	2.46	0.48
1:H:62:ASP:OD1	1:H:63:GLY:N	2.46	0.48
5:L:265:GLN:O	5:L:269:LEU:HG	2.14	0.48
1:G:18:GLN:NE2	1:G:20:SER:O	2.45	0.48
1:G:52:PRO:HB3	1:H:5:VAL:HG21	1.95	0.48
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.95	0.48
3:J:876:SER:O	3:J:876:SER:OG	2.26	0.48
3:J:902:ASP:OD1	3:J:902:ASP:N	2.46	0.48
5:L:604:SER:HB2	5:L:607:LEU:HB2	1.96	0.48
7:Q:66:DG:H2''	7:Q:67:DC:C5	2.49	0.48
8:Z:30:MET:HE3	8:Z:37:TRP:CD1	2.48	0.48
1:G:150:ARG:HG3	1:H:5:VAL:HG23	1.96	0.47
1:H:52:PRO:HA	1:H:149:GLY:O	2.14	0.47
1:H:215:GLU:HA	1:H:218:ARG:NH1	2.28	0.47
1:R:289:LEU:O	1:R:292:THR:OG1	2.32	0.47
2:I:65:ASN:ND2	2:I:106:GLU:O	2.47	0.47
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.96	0.47
3:J:41:PRO:HB2	3:J:270:ARG:HG3	1.95	0.47
5:L:586:ARG:NE	6:P:-36:DG:OP2	2.46	0.47
2:I:233:ARG:HA	2:I:233:ARG:CZ	2.44	0.47
2:I:560:PRO:O	3:J:780:ARG:NH2	2.47	0.47
2:I:629:PHE:O	2:I:647:ARG:NH1	2.46	0.47
2:I:1259:LEU:HD11	5:L:524:GLU:HB3	1.95	0.47
3:J:1072:LYS:O	3:J:1075:ARG:NH1	2.44	0.47
3:J:1261:LEU:O	3:J:1304:ARG:NH2	2.48	0.47
1:H:51:MET:HE2	1:H:51:MET:HB2	1.62	0.47
3:J:1034:PHE:HB2	3:J:1081:VAL:HG23	1.97	0.47
7:Q:78:DG:H2''	7:Q:79:DC:C5	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:995:ASP:OD1	2:I:995:ASP:N	2.48	0.47
3:J:47:ARG:O	3:J:48:THR:OG1	2.27	0.47
5:L:285:ARG:HA	5:L:288:MET:HG2	1.95	0.47
6:P:15:DA:H2'	6:P:16:DT:H71	1.96	0.47
2:I:853:ASP:N	2:I:853:ASP:OD1	2.47	0.47
3:J:120:LEU:HD12	3:J:1330:ARG:HD3	1.97	0.47
3:J:255:LEU:HD11	9:J:1504:1N7:H23	1.97	0.47
3:J:502:PRO:HB3	3:J:506:VAL:HB	1.95	0.47
5:L:268:TYR:HA	5:L:271:ASN:HD21	1.80	0.47
7:Q:20:DC:H2'	7:Q:21:DA:C8	2.50	0.47
8:Z:25:GLU:HG2	8:Z:26:HIS:N	2.29	0.47
1:H:47:LEU:HA	1:H:51:MET:CE	2.45	0.47
2:I:238:GLN:HB2	2:I:284:LEU:CG	2.44	0.47
2:I:1004:ASP:HA	2:I:1007:LYS:O	2.14	0.47
2:I:1246:ARG:NH1	2:I:1258:PRO:HB3	2.29	0.47
3:J:325:LYS:HD2	5:L:508:GLU:HG2	1.97	0.47
2:I:962:GLU:O	2:I:965:GLN:NE2	2.48	0.47
3:J:1184:ASP:OD1	3:J:1184:ASP:N	2.48	0.47
7:Q:68:DG:H2'	7:Q:69:DC:OP2	2.14	0.47
2:I:232:ILE:CG2	2:I:236:LYS:HE2	2.44	0.47
6:P:-25:DT:O2	7:Q:66:DG:N2	2.48	0.47
3:J:1178:THR:HA	3:J:1184:ASP:HB3	1.98	0.46
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.96	0.46
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.16	0.46
3:J:1061:VAL:O	3:J:1104:LYS:N	2.43	0.46
6:P:15:DA:H2'	6:P:15:DA:OP2	2.14	0.46
7:Q:70:DC:C4	7:Q:71:DA:C6	3.03	0.46
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.97	0.46
2:I:979:LEU:HD21	2:I:1000:LEU:HD22	1.97	0.46
6:P:-38:DC:H2'	6:P:-37:DT:H71	1.98	0.46
1:G:8:PHE:HD1	1:G:8:PHE:H	1.64	0.46
2:I:232:ILE:HG23	2:I:236:LYS:HG2	1.98	0.46
2:I:958:LYS:O	2:I:962:GLU:HG2	2.16	0.46
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	2.16	0.46
2:I:256:GLU:HG3	2:I:261:VAL:HA	1.97	0.46
3:J:412:LEU:O	3:J:416:ILE:HG12	2.16	0.46
1:G:76:GLU:OE1	1:G:132:HIS:N	2.46	0.46
2:I:469:VAL:O	2:I:472:GLU:HG3	2.15	0.46
3:J:824:PRO:HD3	3:J:835:LEU:HD12	1.97	0.46
3:J:968:ASN:HD21	3:J:970:SER:HB2	1.81	0.46
1:H:216:ALA:O	1:H:217:ILE:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:903:ARG:O	2:I:907:GLY:N	2.47	0.46
2:I:1000:LEU:HD21	2:I:1011:LEU:HD21	1.96	0.46
3:J:18:ASP:OD1	3:J:18:ASP:N	2.46	0.46
3:J:1169:THR:HB	3:J:1174:ARG:HH11	1.80	0.46
5:L:583:THR:HG21	6:P:-35:DG:H5"	1.98	0.46
1:H:13:LEU:H	1:H:13:LEU:HD22	1.81	0.46
1:G:181:GLU:N	1:G:206:GLU:O	2.41	0.46
1:H:76:GLU:OE1	1:H:132:HIS:N	2.46	0.46
2:I:231:GLU:HB3	2:I:238:GLN:HE21	1.80	0.46
2:I:979:LEU:HA	2:I:1010:GLN:NE2	2.30	0.46
2:I:1006:GLU:H	2:I:1006:GLU:CD	2.24	0.46
3:J:205:LEU:HD23	3:J:205:LEU:HA	1.83	0.46
1:H:222:THR:O	1:H:223:ILE:C	2.58	0.46
2:I:804:PHE:O	3:J:638:SER:OG	2.25	0.46
1:G:45:ARG:NH1	2:I:1084:ASP:OD1	2.42	0.45
1:H:194:GLN:O	1:H:195:ARG:C	2.58	0.45
2:I:472:GLU:HA	2:I:475:VAL:HG12	1.97	0.45
2:I:750:ILE:HD11	2:I:966:ILE:HG21	1.97	0.45
1:H:221:ALA:O	1:H:222:THR:C	2.57	0.45
5:L:283:GLN:NE2	5:L:340:ALA:O	2.40	0.45
8:Z:42:LYS:HD3	8:Z:45:ALA:HB2	1.98	0.45
1:H:61:ILE:HB	1:H:64:VAL:HB	1.98	0.45
2:I:272:ARG:O	2:I:275:ARG:HG3	2.16	0.45
5:L:234:THR:OG1	5:L:248:GLU:OE1	2.34	0.45
3:J:646:ILE:HG12	3:J:764:ARG:HH11	1.81	0.45
3:J:759:ILE:HG12	3:J:771:GLN:HG2	1.99	0.45
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.97	0.45
2:I:742:TYR:HB2	2:I:745:GLU:HG2	1.99	0.45
2:I:819:SER:HB3	2:I:1085:MET:HE2	1.97	0.45
2:I:1003:THR:HA	2:I:1005:GLU:CD	2.42	0.45
3:J:733:SER:O	3:J:737:ILE:HG12	2.16	0.45
1:G:33:ARG:HH22	1:G:197:ASP:C	2.23	0.45
1:G:61:ILE:HB	1:G:64:VAL:HB	1.98	0.45
1:H:29:GLU:CD	1:H:200:LYS:HG3	2.41	0.45
1:H:74:VAL:HG22	1:H:76:GLU:H	1.82	0.45
2:I:56:VAL:CG1	2:I:59:ILE:HD11	2.46	0.45
2:I:979:LEU:HD11	2:I:1011:LEU:HD21	1.98	0.45
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.50	0.45
8:Z:42:LYS:HB3	8:Z:60:THR:HA	1.98	0.45
2:I:989:LEU:HD21	2:I:1002:LEU:HD12	1.99	0.45
3:J:93:THR:OG1	3:J:94:GLN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1032:SER:OG	3:J:1117:SER:N	2.50	0.45
5:L:104:GLU:O	5:L:107:THR:OG1	2.34	0.45
5:L:283:GLN:NE2	5:L:344:LEU:HB2	2.31	0.45
1:H:93:GLN:O	1:H:95:LYS:N	2.50	0.45
6:P:-10:DA:H2''	6:P:-9:DC:OP1	2.16	0.45
2:I:18:ARG:O	2:I:1156:ARG:NH1	2.44	0.45
2:I:962:GLU:OE1	9:I:1401:1N7:H24	2.17	0.45
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.99	0.45
1:G:231:PHE:C	1:G:232:VAL:O	2.57	0.44
1:H:15:ASP:OD1	1:H:15:ASP:N	2.50	0.44
2:I:1001:GLY:HA2	2:I:1011:LEU:HD23	1.99	0.44
2:I:1151:LEU:HD13	2:I:1201:LEU:HD22	1.99	0.44
1:G:13:LEU:HD22	1:G:28:LEU:HD11	1.97	0.44
2:I:235:ASN:OD1	2:I:237:LEU:HB2	2.16	0.44
2:I:743:PRO:O	2:I:974:ARG:NH2	2.51	0.44
3:J:1233:ILE:O	3:J:1237:VAL:HG23	2.18	0.44
7:Q:55:DC:H2'	7:Q:56:DA:C8	2.52	0.44
1:G:23:HIS:CD2	1:G:23:HIS:C	2.95	0.44
1:H:224:LEU:O	1:H:225:ALA:C	2.58	0.44
1:H:225:ALA:O	1:H:226:GLU:C	2.59	0.44
3:J:318:GLY:N	3:J:322:ARG:O	2.40	0.44
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.99	0.44
1:G:93:GLN:O	1:G:95:LYS:N	2.50	0.44
2:I:704:MET:HB3	2:I:704:MET:HE3	1.79	0.44
2:I:990:ASP:OD1	2:I:990:ASP:N	2.41	0.44
3:J:55:GLY:H	3:J:58:CYS:HB2	1.83	0.44
3:J:64:PRO:HG3	3:J:91:GLU:O	2.18	0.44
3:J:576:ARG:HD3	3:J:593:ASN:HA	1.99	0.44
5:L:358:VAL:HG12	5:L:362:ASN:HD21	1.82	0.44
2:I:545:PHE:HZ	3:J:781:LYS:HG2	1.83	0.44
2:I:595:THR:HG22	2:I:598:VAL:O	2.18	0.44
3:J:221:ILE:HD13	3:J:221:ILE:HA	1.87	0.44
5:L:451:ARG:NH2	6:P:-16:DT:OP1	2.51	0.44
6:P:-39:DG:H5'	6:P:-39:DG:H8	1.83	0.44
2:I:1003:THR:HA	2:I:1005:GLU:OE2	2.18	0.44
3:J:530:PRO:HB3	3:J:577:ALA:O	2.18	0.44
3:J:552:ILE:HD11	3:J:570:LYS:HG3	1.99	0.44
3:J:1090:ILE:HD11	3:J:1097:ALA:HB2	1.99	0.44
4:K:12:LYS:HD3	4:K:12:LYS:HA	1.80	0.44
1:G:74:VAL:HG22	1:G:76:GLU:H	1.82	0.44
1:G:180:VAL:HA	1:G:207:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:231:GLU:CB	2:I:238:GLN:HE21	2.31	0.44
2:I:233:ARG:H	2:I:238:GLN:NE2	2.14	0.44
2:I:238:GLN:N	2:I:238:GLN:CD	2.76	0.44
2:I:1010:GLN:HG3	2:I:1011:LEU:CD2	2.43	0.44
1:G:226:GLU:C	1:G:228:LEU:N	2.70	0.44
1:H:41:ASN:O	1:H:45:ARG:HG3	2.18	0.44
2:I:22:LEU:HD13	2:I:603:ILE:HG13	2.00	0.44
2:I:232:ILE:HG23	2:I:236:LYS:HZ3	1.83	0.44
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.86	0.43
9:J:1504:1N7:C17	9:L:701:1N7:H26	2.46	0.43
