



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:15 PM UTC

PDB ID : 6XTX / pdb_00006xtx
EMDB ID : EMD-10619
Title : CryoEM structure of human CMG bound to ATPgammaS and DNA
Authors : Rzechorzek, N.J.; Pellegrini, L.
Deposited on : 2020-01-16
Resolution : 3.29 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:

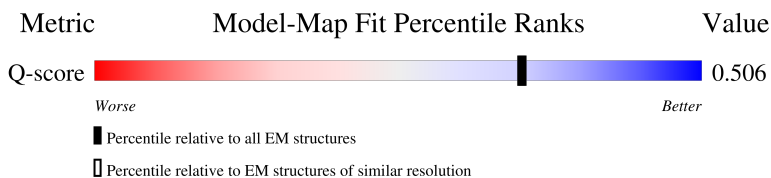
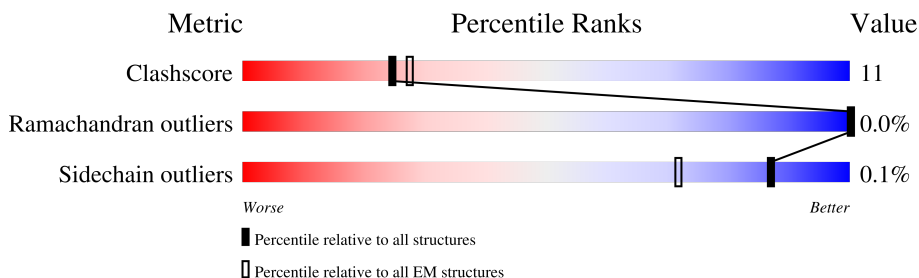
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.29 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	14466 (2.79 - 3.79)

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	2	904	14% 51% 25% 24%
2	3	853	53% 18% 29%
3	4	883	50% 18% 32%
4	5	734	7% 56% 22% 21%

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Mol	Chain	Length	Quality of chain
5	6	821	
6	7	719	
7	A	196	
8	B	222	
9	C	216	
10	D	223	
11	E	566	
12	M	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40834 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	691	Total	C	N	O	S	0	0
			5514	3471	988	1023	32		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	608	Total	C	N	O	S	0	0
			4782	2997	844	916	25		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	598	Total	C	N	O	S	0	0
			4784	3016	850	892	26		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-19	MET	-	initiating methionine	UNP P33991
4	-18	HIS	-	expression tag	UNP P33991
4	-17	HIS	-	expression tag	UNP P33991
4	-16	HIS	-	expression tag	UNP P33991
4	-15	HIS	-	expression tag	UNP P33991
4	-14	HIS	-	expression tag	UNP P33991
4	-13	HIS	-	expression tag	UNP P33991
4	-12	HIS	-	expression tag	UNP P33991
4	-11	HIS	-	expression tag	UNP P33991
4	-10	GLU	-	expression tag	UNP P33991
4	-9	ASN	-	expression tag	UNP P33991
4	-8	LEU	-	expression tag	UNP P33991
4	-7	TYR	-	expression tag	UNP P33991
4	-6	PHE	-	expression tag	UNP P33991
4	-5	GLN	-	expression tag	UNP P33991

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Chain	Residue	Modelled	Actual	Comment	Reference
4	-4	GLY	-	expression tag	UNP P33991
4	-3	SER	-	expression tag	UNP P33991
4	-2	SER	-	expression tag	UNP P33991
4	-1	ALA	-	expression tag	UNP P33991
4	0	THR	-	expression tag	UNP P33991

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	577	Total	C	N	O	S	0	0
			4524	2841	805	843	35		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	679	Total	C	N	O	S	0	0
			5473	3448	965	1033	27		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	598	Total	C	N	O	S	0	0
			4727	2960	837	901	29		

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	196	Total	C	N	O	S	0	0
			1613	1016	290	295	12		

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	176	Total	C	N	O	S	0	0
			1431	916	242	264	9		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	GLU	-	expression tag	UNP Q9Y248
B	187	ASN	-	expression tag	UNP Q9Y248

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Chain	Residue	Modelled	Actual	Comment	Reference
B	188	LEU	-	expression tag	UNP Q9Y248
B	189	TYR	-	expression tag	UNP Q9Y248
B	190	PHE	-	expression tag	UNP Q9Y248
B	191	GLN	-	expression tag	UNP Q9Y248
B	192	GLY	-	expression tag	UNP Q9Y248
B	193	SER	-	expression tag	UNP Q9Y248
B	194	ALA	-	expression tag	UNP Q9Y248
B	195	TRP	-	expression tag	UNP Q9Y248
B	196	SER	-	expression tag	UNP Q9Y248
B	197	HIS	-	expression tag	UNP Q9Y248
B	198	PRO	-	expression tag	UNP Q9Y248
B	199	GLN	-	expression tag	UNP Q9Y248
B	200	PHE	-	expression tag	UNP Q9Y248
B	201	GLU	-	expression tag	UNP Q9Y248
B	202	LYS	-	expression tag	UNP Q9Y248
B	203	GLY	-	expression tag	UNP Q9Y248
B	204	GLY	-	expression tag	UNP Q9Y248
B	205	GLY	-	expression tag	UNP Q9Y248
B	206	SER	-	expression tag	UNP Q9Y248
B	207	GLY	-	expression tag	UNP Q9Y248
B	208	GLY	-	expression tag	UNP Q9Y248
B	209	GLY	-	expression tag	UNP Q9Y248
B	210	SER	-	expression tag	UNP Q9Y248
B	211	GLY	-	expression tag	UNP Q9Y248
B	212	GLY	-	expression tag	UNP Q9Y248
B	213	SER	-	expression tag	UNP Q9Y248
B	214	ALA	-	expression tag	UNP Q9Y248
B	215	TRP	-	expression tag	UNP Q9Y248
B	216	SER	-	expression tag	UNP Q9Y248
B	217	HIS	-	expression tag	UNP Q9Y248
B	218	PRO	-	expression tag	UNP Q9Y248
B	219	GLN	-	expression tag	UNP Q9Y248
B	220	PHE	-	expression tag	UNP Q9Y248
B	221	GLU	-	expression tag	UNP Q9Y248
B	222	LYS	-	expression tag	UNP Q9Y248

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	194	Total	C	N	O	S	0	0
			1552	985	268	293	6		

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	203	Total	C	N	O	S	0	0
			1679	1065	290	314	10		

- Molecule 11 is a protein called Cell division control protein 45 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	538	Total	C	N	O	S	0	0
			4380	2785	751	813	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	346	GLN	GLU	variant	UNP O75419

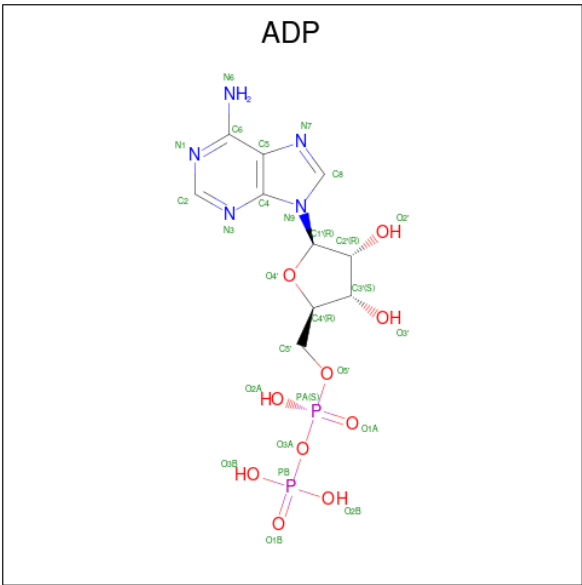
- Molecule 12 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*T P*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	11	Total	C	N	O	P	0	0
			220	110	22	77	11		

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

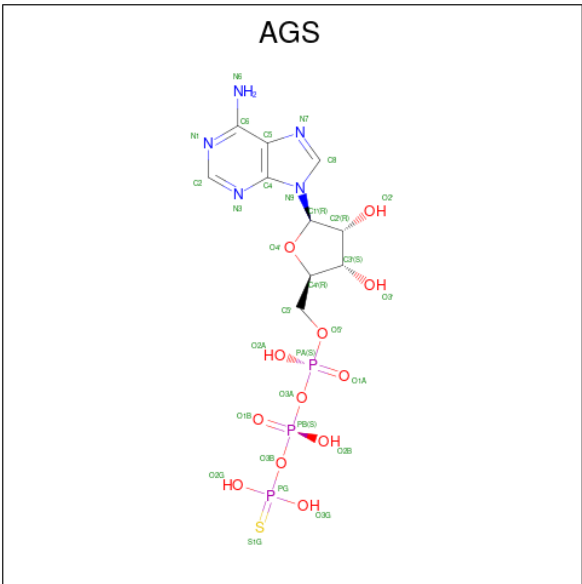
Mol	Chain	Residues	Atoms		AltConf
13	2	1	Total	Zn	0
			1	1	
13	4	1	Total	Zn	0
			1	1	
13	5	1	Total	Zn	0
			1	1	
13	6	1	Total	Zn	0
			1	1	
13	7	1	Total	Zn	0
			1	1	

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
15	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
15	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
15	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

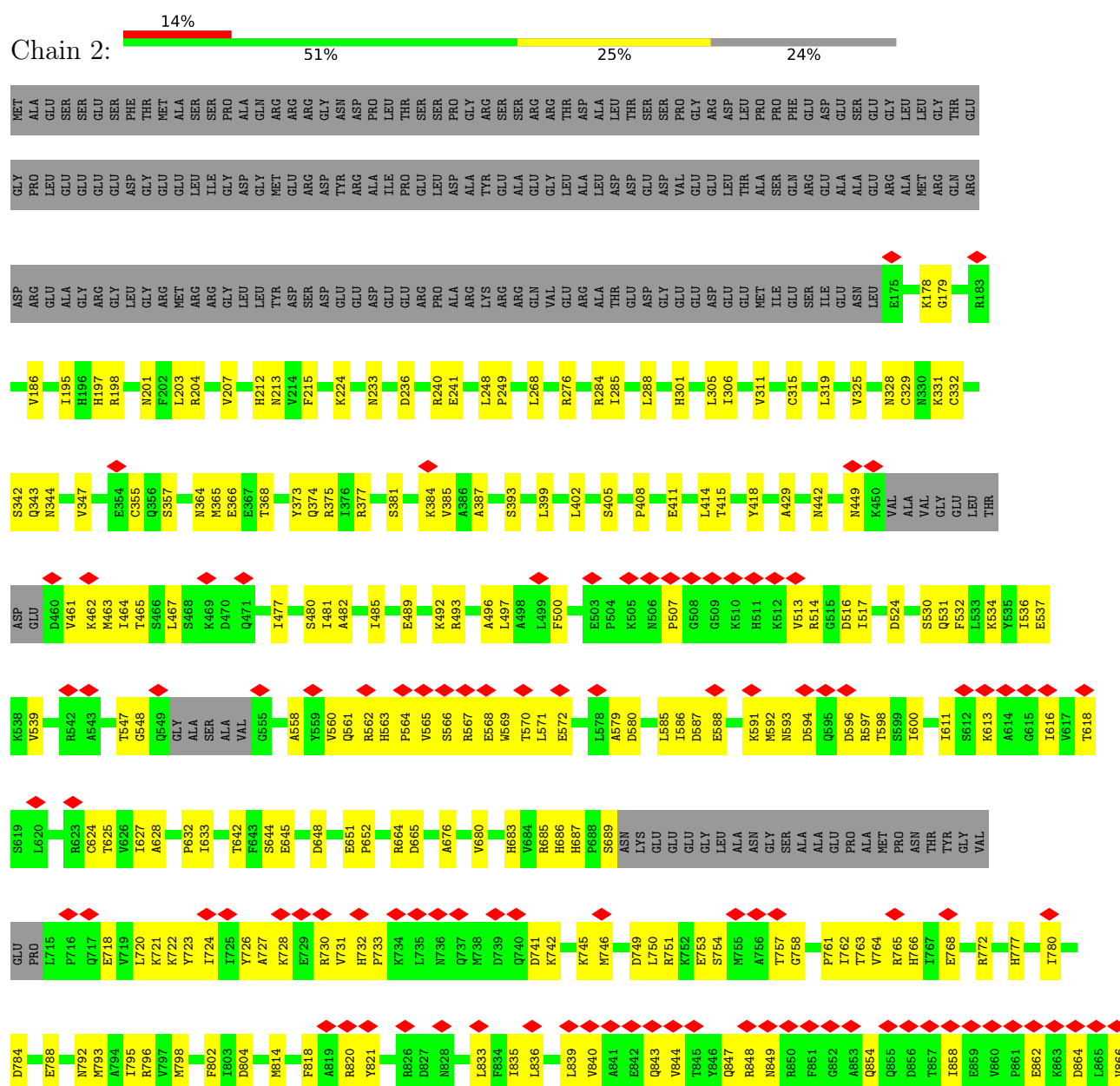
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

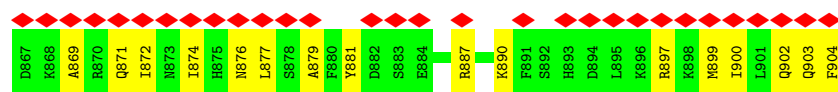
Mol	Chain	Residues	Atoms		AltConf
16	4	1	Total	Mg	0
			1	1	
16	6	1	Total	Mg	0
			1	1	
16	7	1	Total	Mg	0
			1	1	

3 Residue-property plots

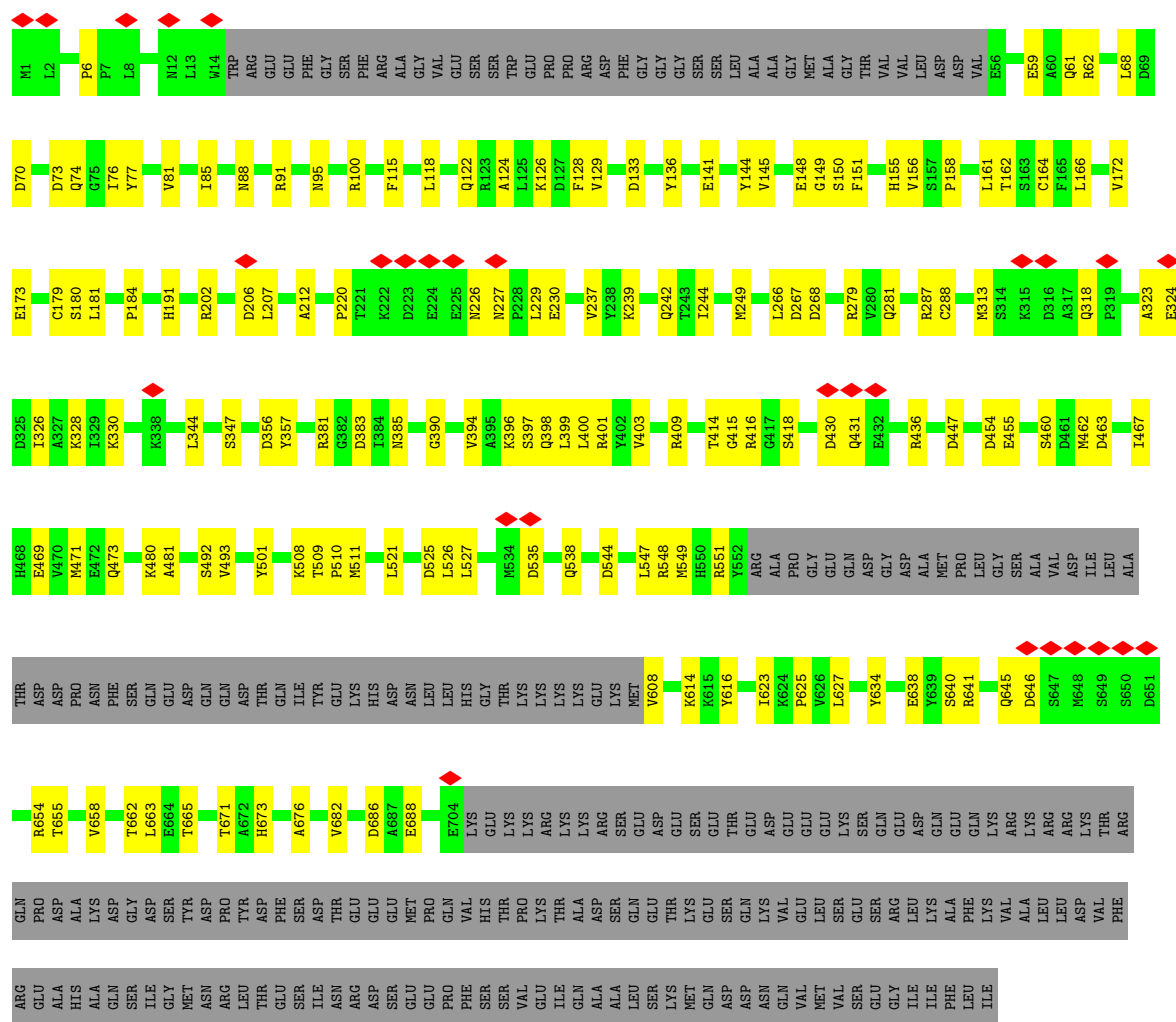
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA replication licensing factor MCM2

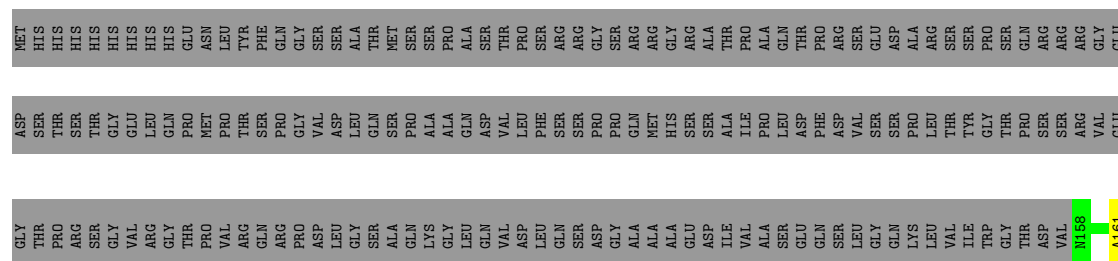


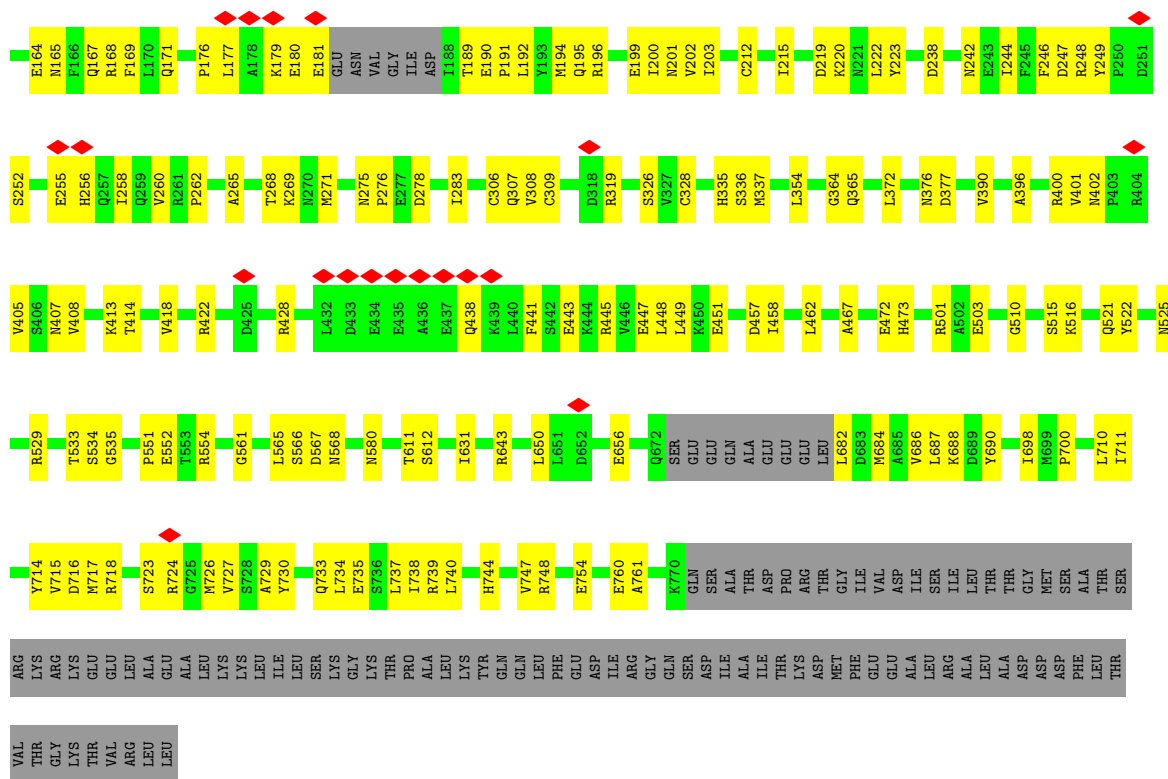


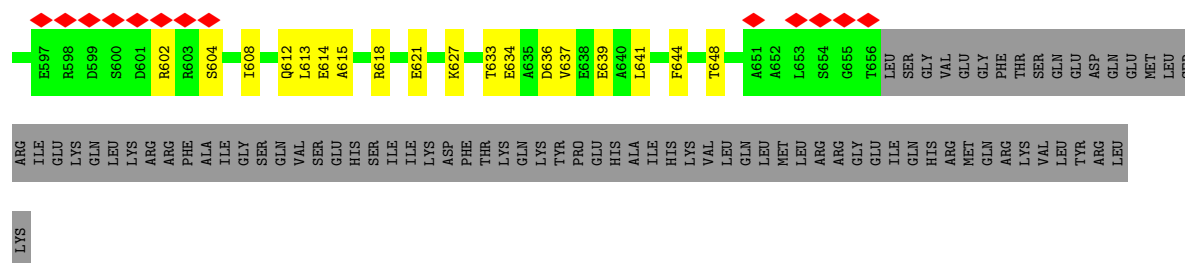
• Molecule 2: DNA replication licensing factor MCM3



