



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:54 PM UTC

PDB ID : 9E2X / pdb_00009e2x
EMDB ID : EMD-47471
Title : Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 2
Authors : Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on : 2024-10-23
Resolution : 3.50 Å(reported)
Based on initial model : .

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:

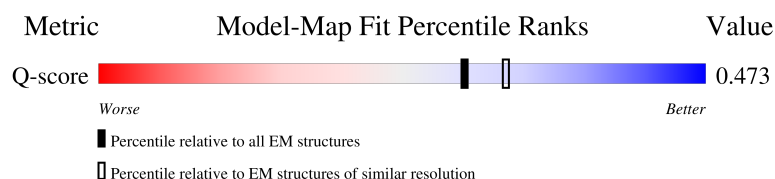
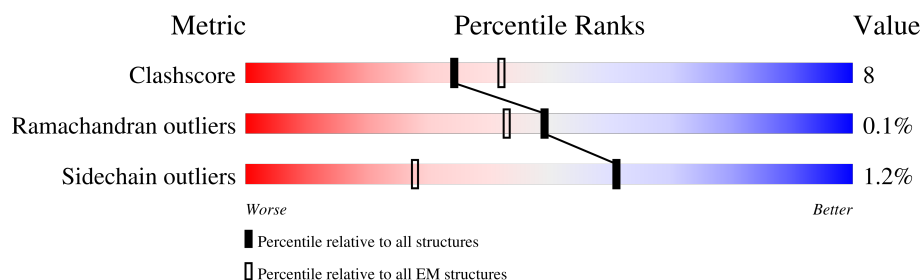
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	208	19% 76% 17% 7%
2	B	213	6% 71% 16% • 11%
3	C	217	10% 67% 12% • 20%
4	D	294	6% 62% 13% 24%

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Mol	Chain	Length	Quality of chain
5	E	650	
6	F	48	
7	G	20	
8	2	868	
9	3	971	
10	4	933	
11	5	775	
12	6	1017	
13	7	845	
14	X	1238	
15	Y	92	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 98329 atoms, of which 49013 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 complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	194	Total	C	H	N	O	S	0	0
			3180	999	1592	273	307	9		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	189	Total	C	H	N	O	S	0	0
			3191	1014	1614	276	282	5		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	174	Total	C	H	N	O	S	0	0
			2813	913	1412	225	257	6		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	222	Total	C	H	N	O	S	0	0
			3671	1170	1844	300	345	12		

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	566	Total	C	H	N	O	S	0	0
			9119	2920	4552	770	863	14		

- Molecule 6 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	48	Total	C	H	N	O	P	0	0
			1548	475	545	182	298	48		

- Molecule 7 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	20	Total	C	H	N	O	P	0	0
			633	194	224	79	116	20		

- Molecule 8 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	655	Total	C	H	N	O	S	0	0
			10454	3271	5250	933	981	19		

- Molecule 9 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	3	644	Total	C	H	N	O	S	0	0
			10097	3173	5073	894	944	13		

- Molecule 10 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4	611	Total	C	H	N	O	S	0	0
			9772	3062	4914	836	932	28		

- Molecule 11 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	5	641	Total	C	H	N	O	S	0	0
			10249	3208	5164	882	973	22		

- Molecule 12 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	6	642	Total	C	H	N	O	S	0	0
			10130	3189	5068	882	966	25		

- Molecule 13 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	7	641	Total	C	H	N	O	S	0	0
			10141	3184	5101	875	953	28		

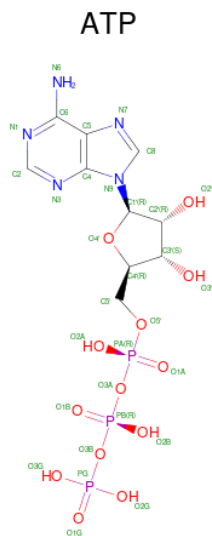
- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	X	705	Total	C	H	N	O	S	0	0
			11536	3691	5821	962	1043	19		

- Molecule 15 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Y	92	Total	C	H	N	O	S	0	0
			1537	495	769	138	131	4		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
16	2	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
16	3	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
16	5	1	Total 41	C 10	H 10	N 5	O 13	P 3	0
16	7	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

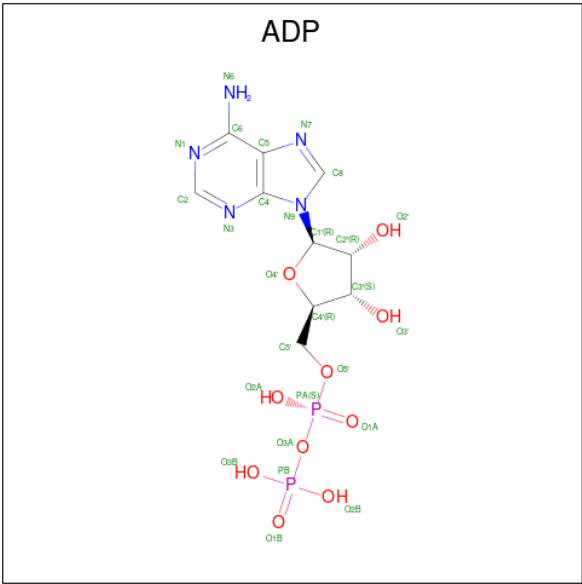
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
17	2	1	Total Mg 1 1	0
17	3	1	Total Mg 1 1	0
17	4	1	Total Mg 1 1	0
17	5	1	Total Mg 1 1	0
17	7	1	Total Mg 1 1	0