3:J:978:ARG:HH12	3:J:1202:GLU:HG3	1.83	0.43
1:H:195:ARG:HE	1:H:195:ARG:HB3	1.51	0.43
2:I:233:ARG:O	2:I:236:LYS:HG3	2.18	0.43
2:I:475:VAL:HG23	2:I:492:MET:HB3	2.00	0.43
2:I:895:LEU:HD12	2:I:895:LEU:HA	1.83	0.43
2:I:971:LEU:HD11	2:I:1014:LEU:HD12	2.00	0.43
3:J:930:LEU:HD22	3:J:1244:GLN:HG3	1.99	0.43
3:J:951:GLN:OE1	3:J:1016:THR:OG1	2.28	0.43
4:K:3:ARG:HD2	4:K:6:VAL:HG12	2.00	0.43
5:L:476:ARG:NH1	5:L:477:GLU:O	2.52	0.43
2:I:12:ARG:HG3	2:I:1181:PRO:HB2	2.01	0.43
2:I:298:ALA:HB3	2:I:334:GLU:HG3	2.00	0.43
3:J:334:LYS:HA	3:J:339:ARG:HD3	2.01	0.43
1:G:97:GLU:OE1	1:G:145:LYS:NZ	2.45	0.43
5:L:138:PRO:O	5:L:142:THR:HG23	2.18	0.43
5:L:471:LEU:HD12	5:L:477:GLU:HA	2.01	0.43
1:H:226:GLU:HA	1:H:229:GLU:HG2	2.00	0.43
2:I:624:ASP:OD1	2:I:624:ASP:N	2.47	0.43
3:J:326:SER:OG	3:J:329:ASP:OD2	2.37	0.43
5:L:360:ASP:O	5:L:363:ARG:HD3	2.18	0.43
7:Q:60:DT:H2"	7:Q:61:DT:C4	2.53	0.43
2:I:225:PHE:HZ	2:I:345:PRO:HA	1.83	0.43
2:I:1000:LEU:C	2:I:1002:LEU:N	2.75	0.43
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	2.01	0.43
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.01	0.43
3:J:1075:ARG:HD3	3:J:1075:ARG:HA	1.87	0.43
7:Q:23:DA:H2"	7:Q:24:DA:C8	2.54	0.43
8:Z:39:LEU:N	8:Z:43:TYR:O	2.51	0.43
2:I:268:ARG:HA	2:I:268:ARG:HD2	1.88	0.43
2:I:799:ASN:ND2	2:I:799:ASN:H	2.17	0.43
3:J:842:ARG:HD3	3:J:882:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1169:THR:HB	3:J:1174:ARG:NH1	2.34	0.43
4:K:80:LEU:HD23	4:K:80:LEU:HA	1.92	0.43
5:L:137:TYR:HD2	5:L:139:GLU:HB2	1.84	0.43
1:R:265:ARG:HD2	1:R:294:ASN:HB3	2.01	0.43
3:J:733:SER:OG	3:J:736:GLN:OE1	2.29	0.42
5:L:358:VAL:O	5:L:362:ASN:ND2	2.52	0.42
8:Z:64:SER:O	8:Z:67:ARG:HD3	2.18	0.42
3:J:255:LEU:N	3:J:259:ARG:O	2.51	0.42
3:J:650:LYS:NZ	3:J:760:THR:O	2.41	0.42
5:L:595:LEU:O	5:L:599:ARG:HD3	2.19	0.42
1:H:205:MET:HE2	1:H:205:MET:HB2	1.79	0.42
2:I:59:ILE:HG21	2:I:475:VAL:HG13	2.01	0.42
2:I:1021:LEU:O	2:I:1024:GLU:HG3	2.19	0.42
2:I:203:LYS:O	2:I:204:LEU:HD23	2.19	0.42
2:I:501:ALA:O	2:I:504:GLU:HG3	2.19	0.42
3:J:977:SER:OG	3:J:980:THR:OG1	2.36	0.42
3:J:1313:SER:O	3:J:1316:THR:OG1	2.37	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.54	0.42
1:G:224:LEU:O	1:G:225:ALA:C	2.61	0.42
2:I:972:PHE:CZ	2:I:998:LEU:HD22	2.55	0.42
1:G:33:ARG:HA	1:G:33:ARG:NE	2.35	0.42
1:H:149:GLY:O	1:H:177:TYR:HB3	2.20	0.42
2:I:263:VAL:HG13	2:I:267:ARG:HB2	2.02	0.42
3:J:136:GLU:HG2	3:J:312:ARG:HH21	1.84	0.42
5:L:220:LYS:HD2	5:L:220:LYS:HA	1.84	0.42
1:G:51:MET:HE2	1:G:216:ALA:HB1	2.02	0.42
2:I:61:SER:O	2:I:63:SER:N	2.49	0.42
2:I:340:ASP:OD1	2:I:340:ASP:N	2.46	0.42
2:I:965:GLN:NE2	2:I:966:ILE:HG12	2.35	0.42
3:J:1357:ILE:HD12	3:J:1359:ALA:HB3	2.02	0.42
8:Z:68:TRP:O	8:Z:71:GLN:HG3	2.19	0.42
1:H:233:ASP:HB2	1:H:234:LEU:H	1.47	0.42
2:I:1032:LYS:HB2	2:I:1032:LYS:HE3	1.68	0.42
1:H:25:LYS:HE2	1:H:25:LYS:HB3	1.76	0.42
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.55	0.42
6:P:-41:DA:H2''	6:P:-40:DG:H8	1.84	0.42
2:I:519:ASN:HD21	2:I:796:LEU:HD22	1.85	0.42
6:P:-39:DG:H1'	6:P:-38:DC:O4'	2.20	0.42
1:R:265:ARG:HA	1:R:268:ASN:ND2	2.35	0.42
1:G:23:HIS:CD2	1:G:23:HIS:O	2.73	0.41
1:H:226:GLU:O	1:H:229:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:960:LEU:O	2:I:963:GLU:HG3	2.20	0.41
4:K:35:LYS:HD3	4:K:35:LYS:HA	1.83	0.41
5:L:103:ARG:O	5:L:107:THR:HG23	2.19	0.41
7:Q:67:DC:H1'	7:Q:68:DG:H5'	2.02	0.41
1:R:266:SER:O	1:R:270:LEU:HG	2.20	0.41
3:J:1062:LEU:O	3:J:1067:ARG:NH2	2.53	0.41
5:L:137:TYR:CD2	5:L:139:GLU:HB2	2.55	0.41
1:G:231:PHE:O	1:G:232:VAL:C	2.62	0.41
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.94	0.41
2:I:256:GLU:O	2:I:286:GLU:HG2	2.20	0.41
2:I:1270:PHE:CZ	2:I:1274:GLU:HB3	2.55	0.41
1:H:83:LEU:HD21	3:J:526:VAL:CG2	2.50	0.41
1:H:136:GLU:HG2	1:H:137:ASN:H	1.85	0.41
2:I:229:ILE:HG21	2:I:332:ARG:HH11	1.85	0.41
2:I:596:ASP:OD1	2:I:596:ASP:N	2.51	0.41
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.20	0.41
3:J:1167:LYS:O	3:J:1168:GLU:C	2.63	0.41
1:G:8:PHE:CE2	1:H:150:ARG:CZ	3.04	0.41
1:H:86:LYS:NZ	3:J:532:GLU:OE2	2.54	0.41
1:H:198:LEU:N	1:H:198:LEU:HD23	2.34	0.41
2:I:236:LYS:HE3	8:Z:48:LEU:HD11	2.03	0.41
3:J:847:ASP:OD1	3:J:847:ASP:N	2.53	0.41
3:J:1207:GLY:HA2	3:J:1223:LEU:HD13	2.02	0.41
6:P:-30:DG:H2''	6:P:-29:DG:C8	2.56	0.41
7:Q:69:DC:H2''	7:Q:70:DC:C4	2.55	0.41
2:I:221:LEU:HD11	2:I:314:ASN:HB2	2.02	0.41
2:I:236:LYS:HD2	8:Z:48:LEU:HD11	2.01	0.41
1:G:33:ARG:HA	1:G:33:ARG:HE	1.85	0.41
1:G:136:GLU:HG2	1:G:137:ASN:H	1.85	0.41
1:H:232:VAL:HG22	1:H:233:ASP:N	2.34	0.41
2:I:234:ASP:C	2:I:236:LYS:H	2.29	0.41
2:I:678:ARG:HA	2:I:678:ARG:HD3	1.83	0.41
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.53	0.41
2:I:1303:LYS:HB2	2:I:1303:LYS:HE3	1.90	0.41
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.54	0.41
3:J:978:ARG:NH2	3:J:1197:ASN:O	2.53	0.41
3:J:1253:ILE:H	3:J:1253:ILE:HG13	1.71	0.41
2:I:325:LEU:O	2:I:330:HIS:HB2	2.21	0.41
2:I:367:TYR:OH	2:I:374:GLU:OE2	2.36	0.41
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.55	0.41
2:I:1252:SER:HB3	2:I:1255:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1283:ALA:HB1	2:I:1286:THR:HB	2.03	0.41
2:I:1316:GLU:HA	2:I:1317:PRO:HD3	1.94	0.41
3:J:1138:LEU:N	3:J:1139:PRO:HD3	2.36	0.41
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.35	0.41
5:L:161:LEU:HG	5:L:162:ILE:HG12	2.02	0.41
5:L:426:LYS:HE2	6:P:-9:DC:H3'	2.02	0.41
1:R:300:LEU:HG	1:R:304:LYS:HE2	2.02	0.41
1:G:12:ARG:O	1:G:14:VAL:HG13	2.21	0.41
1:H:207:THR:HG22	1:H:213:PRO:HG3	2.01	0.41
2:I:404:LYS:HA	2:I:404:LYS:HD2	1.89	0.41
7:Q:53:DA:H2'	7:Q:54:DC:C6	2.56	0.41
1:H:52:PRO:N	1:H:150:ARG:HG2	2.36	0.40
2:I:236:LYS:C	2:I:238:GLN:HE22	2.29	0.40
2:I:1045:GLY:HA2	5:L:499:LYS:HE3	2.03	0.40
2:I:1246:ARG:HH12	2:I:1258:PRO:HB3	1.85	0.40
2:I:1272:GLU:OE2	3:J:343:LEU:HD13	2.22	0.40
2:I:65:ASN:CB	2:I:105:TYR:HB2	2.51	0.40
2:I:232:ILE:HD11	2:I:333:ILE:HD11	2.03	0.40
2:I:971:LEU:CD1	2:I:1014:LEU:HD12	2.51	0.40
3:J:1140:ARG:NH2	3:J:1236:GLU:OE1	2.36	0.40
4:K:15:ASN:C	4:K:17:PHE:H	2.29	0.40
1:R:262:LEU:HB3	1:R:266:SER:HB2	2.03	0.40
6:P:-40:DG:H2''	6:P:-39:DG:H8	1.87	0.40
1:H:18:GLN:HG3	1:H:20:SER:O	2.21	0.40
1:H:39:LEU:HD13	1:H:39:LEU:HA	1.92	0.40
1:H:211:ILE:O	1:H:211:ILE:HG13	2.18	0.40
3:J:1181:ASP:OD1	3:J:1181:ASP:N	2.53	0.40
5:L:385:ARG:HB3	6:P:-7:DT:H1'	2.04	0.40
1:G:12:ARG:NH2	1:H:230:ALA:HB2	2.36	0.40
1:H:37:HIS:CD2	1:H:187:VAL:CG1	2.92	0.40
2:I:1012:GLU:CD	2:I:1012:GLU:C	2.90	0.40
3:J:1159:ILE:HG22	3:J:1177:ILE:HD12	2.04	0.40
3:J:1166:GLY:N	3:J:1174:ARG:O	2.55	0.40
3:J:1167:LYS:HE2	3:J:1167:LYS:HB2	1.71	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	G	229/329 (70%)	214 (93%)	15 (7%)	0	100	100
1	H	215/329 (65%)	189 (88%)	25 (12%)	1 (0%)	24	43
1	R	71/329 (22%)	71 (100%)	0	0	100	100
2	I	1339/1342 (100%)	1284 (96%)	53 (4%)	2 (0%)	48	71
3	J	1331/1407 (95%)	1282 (96%)	49 (4%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	L	464/608 (76%)	451 (97%)	13 (3%)	0	100	100
8	Z	71/80 (89%)	60 (84%)	11 (16%)	0	100	100
All	All	3797/4515 (84%)	3625 (96%)	169 (4%)	3 (0%)	49	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	30	PRO
2	I	236	LYS
2	I	232	ILE