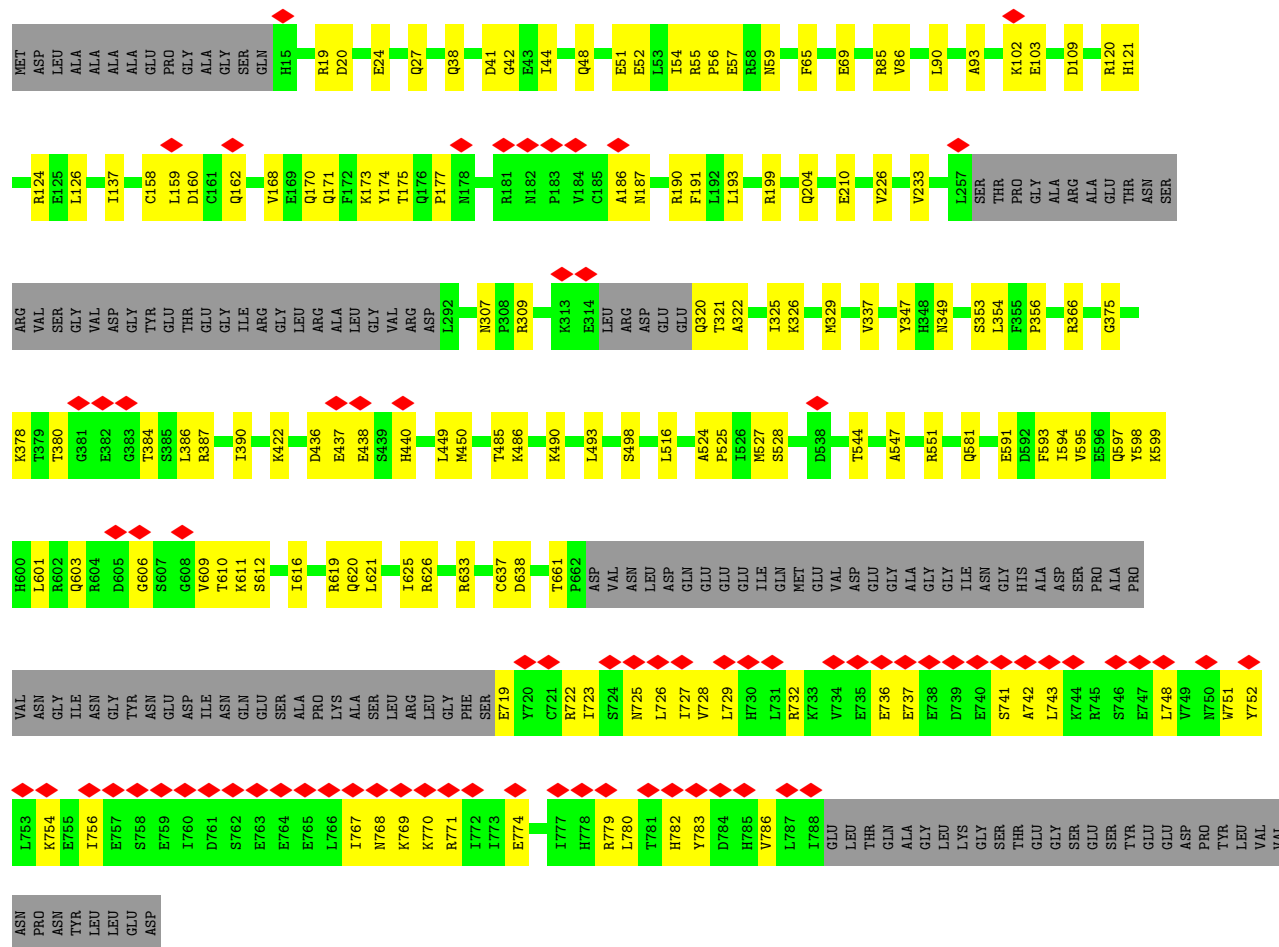
• Molecule 3: DNA replication licensing factor MCM4





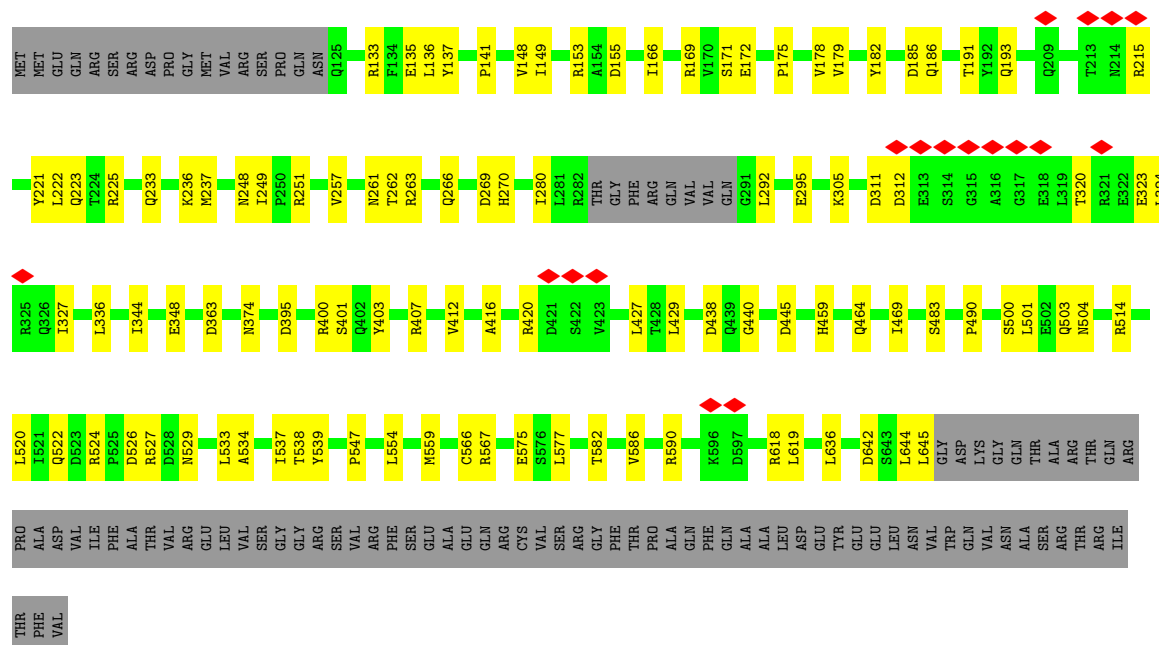


• Molecule 5: DNA replication licensing factor MCM6



• Molecule 6: DNA replication licensing factor MCM7



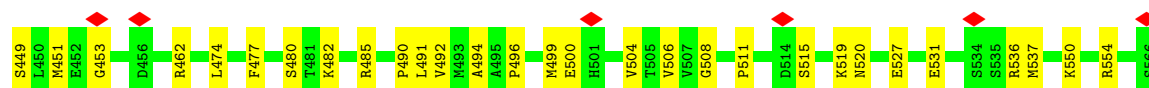
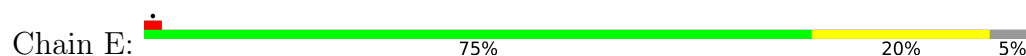




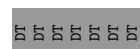
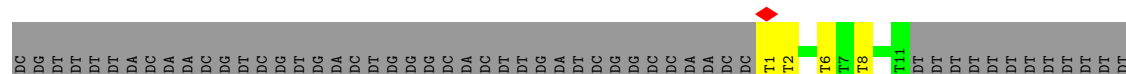
- Molecule 10: DNA replication complex GINS protein SLD5



- Molecule 11: Cell division control protein 45 homolog



- Molecule 12: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: ZN, MG, ADP, AGS

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	2	0.31	0/5616	0.42	0/7576
2	3	0.36	0/4859	0.45	0/6563
3	4	0.43	0/4870	0.47	1/6579 (0.0%)
4	5	0.38	0/4590	0.45	0/6171
5	6	0.38	0/5563	0.47	0/7502
6	7	0.39	0/4801	0.44	0/6482
7	A	0.36	0/1645	0.46	0/2210
8	B	0.44	0/1462	0.45	0/1981
9	C	0.41	0/1587	0.43	0/2143
10	D	0.41	0/1711	0.45	0/2305
11	E	0.39	0/4472	0.42	0/6037
12	M	0.51	0/241	0.52	0/370
All	All	0.38	0/41417	0.45	1/55919 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	458	ILE	N-CA-C	-5.08	105.92	113.39

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	2	5514	0	5526	164	0
2	3	4782	0	4829	107	0
3	4	4784	0	4824	107	0
4	5	4524	0	4608	122	0
5	6	5473	0	5506	104	0
6	7	4727	0	4757	96	0
7	A	1613	0	1606	51	0
8	B	1431	0	1456	30	0
9	C	1552	0	1504	35	0
10	D	1679	0	1700	36	0
11	E	4380	0	4332	76	0
12	M	220	0	133	4	0
13	2	1	0	0	0	0
13	4	1	0	0	0	0
13	5	1	0	0	0	0
13	6	1	0	0	0	0
13	7	1	0	0	0	0
14	2	27	0	12	1	0
14	3	27	0	12	0	0
15	4	62	0	24	3	0
15	7	31	0	12	2	0
16	4	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
All	All	40834	0	40841	863	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 11.