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	Zn	0
			1	1	
18	4	1	Total	Zn	0
			1	1	
18	5	1	Total	Zn	0
			1	1	
18	6	1	Total	Zn	0
			1	1	
18	7	1	Total	Zn	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

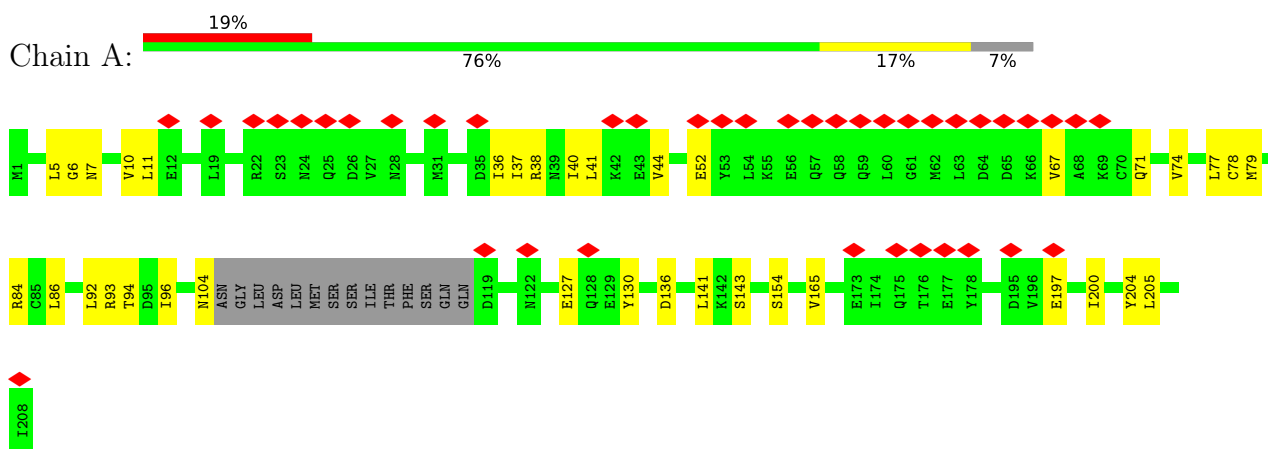


Mol	Chain	Residues	Atoms						AltConf
19	4	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
19	4	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

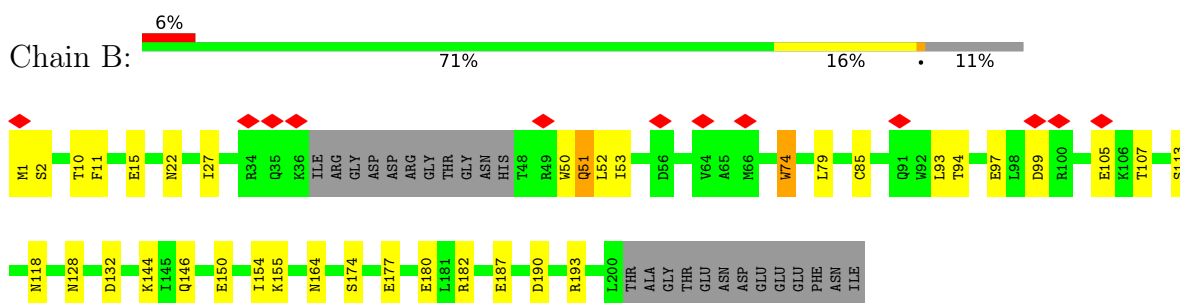
3 Residue-property plots

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.

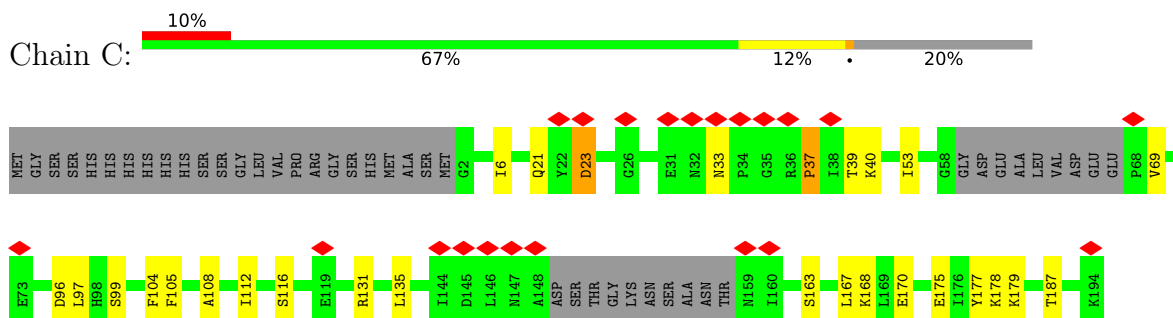
- Molecule 1: DNA replication complex GINS protein PSF1