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	G	197/286 (69%)	187 (95%)	10 (5%)	21	40
1	H	186/286 (65%)	154 (83%)	32 (17%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1126 (98%)	29 (2%)	42	64
3	J	1118/1168 (96%)	1097 (98%)	21 (2%)	50	70
4	K	67/75 (89%)	67 (100%)	0	100	100
5	L	414/537 (77%)	413 (100%)	1 (0%)	87	95
8	Z	64/71 (90%)	63 (98%)	1 (2%)	55	73
All	All	3266/3866 (84%)	3172 (97%)	94 (3%)	38	61

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	7	GLU
1	G	8	PHE
1	G	10	LYS
1	G	12	ARG
1	G	13	LEU
1	G	15	ASP
1	G	26	VAL
1	G	28	LEU
1	G	29	GLU
1	G	156	SER
1	H	6	THR
1	H	9	LEU
1	H	13	LEU
1	H	15	ASP
1	H	16	ILE
1	H	17	GLU
1	H	19	VAL
1	H	30	PRO
1	H	33	ARG
1	H	39	LEU
1	H	46	ILE
1	H	48	LEU
1	H	49	SER
1	H	51	MET
1	H	57	THR
1	H	58	GLU
1	H	156	SER
1	H	180	VAL
1	H	191	ARG

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Mol	Chain	Res	Type
1	H	192	VAL
1	H	193	GLU
1	H	194	GLN
1	H	195	ARG
1	H	196	THR
1	H	198	LEU
1	H	205	MET
1	H	206	GLU
1	H	211	ILE
1	H	212	ASP
1	H	226	GLU
1	H	232	VAL
1	H	233	ASP
2	I	235	ASN
2	I	346	TYR
2	I	419	ILE
2	I	481	LEU
2	I	680	LEU
2	I	717	VAL
2	I	730	SER
2	I	731	ARG
2	I	755	LYS
2	I	799	ASN
2	I	853	ASP
2	I	968	GLU
2	I	998	LEU
2	I	999	GLU
2	I	1000	LEU
2	I	1002	LEU
2	I	1003	THR
2	I	1005	GLU
2	I	1006	GLU
2	I	1007	LYS
2	I	1008	GLN
2	I	1011	LEU
2	I	1013	GLN
2	I	1014	LEU
2	I	1020	GLU
2	I	1060	ILE
2	I	1077	SER
2	I	1101	LEU
2	I	1105	SER