All (863) 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)
4:5:531:MET:HA	4:5:534:LYS:HE2	1.58	0.85
11:E:389:LYS:HZ1	11:E:462:ARG:HD2	1.47	0.80
7:A:98:LEU:H	7:A:103:ARG:HH21	1.31	0.79
2:3:347:SER:HG	2:3:608:VAL:N	1.82	0.78
8:B:129:ARG:NH2	9:C:151:ASP:OD2	2.16	0.78
5:6:159:LEU:HB3	5:6:187:ASN:HD21	1.48	0.78
9:C:34:VAL:HG12	9:C:86:VAL:HG12	1.65	0.77
2:3:397:SER:HB3	4:5:464:GLN:HE22	1.50	0.77
3:4:161:ALA:O	3:4:165:ASN:ND2	2.18	0.77
1:2:561:GLN:HE22	1:2:564:PRO:HD3	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:100:ARG:NH2	2:3:150:SER:O	2.20	0.74
3:4:191:PRO:HB2	3:4:194:MET:HB2	1.70	0.73
4:5:537:ILE:HA	4:5:540:HIS:HB3	1.70	0.73
11:E:99:ASP:OD1	11:E:100:THR:N	2.22	0.73
2:3:658:VAL:HG23	2:3:662:THR:HG21	1.71	0.73
5:6:54:ILE:HD11	5:6:103:GLU:HB2	1.71	0.73
7:A:179:ARG:NH2	7:A:183:GLU:OE2	2.23	0.72
5:6:187:ASN:ND2	5:6:190:ARG:O	2.23	0.72
5:6:27:GLN:HG3	5:6:93:ALA:HB2	1.73	0.71
4:5:40:ARG:NH2	8:B:119:ASP:OD2	2.24	0.70
5:6:307:ASN:O	5:6:309:ARG:NH1	2.23	0.70
8:B:7:GLU:OE1	9:C:189:TRP:NE1	2.21	0.70
2:3:230:GLU:OE1	6:7:72:ARG:NH2	2.25	0.70
1:2:890:LYS:O	1:2:902:GLN:NE2	2.25	0.70
11:E:287:HIS:HB2	11:E:325:VAL:HG12	1.73	0.69
11:E:263:LEU:HD23	11:E:269:ARG:HH21	1.57	0.69
14:2:1001:ADP:O3A	5:6:619:ARG:NH2	2.26	0.69
2:3:70:ASP:OD2	2:3:77:TYR:N	2.26	0.69
8:B:136:VAL:HG13	8:B:167:MET:HE1	1.74	0.68
1:2:580:ASP:HB3	4:5:238:HIS:CD2	2.28	0.68
1:2:848:ARG:HH21	5:6:609:VAL:HG12	1.58	0.68
1:2:325:VAL:HA	1:2:368:THR:HG23	1.74	0.68
4:5:56:ARG:NH2	8:B:119:ASP:OD1	2.24	0.68
5:6:752:TYR:HE1	5:6:756:ILE:HD12	1.59	0.68
1:2:593:ASN:ND2	1:2:596:ASP:OD2	2.27	0.68
3:4:219:ASP:OD1	3:4:220:LYS:N	2.26	0.68
1:2:818:PHE:HA	1:2:821:TYR:HB3	1.75	0.68
3:4:335:HIS:O	3:4:335:HIS:ND1	2.27	0.68
5:6:390:ILE:O	5:6:498:SER:OG	2.12	0.67
1:2:365:MET:HB2	4:5:273:LYS:HZ1	1.60	0.67
1:2:301:HIS:HB3	1:2:306:ILE:HD11	1.77	0.67
11:E:447:TYR:OH	11:E:554:ARG:NH2	2.28	0.67
1:2:328:ASN:HD22	1:2:364:ASN:HB2	1.60	0.67
1:2:757:THR:HG22	1:2:758:GLY:H	1.60	0.67
5:6:725:ASN:HA	5:6:728:VAL:HG12	1.74	0.67
3:4:400:ARG:HG2	3:4:408:VAL:HG12	1.76	0.66
5:6:20:ASP:OD1	5:6:85:ARG:NH2	2.28	0.66
2:3:91:ARG:NH2	2:3:268:ASP:OD1	2.28	0.66
2:3:645:GLN:OE1	2:3:654:ARG:NH2	2.29	0.66
7:A:144:LYS:NZ	8:B:11:GLU:OE2	2.28	0.66
2:3:151:PHE:H	2:3:155:HIS:HE1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:198:ARG:NH2	1:2:241:GLU:OE2	2.29	0.66
1:2:507:PRO:HD3	1:2:513:VAL:HG12	1.77	0.66
7:A:149:GLU:OE2	7:A:174:GLN:NE2	2.28	0.66
1:2:754:SER:HB2	1:2:761:PRO:HB3	1.75	0.66
3:4:726:MET:HG3	3:4:727:VAL:H	1.59	0.66
10:D:22:THR:HG22	10:D:24:ALA:H	1.60	0.65
1:2:514:ARG:O	1:2:772:ARG:NH1	2.30	0.65
10:D:71:GLU:OE1	10:D:73:LEU:N	2.25	0.65
7:A:74:ARG:NH2	9:C:18:ASN:O	2.29	0.65
1:2:733:PRO:HA	1:2:784:ASP:HB3	1.79	0.65
8:B:51:ASN:ND2	10:D:80:MET:SD	2.70	0.65
11:E:323:LYS:HG3	11:E:324:GLN:HE21	1.62	0.65
1:2:204:ARG:O	1:2:213:ASN:ND2	2.28	0.65
8:B:23:LEU:HB3	8:B:36:PHE:HD2	1.61	0.65
11:E:28:ASP:OD1	11:E:197:SER:OG	2.15	0.65
3:4:643:ARG:NH2	15:4:904:AGS:S1G	2.70	0.64
2:3:162:THR:OG1	2:3:164:CYS:SG	2.54	0.64
3:4:246:PHE:HA	3:4:249:TYR:CD2	2.32	0.64
4:5:441:VAL:HG22	4:5:483:SER:HB2	1.78	0.64
1:2:876:ASN:HD21	1:2:879:ALA:HB3	1.62	0.64
11:E:448:CYS:SG	11:E:449:SER:N	2.70	0.64
5:6:436:ASP:O	5:6:440:HIS:N	2.31	0.64
5:6:723:ILE:HG13	5:6:726:LEU:HD12	1.79	0.64
8:B:175:GLN:HB2	10:D:188:THR:HG21	1.80	0.64
4:5:421:ASP:HB3	4:5:424:SER:OG	1.98	0.63
10:D:21:LEU:HD21	10:D:29:ARG:HH12	1.63	0.63
2:3:544:ASP:OD2	2:3:548:ARG:NH2	2.31	0.63
9:C:35:ARG:NH1	9:C:37:GLU:OE2	2.30	0.63
2:3:381:ARG:NH2	2:3:385:ASN:OD1	2.28	0.63
2:3:61:GLN:HG3	2:3:124:ALA:HB2	1.79	0.63
1:2:402:LEU:O	1:2:405:SER:OG	2.12	0.63
1:2:489:GLU:HA	1:2:492:LYS:HD2	1.81	0.63
5:6:768:ASN:OD1	5:6:771:ARG:NH1	2.32	0.63
6:7:416:ALA:HB3	6:7:469:ILE:HD11	1.80	0.63
7:A:149:GLU:OE1	11:E:41:GLN:NE2	2.32	0.63
4:5:416:ALA:HA	4:5:430:GLU:O	1.97	0.62
4:5:347:THR:O	4:5:351:LYS:N	2.32	0.62
1:2:742:LYS:HD2	1:2:788:GLU:HG3	1.82	0.62
4:5:528:ARG:HA	4:5:531:MET:HE2	1.80	0.62
1:2:485:ILE:HD11	1:2:531:GLN:HB2	1.80	0.62
5:6:187:ASN:HB2	5:6:190:ARG:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:500:PHE:O	1:2:728:LYS:NZ	2.33	0.62
3:4:365:GLN:NE2	6:7:266:GLN:OE1	2.32	0.62
5:6:594:ILE:HD13	5:6:625:ILE:HG22	1.82	0.62
1:2:664:ARG:NH1	1:2:665:ASP:O	2.33	0.62
1:2:683:HIS:CE1	5:6:386:LEU:HD13	2.35	0.62
4:5:167:ARG:HH11	4:5:181:ASN:HA	1.63	0.62
6:7:520:LEU:HD23	6:7:644:LEU:HD11	1.82	0.62
6:7:311:ASP:OD1	6:7:312:ASP:N	2.32	0.61
2:3:663:LEU:HD23	6:7:537:ILE:HD12	1.83	0.61
5:6:124:ARG:NH2	5:6:210:GLU:OE2	2.34	0.61
6:7:56:ALA:HB2	6:7:63:VAL:HG21	1.82	0.61
9:C:7:ARG:NH2	9:C:23:ASP:OD2	2.33	0.61
6:7:403:TYR:OH	6:7:445:ASP:OD2	2.19	0.60
10:D:175:VAL:HG12	10:D:220:VAL:HG12	1.83	0.60
1:2:872:ILE:HG23	1:2:874:ILE:HG12	1.83	0.60
2:3:115:PHE:CZ	2:3:287:ARG:HD3	2.35	0.60
4:5:174:SER:OG	4:5:207:CYS:SG	2.60	0.60
1:2:477:ILE:O	1:2:480:SER:OG	2.19	0.60
1:2:580:ASP:HB3	4:5:238:HIS:HD2	1.67	0.60
3:4:718:ARG:NH1	3:4:729:ALA:O	2.31	0.60
5:6:159:LEU:HB3	5:6:187:ASN:ND2	2.16	0.60
5:6:598:TYR:HB2	5:6:621:LEU:HD13	1.84	0.60
2:3:344:LEU:HD11	2:3:616:TYR:HE2	1.67	0.60
5:6:109:ASP:OD1	5:6:109:ASP:N	2.34	0.60
2:3:212:ALA:HB2	2:3:287:ARG:HH22	1.67	0.59
6:7:324:LEU:HA	6:7:327:ILE:HG22	1.84	0.59
1:2:355:CYS:SG	1:2:357:SER:OG	2.59	0.59
1:2:897:ARG:HB3	1:2:899:MET:HG2	1.83	0.59
1:2:762:ILE:HG23	1:2:766:HIS:HB2	1.84	0.59
2:3:6:PRO:HD2	2:3:149:GLY:O	2.02	0.59
5:6:611:LYS:NZ	5:6:612:SER:O	2.35	0.59
6:7:374:ASN:HB3	6:7:483:SER:HB3	1.84	0.59
2:3:173:GLU:HG3	2:3:281:GLN:HG2	1.83	0.59
6:7:222:LEU:HD12	6:7:223:GLN:H	1.66	0.59
1:2:329:CYS:HB3	1:2:332:CYS:SG	2.42	0.59
3:4:402:ASN:HB2	3:4:405:VAL:HG22	1.83	0.59
2:3:173:GLU:N	2:3:173:GLU:OE1	2.36	0.59
5:6:752:TYR:CE1	5:6:756:ILE:HD12	2.37	0.59
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.84	0.59
1:2:463:MET:O	1:2:467:LEU:HG	2.03	0.59
1:2:562:ARG:HD3	12:M:2:DT:H3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:247:ASP:HB2	3:4:248:ARG:HD2	1.85	0.59
9:C:204:GLN:N	9:C:204:GLN:OE1	2.36	0.59
1:2:343:GLN:HA	4:5:287:VAL:HG11	1.84	0.59
7:A:43:ASN:O	7:A:47:VAL:HG23	2.02	0.59
1:2:514:ARG:NH2	1:2:516:ASP:O	2.36	0.58
2:3:641:ARG:HA	6:7:527:ARG:HH12	1.68	0.58
11:E:257:GLU:HG2	11:E:258:ASP:N	2.19	0.58
1:2:563:HIS:HD2	1:2:565:VAL:H	1.49	0.58
5:6:52:GLU:OE2	5:6:55:ARG:NH1	2.35	0.58
9:C:106:VAL:O	9:C:167:ARG:NH2	2.36	0.58
10:D:29:ARG:HE	10:D:50:ILE:HD11	1.68	0.58
1:2:731:VAL:O	1:2:732:HIS:ND1	2.36	0.58
4:5:507:MET:HB2	4:5:510:ILE:HG22	1.83	0.58
4:5:528:ARG:O	4:5:532:LEU:HG	2.02	0.58
1:2:848:ARG:HH12	5:6:606:GLY:HA3	1.68	0.58
2:3:409:ARG:NH2	2:3:447:ASP:O	2.24	0.58
7:A:62:ILE:O	7:A:66:HIS:N	2.34	0.58
2:3:430:ASP:O	4:5:425:ARG:NH2	2.36	0.58
4:5:439:GLY:N	4:5:481:ARG:O	2.37	0.58
7:A:111:MET:O	7:A:115:ASN:ND2	2.29	0.58
11:E:385:GLU:OE1	11:E:462:ARG:NE	2.37	0.58
6:7:171:SER:OG	6:7:172:GLU:N	2.35	0.58
1:2:315:CYS:HB2	1:2:374:GLN:HE21	1.69	0.58
3:4:278:ASP:HB3	3:4:283:ILE:HD11	1.85	0.58
4:5:231:GLU:OE2	4:5:243:ARG:N	2.28	0.58
4:5:170:ILE:HG22	4:5:214:ILE:HD13	1.86	0.57
1:2:763:THR:HG22	1:2:764:VAL:H	1.69	0.57
8:B:2:ASP:N	8:B:2:ASP:OD1	2.35	0.57
1:2:517:ILE:O	1:2:625:THR:OG1	2.21	0.57
7:A:194:ILE:HG13	7:A:195:LEU:H	1.70	0.57
2:3:141:GLU:OE1	2:3:237:VAL:HG11	2.03	0.57
2:3:527:LEU:HD23	2:3:655:THR:HB	1.87	0.57
4:5:325:LEU:HA	4:5:328:LEU:HD23	1.86	0.57
10:D:37:GLU:HG3	10:D:92:TYR:HE1	1.70	0.57
3:4:306:CYS:SG	3:4:308:VAL:N	2.67	0.57
3:4:510:GLY:O	3:4:516:LYS:NZ	2.36	0.57
8:B:78:GLU:OE1	8:B:85:THR:OG1	2.22	0.57
9:C:168:LEU:O	9:C:173:ARG:NH1	2.38	0.57
1:2:384:LYS:HG2	1:2:385:VAL:HG23	1.85	0.57
1:2:835:ILE:O	1:2:839:LEU:HG	2.05	0.57
3:4:390:VAL:HG23	3:4:418:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:567:ARG:O	6:7:618:ARG:NH1	2.38	0.57
9:C:169:ASP:OD1	9:C:169:ASP:N	2.37	0.57
2:3:462:MET:O	6:7:407:ARG:NH1	2.38	0.56
3:4:200:ILE:HG21	3:4:258:ILE:HD11	1.87	0.56
1:2:377:ARG:NH2	1:2:393:SER:OG	2.37	0.56
6:7:5:ASP:OD1	6:7:6:TYR:N	2.36	0.56
6:7:178:VAL:HG12	6:7:179:VAL:HG23	1.87	0.56
11:E:386:SER:O	11:E:389:LYS:NZ	2.33	0.56
3:4:566:SER:OG	3:4:567:ASP:N	2.34	0.56
4:5:377:LEU:HB2	4:5:485:LEU:HD12	1.87	0.56
11:E:536:ARG:HE	11:E:550:LYS:HE2	1.69	0.56
5:6:329:MET:HE1	5:6:337:VAL:HG21	1.88	0.56
10:D:123:SER:HB3	10:D:126:GLU:HG3	1.87	0.56
7:A:135:ASP:OD2	7:A:138:GLN:NE2	2.32	0.56
9:C:78:ASP:CG	9:C:82:ARG:H	2.14	0.56
1:2:840:VAL:O	1:2:844:VAL:HG23	2.05	0.56
1:2:325:VAL:HG11	1:2:347:VAL:HG11	1.88	0.56
2:3:640:SER:O	6:7:527:ARG:NH1	2.39	0.56
5:6:174:TYR:OH	5:6:193:LEU:HD22	2.06	0.56
2:3:662:THR:O	2:3:665:THR:HG22	2.06	0.56
3:4:199:GLU:HA	3:4:202:VAL:HG12	1.88	0.56
4:5:586:TYR:CZ	4:5:590:ARG:HD2	2.40	0.56
4:5:380:LEU:HA	4:5:488:ALA:HB3	1.88	0.55
2:3:73:ASP:OD1	2:3:74:GLN:N	2.37	0.55
3:4:716:ASP:OD1	3:4:717:MET:N	2.39	0.55
4:5:172:CYS:HB3	4:5:177:ASN:H	1.70	0.55
4:5:380:LEU:O	4:5:520:VAL:N	2.31	0.55
4:5:565:TYR:CE1	4:5:569:LYS:HG3	2.41	0.55
1:2:680:VAL:HG11	5:6:591:GLU:HG3	1.88	0.55
1:2:765:ARG:HG3	1:2:765:ARG:O	2.06	0.55
5:6:601:LEU:HG	5:6:616:ILE:HD13	1.88	0.55
6:7:40:LEU:HD23	6:7:45:GLN:HB3	1.87	0.55
6:7:459:HIS:O	6:7:514:ARG:NH1	2.32	0.55
3:4:242:ASN:O	3:4:249:TYR:OH	2.16	0.55
11:E:282:GLN:O	11:E:330:GLN:NE2	2.39	0.55
11:E:443:GLY:O	11:E:485:ARG:NH2	2.39	0.55
3:4:328:CYS:SG	3:4:336:SER:OG	2.65	0.55
3:4:533:THR:HG22	3:4:534:SER:H	1.70	0.55
2:3:244:ILE:HD13	2:3:266:LEU:HD11	1.89	0.55
3:4:189:THR:HB	3:4:195:GLN:HE22	1.71	0.55
3:4:405:VAL:HG23	3:4:407:ASN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:37:GLU:OE1	4:5:41:GLN:NE2	2.40	0.55
2:3:385:ASN:HD22	2:3:493:VAL:H	1.54	0.55
1:2:592:MET:HE3	1:2:597:ARG:HG2	1.89	0.55
2:3:509:THR:HG23	2:3:511:MET:H	1.71	0.55
5:6:170:GLN:OE1	5:6:170:GLN:N	2.40	0.55
1:2:741:ASP:O	1:2:745:LYS:NZ	2.30	0.54
4:5:372:ARG:HB2	4:5:618:ARG:NH2	2.22	0.54
5:6:719:GLU:OE2	5:6:722:ARG:NH1	2.40	0.54
6:7:169:ARG:HH11	6:7:236:LYS:HD3	1.71	0.54
7:A:162:ASP:OD2	7:A:181:LYS:NZ	2.39	0.54
1:2:570:THR:OG1	1:2:571:LEU:N	2.41	0.54
2:3:397:SER:CB	4:5:464:GLN:HE22	2.20	0.54
2:3:416:ARG:HG2	4:5:456:VAL:HG11	1.88	0.54
3:4:656:GLU:OE2	6:7:590:ARG:NH2	2.40	0.54
2:3:267:ASP:OD2	2:3:268:ASP:N	2.40	0.54
6:7:500:SER:O	6:7:504:ASN:ND2	2.41	0.54
11:E:230:GLN:NE2	11:E:381:MET:SD	2.79	0.54
4:5:380:LEU:HD23	4:5:381:GLY:N	2.23	0.54
6:7:135:GLU:HG3	6:7:137:TYR:CZ	2.43	0.54
10:D:106:HIS:NE2	10:D:162:VAL:O	2.39	0.54
2:3:638:GLU:OE1	2:3:641:ARG:NH2	2.35	0.54
1:2:877:LEU:O	1:2:881:TYR:N	2.36	0.54
2:3:469:GLU:HA	2:3:473:GLN:OE1	2.08	0.54
3:4:354:LEU:HD13	3:4:372:LEU:HD11	1.88	0.54
6:7:269:ASP:OD1	6:7:270:HIS:N	2.40	0.54
7:A:124:TYR:O	7:A:127:SER:OG	2.26	0.54
2:3:191:HIS:HB3	2:3:229:LEU:HD22	1.90	0.53
5:6:737:GLU:HG2	5:6:742:ALA:HA	1.90	0.53
9:C:90:LYS:HA	9:C:93:GLN:HB2	1.89	0.53
10:D:178:ARG:NE	10:D:180:GLU:OE2	2.39	0.53
5:6:320:GLN:O	5:6:581:GLN:NE2	2.41	0.53
6:7:51:ASP:OD1	6:7:52:LEU:N	2.41	0.53
3:4:515:SER:HA	15:4:902:AGS:O1A	2.08	0.53
5:6:525:PRO:O	5:6:528:SER:OG	2.22	0.53
2:3:460:SER:OG	2:3:463:ASP:OD2	2.25	0.53
3:4:457:ASP:N	3:4:457:ASP:OD1	2.38	0.53
3:4:748:ARG:HH22	3:4:754:GLU:HG2	1.74	0.53
4:5:589:MET:HE1	4:5:644:PHE:HE2	1.72	0.53
7:A:129:GLY:H	7:A:133:GLY:HA2	1.73	0.53
3:4:501:ARG:O	3:4:739:ARG:NH2	2.41	0.53
3:4:179:LYS:HG3	3:4:180:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:390:GLY:O	2:3:396:LYS:NZ	2.41	0.53
2:3:627:LEU:HA	2:3:682:VAL:HG22	1.91	0.53
5:6:736:GLU:HB2	5:6:743:LEU:HD11	1.91	0.53
11:E:28:ASP:OD2	11:E:76:ASN:ND2	2.36	0.53
1:2:644:SER:OG	1:2:651:GLU:OE1	2.25	0.53
4:5:525:ASN:O	4:5:529:ASP:N	2.37	0.53
4:5:96:LEU:HD22	4:5:297:LEU:HD22	1.91	0.52
6:7:223:GLN:HE21	6:7:225:ARG:HB2	1.75	0.52
1:2:792:ASN:O	1:2:796:ARG:HB2	2.09	0.52
5:6:171:GLN:H	5:6:175:THR:HG21	1.74	0.52
1:2:366:GLU:N	1:2:366:GLU:OE2	2.42	0.52
3:4:448:LEU:O	3:4:451:GLU:HG3	2.09	0.52
5:6:743:LEU:HD22	5:6:748:LEU:HD22	1.91	0.52
8:B:144:LYS:HE2	10:D:204:HIS:CE1	2.44	0.52
5:6:109:ASP:OD2	5:6:199:ARG:NH2	2.42	0.52
8:B:144:LYS:HE2	10:D:204:HIS:HE1	1.75	0.52
1:2:687:HIS:O	1:2:689:SER:N	2.41	0.52
1:2:820:ARG:HH22	1:2:871:GLN:HB3	1.74	0.52
2:3:616:TYR:OH	2:3:676:ALA:O	2.21	0.52
6:7:280:ILE:HD12	6:7:295:GLU:HG3	1.92	0.52
7:A:161:VAL:HG13	7:A:181:LYS:NZ	2.25	0.52
1:2:592:MET:HE1	1:2:600:ILE:HG21	1.92	0.52
2:3:673:HIS:HD2	2:3:686:ASP:HA	1.74	0.52
4:5:363:LYS:NZ	4:5:621:GLU:OE2	2.42	0.52
6:7:445:ASP:OD1	6:7:445:ASP:N	2.33	0.52
6:7:642:ASP:C	6:7:644:LEU:H	2.18	0.52
11:E:496:PRO:HA	11:E:504:VAL:HG12	1.90	0.52
1:2:777:HIS:HA	1:2:780:ILE:HG22	1.92	0.52
6:7:412:VAL:HG11	12:M:8:DT:H3'	1.91	0.52
7:A:170:LYS:NZ	11:E:64:GLU:OE2	2.43	0.52
4:5:156:ILE:HD12	4:5:230:GLN:HB2	1.90	0.52
4:5:332:TYR:HE2	4:5:351:LYS:HE2	1.75	0.52
4:5:633:THR:OG1	4:5:634:GLU:N	2.38	0.52
6:7:186:GLN:HE21	6:7:215:ARG:HH11	1.55	0.52
4:5:319:GLU:O	4:5:323:ARG:HG2	2.10	0.52
4:5:634:GLU:HA	4:5:637:VAL:HG12	1.91	0.52
7:A:158:GLU:HG3	7:A:166:SER:HB3	1.92	0.51
8:B:100:LEU:O	8:B:104:SER:HB2	2.11	0.51
10:D:199:GLU:HG3	10:D:200:LYS:H	1.75	0.51
5:6:779:ARG:HD2	5:6:782:HIS:NE2	2.26	0.51
6:7:363:ASP:OD1	6:7:363:ASP:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:83:ARG:HH21	7:A:110:GLU:CD	2.18	0.51
11:E:25:SER:OG	11:E:384:MET:SD	2.66	0.51
2:3:623:ILE:HG22	2:3:625:PRO:HD3	1.92	0.51
5:6:767:ILE:HD12	5:6:770:LYS:HB2	1.91	0.51
11:E:98:CYS:HB2	11:E:118:LEU:HD12	1.92	0.51
4:5:526:GLU:HA	4:5:529:ASP:HB2	1.91	0.51
6:7:257:VAL:HG13	6:7:261:ASN:HB2	1.93	0.51
4:5:172:CYS:SG	4:5:173:ARG:N	2.82	0.51
3:4:167:GLN:HG2	3:4:244:ILE:HD11	1.93	0.51
3:4:199:GLU:O	3:4:203:ILE:HG12	2.10	0.51
4:5:236:VAL:HG21	4:5:242:PRO:HG3	1.93	0.51
4:5:585:ARG:HG2	4:5:641:LEU:HD22	1.93	0.51
8:B:103:ALA:O	8:B:107:ILE:HG12	2.11	0.51
1:2:862:GLU:HA	1:2:900:ILE:HD11	1.93	0.51
3:4:364:GLY:N	6:7:438:ASP:OD2	2.43	0.51
4:5:87:TYR:HB3	4:5:95:HIS:CE1	2.45	0.51
1:2:903:GLN:HG2	1:2:904:PHE:H	1.76	0.51
11:E:368:LYS:O	11:E:369:HIS:ND1	2.44	0.51
11:E:527:GLU:O	11:E:531:GLU:HG3	2.11	0.51
1:2:315:CYS:SG	1:2:408:PRO:HD3	2.51	0.51
2:3:133:ASP:OD1	2:3:136:TYR:N	2.34	0.51
4:5:590:ARG:HG2	4:5:608:ILE:HG21	1.93	0.51
5:6:321:THR:OG1	5:6:322:ALA:N	2.42	0.51
7:A:39:LEU:HD22	7:A:65:ARG:HG2	1.93	0.51
3:4:401:VAL:HG12	3:4:407:ASN:O	2.11	0.50
3:4:698:ILE:HG22	3:4:700:PRO:HD3	1.92	0.50
8:B:49:ALA:HB1	8:B:60:LEU:HD21	1.94	0.50
1:2:462:LYS:HG3	1:2:463:MET:SD	2.51	0.50
3:4:171:GLN:HE21	3:4:244:ILE:HD12	1.75	0.50
3:4:682:LEU:HG	3:4:686:VAL:HG11	1.94	0.50
5:6:609:VAL:HG22	5:6:610:THR:HG23	1.93	0.50
1:2:633:ILE:HB	1:2:648:ASP:OD2	2.12	0.50
2:3:122:GLN:HG2	2:3:145:VAL:HG12	1.94	0.50
4:5:590:ARG:HG2	4:5:608:ILE:CG2	2.42	0.50
4:5:387:LYS:O	4:5:391:LEU:HG	2.12	0.50
4:5:453:ASP:OD2	4:5:454:ASP:N	2.45	0.50
5:6:380:THR:HG1	5:6:384:THR:HG1	1.42	0.50
1:2:449:ASN:HD21	1:2:721:LYS:HE2	1.76	0.50
4:5:134:PRO:HB2	4:5:152:PRO:HD3	1.93	0.50
5:6:751:TRP:HA	5:6:754:LYS:HB2	1.92	0.50
7:A:161:VAL:HG13	7:A:181:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:88:ASN:HA	2:3:136:TYR:OH	2.10	0.50
6:7:420:ARG:NH1	12:M:6:DT:O2	2.44	0.50
7:A:58:LEU:HD23	9:C:41:PRO:HG2	1.94	0.50
8:B:26:ILE:HG13	8:B:33:LEU:HB2	1.93	0.50
11:E:451:MET:HG2	11:E:453:GLY:H	1.76	0.50
1:2:548:GLY:N	1:2:587:ASP:O	2.44	0.50
2:3:81:VAL:HG21	2:3:128:PHE:HE2	1.77	0.50
2:3:85:ILE:HD11	2:3:129:VAL:HG23	1.93	0.50
4:5:156:ILE:HG22	4:5:228:LYS:HB3	1.94	0.50
1:2:676:ALA:HB3	5:6:595:VAL:HG23	1.94	0.50
1:2:843:GLN:HE22	1:2:847:GLN:HG3	1.77	0.50
6:7:155:ASP:OD2	6:7:155:ASP:N	2.44	0.50
11:E:490:PRO:HD3	11:E:511:PRO:HG3	1.94	0.50
11:E:515:SER:O	11:E:515:SER:OG	2.25	0.50
1:2:373:TYR:CE1	4:5:289:ILE:HD11	2.47	0.50
5:6:19:ARG:NH1	5:6:24:GLU:OE2	2.45	0.50
9:C:100:PHE:CE1	9:C:107:VAL:HG11	2.47	0.50
10:D:202:SER:OG	10:D:204:HIS:NE2	2.35	0.50
1:2:750:LEU:HD21	1:2:762:ILE:HG12	1.94	0.49
2:3:179:CYS:HB3	2:3:242:GLN:NE2	2.28	0.49
2:3:467:ILE:HG22	2:3:471:MET:HG3	1.94	0.49
3:4:740:LEU:HB3	3:4:761:ALA:HB1	1.94	0.49
5:6:160:ASP:OD2	5:6:186:ALA:N	2.29	0.49
2:3:646:ASP:N	2:3:646:ASP:OD1	2.44	0.49
3:4:396:ALA:HB2	3:4:414:THR:HG22	1.93	0.49
3:4:428:ARG:O	3:4:688:LYS:HE2	2.13	0.49
5:6:752:TYR:CZ	5:6:769:LYS:HE2	2.48	0.49
6:7:153:ARG:HH12	6:7:251:ARG:NH1	2.10	0.49
4:5:515:ASP:OD1	4:5:515:ASP:N	2.43	0.49
6:7:36:GLN:HE22	6:7:39:ARG:CZ	2.25	0.49
7:A:10:ILE:HD12	9:C:22:LEU:HD22	1.94	0.49
4:5:390:LEU:O	4:5:394:VAL:HG23	2.11	0.49
9:C:128:SER:OG	9:C:129:PRO:HD2	2.12	0.49
10:D:187:ASP:OD1	10:D:188:THR:N	2.38	0.49
3:4:319:ARG:HG2	6:7:221:TYR:CE2	2.48	0.49
5:6:86:VAL:O	5:6:90:LEU:HG	2.13	0.49
5:6:485:THR:HG23	5:6:490:LYS:HE2	1.94	0.49
7:A:194:ILE:HG13	7:A:195:LEU:N	2.27	0.49
1:2:804:ASP:N	1:2:804:ASP:OD1	2.35	0.49
11:E:172:ARG:O	11:E:176:GLU:HG3	2.13	0.49
11:E:389:LYS:NZ	11:E:462:ARG:HD2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:558:ALA:HB3	1:2:611:ILE:HD13	1.93	0.49
1:2:903:GLN:OE1	1:2:903:GLN:N	2.42	0.49
4:5:614:GLU:HG2	4:5:618:ARG:NH1	2.28	0.49
6:7:575:GLU:CD	6:7:575:GLU:H	2.20	0.49
11:E:133:ILE:O	11:E:181:ARG:HD2	2.13	0.49
1:2:500:PHE:CZ	1:2:724:ILE:HG22	2.48	0.49
1:2:560:VAL:H	1:2:613:LYS:HE2	1.77	0.49
1:2:207:VAL:O	1:2:240:ARG:NH2	2.46	0.49
3:4:580:ASN:N	3:4:580:ASN:OD1	2.45	0.49
6:7:526:ASP:HB3	6:7:529:ASN:HB3	1.93	0.49
1:2:547:THR:OG1	1:2:588:GLU:OE1	2.30	0.48
3:4:376:ASN:OD1	3:4:377:ASP:N	2.45	0.48
6:7:153:ARG:HH12	6:7:251:ARG:HH12	1.60	0.48
7:A:88:ARG:NH2	10:D:101:GLU:OE1	2.45	0.48
10:D:197:ASP:OD1	10:D:197:ASP:N	2.46	0.48
1:2:642:THR:HG23	1:2:645:GLU:HG2	1.94	0.48
2:3:95:ASN:HA	2:3:148:GLU:O	2.14	0.48
2:3:436:ARG:NH1	2:3:481:ALA:HB3	2.28	0.48
3:4:723:SER:OG	3:4:724:ARG:NH1	2.46	0.48
1:2:207:VAL:HA	1:2:212:HIS:O	2.14	0.48
1:2:462:LYS:O	1:2:465:THR:OG1	2.31	0.48
2:3:400:LEU:HD12	2:3:454:ASP:HB3	1.95	0.48
5:6:159:LEU:O	5:6:162:GLN:NE2	2.45	0.48
5:6:378:LYS:HB2	5:6:386:LEU:HD12	1.95	0.48
7:A:83:ARG:NH2	7:A:110:GLU:OE1	2.46	0.48
1:2:844:VAL:HG22	1:2:858:ILE:HG12	1.94	0.48
2:3:249:MET:HE2	2:3:279:ARG:HH21	1.79	0.48
3:4:726:MET:HG3	3:4:727:VAL:N	2.28	0.48
8:B:66:MET:HE2	8:B:96:THR:HG22	1.96	0.48
11:E:74:LEU:HD11	11:E:95:PHE:HD1	1.79	0.48
5:6:349:ASN:O	5:6:353:SER:OG	2.23	0.48
11:E:343:MET:SD	11:E:343:MET:N	2.87	0.48
1:2:248:LEU:HD21	1:2:285:ILE:HD13	1.95	0.48
1:2:720:LEU:O	1:2:724:ILE:HG23	2.14	0.48
2:3:151:PHE:H	2:3:155:HIS:CE1	2.27	0.48
4:5:143:ASP:OD1	4:5:143:ASP:N	2.45	0.48
6:7:336:LEU:HD22	6:7:559:MET:HE3	1.96	0.48
3:4:190:GLU:O	3:4:192:LEU:N	2.45	0.48
6:7:500:SER:H	6:7:503:GLN:NE2	2.11	0.48
11:E:126:GLU:N	11:E:126:GLU:OE1	2.47	0.48
11:E:265:VAL:HG13	11:E:266:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:890:LYS:HB3	1:2:903:GLN:HG2	1.95	0.48
1:2:178:LYS:HD3	1:2:179:GLY:N	2.28	0.48
1:2:802:PHE:HE2	1:2:814:MET:HE1	1.77	0.48
6:7:320:THR:OG1	6:7:323:GLU:HG2	2.14	0.48
1:2:381:SER:HB3	1:2:384:LYS:HE2	1.94	0.47
4:5:356:LEU:HD13	4:5:377:LEU:HD12	1.95	0.47
4:5:387:LYS:HD3	4:5:520:VAL:HG11	1.96	0.47
1:2:594:ASP:O	1:2:598:THR:HG23	2.14	0.47
2:3:118:LEU:HD23	2:3:118:LEU:HA	1.69	0.47
5:6:637:CYS:SG	5:6:638:ASP:N	2.86	0.47
11:E:477:PHE:O	11:E:480:SER:N	2.43	0.47
3:4:201:ASN:OD1	3:4:252:SER:OG	2.18	0.47
4:5:380:LEU:N	4:5:518:PHE:O	2.48	0.47
10:D:112:LYS:HE2	10:D:112:LYS:HB3	1.70	0.47
11:E:133:ILE:HG13	11:E:181:ARG:HG3	1.97	0.47
1:2:343:GLN:NE2	1:2:399:LEU:HD11	2.30	0.47
1:2:385:VAL:O	1:2:387:ALA:N	2.46	0.47
1:2:586:ILE:HB	1:2:628:ALA:HB2	1.96	0.47
2:3:418:SER:HA	4:5:470:ALA:O	2.14	0.47
3:4:714:TYR:HB2	3:4:734:LEU:HD13	1.96	0.47
9:C:201:ASN:HA	9:C:204:GLN:CD	2.40	0.47
10:D:71:GLU:OE1	10:D:74:LYS:N	2.44	0.47
10:D:104:PHE:CD2	10:D:105:PRO:HD3	2.49	0.47
11:E:5:ASP:OD1	11:E:5:ASP:N	2.45	0.47