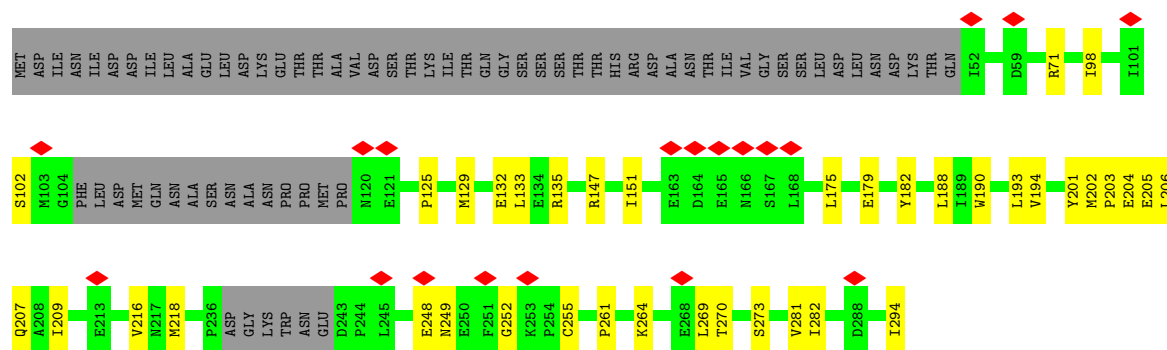
- Molecule 2: DNA replication complex GINS protein PSF2



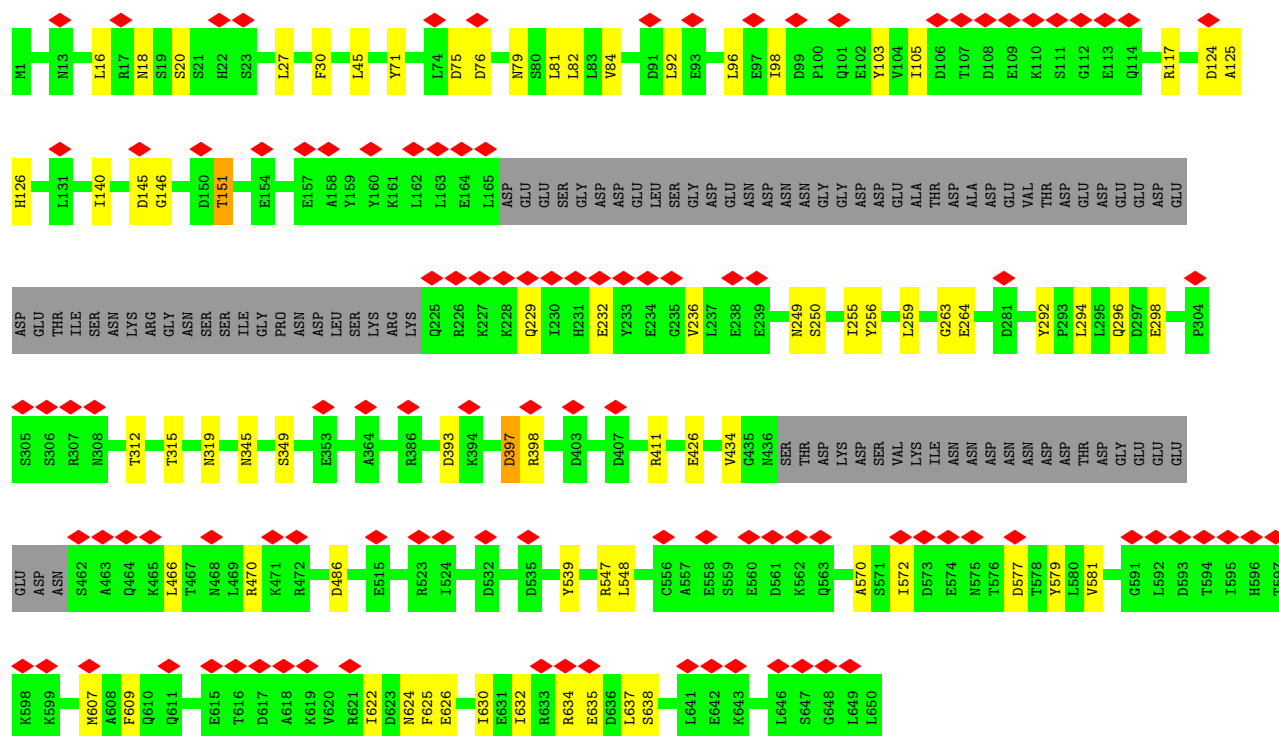
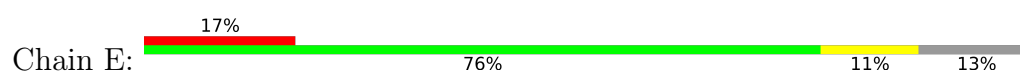
- Molecule 3: DNA replication complex GINS protein PSF3