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Mol	Chain	Res	Type
3	J	26	SER
3	J	60	ARG
3	J	100	GLU
3	J	221	ILE
3	J	242	LEU
3	J	352	ARG
3	J	357	VAL
3	J	441	LEU
3	J	510	LEU
3	J	592	VAL
3	J	654	ILE
3	J	708	ASN
3	J	728	SER
3	J	831	VAL
3	J	844	THR
3	J	876	SER
3	J	1009	GLU
3	J	1017	VAL
3	J	1167	LYS
3	J	1361	THR
3	J	1371	ARG
5	L	244	THR
8	Z	44	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	66	HIS
1	H	41	ASN
2	I	60	GLN
2	I	150	HIS
2	I	235	ASN
2	I	238	GLN
2	I	494	ASN
2	I	573	ASN
2	I	752	ASN
2	I	808	ASN
2	I	834	GLN
2	I	856	ASN
2	I	952	GLN
2	I	965	GLN
2	I	1288	GLN

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Mol	Chain	Res	Type
3	J	158	GLN
3	J	232	ASN
3	J	294	ASN
3	J	469	HIS
3	J	720	ASN
3	J	739	GLN
3	J	1010	GLN
3	J	1019	ASN
3	J	1023	HIS
3	J	1259	GLN
4	K	72	GLN
5	L	227	GLN
5	L	472	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
9	1N7	J	1504	-	32,32,46	0.59	0	51,51,72	0.83	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	1N7	L	701	-	32,32,46	0.60	1 (3%)	51,51,72	0.82	1 (1%)
9	1N7	I	1401	-	32,32,46	0.59	1 (3%)	51,51,72	0.83	1 (1%)

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	1N7	J	1504	-	-	0/9/74/92	0/4/4/4
9	1N7	L	701	-	-	0/9/74/92	0/4/4/4
9	1N7	I	1401	-	-	0/9/74/92	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1401	1N7	C5-C6	-2.02	1.52	1.55
9	L	701	1N7	C5-C6	-2.02	1.52	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C6-C5-C4	-2.30	105.31	107.42
9	L	701	1N7	C6-C5-C4	-2.28	105.33	107.42
9	I	1401	1N7	C6-C5-C4	-2.25	105.36	107.42

There are no chirality outliers.

There are no torsion outliers.

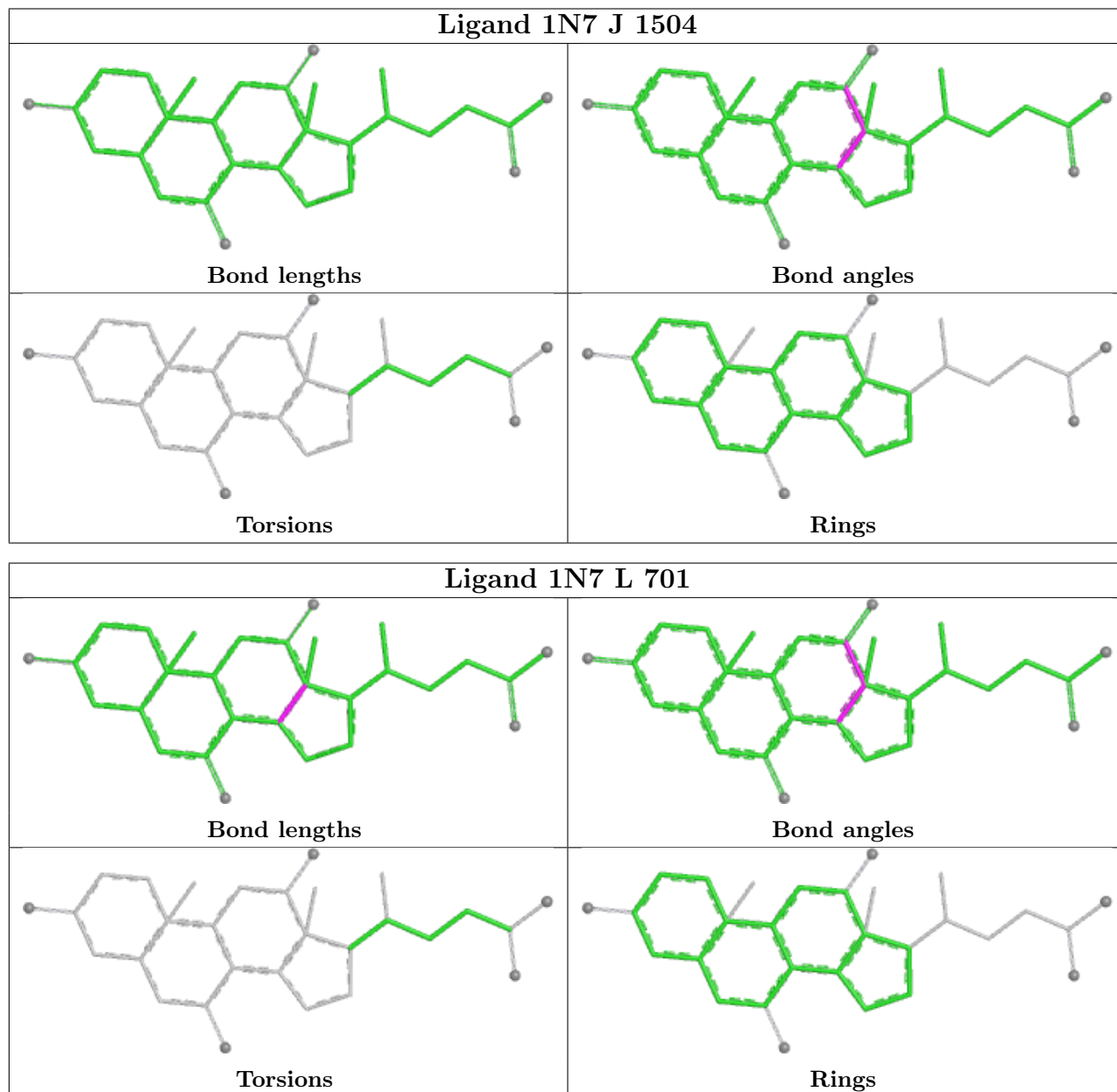
There are no ring outliers.

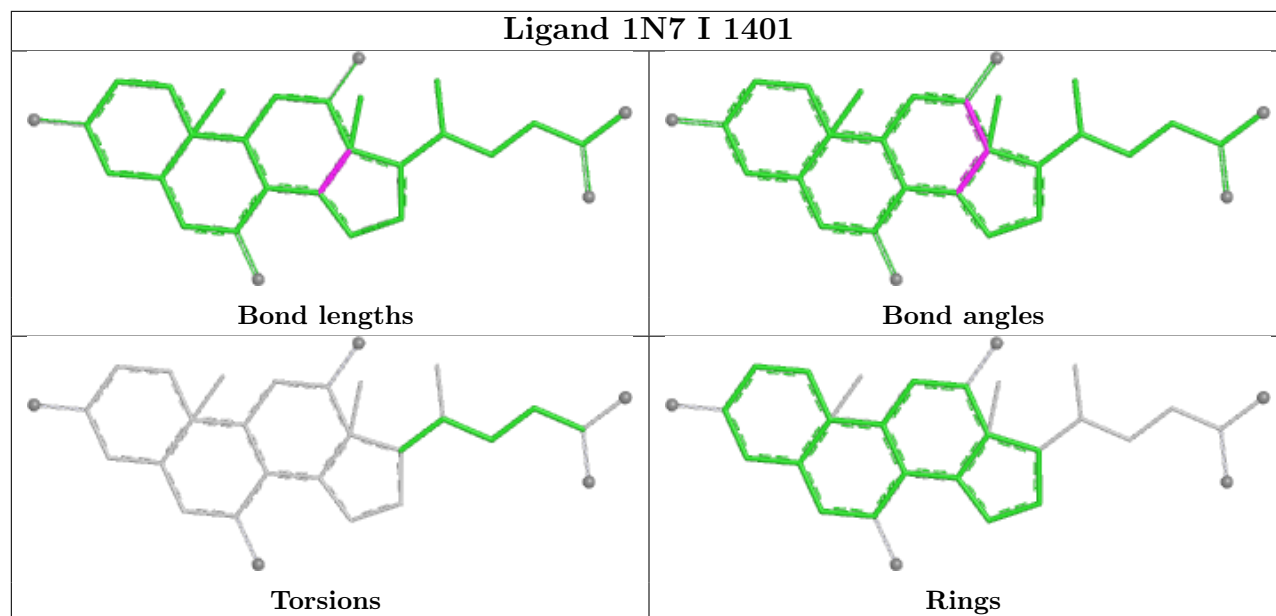
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1504	1N7	5	0
9	L	701	1N7	6	0
9	I	1401	1N7	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

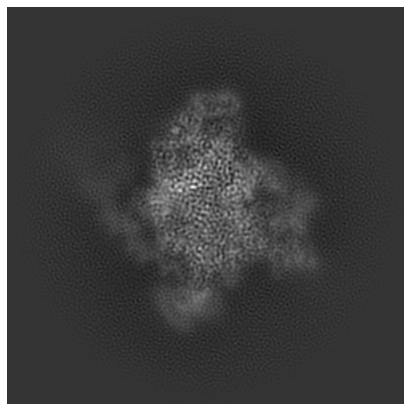
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29423. These allow visual inspection of the internal detail of the map and identification of artifacts.