1:2:849:ASN:ND2	5:6:727:ILE:HB	2.30	0.47
4:5:608:ILE:HD12	4:5:612:GLN:OE1	2.15	0.47
5:6:44:ILE:H	5:6:44:ILE:HD12	1.79	0.47
6:7:420:ARG:HG2	6:7:427:LEU:HG	1.96	0.47
6:7:501:LEU:C	6:7:503:GLN:H	2.21	0.47
10:D:175:VAL:HG11	10:D:198:LEU:HD13	1.95	0.47
11:E:257:GLU:HG2	11:E:258:ASP:H	1.77	0.47
5:6:770:LYS:O	5:6:774:GLU:HG3	2.14	0.47
1:2:854:GLN:OE1	5:6:603:GLN:HB2	2.15	0.47
2:3:184:PRO:HA	2:3:239:LYS:O	2.15	0.47
3:4:220:LYS:HE2	3:4:220:LYS:HB3	1.81	0.47
4:5:32:GLN:NE2	4:5:105:GLU:OE2	2.48	0.47
5:6:38:GLN:CD	5:6:42:GLY:HA2	2.40	0.47
1:2:463:MET:SD	1:2:463:MET:N	2.88	0.47
3:4:650:LEU:HD12	3:4:650:LEU:H	1.78	0.47
4:5:237:PRO:HG2	4:5:240:GLU:OE1	2.15	0.47
8:B:17:ILE:HG22	8:B:60:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:88:LEU:HD22	9:C:123:LEU:HD23	1.97	0.47
3:4:521:GLN:O	3:4:525:ASN:ND2	2.48	0.47
7:A:94:TYR:CE2	9:C:202:LEU:HD11	2.50	0.47
5:6:120:ARG:O	5:6:121:HIS:ND1	2.48	0.47
1:2:288:LEU:HD21	1:2:305:LEU:HD23	1.96	0.46
2:3:226:ASN:OD1	2:3:227:ASN:N	2.45	0.46
4:5:94:GLU:HG3	4:5:95:HIS:HD2	1.79	0.46
4:5:577:GLU:HA	4:5:580:GLU:OE2	2.14	0.46
1:2:616:ILE:HD12	1:2:616:ILE:HA	1.78	0.46
4:5:381:GLY:HA3	4:5:520:VAL:HG12	1.97	0.46
5:6:780:LEU:HB3	5:6:786:VAL:HB	1.97	0.46
1:2:897:ARG:NH2	1:2:899:MET:SD	2.88	0.46
2:3:326:ILE:HG12	2:3:330:LYS:HE3	1.98	0.46
5:6:187:ASN:OD1	5:6:187:ASN:N	2.49	0.46
5:6:780:LEU:HA	5:6:783:TYR:CD2	2.50	0.46
8:B:81:GLU:HG3	8:B:83:THR:H	1.81	0.46
1:2:186:VAL:HG13	1:2:195:ILE:HD12	1.97	0.46
1:2:751:ARG:HD3	4:5:532:LEU:HD13	1.97	0.46
2:3:501:TYR:OH	2:3:508:LYS:NZ	2.47	0.46
3:4:521:GLN:HE21	6:7:464:GLN:HG2	1.80	0.46
6:7:223:GLN:HG2	6:7:225:ARG:H	1.81	0.46
8:B:96:THR:HG21	8:B:117:VAL:HG21	1.97	0.46
11:E:181:ARG:HA	11:E:184:ILE:HG22	1.97	0.46
1:2:481:ILE:HD11	1:2:496:ALA:HB2	1.97	0.46
1:2:585:LEU:HD23	1:2:627:ILE:HB	1.98	0.46
1:2:587:ASP:OD1	1:2:588:GLU:N	2.49	0.46
3:4:306:CYS:HB2	3:4:337:MET:SD	2.55	0.46
3:4:735:GLU:OE2	15:4:904:AGS:O3'	2.19	0.46
4:5:570:CYS:SG	4:5:572:PRO:HD3	2.56	0.46
3:4:265:ALA:O	3:4:422:ARG:NH1	2.48	0.46
3:4:306:CYS:SG	3:4:307:GLN:N	2.89	0.46
4:5:145:MET:O	4:5:146:SER:OG	2.24	0.46
5:6:56:PRO:O	5:6:57:GLU:HG2	2.16	0.46
7:A:20:GLN:NE2	9:C:205:ASN:OD1	2.49	0.46
7:A:109:GLU:OE2	7:A:109:GLU:N	2.40	0.46
11:E:491:LEU:HD23	11:E:492:VAL:N	2.30	0.46
1:2:726:TYR:CE2	1:2:730:ARG:HD2	2.50	0.46
2:3:673:HIS:CD2	2:3:686:ASP:HA	2.50	0.46
4:5:49:THR:OG1	4:5:50:GLY:N	2.49	0.46
6:7:539:TYR:CG	6:7:547:PRO:HG3	2.51	0.46
7:A:73:ARG:HG3	10:D:149:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:324:GLU:HG2	2:3:328:LYS:HE3	1.98	0.46
2:3:431:GLN:NE2	4:5:424:SER:O	2.49	0.46
6:7:554:LEU:H	6:7:554:LEU:HD12	1.81	0.46
10:D:29:ARG:NE	10:D:50:ILE:HD11	2.31	0.46
11:E:250:SER:O	11:E:254:HIS:HB3	2.15	0.46
1:2:566:SER:OG	1:2:568:GLU:HG2	2.16	0.46
2:3:202:ARG:NH2	2:3:220:PRO:HG3	2.31	0.46
4:5:335:ILE:O	4:5:339:ILE:HG23	2.16	0.46
5:6:616:ILE:HG23	5:6:620:GLN:HG3	1.98	0.46
6:7:534:ALA:O	6:7:538:THR:HG23	2.16	0.46
9:C:78:ASP:OD1	9:C:82:ARG:N	2.38	0.46
2:3:436:ARG:HH12	2:3:481:ALA:HB3	1.80	0.45
3:4:191:PRO:O	3:4:195:GLN:N	2.44	0.45
3:4:413:LYS:HB3	3:4:413:LYS:HE2	1.76	0.45
3:4:438:GLN:HG2	3:4:441:PHE:CE2	2.51	0.45
5:6:173:LYS:HG2	5:6:174:TYR:H	1.80	0.45
11:E:36:LEU:HD12	11:E:36:LEU:HA	1.63	0.45
6:7:148:VAL:HG12	6:7:149:ILE:H	1.81	0.45
10:D:104:PHE:CG	10:D:105:PRO:HD3	2.51	0.45
11:E:130:TYR:HE1	11:E:134:PHE:HD2	1.65	0.45
1:2:862:GLU:O	1:2:864:ASP:N	2.50	0.45
4:5:358:PHE:CE1	4:5:563:ILE:HG12	2.52	0.45
5:6:375:GLY:O	5:6:633:ARG:NH2	2.48	0.45
6:7:522:GLN:OE1	6:7:524:ARG:NH2	2.50	0.45
1:2:284:ARG:HD2	1:2:442:ASN:O	2.15	0.45
6:7:185:ASP:OD1	6:7:185:ASP:N	2.49	0.45
3:4:275:ASN:OD1	6:7:263:ARG:NH2	2.41	0.45
3:4:730:TYR:H	3:4:733:GLN:NE2	2.15	0.45
4:5:338:SER:O	4:5:338:SER:OG	2.27	0.45
8:B:27:TYR:HA	8:B:32:ASP:OD1	2.16	0.45
10:D:152:ASN:N	10:D:152:ASN:OD1	2.50	0.45
11:E:451:MET:HE2	11:E:453:GLY:HA3	1.99	0.45
1:2:750:LEU:HB2	1:2:818:PHE:CE2	2.51	0.45
2:3:521:LEU:HD12	2:3:521:LEU:HA	1.77	0.45
2:3:547:LEU:O	2:3:551:ARG:HG3	2.15	0.45
3:4:164:GLU:O	3:4:168:ARG:HG3	2.16	0.45
3:4:238:ASP:OD2	3:4:260:VAL:HG12	2.17	0.45
4:5:636:ASP:O	4:5:639:GLU:HG3	2.16	0.45
5:6:599:LYS:HB2	5:6:599:LYS:HE3	1.74	0.45
10:D:173:LEU:HD13	10:D:211:ILE:HD12	1.99	0.45
1:2:562:ARG:NH1	1:2:567:ARG:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:171:GLN:NE2	3:4:244:ILE:HD12	2.32	0.45
3:4:222:LEU:HD12	3:4:223:TYR:N	2.32	0.45
4:5:401:GLY:HA2	4:5:441:VAL:O	2.16	0.45
4:5:468:SER:HB3	4:5:477:THR:HG22	1.98	0.45
4:5:526:GLU:O	4:5:530:VAL:HG23	2.17	0.45
4:5:615:ALA:HA	4:5:618:ARG:HG2	1.98	0.45
8:B:66:MET:HG2	8:B:113:ILE:HD13	1.99	0.45
1:2:203:LEU:HD23	1:2:215:PHE:CD2	2.52	0.45
1:2:530:SER:O	1:2:534:LYS:HG2	2.17	0.45
5:6:768:ASN:HA	5:6:771:ARG:HH11	1.81	0.45
1:2:342:SER:OG	1:2:344:ASN:OD1	2.29	0.45
1:2:493:ARG:O	1:2:497:LEU:HG	2.16	0.45
1:2:720:LEU:HA	1:2:723:TYR:HB3	1.99	0.45
4:5:581:LYS:HG3	4:5:634:GLU:HG2	1.99	0.45
5:6:168:VAL:HB	5:6:177:PRO:HG3	1.98	0.45
6:7:582:THR:O	6:7:586:VAL:HG23	2.17	0.45
7:A:46:ASP:HA	7:A:49:GLU:HB3	1.98	0.45
11:E:62:PHE:O	11:E:66:LYS:HB3	2.17	0.45
11:E:132:ASP:OD2	11:E:132:ASP:N	2.50	0.45
1:2:795:ILE:O	1:2:798:MET:HG3	2.17	0.44
3:4:271:MET:HE1	3:4:354:LEU:HB3	1.99	0.44
4:5:463:GLU:HG3	4:5:513:ARG:CZ	2.47	0.44
6:7:182:TYR:HE2	6:7:193:GLN:HG2	1.81	0.44
6:7:400:ARG:HE	6:7:400:ARG:HB3	1.64	0.44
6:7:559:MET:HB3	6:7:559:MET:HE2	1.67	0.44
6:7:636:LEU:HD23	6:7:636:LEU:HA	1.76	0.44
7:A:9:LEU:HB3	7:A:79:TYR:CD2	2.51	0.44
11:E:203:PHE:HE2	11:E:248:HIS:CD2	2.35	0.44
2:3:148:GLU:HG2	2:3:149:GLY:N	2.32	0.44
3:4:255:GLU:OE1	3:4:255:GLU:N	2.50	0.44
3:4:255:GLU:HG2	3:4:256:HIS:N	2.32	0.44
4:5:210:ASP:OD1	4:5:210:ASP:N	2.43	0.44
1:2:248:LEU:HB3	1:2:249:PRO:HD3	2.00	0.44
1:2:532:PHE:O	1:2:536:ILE:HG12	2.17	0.44
1:2:536:ILE:HA	1:2:539:VAL:HG12	1.99	0.44
2:3:206:ASP:HB2	6:7:292:LEU:HD12	1.99	0.44
2:3:535:ASP:HB3	2:3:538:GLN:HE22	1.82	0.44
3:4:533:THR:HG22	3:4:534:SER:N	2.31	0.44
5:6:732:ARG:O	5:6:736:GLU:HG3	2.17	0.44
6:7:236:LYS:HB3	6:7:236:LYS:HE3	1.80	0.44
9:C:35:ARG:HA	9:C:64:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:474:LEU:HD12	11:E:474:LEU:HA	1.81	0.44
1:2:306:ILE:HD12	1:2:418:TYR:HB2	2.00	0.44
1:2:319:LEU:HD13	4:5:289:ILE:HG21	1.99	0.44
2:3:59:GLU:OE1	2:3:62:ARG:NH2	2.51	0.44
2:3:158:PRO:HD3	2:3:172:VAL:HG13	2.00	0.44
3:4:551:PRO:HG2	3:4:552:GLU:CD	2.42	0.44
4:5:331:VAL:HG11	4:5:627:LYS:HG2	1.99	0.44
5:6:126:LEU:HD21	5:6:137:ILE:HD11	2.00	0.44
6:7:566:CYS:SG	6:7:619:LEU:HA	2.57	0.44
8:B:148:LEU:HD23	8:B:148:LEU:HA	1.79	0.44
1:2:618:THR:HB	4:5:156:ILE:HD11	2.00	0.44
2:3:480:LYS:HD3	2:3:480:LYS:HA	1.80	0.44
4:5:378:LEU:HD23	4:5:517:ILE:HD12	1.98	0.44
6:7:153:ARG:HB2	6:7:155:ASP:OD2	2.17	0.44
4:5:579:ALA:O	4:5:583:LYS:HG3	2.17	0.44
4:5:614:GLU:HG2	4:5:618:ARG:HH12	1.83	0.44
1:2:332:CYS:HB3	1:2:355:CYS:SG	2.58	0.44
1:2:375:ARG:HD3	1:2:565:VAL:HG11	1.98	0.44
2:3:126:LYS:HA	2:3:129:VAL:HG12	1.98	0.44
4:5:582:LEU:HD23	4:5:582:LEU:HA	1.83	0.44
4:5:613:LEU:HD12	4:5:613:LEU:HA	1.85	0.44
6:7:24:ASP:C	6:7:26:LEU:H	2.25	0.44
11:E:275:ASP:OD1	11:E:276:LEU:N	2.42	0.44
1:2:651:GLU:HB3	1:2:652:PRO:HD3	1.99	0.44
2:3:91:ARG:HB3	2:3:144:TYR:HB2	1.99	0.44
2:3:526:LEU:HD23	2:3:526:LEU:HA	1.85	0.44
2:3:627:LEU:HD23	2:3:682:VAL:HG21	2.00	0.44
10:D:108:LEU:HD23	10:D:108:LEU:HA	1.85	0.44
11:E:125:LEU:HD23	11:E:125:LEU:HA	1.87	0.44
11:E:299:ARG:HG2	11:E:353:MET:HG2	2.00	0.44
4:5:462:MET:HE1	4:5:514:PHE:CE2	2.53	0.44
4:5:507:MET:HE2	4:5:510:ILE:HG21	1.99	0.44
8:B:67:ASP:OD1	8:B:68:VAL:N	2.51	0.44
11:E:305:VAL:HG12	11:E:309:LYS:NZ	2.33	0.44
2:3:81:VAL:HG21	2:3:128:PHE:CE2	2.53	0.43
4:5:317:GLN:NE2	4:5:318:GLU:HG2	2.33	0.43
6:7:148:VAL:HG12	6:7:149:ILE:N	2.34	0.43
1:2:757:THR:HG22	1:2:758:GLY:N	2.30	0.43
4:5:197:CYS:HB2	4:5:211:PRO:HG3	2.00	0.43
6:7:48:LEU:HD23	6:7:136:LEU:HD12	1.99	0.43
9:C:93:GLN:O	9:C:97:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:348:ASP:HA	4:5:351:LYS:HB2	2.00	0.43
6:7:43:ARG:HH22	6:7:133:ARG:HH11	1.66	0.43
3:4:258:ILE:HD12	3:4:258:ILE:HA	1.77	0.43
1:2:365:MET:SD	4:5:270:SER:HB2	2.58	0.43
3:4:326:SER:O	3:4:326:SER:OG	2.35	0.43
5:6:661:THR:HB	5:6:719:GLU:N	2.32	0.43
7:A:28:GLY:O	7:A:32:VAL:HG13	2.18	0.43
7:A:102:LEU:C	7:A:104:PHE:H	2.26	0.43
2:3:671:THR:HG22	2:3:682:VAL:HG11	1.99	0.43
3:4:212:CYS:HB3	3:4:262:PRO:HB3	2.01	0.43
9:C:167:ARG:C	9:C:168:LEU:HD12	2.43	0.43
11:E:398:ILE:HD13	11:E:398:ILE:HA	1.86	0.43
3:4:711:ILE:O	3:4:715:VAL:HG23	2.19	0.43
6:7:233:GLN:HG2	6:7:262:THR:HG22	2.00	0.43
9:C:40:MET:HB3	9:C:60:VAL:HB	1.99	0.43
10:D:33:ALA:O	10:D:37:GLU:HG2	2.18	0.43
11:E:445:PHE:HD1	11:E:446:LEU:O	2.01	0.43
2:3:415:GLY:HA3	2:3:455:GLU:O	2.19	0.43
2:3:525:ASP:OD2	2:3:665:THR:OG1	2.36	0.43
4:5:602:ARG:C	4:5:604:SER:H	2.27	0.43
5:6:741:SER:OG	5:6:742:ALA:N	2.52	0.43
10:D:82:MET:HE2	10:D:82:MET:HB3	1.75	0.43
1:2:876:ASN:ND2	1:2:879:ALA:HB3	2.31	0.43
3:4:169:PHE:CZ	3:4:215:ILE:HG22	2.54	0.43
3:4:238:ASP:O	3:4:242:ASN:ND2	2.52	0.43
3:4:551:PRO:HG2	3:4:552:GLU:OE1	2.19	0.43
5:6:450:MET:HE3	5:6:450:MET:HB2	1.87	0.43
6:7:645:LEU:HD23	6:7:645:LEU:HA	1.91	0.43
7:A:41:GLU:HG3	7:A:42:GLN:N	2.34	0.43
1:2:464:ILE:HD13	1:2:467:LEU:HD12	2.01	0.43
1:2:500:PHE:HE1	1:2:727:ALA:HB3	1.83	0.43
3:4:268:THR:HG22	3:4:269:LYS:HG3	1.99	0.43
3:4:462:LEU:HD23	3:4:462:LEU:HA	1.90	0.43
3:4:735:GLU:O	3:4:738:ILE:HB	2.19	0.43
5:6:347:TYR:OH	5:6:366:ARG:HB3	2.18	0.43
5:6:387:ARG:O	5:6:626:ARG:NH1	2.50	0.43
11:E:200:MET:O	11:E:204:GLU:HG2	2.19	0.43
2:3:318:GLN:HE22	2:3:614:LYS:HB3	1.83	0.42
3:4:276:PRO:HB3	6:7:175:PRO:HB3	2.00	0.42
5:6:390:ILE:HG22	5:6:626:ARG:HD2	2.00	0.42
5:6:544:THR:O	5:6:547:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:21:LEU:HD12	7:A:22:PRO:HD2	2.01	0.42
7:A:30:ARG:HH21	7:A:31:GLN:HG3	1.83	0.42
7:A:33:LEU:HD13	10:D:148:HIS:HB2	2.01	0.42
7:A:188:GLN:O	9:C:202:LEU:HG	2.19	0.42
8:B:173:ASN:OD1	9:C:135:SER:OG	2.28	0.42
9:C:27:MET:HE1	9:C:122:GLN:HG3	2.01	0.42
11:E:499:MET:SD	11:E:500:GLU:N	2.92	0.42
1:2:197:HIS:CE1	1:2:201:ASN:HD21	2.37	0.42
1:2:524:ASP:HA	1:2:632:PRO:HG3	2.01	0.42
1:2:820:ARG:NH2	1:2:871:GLN:HB3	2.34	0.42
2:3:166:LEU:HD11	2:3:288:CYS:HB3	2.00	0.42
4:5:74:MET:HE2	4:5:89:TYR:CE1	2.54	0.42
5:6:449:LEU:HD23	5:6:449:LEU:HA	1.74	0.42
5:6:486:LYS:HA	5:6:486:LYS:HD3	1.74	0.42
7:A:190:VAL:HG12	7:A:191:LEU:HD12	2.01	0.42
10:D:37:GLU:HG3	10:D:92:TYR:CE1	2.50	0.42
1:2:749:ASP:O	1:2:753:GLU:HG2	2.19	0.42
2:3:398:GLN:NE2	4:5:369:LEU:HD22	2.33	0.42
3:4:306:CYS:HB3	3:4:309:CYS:SG	2.59	0.42
3:4:611:THR:OG1	3:4:612:SER:N	2.52	0.42
11:E:537:MET:HE2	11:E:537:MET:HB3	1.88	0.42
1:2:762:ILE:HA	1:2:766:HIS:ND1	2.34	0.42
2:3:394:VAL:HG12	2:3:394:VAL:O	2.19	0.42
2:3:399:LEU:O	2:3:403:VAL:HG23	2.20	0.42
5:6:48:GLN:HA	5:6:51:GLU:HG2	2.01	0.42
10:D:206:ILE:HG22	10:D:207:ARG:N	2.34	0.42
11:E:106:VAL:HG11	11:E:133:ILE:HG21	2.00	0.42
1:2:793:MET:HE3	1:2:793:MET:HB3	1.80	0.42
2:3:74:GLN:HG3	2:3:76:ILE:HG12	2.02	0.42
4:5:184:MET:HE1	4:5:191:TYR:CG	2.54	0.42
4:5:348:ASP:OD1	4:5:351:LYS:HD2	2.19	0.42
5:6:326:LYS:HA	5:6:329:MET:HG3	2.01	0.42
6:7:182:TYR:OH	6:7:193:GLN:NE2	2.51	0.42
6:7:344:ILE:HA	15:7:1001:AGS:H2	2.01	0.42
7:A:3:CYS:SG	7:A:72:ASN:ND2	2.92	0.42
11:E:2:PHE:HE1	11:E:117:LEU:HD12	1.84	0.42
1:2:399:LEU:HD23	1:2:399:LEU:HA	1.69	0.42
3:4:561:GLY:O	3:4:565:LEU:HG	2.19	0.42
4:5:555:ASP:OD1	4:5:555:ASP:N	2.52	0.42
5:6:593:PHE:O	5:6:597:GLN:HG2	2.20	0.42
5:6:736:GLU:CB	5:6:743:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:395:ASP:OD1	6:7:401:SER:OG	2.24	0.42
8:B:19:PRO:HD2	8:B:40:LEU:O	2.19	0.42
9:C:161:THR:HG21	9:C:180:GLN:NE2	2.34	0.42
10:D:187:ASP:CG	10:D:188:THR:H	2.26	0.42
1:2:429:ALA:HB1	5:6:438:GLU:HB3	2.02	0.42
1:2:569:TRP:CZ2	12:M:1:DT:H2"	2.55	0.42
1:2:723:TYR:CE1	1:2:727:ALA:HB2	2.55	0.42
2:3:344:LEU:HD11	2:3:616:TYR:CE2	2.52	0.42
11:E:67:GLU:OE2	11:E:67:GLU:N	2.53	0.42
11:E:508:GLY:O	11:E:520:ASN:ND2	2.45	0.42
1:2:534:LYS:O	1:2:537:GLU:HB3	2.20	0.42
2:3:401:ARG:HD2	4:5:464:GLN:OE1	2.19	0.42
3:4:443:GLU:O	3:4:447:GLU:HG3	2.19	0.42
3:4:467:ALA:HB2	3:4:522:TYR:CD2	2.55	0.42
3:4:566:SER:C	3:4:568:ASN:H	2.26	0.42
4:5:334:VAL:HG22	4:5:554:ILE:HG13	2.02	0.42
6:7:237:MET:HE2	6:7:237:MET:HB3	1.80	0.42
1:2:331:LYS:HD2	1:2:357:SER:HB3	2.02	0.42
1:2:723:TYR:OH	1:2:780:ILE:O	2.37	0.42
9:C:40:MET:HE2	9:C:43:LEU:HD12	2.02	0.42
3:4:744:HIS:CE1	3:4:760:GLU:HG2	2.55	0.42
4:5:644:PHE:O	4:5:648:THR:HG22	2.20	0.42
5:6:102:LYS:HD2	5:6:102:LYS:HA	1.91	0.42
7:A:31:GLN:O	7:A:35:GLU:HG2	2.19	0.42
10:D:21:LEU:HA	10:D:21:LEU:HD23	1.79	0.42
11:E:494:ALA:HB2	11:E:506:VAL:HG22	2.02	0.42
1:2:224:LYS:HE2	11:E:313:GLU:HG2	2.02	0.41
1:2:276:ARG:HH21	11:E:319:GLY:C	2.27	0.41
3:4:181:GLU:CD	3:4:445:ARG:HG3	2.45	0.41
3:4:684:MET:O	3:4:687:LEU:N	2.53	0.41
4:5:59:LEU:HD22	4:5:107:ALA:HB2	2.02	0.41
5:6:65:PHE:O	5:6:69:GLU:HG3	2.19	0.41
5:6:422:LYS:HD2	5:6:422:LYS:HA	1.75	0.41
7:A:37:LYS:HE2	7:A:37:LYS:HB2	1.82	0.41
2:3:509:THR:OG1	2:3:510:PRO:HD2	2.20	0.41
4:5:238:HIS:O	4:5:238:HIS:CG	2.72	0.41
4:5:397:CYS:C	4:5:560:LYS:HE3	2.45	0.41
4:5:455:ARG:O	4:5:458:ILE:HG22	2.20	0.41
5:6:325:ILE:O	5:6:329:MET:HG2	2.20	0.41
7:A:84:LEU:HD12	7:A:84:LEU:HA	1.91	0.41
1:2:685:ARG:HG3	1:2:686:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:356:ASP:OD1	2:3:357:TYR:N	2.53	0.41
3:4:196:ARG:O	3:4:200:ILE:HG12	2.20	0.41
3:4:551:PRO:O	3:4:554:ARG:HD3	2.21	0.41
3:4:737:LEU:HD23	3:4:737:LEU:HA	1.87	0.41
4:5:507:MET:SD	4:5:507:MET:N	2.94	0.41
6:7:269:ASP:OD2	6:7:305:LYS:HE3	2.19	0.41
6:7:427:LEU:HD12	6:7:427:LEU:H	1.85	0.41
1:2:561:GLN:HB3	1:2:572:GLU:HG2	2.01	0.41
1:2:765:ARG:HD3	1:2:768:GLU:OE1	2.20	0.41
2:3:641:ARG:HA	6:7:527:ARG:NH1	2.34	0.41
3:4:176:PRO:O	3:4:177:LEU:HD23	2.21	0.41
3:4:631:ILE:HG13	3:4:631:ILE:O	2.20	0.41
5:6:158:CYS:HA	5:6:191:PHE:HD1	1.86	0.41
6:7:344:ILE:HA	15:7:1001:AGS:C2	2.51	0.41
6:7:400:ARG:O	6:7:440:GLY:HA3	2.20	0.41
1:2:588:GLU:HB3	1:2:591:LYS:HD2	2.02	0.41
4:5:167:ARG:NH1	4:5:181:ASN:HD22	2.18	0.41
5:6:120:ARG:HG2	5:6:121:HIS:H	1.86	0.41
6:7:14:LYS:NZ	6:7:83:GLU:OE1	2.44	0.41
6:7:77:PHE:O	6:7:81:VAL:HG23	2.20	0.41
7:A:24:PHE:CG	7:A:107:ALA:HB2	2.55	0.41
9:C:88:LEU:HD13	9:C:134:ILE:HD11	2.02	0.41
2:3:151:PHE:N	2:3:155:HIS:HE1	2.13	0.41
5:6:59:ASN:OD1	5:6:59:ASN:N	2.53	0.41
5:6:437:GLU:C	5:6:440:HIS:H	2.29	0.41
6:7:135:GLU:HG3	6:7:137:TYR:OH	2.21	0.41
6:7:248:ASN:OD1	6:7:249:ILE:N	2.49	0.41
6:7:348:GLU:OE2	6:7:348:GLU:N	2.36	0.41
1:2:233:ASN:HB3	1:2:236:ASP:OD1	2.21	0.41
6:7:577:LEU:HD23	6:7:577:LEU:HA	1.88	0.41
7:A:161:VAL:HA	7:A:181:LYS:HZ2	1.85	0.41
8:B:81:GLU:HG2	8:B:85:THR:HG22	2.01	0.41
1:2:833:LEU:HD23	1:2:836:LEU:HD21	2.02	0.41
2:3:206:ASP:CG	2:3:207:LEU:H	2.28	0.41
3:4:529:ARG:HD2	3:4:529:ARG:HA	1.82	0.41
3:4:534:SER:OG	3:4:535:GLY:N	2.52	0.41
5:6:354:LEU:HD12	5:6:354:LEU:HA	1.80	0.41
6:7:166:ILE:HA	6:7:269:ASP:O	2.20	0.41
6:7:533:LEU:O	6:7:537:ILE:HG13	2.20	0.41
9:C:92:TYR:O	9:C:97:ARG:NH1	2.54	0.41
11:E:122:ASP:OD1	11:E:122:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:461:VAL:O	1:2:464:ILE:N	2.54	0.41
1:2:718:GLU:HG3	1:2:722:LYS:NZ	2.35	0.41
2:3:180:SER:OG	2:3:181:LEU:N	2.54	0.41
2:3:281:GLN:HG3	2:3:313:MET:HG3	2.02	0.41
5:6:356:PRO:O	5:6:551:ARG:NH1	2.53	0.41
5:6:723:ILE:HA	5:6:726:LEU:HD12	2.02	0.41
6:7:182:TYR:HB2	6:7:191:THR:HG23	2.03	0.41
7:A:98:LEU:HB3	7:A:102:LEU:HD12	2.02	0.41
7:A:152:CYS:SG	7:A:169:LEU:HG	2.61	0.41
7:A:165:THR:O	7:A:165:THR:OG1	2.37	0.41
9:C:201:ASN:HA	9:C:204:GLN:NE2	2.36	0.41
11:E:83:LEU:HA	11:E:83:LEU:HD12	1.86	0.41
11:E:165:VAL:HG22	11:E:169:MET:HG3	2.03	0.41
11:E:536:ARG:HH21	11:E:550:LYS:HE2	1.84	0.41
1:2:268:LEU:HD23	1:2:268:LEU:HA	1.85	0.41
1:2:311:VAL:HG22	1:2:411:GLU:HG3	2.03	0.41
1:2:726:TYR:CZ	1:2:730:ARG:HD2	2.56	0.41
1:2:866:VAL:HA	1:2:869:ALA:HB3	2.03	0.41
3:4:710:LEU:HA	3:4:710:LEU:HD23	1.88	0.41
4:5:56:ARG:HE	4:5:56:ARG:HB3	1.70	0.41
9:C:40:MET:O	9:C:59:ALA:HA	2.21	0.41
1:2:482:ALA:HB3	1:2:492:LYS:NZ	2.36	0.40
2:3:323:ALA:HA	2:3:326:ILE:HG22	2.04	0.40
2:3:383:ASP:HB3	2:3:492:SER:HB3	2.02	0.40
2:3:549:MET:HE2	4:5:365:LEU:HD13	2.04	0.40
3:4:503:GLU:HB3	3:4:612:SER:HB3	2.02	0.40
3:4:690:TYR:OH	3:4:747:VAL:O	2.30	0.40
4:5:266:MET:HB3	4:5:266:MET:HE2	1.78	0.40
4:5:529:ASP:HA	4:5:532:LEU:HD12	2.03	0.40
5:6:516:LEU:HA	5:6:516:LEU:HD12	1.90	0.40
5:6:527:MET:HB3	5:6:527:MET:HE2	1.77	0.40
6:7:51:ASP:OD1	6:7:53:ASP:N	2.45	0.40
8:B:52:LEU:HD23	8:B:52:LEU:HA	1.89	0.40
11:E:350:LYS:HB2	11:E:350:LYS:HE3	1.84	0.40
11:E:364:HIS:CD2	11:E:370:LYS:HD2	2.56	0.40
1:2:414:LEU:HD23	1:2:414:LEU:HA	1.90	0.40
1:2:507:PRO:HB3	4:5:542:SER:O	2.21	0.40
3:4:445:ARG:O	3:4:449:LEU:HG	2.20	0.40
5:6:450:MET:HE1	5:6:493:LEU:HD13	2.03	0.40
7:A:43:ASN:HB2	7:A:65:ARG:HD3	2.02	0.40
11:E:254:HIS:O	11:E:254:HIS:ND1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:68:LEU:HD23	2:3:68:LEU:HA	1.95	0.40
2:3:634:TYR:OH	2:3:688:GLU:OE1	2.14	0.40
3:4:472:GLU:HG3	3:4:473:HIS:H	1.86	0.40
3:4:566:SER:O	3:4:568:ASN:N	2.51	0.40
4:5:128:LEU:O	4:5:128:LEU:HD12	2.21	0.40
5:6:41:ASP:OD1	5:6:41:ASP:N	2.53	0.40
5:6:204:GLN:HB2	5:6:233:VAL:HG22	2.04	0.40
5:6:524:ALA:HB3	5:6:525:PRO:HD3	2.02	0.40
6:7:429:LEU:HA	6:7:429:LEU:HD12	1.78	0.40
6:7:642:ASP:C	6:7:644:LEU:N	2.79	0.40
11:E:263:LEU:HB3	11:E:269:ARG:HH21	1.87	0.40
11:E:482:LYS:HD3	11:E:482:LYS:HA	1.88	0.40
1:2:746:MET:HE2	1:2:795:ILE:HG23	2.02	0.40
1:2:887:ARG:NH1	1:2:887:ARG:HA	2.37	0.40
2:3:156:VAL:HG21	2:3:161:LEU:HD13	2.03	0.40
3:4:202:VAL:HG13	3:4:203:ILE:HG23	2.03	0.40
4:5:171:GLN:HG3	4:5:178:THR:HG22	2.03	0.40
7:A:7:MET:HE3	7:A:7:MET:HB3	1.89	0.40
11:E:191:TYR:HB3	11:E:519:LYS:HB3	2.04	0.40
11:E:284:TRP:HE1	11:E:424:ARG:NH2	2.20	0.40
1:2:415:THR:O	1:2:442:ASN:HB3	2.21	0.40
1:2:579:ALA:O	1:2:624:CYS:HB3	2.22	0.40
1:2:721:LYS:O	1:2:724:ILE:HG12	2.22	0.40
2:3:398:GLN:HE22	4:5:369:LEU:HD22	1.87	0.40
2:3:414:THR:HA	2:3:454:ASP:OD1	2.22	0.40
5:6:729:LEU:HD12	5:6:751:TRP:HZ3	1.86	0.40
6:7:459:HIS:HB3	6:7:514:ARG:NH2	2.37	0.40
7:A:148:ILE:HB	7:A:179:ARG:HB3	2.03	0.40
8:B:60:LEU:HD12	8:B:103:ALA:HB2	2.04	0.40
9:C:32:LEU:HA	9:C:33:PRO:HD3	1.90	0.40
10:D:21:LEU:HD21	10:D:29:ARG:NH1	2.35	0.40
11:E:23:VAL:HG12	11:E:24:ALA:O	2.21	0.40
11:E:39:LEU:HD23	11:E:39:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2	683/904 (76%)	596 (87%)	87 (13%)	0	100	100
2	3	602/853 (71%)	534 (89%)	68 (11%)	0	100	100
3	4	592/883 (67%)	514 (87%)	78 (13%)	0	100	100
4	5	563/734 (77%)	504 (90%)	58 (10%)	1 (0%)	43	71
5	6	671/821 (82%)	602 (90%)	69 (10%)	0	100	100
6	7	592/719 (82%)	531 (90%)	60 (10%)	1 (0%)	43	71
7	A	194/196 (99%)	169 (87%)	25 (13%)	0	100	100
8	B	174/222 (78%)	161 (92%)	13 (8%)	0	100	100
9	C	190/216 (88%)	173 (91%)	17 (9%)	0	100	100
10	D	201/223 (90%)	186 (92%)	15 (8%)	0	100	100
11	E	534/566 (94%)	480 (90%)	54 (10%)	0	100	100
All	All	4996/6337 (79%)	4450 (89%)	544 (11%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	5	115	PRO
6	7	490	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	610/781 (78%)	610 (100%)	0	100	100
2	3	527/742 (71%)	527 (100%)	0	100	100
3	4	530/771 (69%)	530 (100%)	0	100	100
4	5	494/625 (79%)	493 (100%)	1 (0%)	87	88
5	6	614/724 (85%)	613 (100%)	1 (0%)	87	88
6	7	514/619 (83%)	514 (100%)	0	100	100
7	A	174/174 (100%)	173 (99%)	1 (1%)	78	81
8	B	160/195 (82%)	160 (100%)	0	100	100
9	C	167/186 (90%)	167 (100%)	0	100	100
10	D	188/205 (92%)	188 (100%)	0	100	100
11	E	491/517 (95%)	489 (100%)	2 (0%)	84	84
All	All	4469/5539 (81%)	4464 (100%)	5 (0%)	87	90