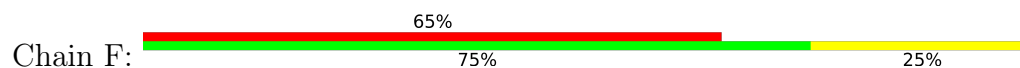
- Molecule 4: DNA replication complex GINS protein SLD5



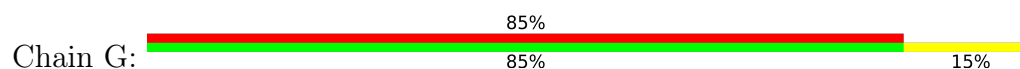
• Molecule 5: Cell division control protein 45

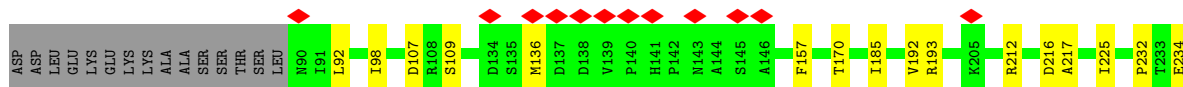
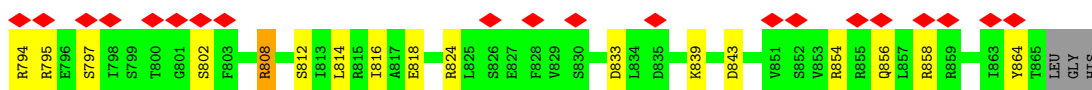


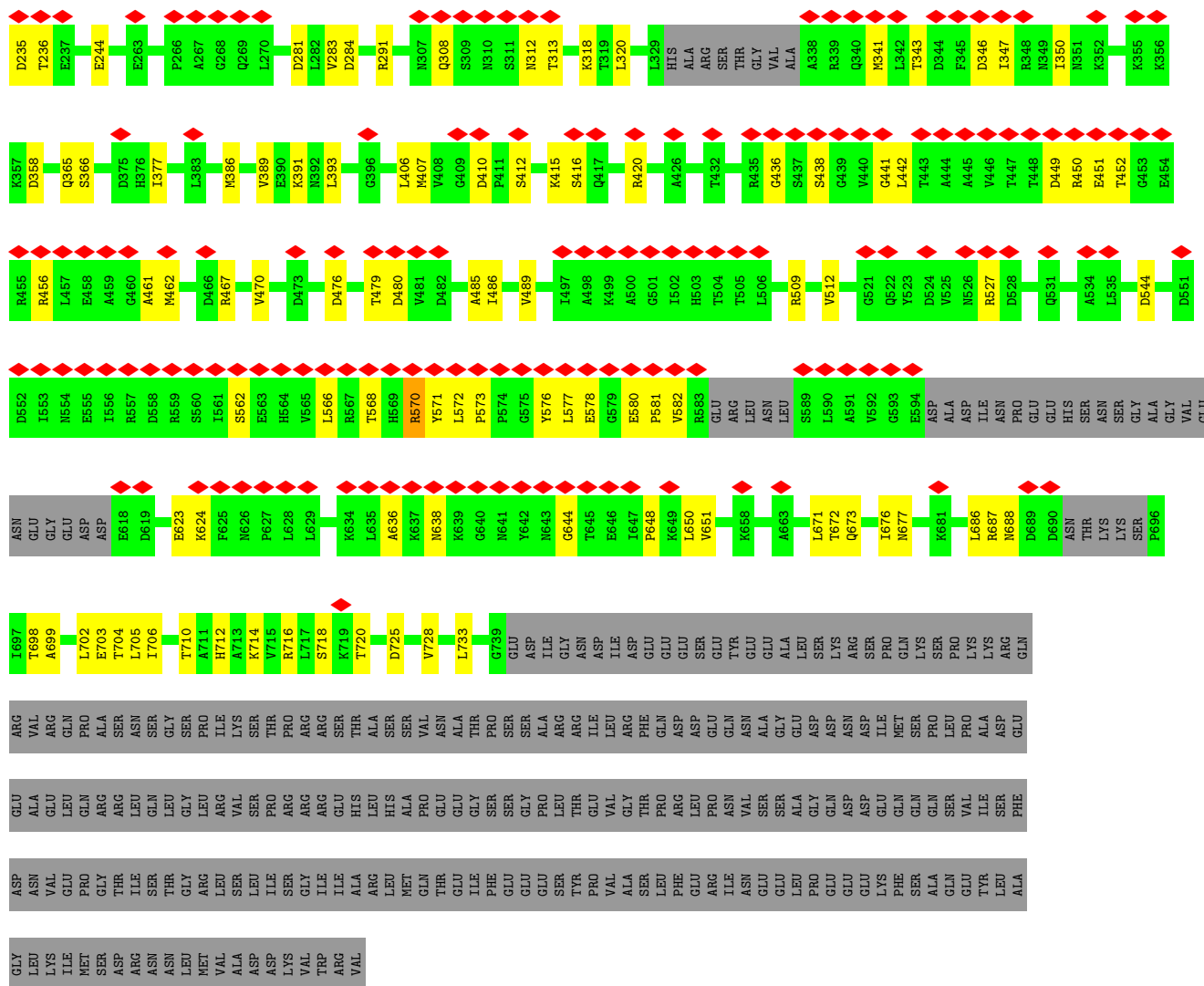
• Molecule 6: Leading strand DNA template