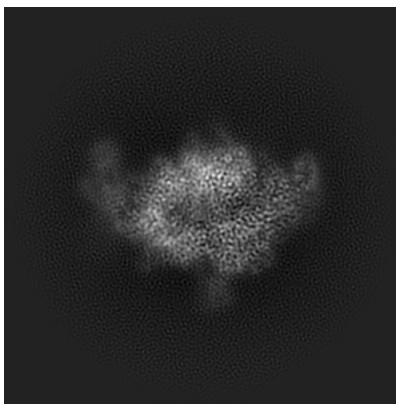
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

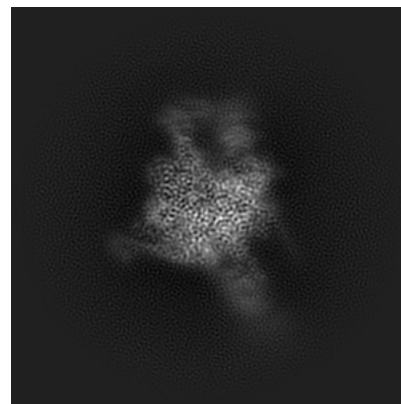
6.1.1 Primary map



X

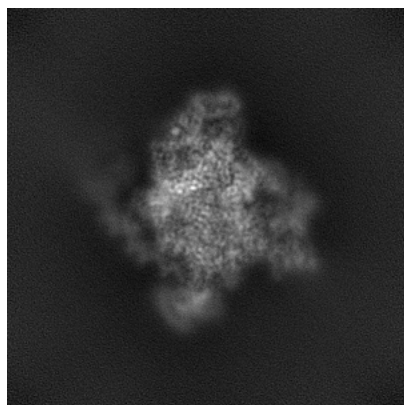


Y

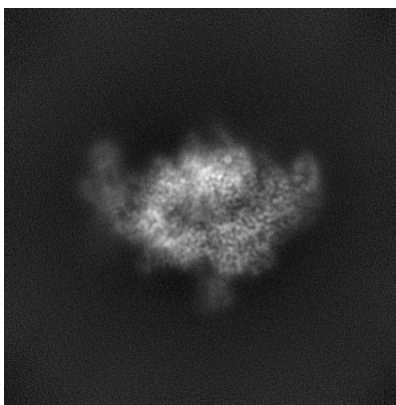


Z

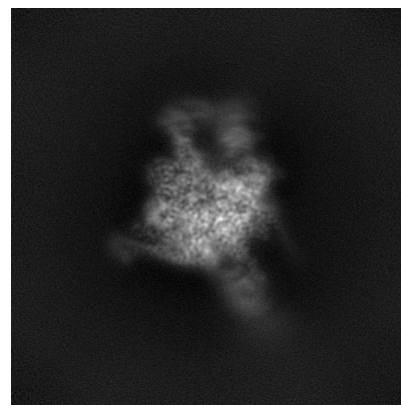
6.1.2 Raw map



X



Y

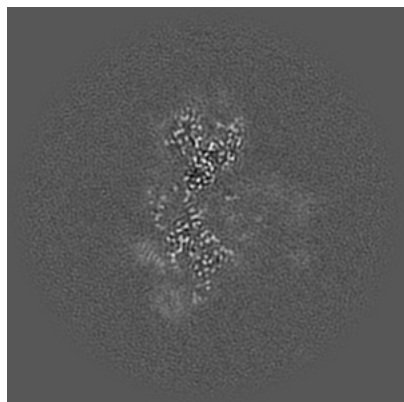


Z

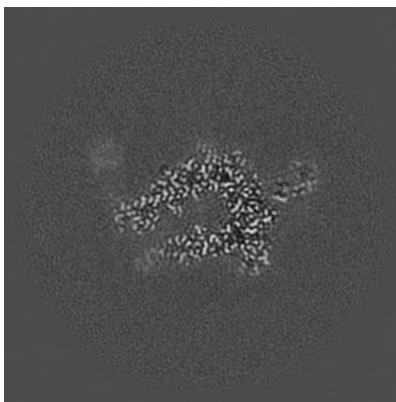
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

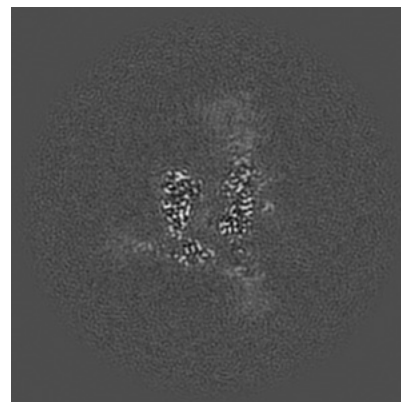
6.2.1 Primary map



X Index: 180

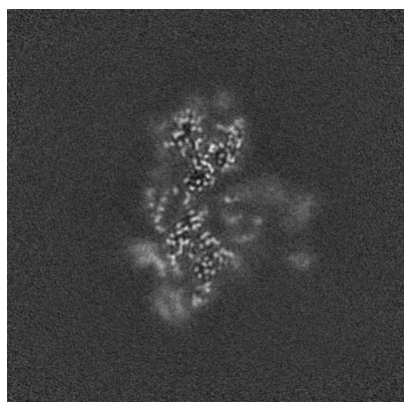


Y Index: 180

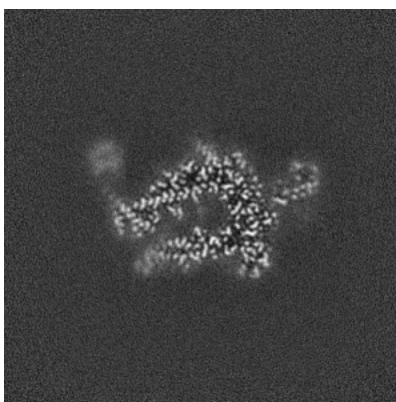


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

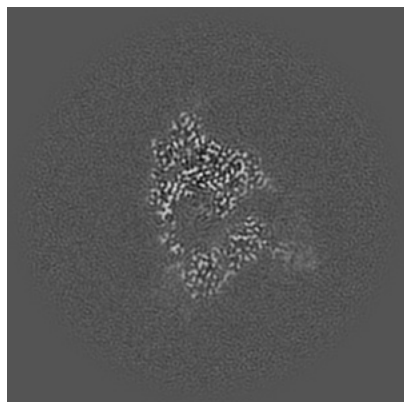


Z Index: 180

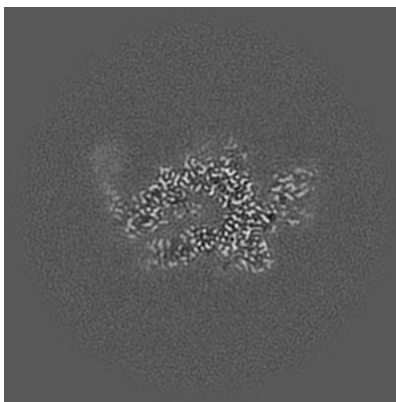
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