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

Mol	Chain	Res	Type
4	5	271	ILE
5	6	226	VAL
7	A	80	LEU
11	E	132	ASP
11	E	284	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	180	HIS
1	2	196	HIS
1	2	197	HIS
1	2	201	ASN
1	2	206	HIS
1	2	282	HIS
1	2	328	ASN
1	2	419	HIS
1	2	443	HIS
1	2	488	HIS
1	2	531	GLN
1	2	563	HIS
1	2	601	HIS

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Mol	Chain	Res	Type
1	2	607	GLN
1	2	683	HIS
1	2	838	GLN
1	2	843	GLN
1	2	889	ASN
1	2	893	HIS
2	3	112	ASN
2	3	155	HIS
2	3	241	HIS
2	3	398	GLN
2	3	513	ASN
3	4	165	ASN
3	4	171	GLN
3	4	195	GLN
3	4	214	HIS
3	4	256	HIS
3	4	365	GLN
3	4	368	HIS
3	4	415	HIS
3	4	521	GLN
3	4	525	ASN
3	4	594	GLN
3	4	633	ASN
3	4	733	GLN
3	4	744	HIS
4	5	95	HIS
4	5	181	ASN
4	5	244	HIS
4	5	426	ASN
4	5	464	GLN
4	5	525	ASN
5	6	27	GLN
5	6	70	GLN
5	6	342	GLN
5	6	349	ASN
5	6	359	HIS
5	6	509	HIS
6	7	36	GLN
6	7	186	GLN
6	7	223	GLN
6	7	243	GLN
6	7	503	GLN