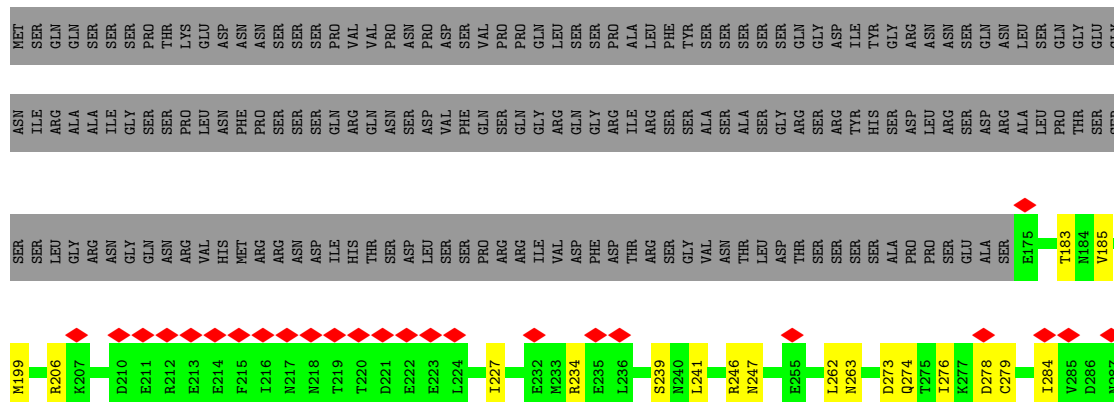
• Molecule 7: Lagging strand DNA template