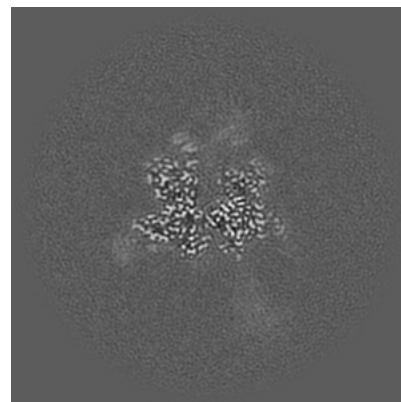
6.3.1 Primary map



X Index: 163

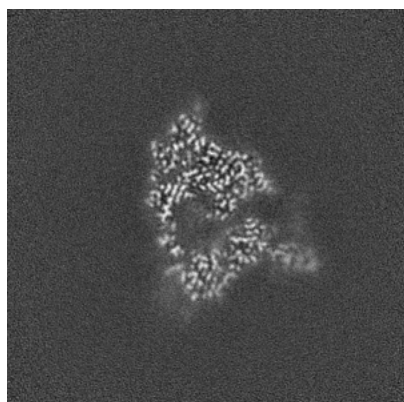


Y Index: 174

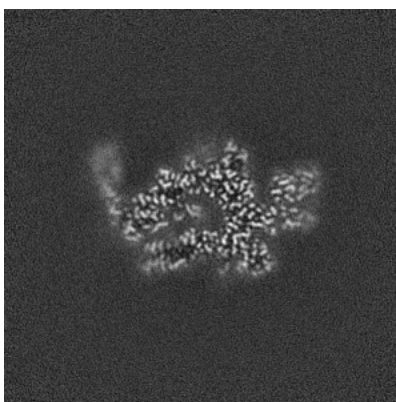


Z Index: 199

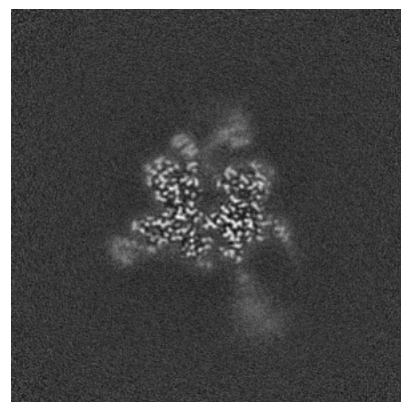
6.3.2 Raw map



X Index: 163



Y Index: 173

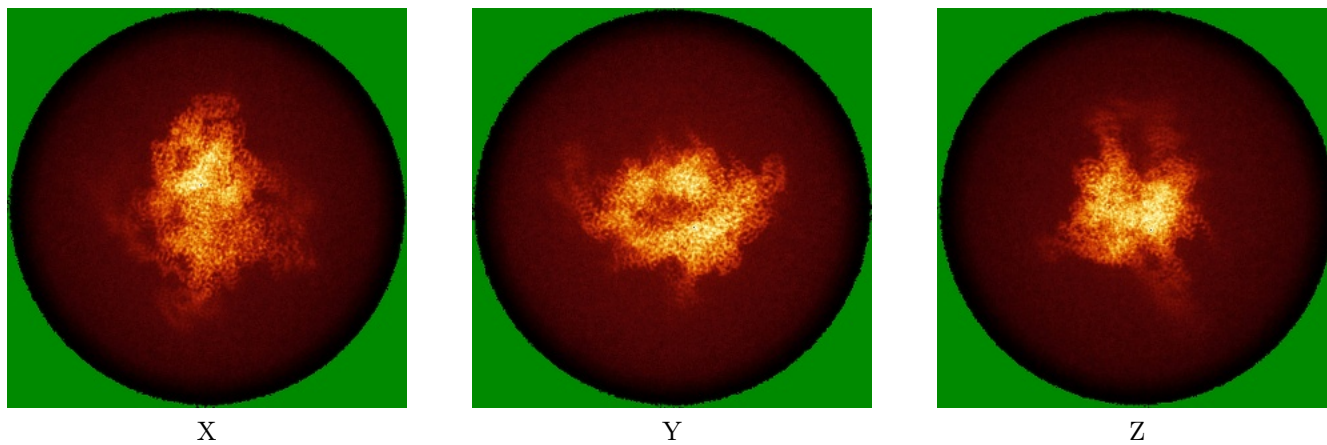


Z Index: 198

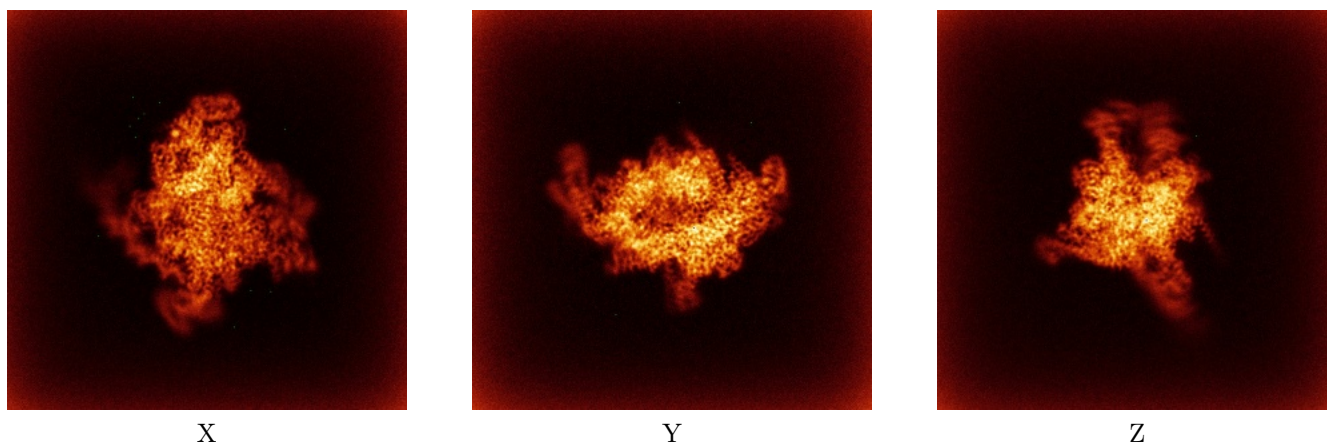
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

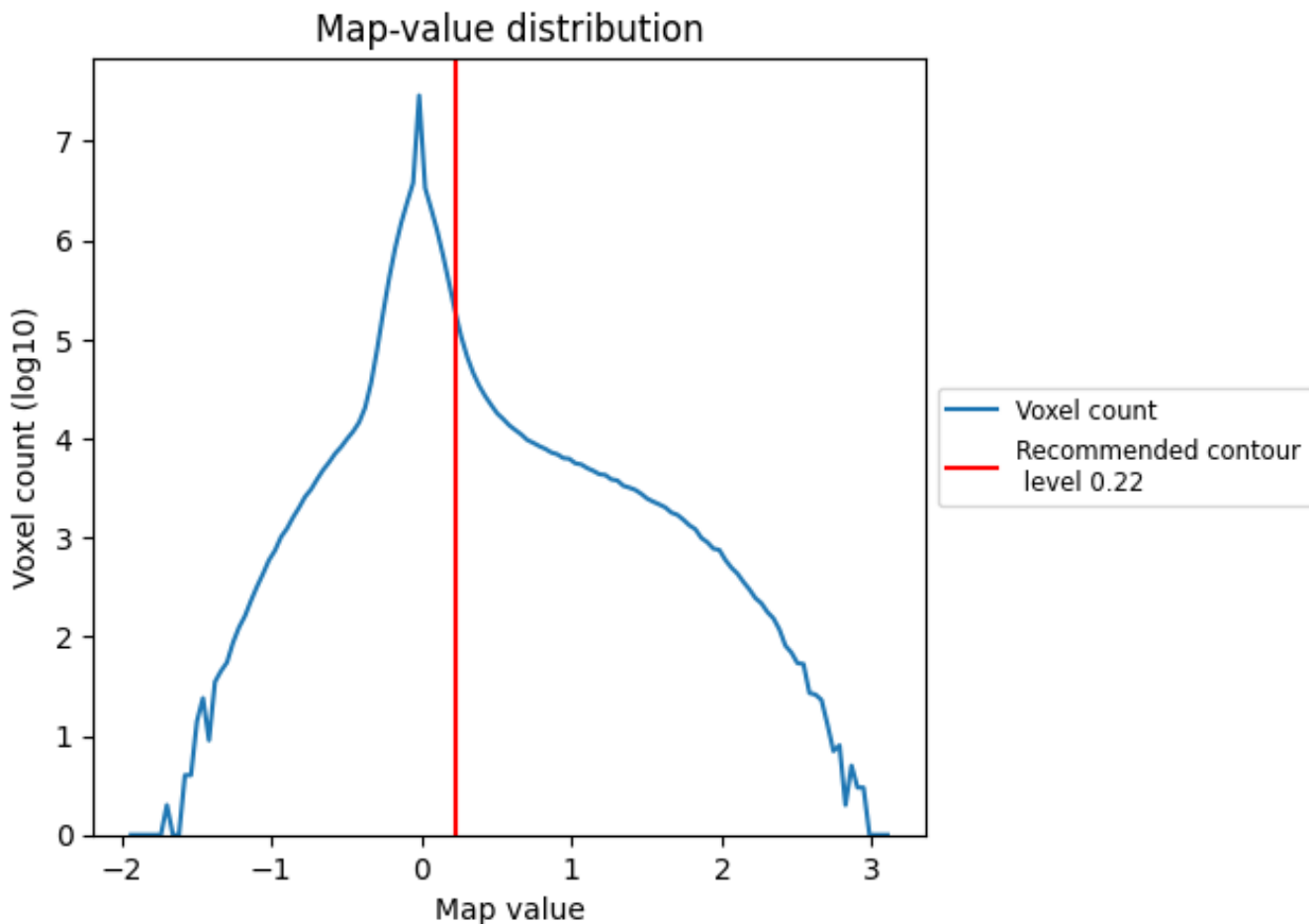
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

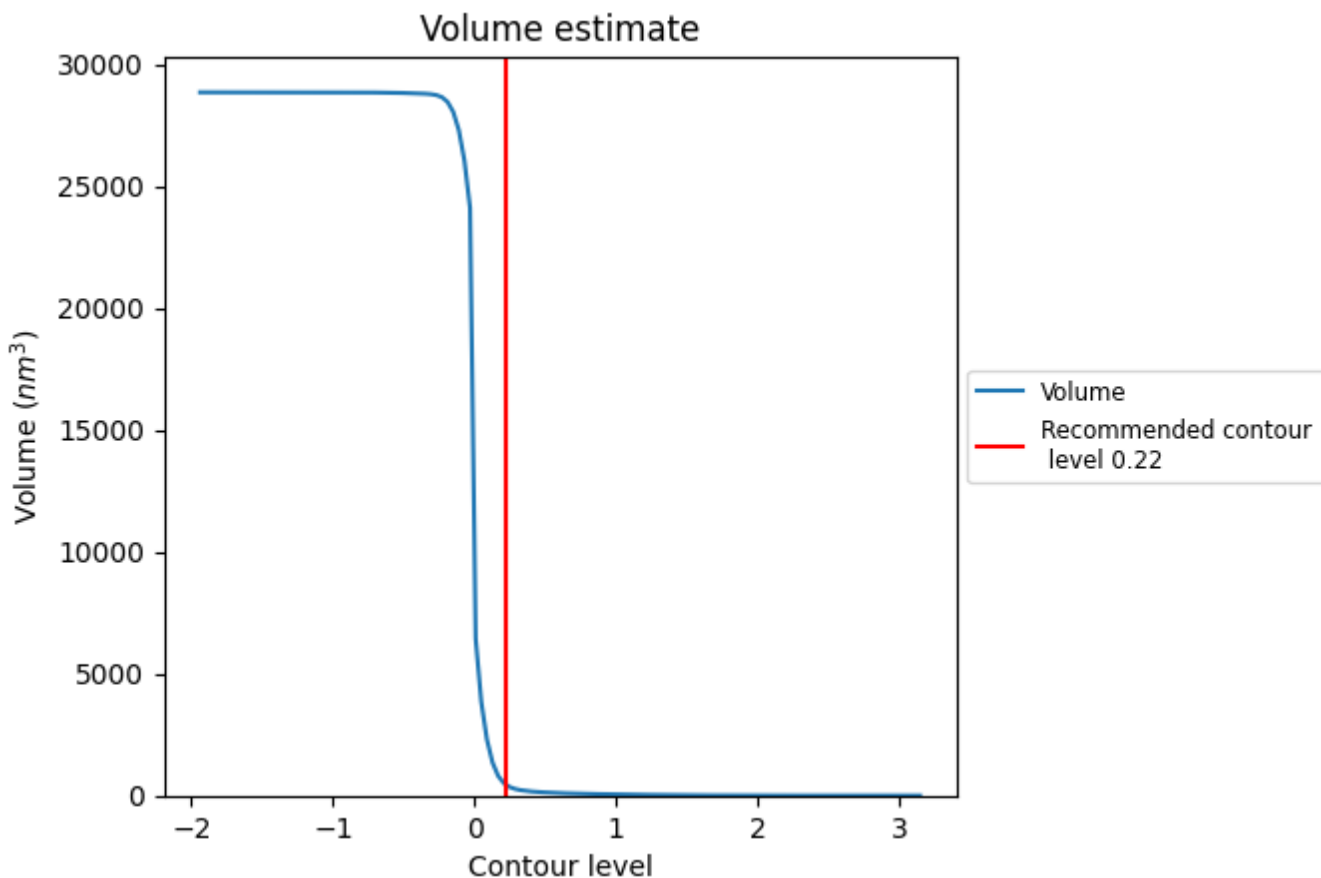
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