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Mol	Chain	Res	Type
6	7	504	ASN
6	7	543	HIS
7	A	20	GLN
7	A	72	ASN
7	A	174	GLN
7	A	188	GLN
8	B	56	GLN
8	B	102	HIS
8	B	166	HIS
9	C	18	ASN
9	C	136	GLN
9	C	177	GLN
9	C	180	GLN
10	D	78	HIS
10	D	136	ASN
11	E	15	GLN
11	E	248	HIS
11	E	253	ASN
11	E	324	GLN
11	E	339	ASN
11	E	364	HIS
11	E	414	HIS
11	E	483	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
15	AGS	7	1001	16	32,33,33	0.48	0	45,52,52	0.35	0
14	ADP	2	1001	-	28,29,29	1.38	4 (14%)	43,45,45	1.94	8 (18%)
15	AGS	4	904	16	32,33,33	0.58	0	45,52,52	0.37	0
14	ADP	3	1001	-	28,29,29	1.35	5 (17%)	43,45,45	1.83	8 (18%)
15	AGS	4	902	16	32,33,33	0.56	0	45,52,52	0.42	0

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
15	AGS	7	1001	16	-	4/21/38/38	0/3/3/3
14	ADP	2	1001	-	-	4/16/32/32	0/3/3/3
15	AGS	4	904	16	-	8/21/38/38	0/3/3/3
14	ADP	3	1001	-	-	4/16/32/32	0/3/3/3
15	AGS	4	902	16	-	2/21/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	1001	ADP	C5-C4	4.65	1.47	1.39
14	3	1001	ADP	C5-C4	4.31	1.46	1.39
14	3	1001	ADP	C5-N7	-2.65	1.34	1.39
14	2	1001	ADP	C5-N7	-2.59	1.34	1.39
14	2	1001	ADP	C5-C6	2.53	1.48	1.41
14	3	1001	ADP	C4-N9	-2.24	1.33	1.37
14	3	1001	ADP	C5-C6	2.23	1.47	1.41
14	2	1001	ADP	C8-N7	2.15	1.35	1.31
14	3	1001	ADP	C8-N7	2.05	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	1001	ADP	C5-C4-N3	-6.69	117.50	126.72
14	3	1001	ADP	C5-C4-N3	-5.60	119.01	126.72
14	2	1001	ADP	N3-C4-N9	5.36	136.29	127.17
14	3	1001	ADP	N3-C4-N9	4.75	135.25	127.17
14	2	1001	ADP	C2-N3-C4	3.93	121.44	111.83
14	3	1001	ADP	C2-N3-C4	3.58	120.58	111.83
14	3	1001	ADP	N3-C2-N1	-3.32	123.56	128.58
14	2	1001	ADP	C4-C5-N7	-3.17	106.96	110.58
14	3	1001	ADP	C4-N9-C8	3.08	108.98	105.74
14	2	1001	ADP	N3-C2-N1	-3.06	123.95	128.58
14	3	1001	ADP	C4-C5-N7	-2.99	107.17	110.58
14	2	1001	ADP	C3'-C2'-C1'	2.95	107.03	101.46
14	2	1001	ADP	C5-N7-C8	2.33	107.11	103.45
14	3	1001	ADP	C5-N7-C8	2.29	107.05	103.45
14	2	1001	ADP	C4-N9-C8	2.04	107.88	105.74
14	3	1001	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (22) torsion outliers are listed below:

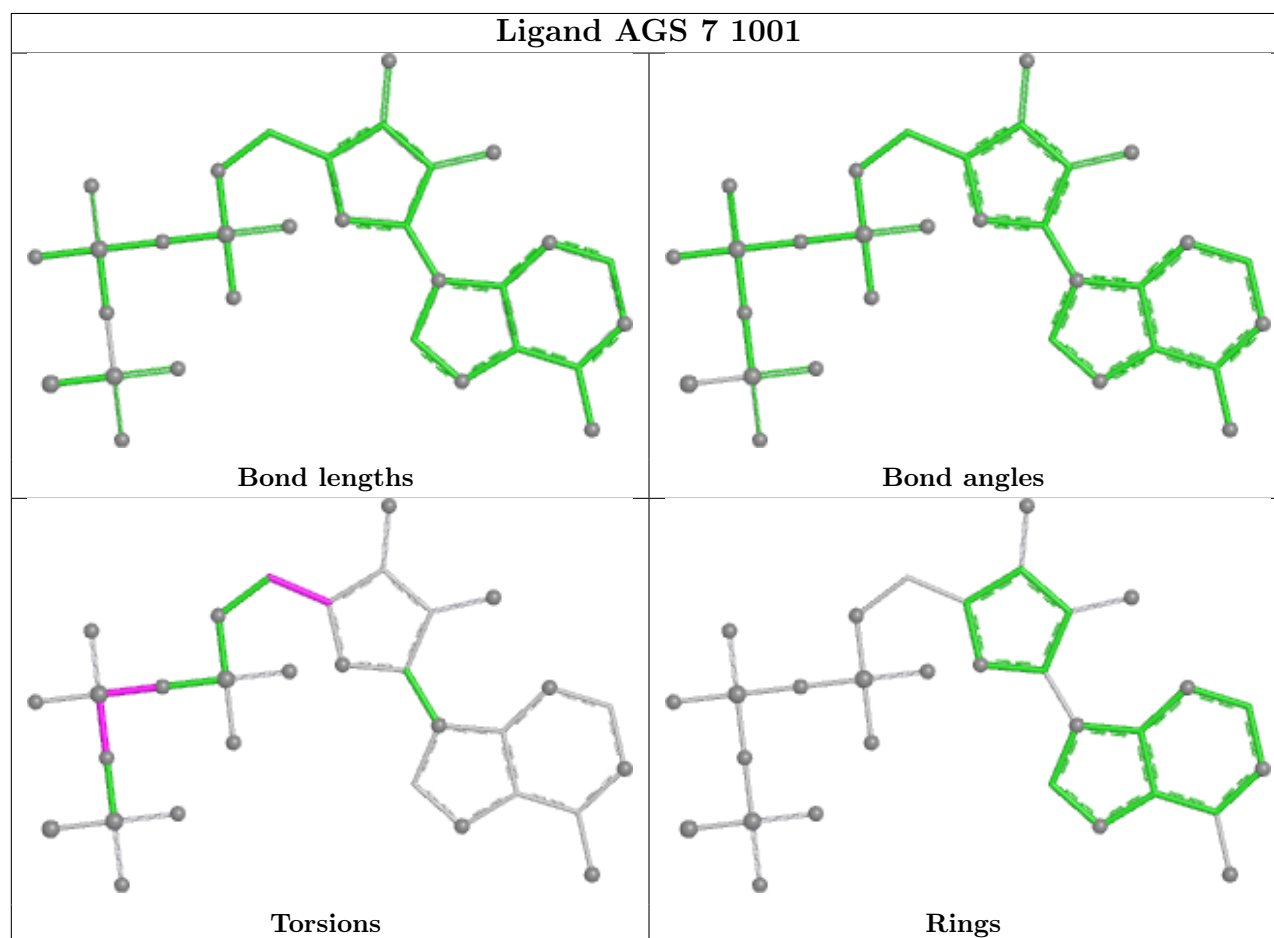
Mol	Chain	Res	Type	Atoms
14	3	1001	ADP	C5'-O5'-PA-O1A
14	3	1001	ADP	C5'-O5'-PA-O2A
14	3	1001	ADP	C5'-O5'-PA-O3A
15	4	904	AGS	PB-O3B-PG-O2G
15	4	904	AGS	PB-O3B-PG-O3G
15	4	904	AGS	C5'-O5'-PA-O1A
15	4	904	AGS	C5'-O5'-PA-O3A
14	2	1001	ADP	C5'-O5'-PA-O1A
15	4	904	AGS	C5'-O5'-PA-O2A
15	4	904	AGS	O4'-C4'-C5'-O5'
15	4	902	AGS	PA-O3A-PB-O2B
14	2	1001	ADP	C2'-C1'-N9-C4
14	2	1001	ADP	C2'-C1'-N9-C8
14	2	1001	ADP	C3'-C4'-C5'-O5'
15	4	904	AGS	C3'-C4'-C5'-O5'
15	4	902	AGS	PB-O3B-PG-O2G
15	7	1001	AGS	PG-O3B-PB-O1B
15	7	1001	AGS	PA-O3A-PB-O1B
15	7	1001	AGS	PA-O3A-PB-O2B
15	7	1001	AGS	O4'-C4'-C5'-O5'
14	3	1001	ADP	O4'-C4'-C5'-O5'
15	4	904	AGS	PB-O3A-PA-O2A

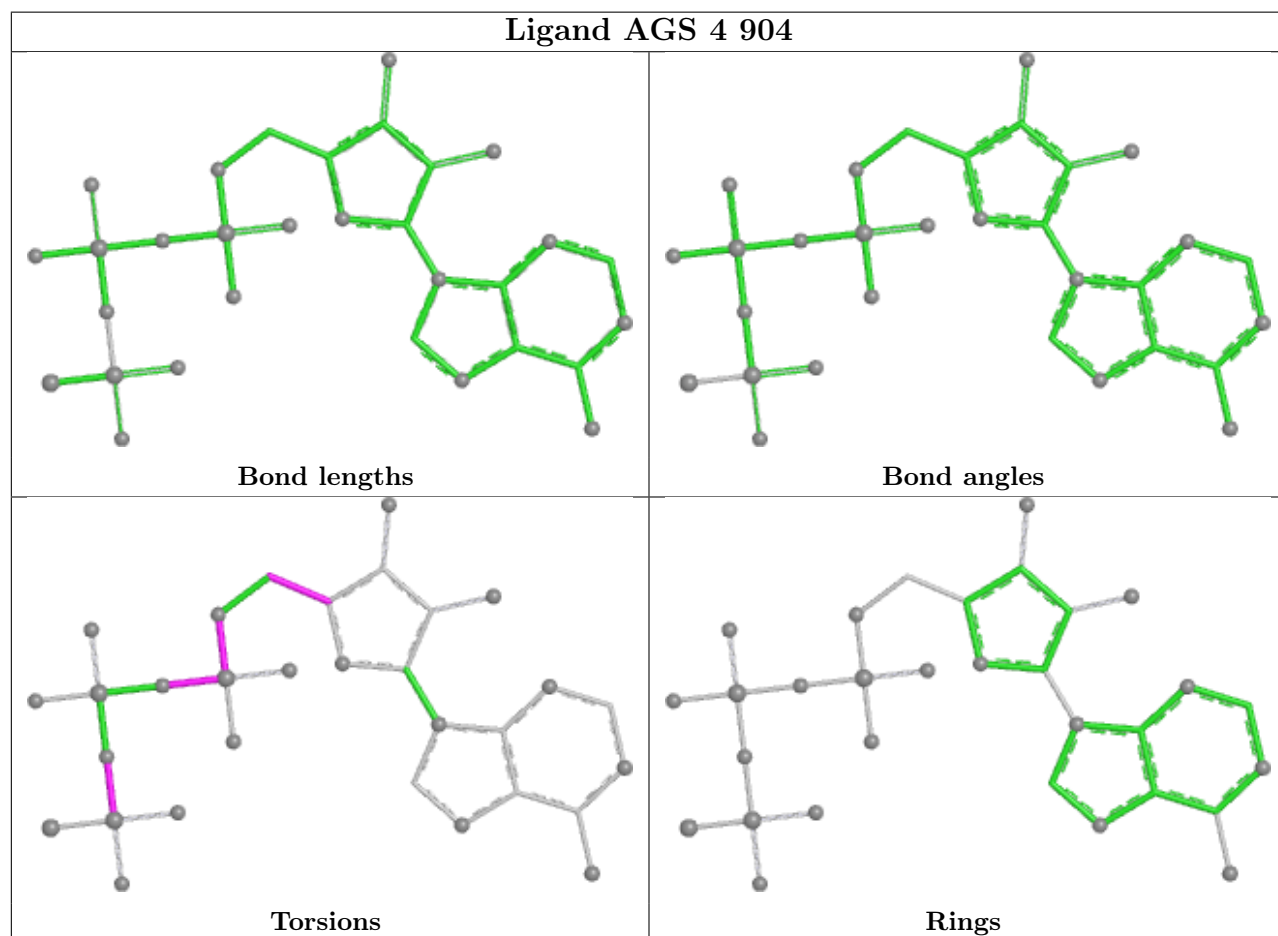
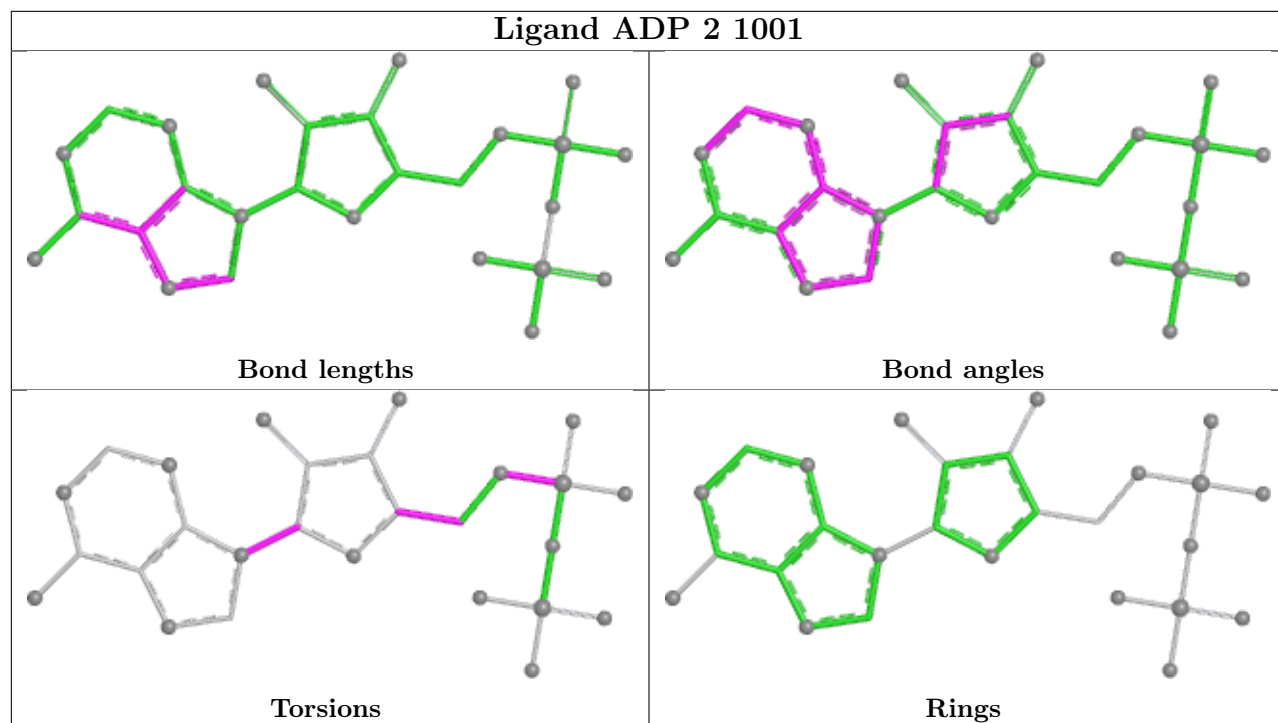
There are no ring outliers.

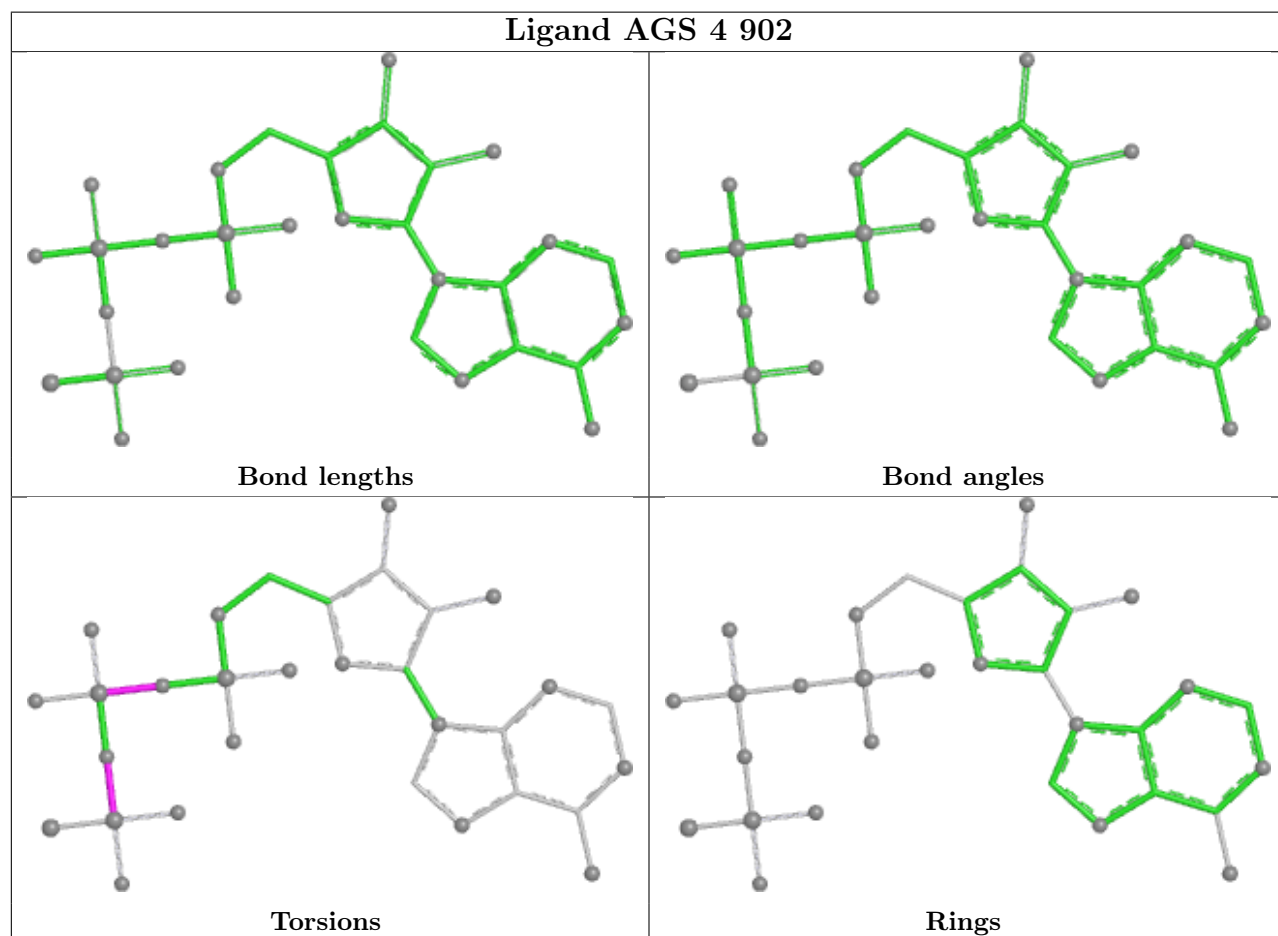
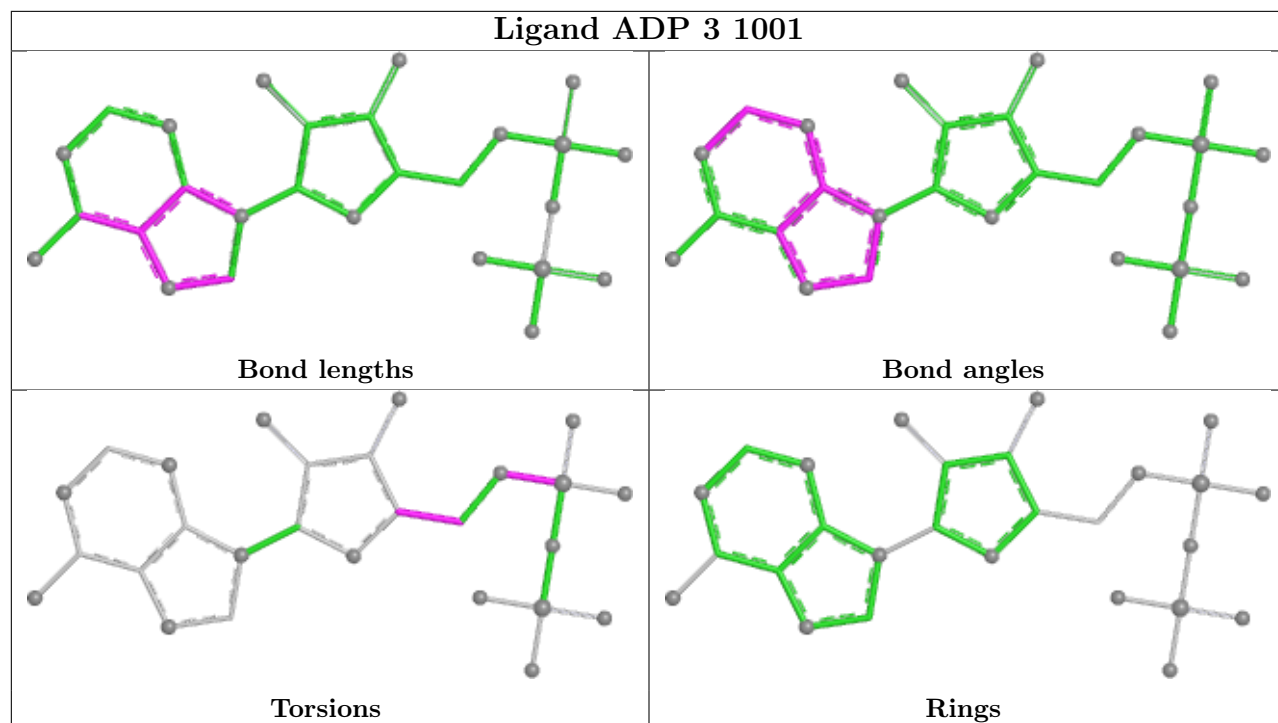
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	7	1001	AGS	2	0
14	2	1001	ADP	1	0
15	4	904	AGS	2	0
15	4	902	AGS	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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

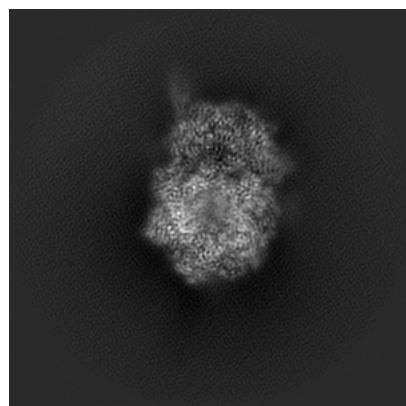
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10619. These allow visual inspection of the internal detail of the map and identification of artifacts.