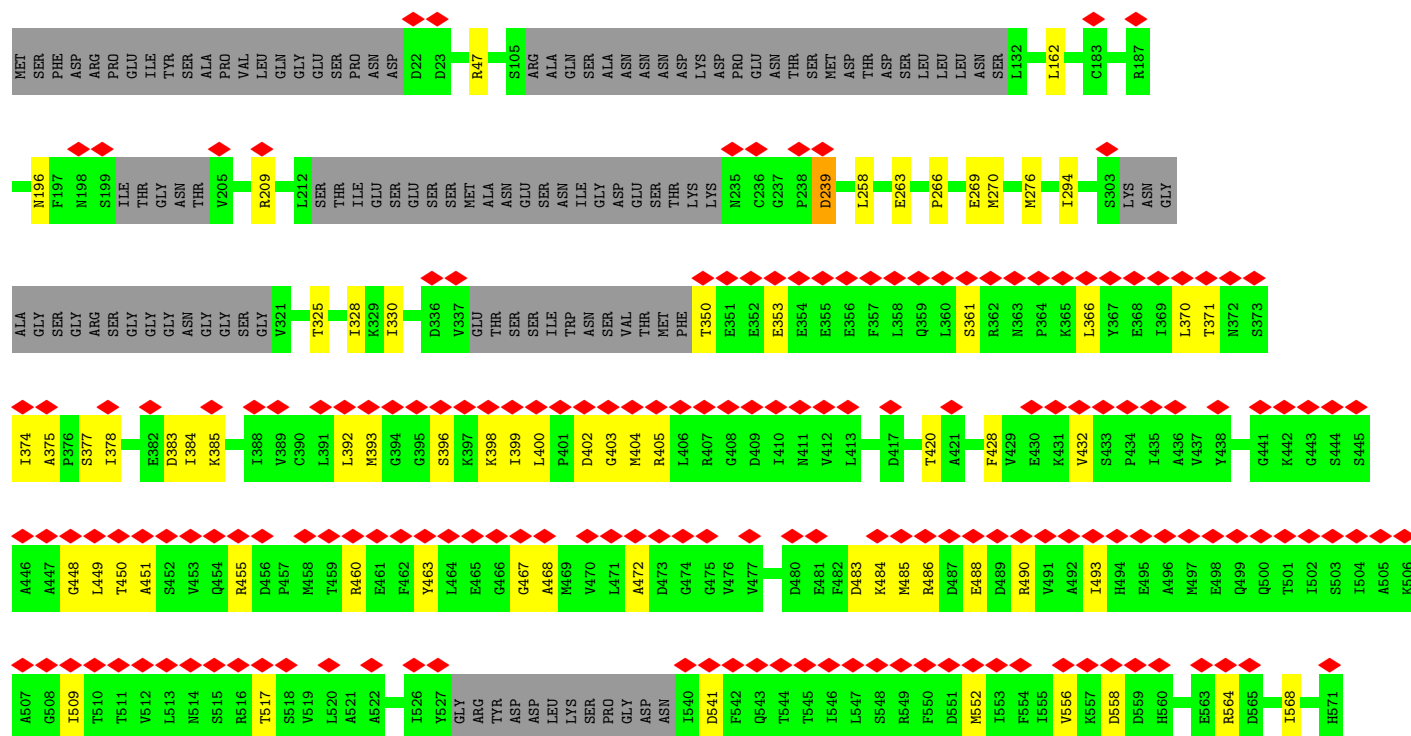


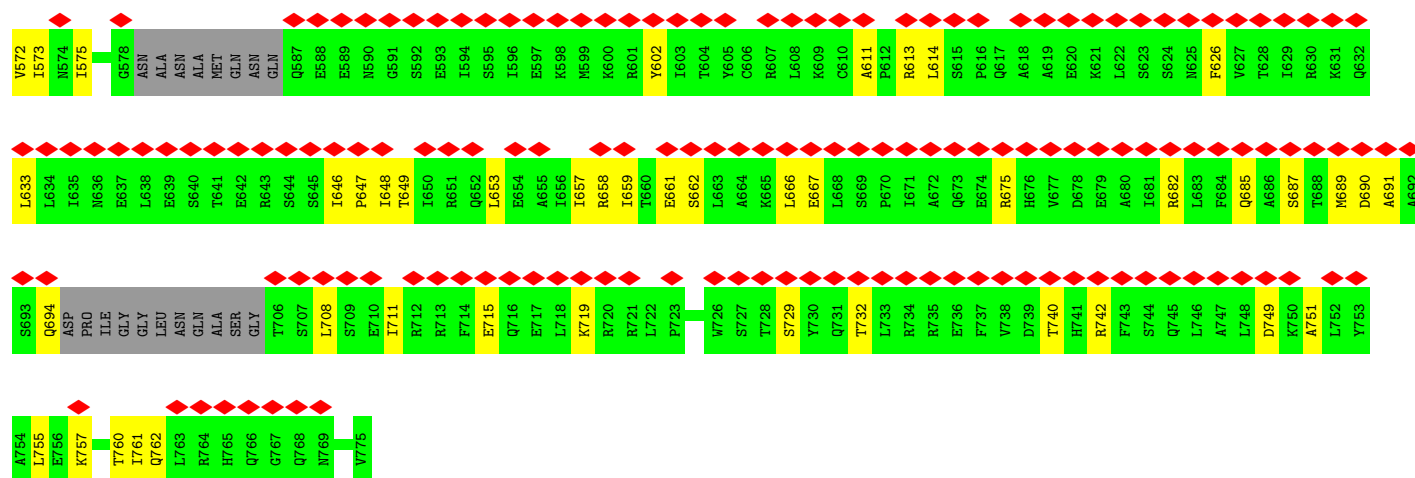