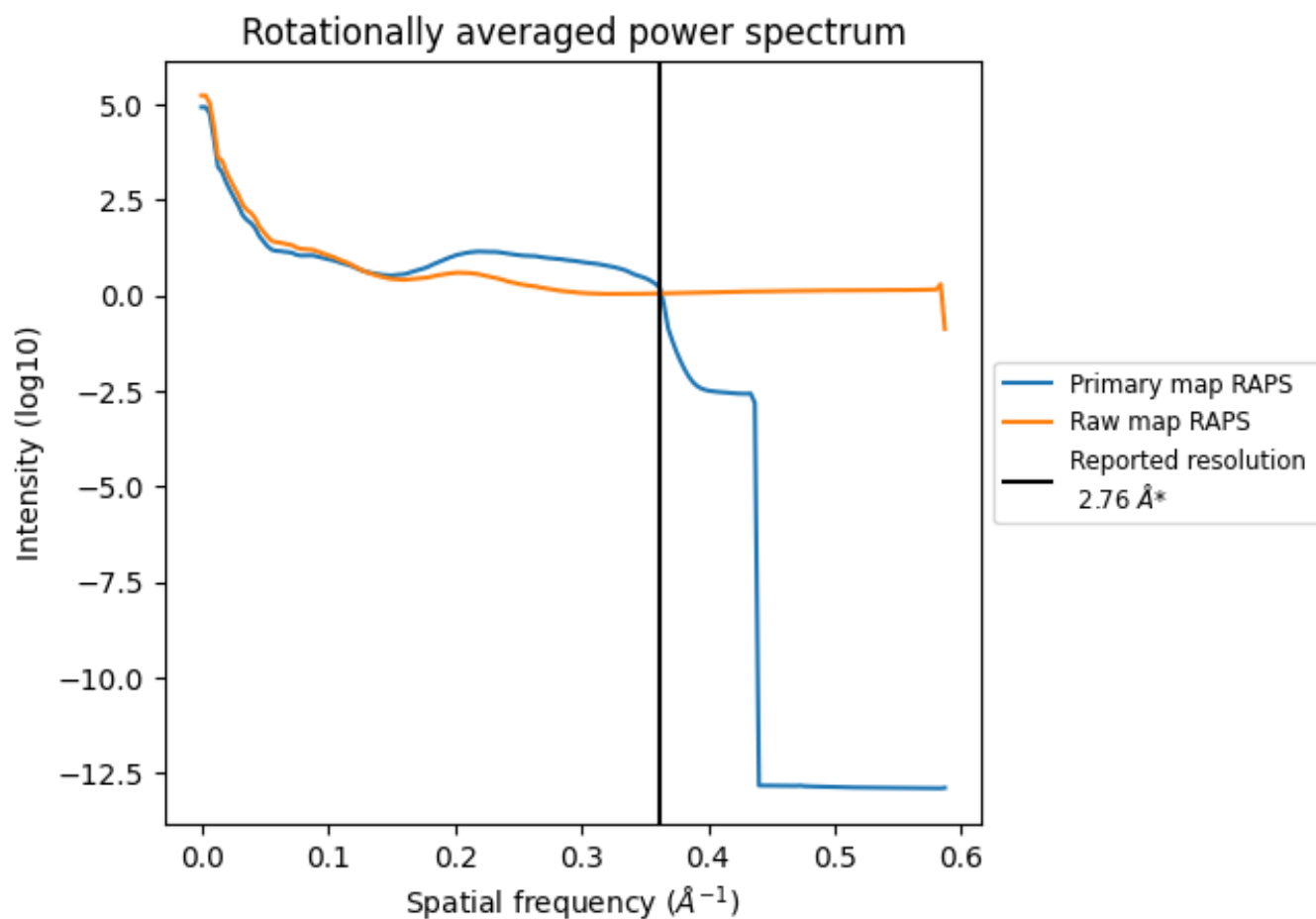
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 457 nm³; this corresponds to an approximate mass of 413 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](#)