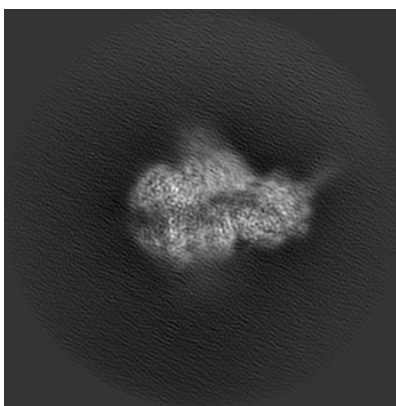
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

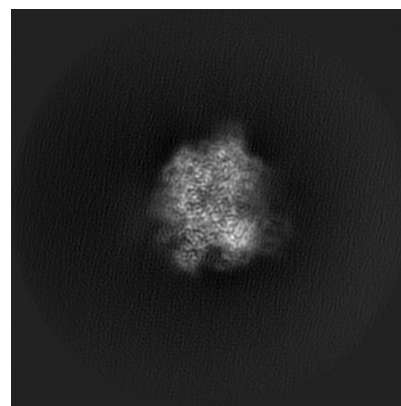
6.1.1 Primary map



X

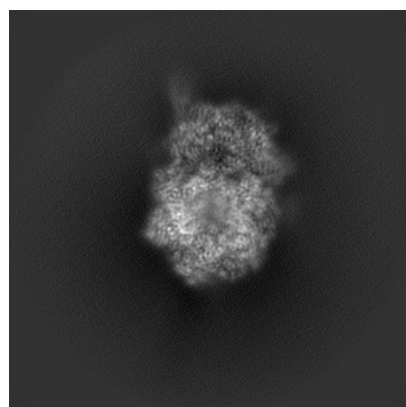


Y

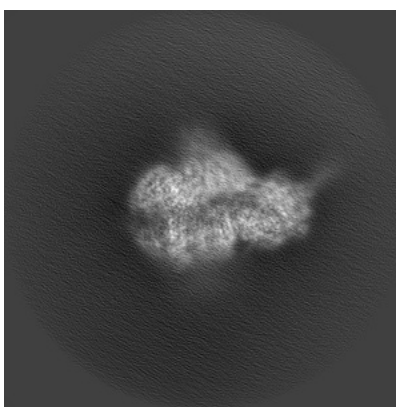


Z

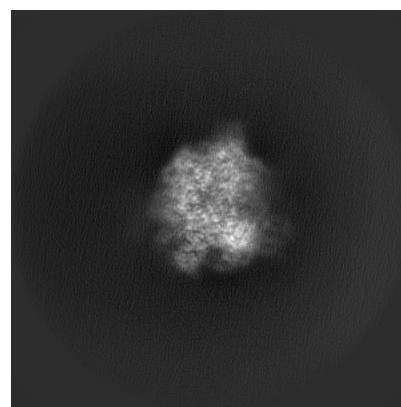
6.1.2 Raw map



X



Y

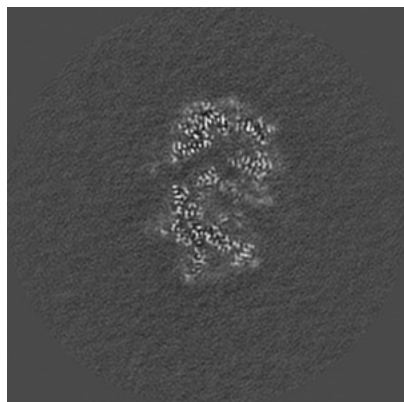


Z

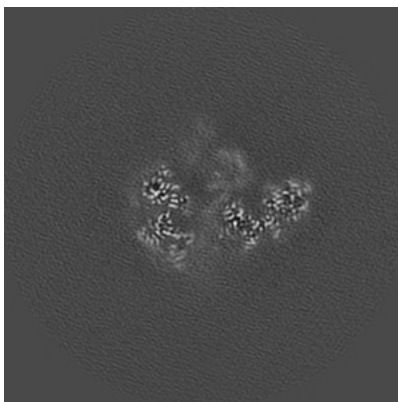
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

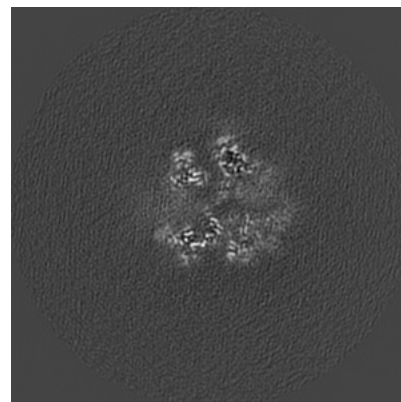
6.2.1 Primary map



X Index: 180

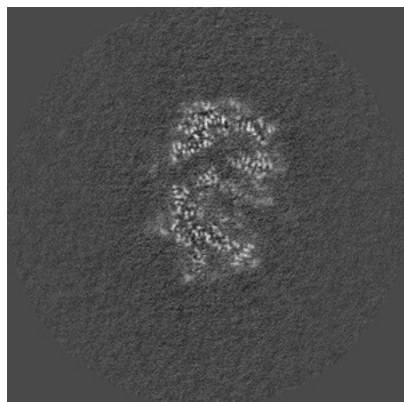


Y Index: 180

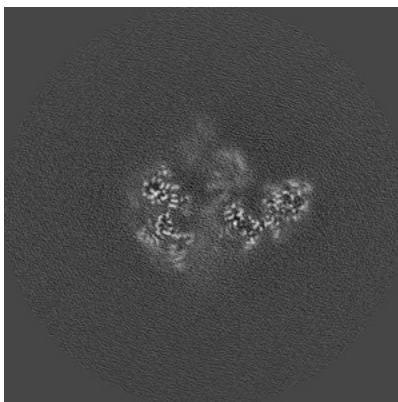


Z Index: 180

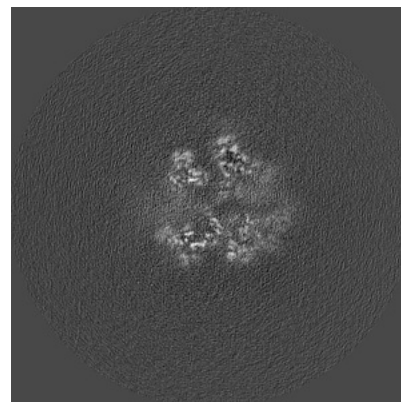
6.2.2 Raw map



X Index: 180



Y Index: 180

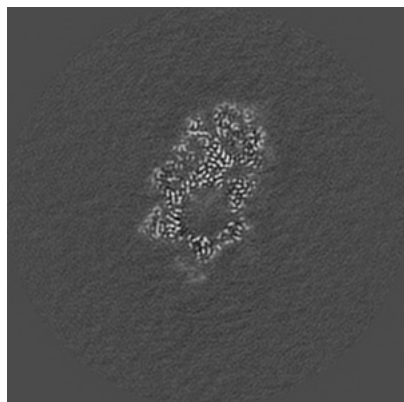


Z Index: 180

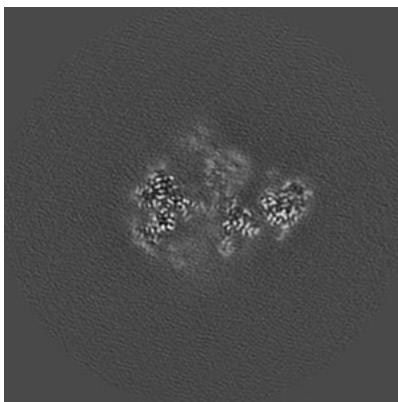
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

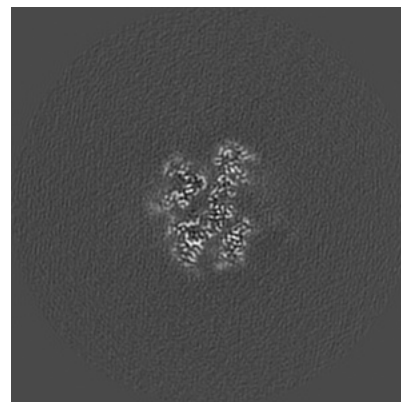
6.3.1 Primary map



X Index: 165

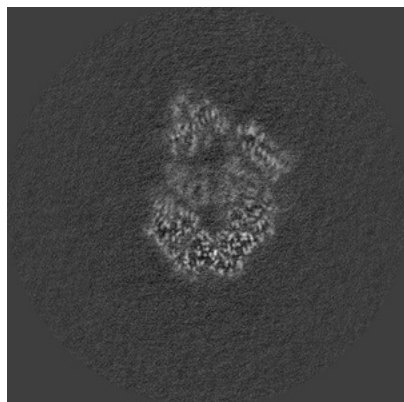


Y Index: 173

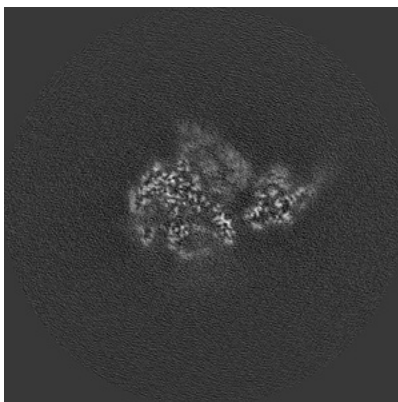


Z Index: 154

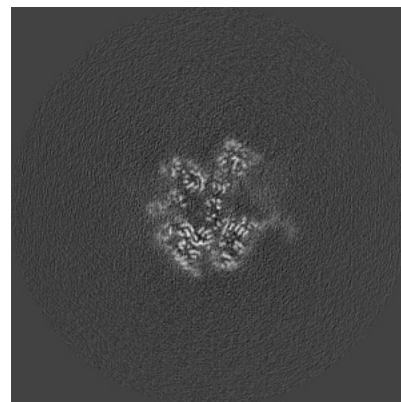
6.3.2 Raw map



X Index: 198



Y Index: 162

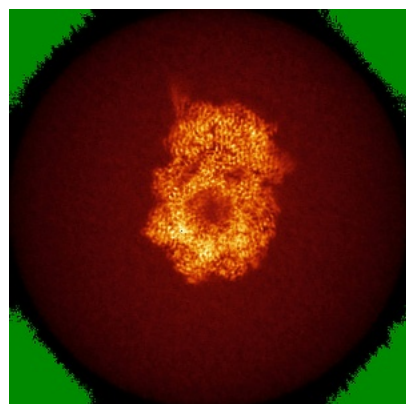


Z Index: 159

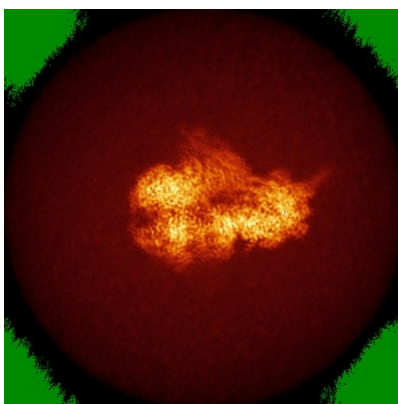
The images above show the largest variance slices of the map in three orthogonal directions.

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

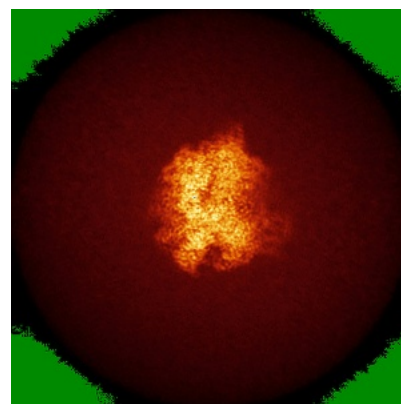
6.4.1 Primary map



X

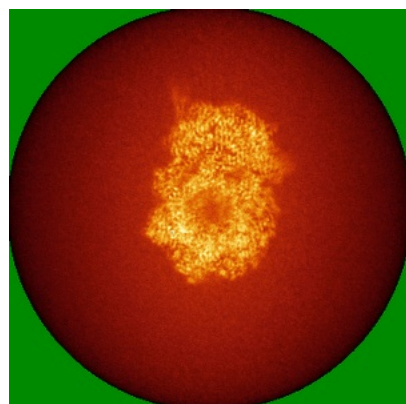


Y

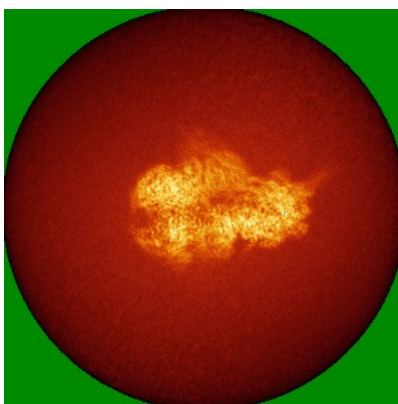


Z

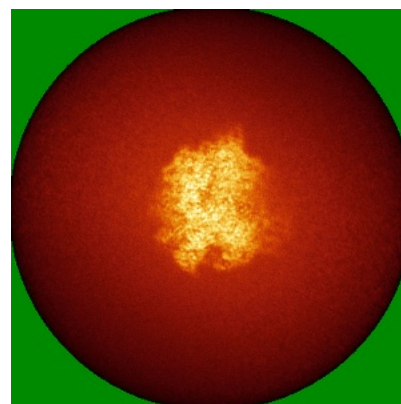
6.4.2 Raw map



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.

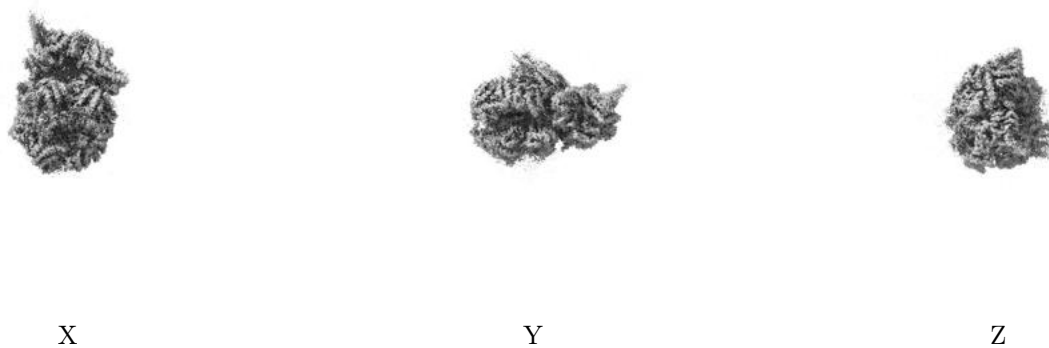
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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



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.

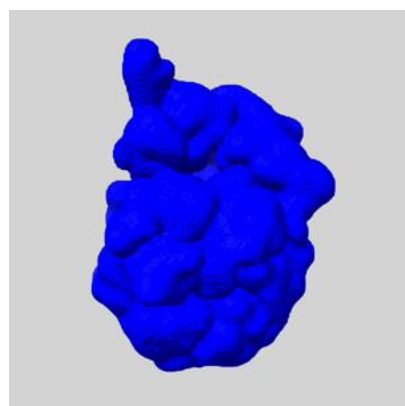
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

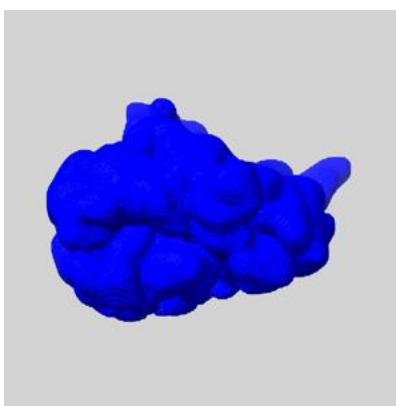
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

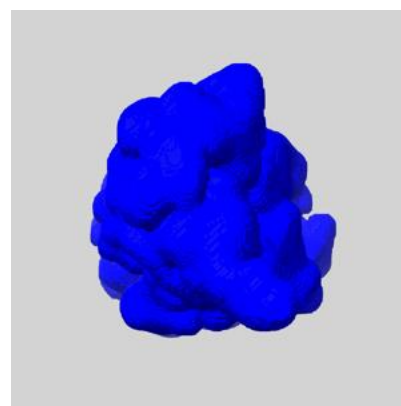
6.6.1 emd_10619_msk_1.map [i](#)