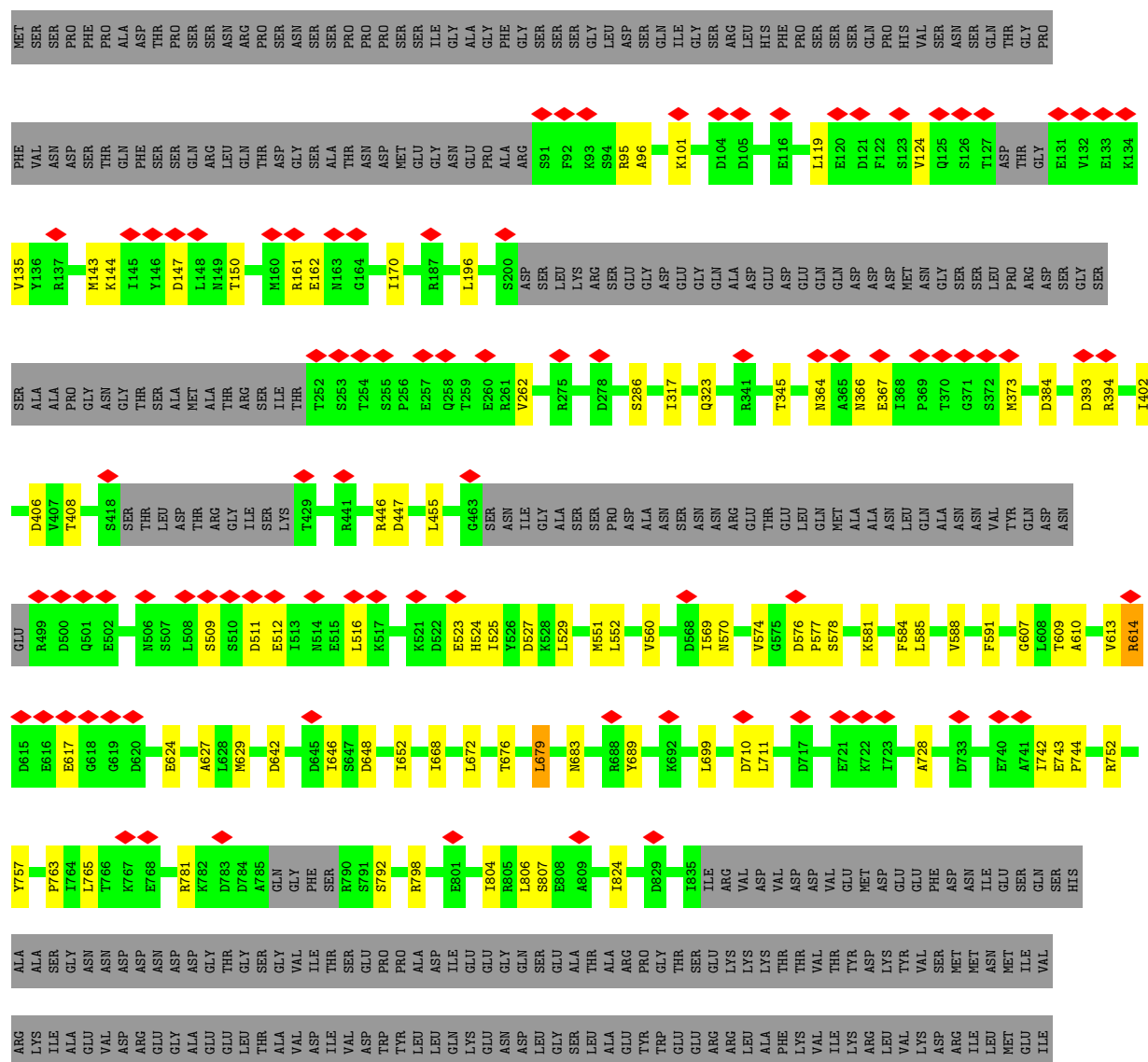
• Molecule 10: DNA replication licensing factor MCM4