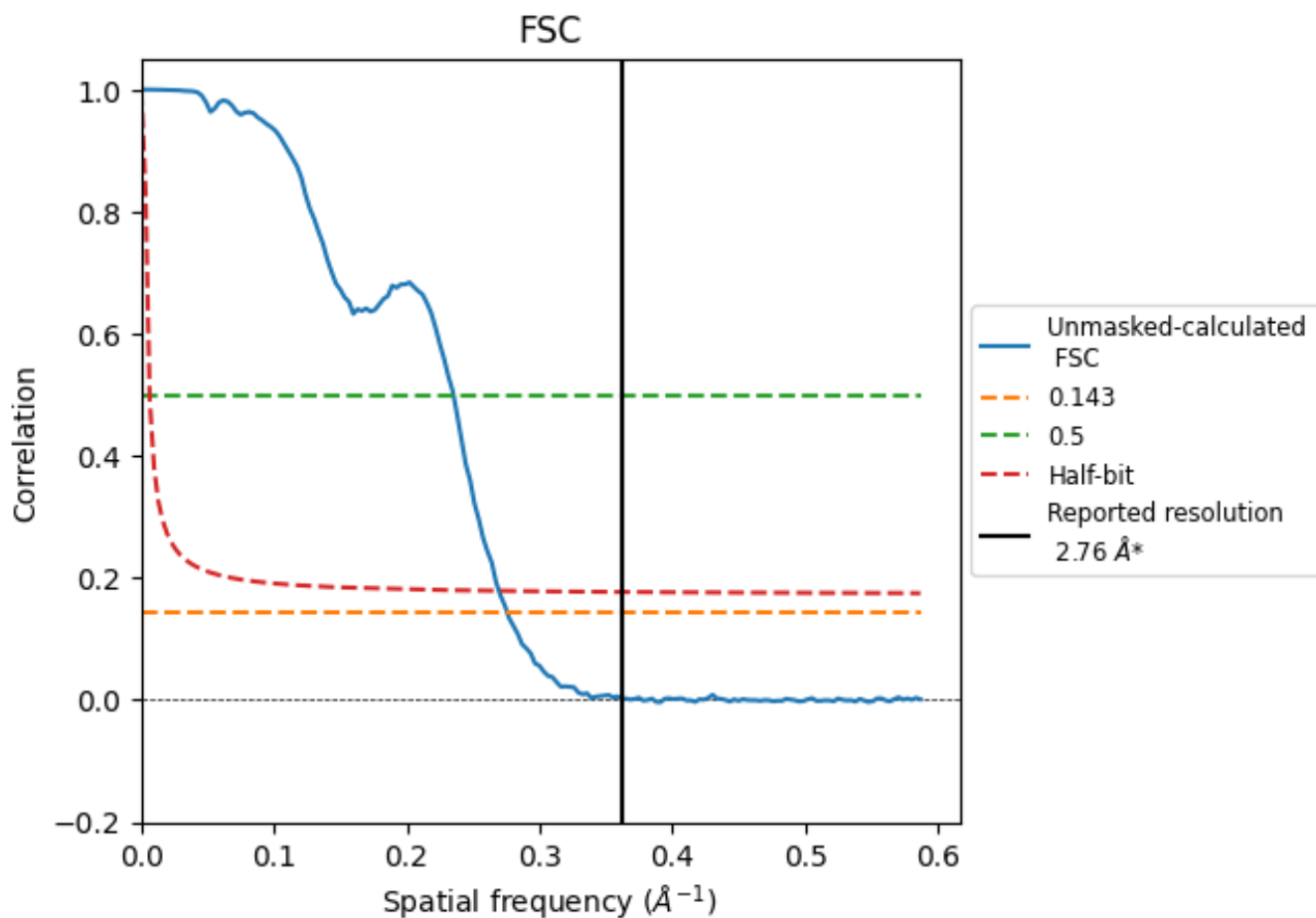


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

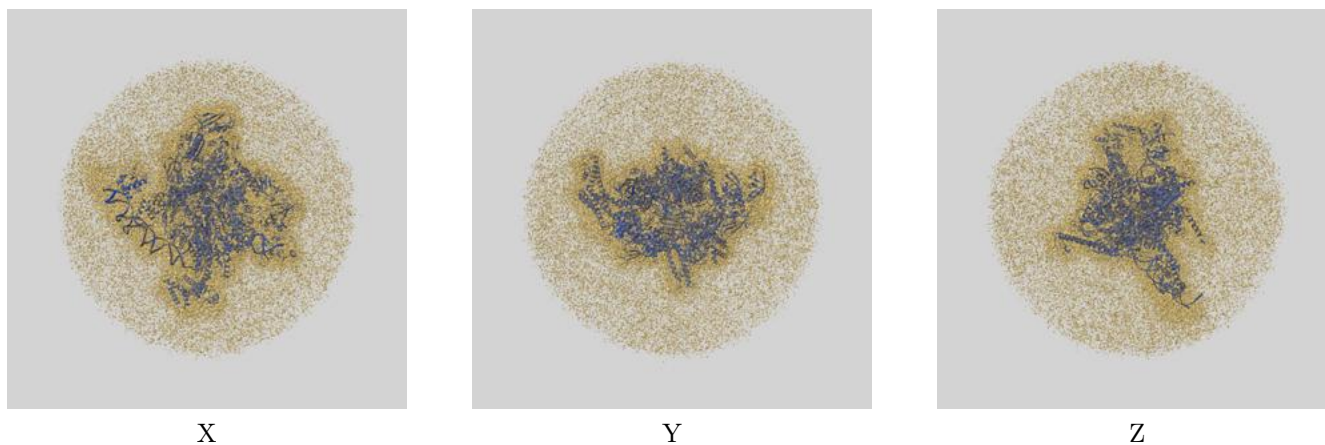
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.25	3.71

*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 3.63 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

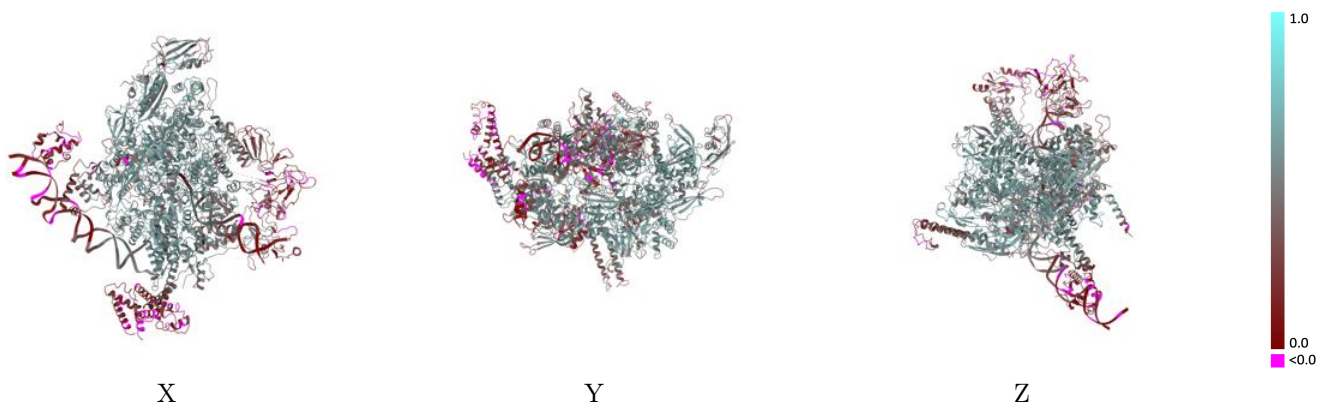
This section contains information regarding the fit between EMDB map EMD-29423 and PDB model 8FTD. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



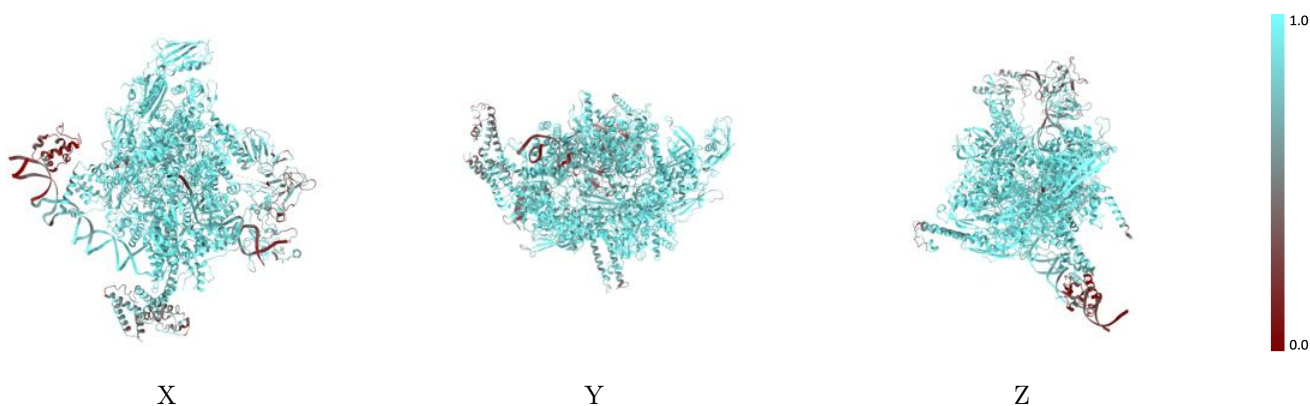
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



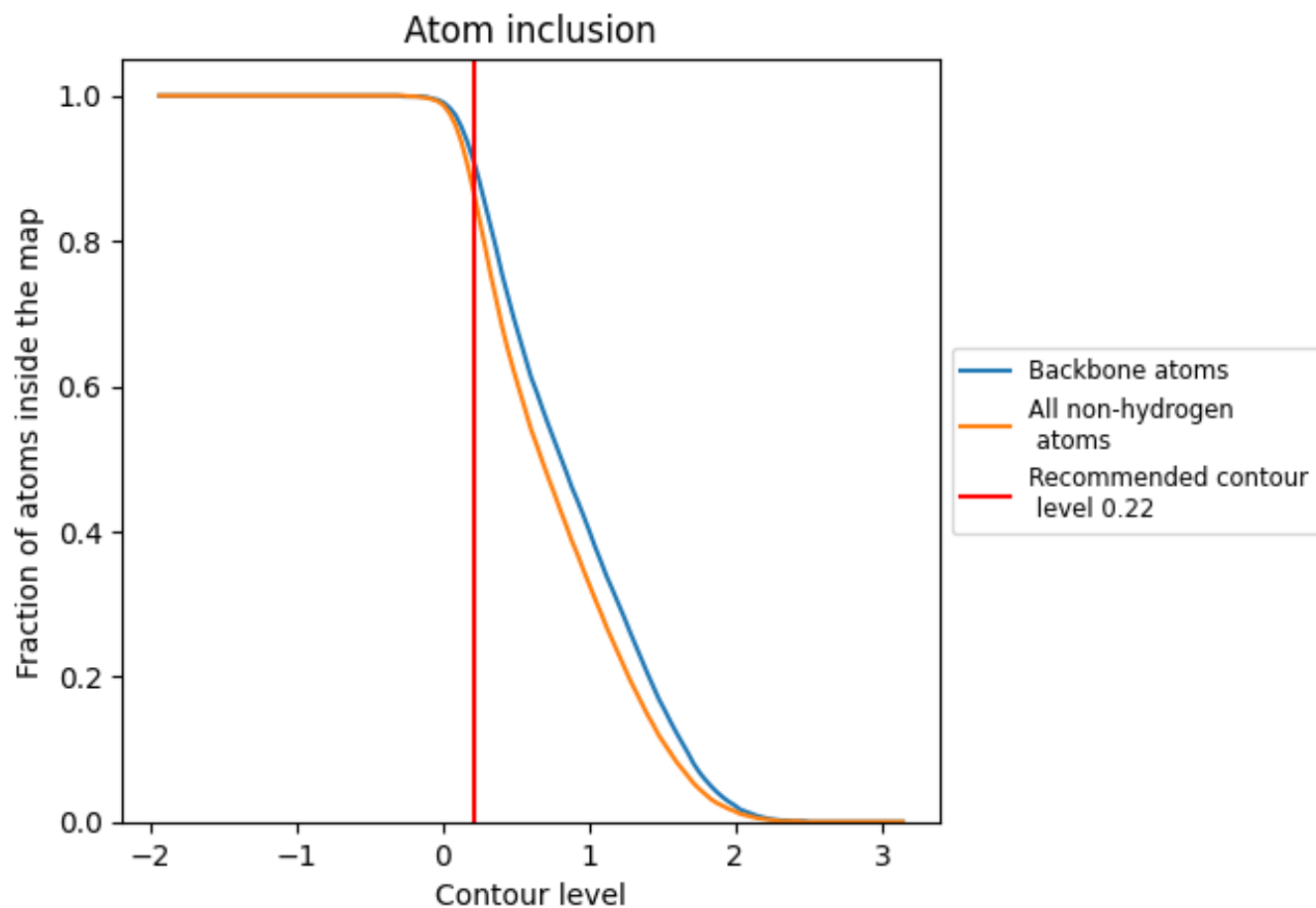
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).























9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.4560
G	 0.9340	 0.5380
H	 0.9100	 0.4930
I	 0.9210	 0.5250
J	 0.8870	 0.4850
K	 0.8950	 0.5160
L	 0.7870	 0.3300
P	 0.6980	 0.2840
Q	 0.6470	 0.2420
R	 0.2250	 0.1140
Z	 0.6690	 0.2270