X



Y

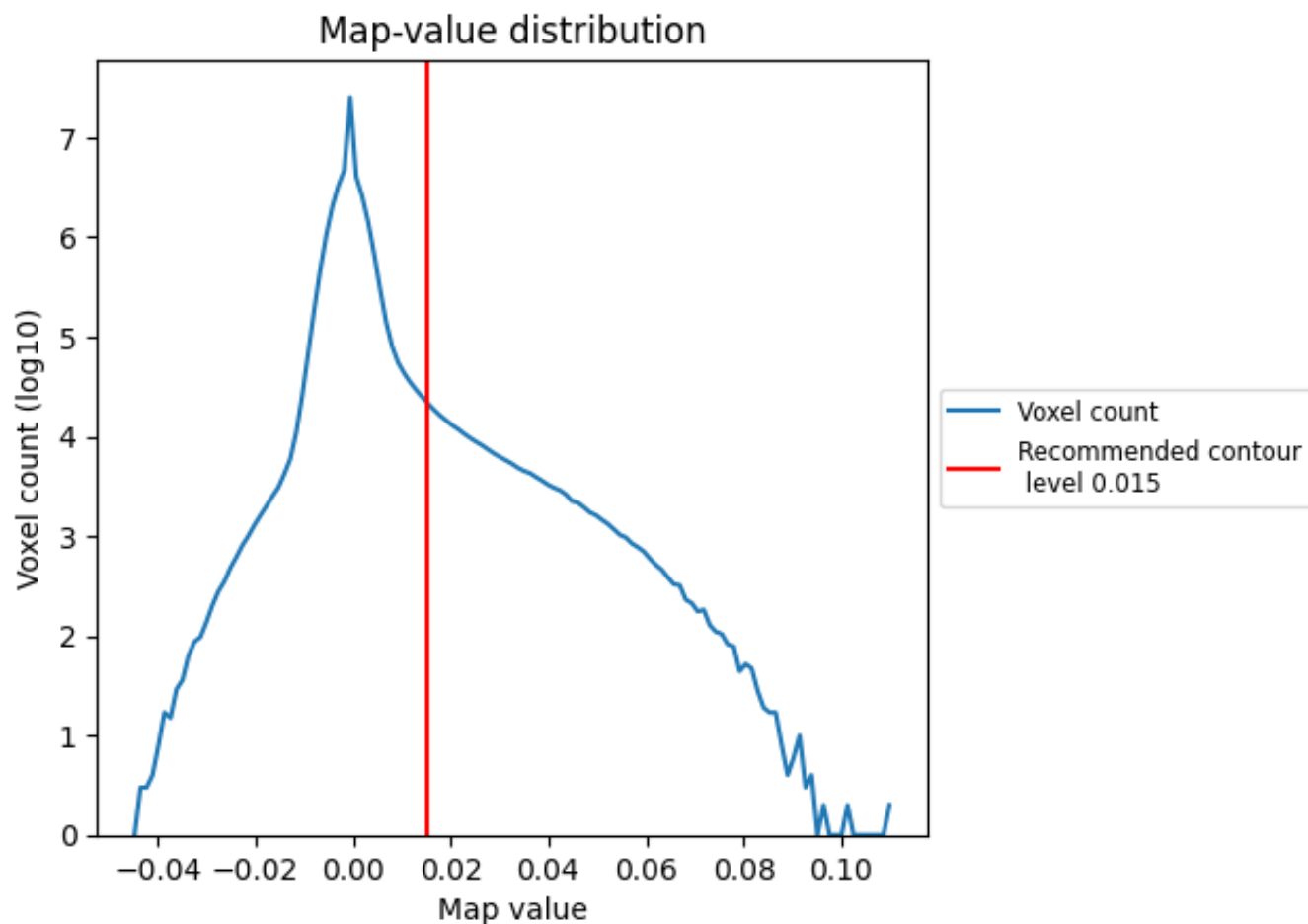


Z

7 Map analysis [i](#)

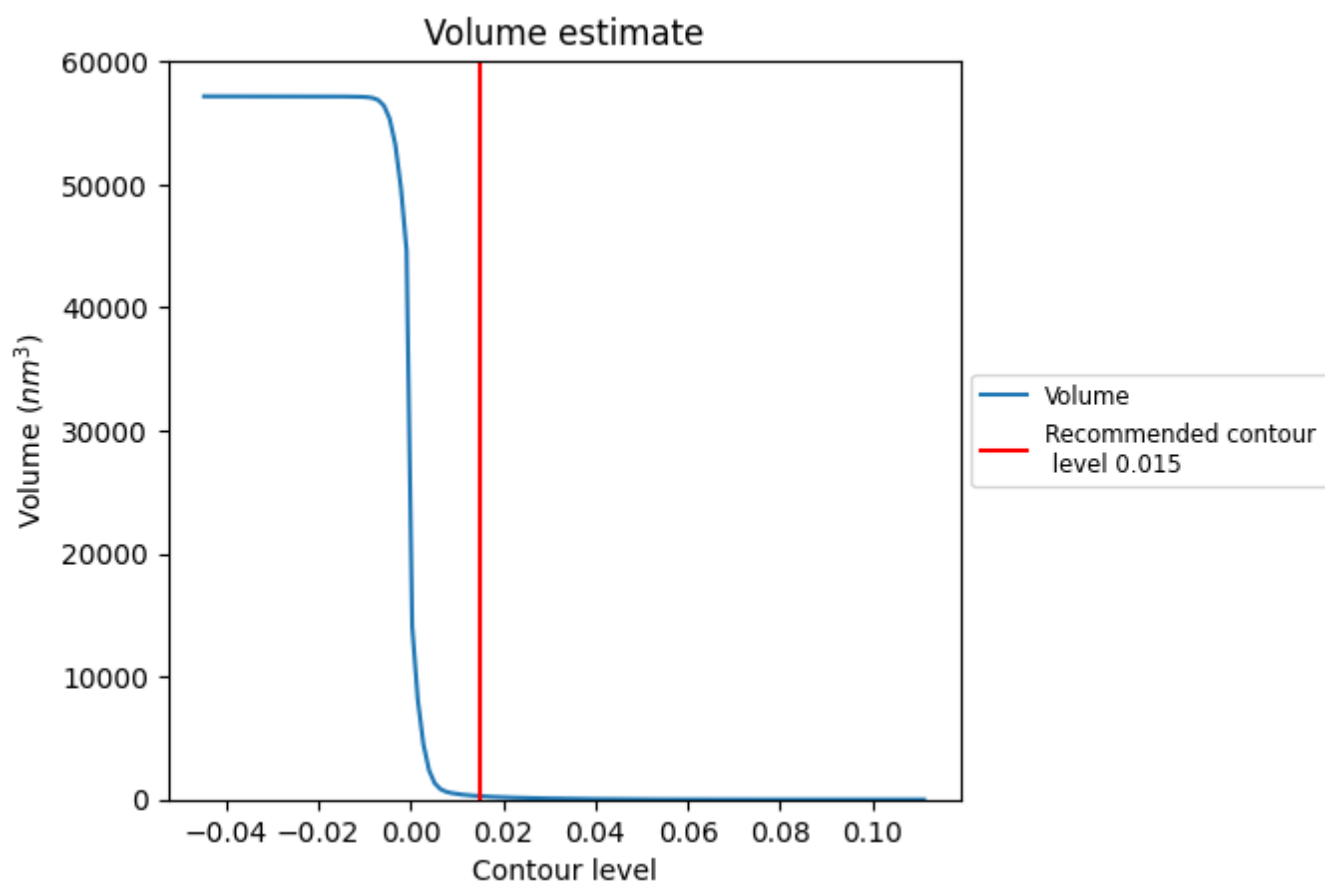
This section contains the results of statistical analysis of the map.

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.

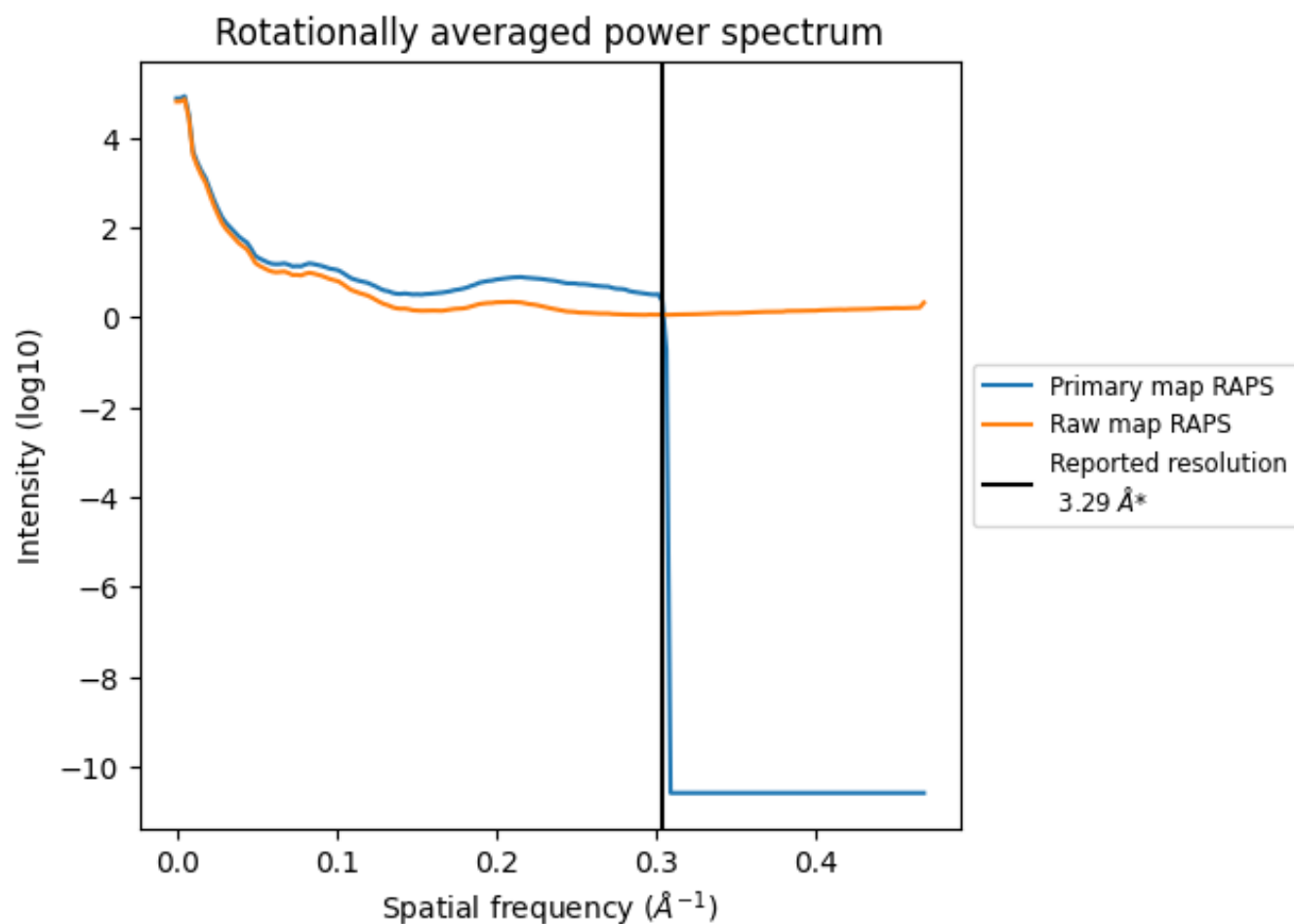
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 251 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

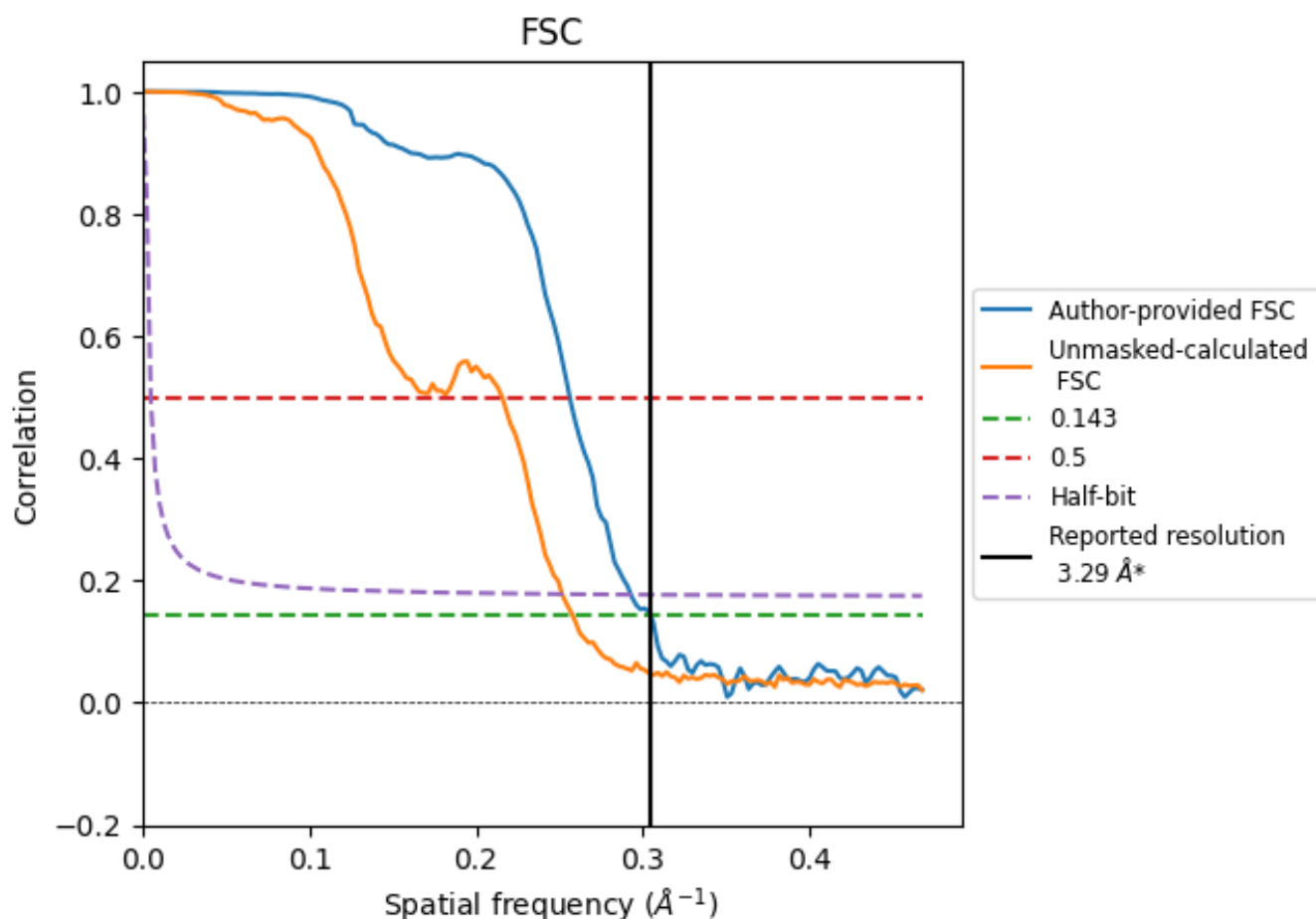


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

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 $0.304 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

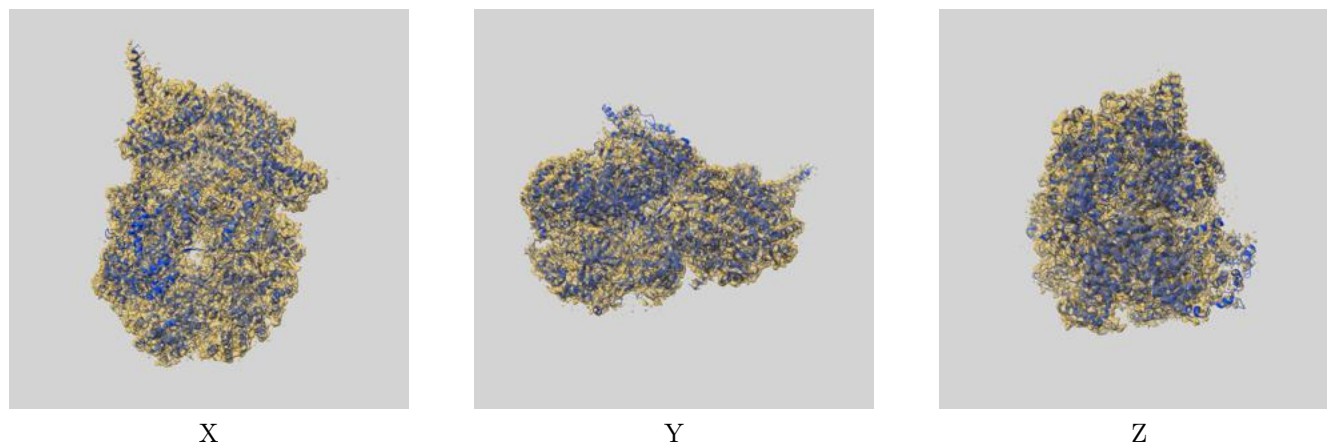
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.28	3.90	3.42
Unmasked-calculated*	3.88	4.64	3.97

*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 3.88 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

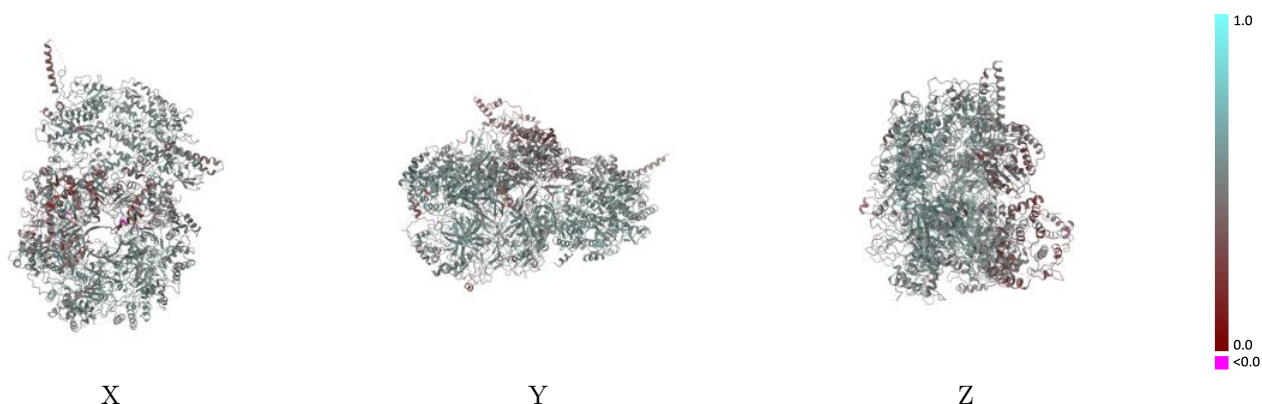
This section contains information regarding the fit between EMDB map EMD-10619 and PDB model 6XTX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



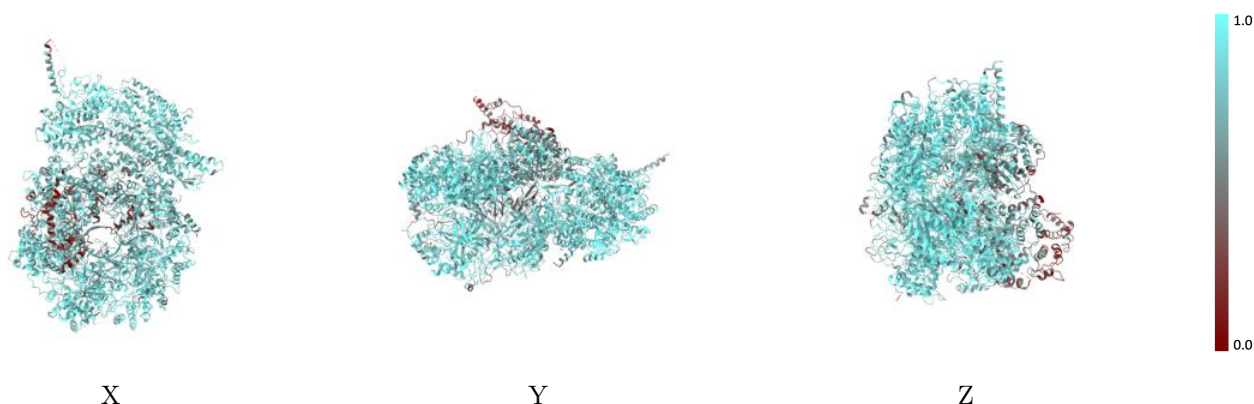
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



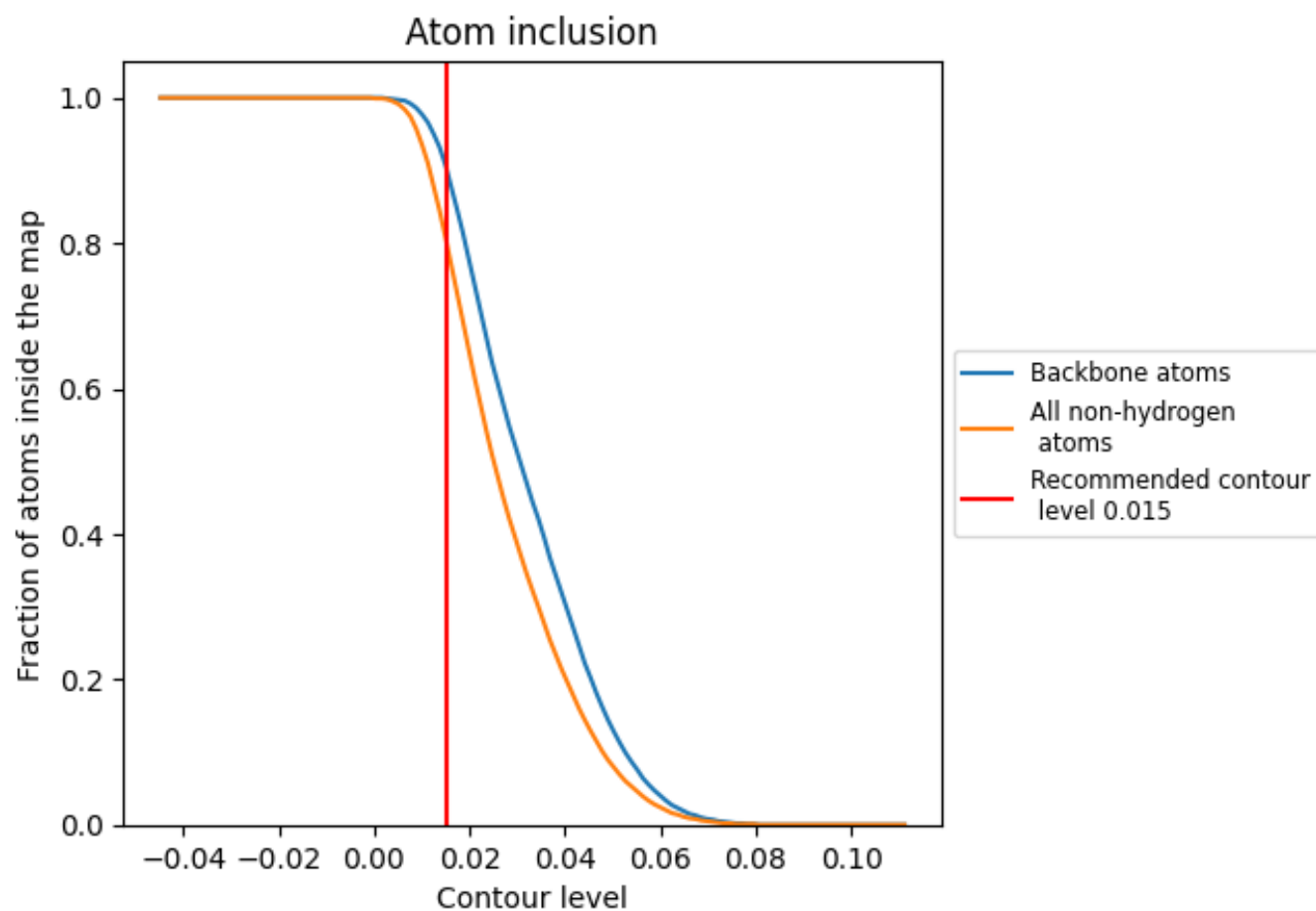
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.5060
2	0.6860	0.4620
3	0.8140	0.5150
4	0.8580	0.5280
5	0.7400	0.4830
6	0.7760	0.4990
7	0.8490	0.5220
A	0.8370	0.5020
B	0.9070	0.5440
C	0.8620	0.5300
D	0.8590	0.5270
E	0.8570	0.5150
M	0.9000	0.5640

1.0

0.0

<0.0