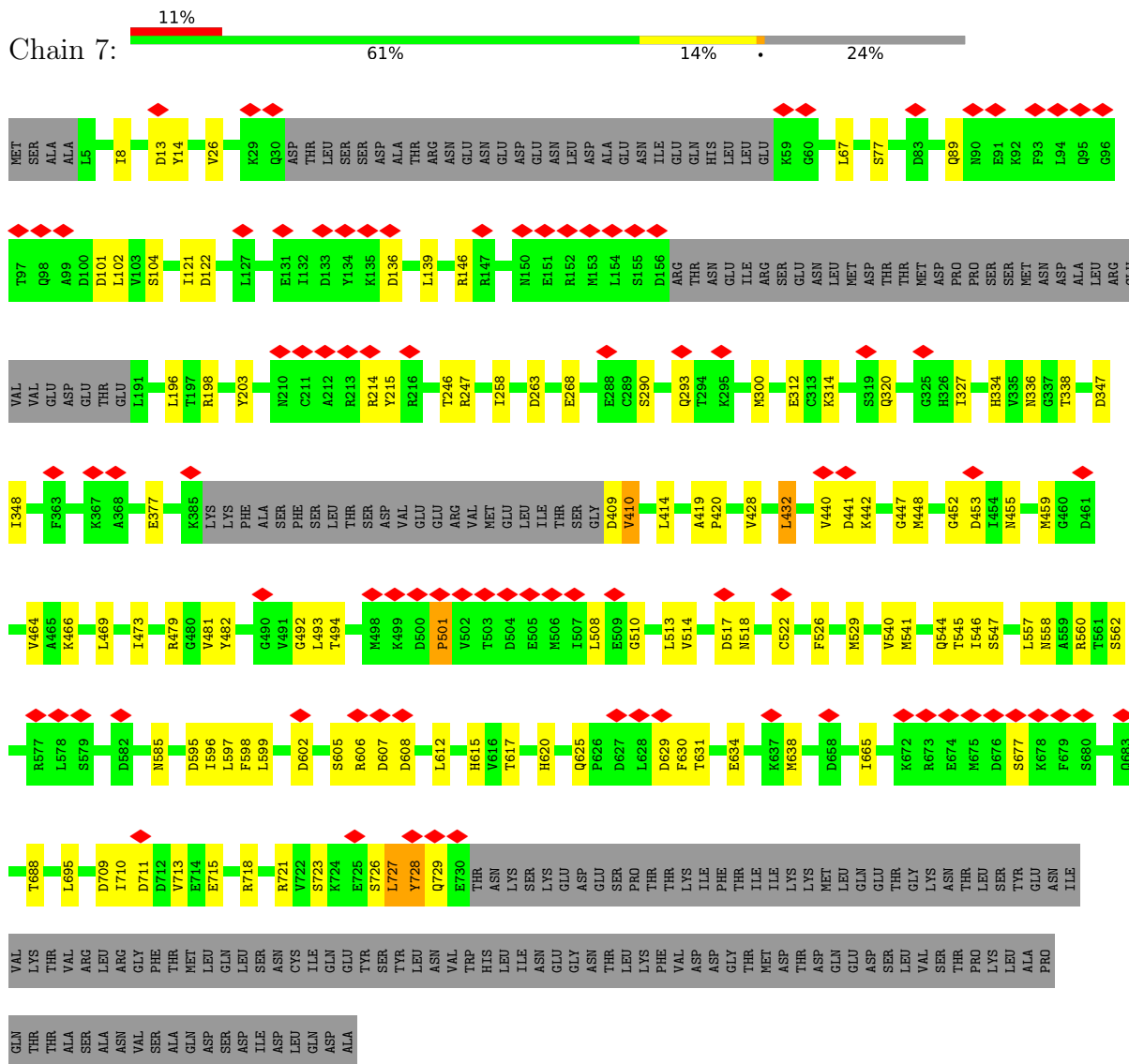




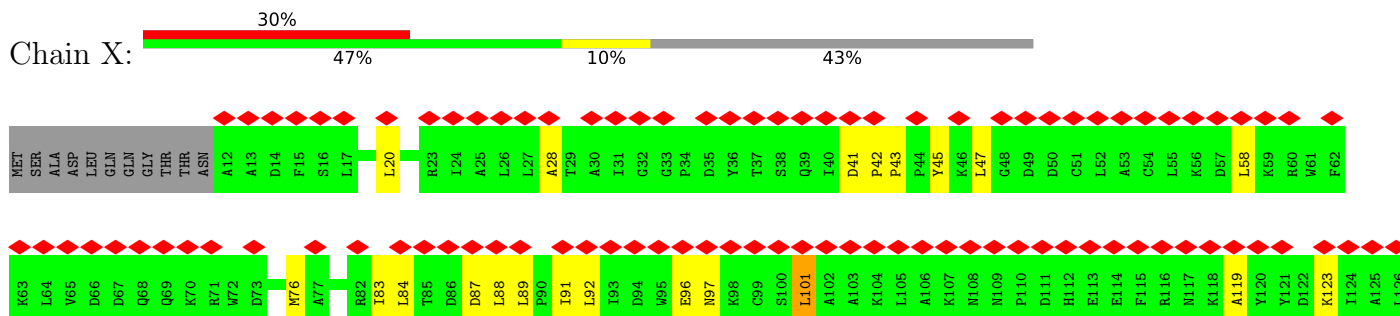
• Molecule 12: DNA replication licensing factor MCM6



Chain 7:

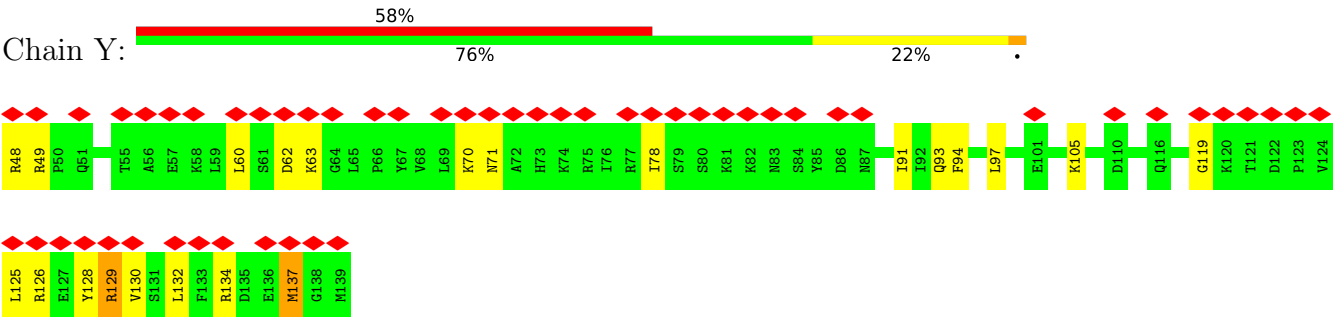


Chain X:





● Molecule 15: Chromosome segregation in meiosis protein 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40714	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	25.215	Depositor
Minimum map value	-11.847	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.450	Depositor
Recommended contour level	3	Depositor
Map size (Å)	370.04797, 370.04797, 370.04797	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8259999, 0.8259999, 0.8259999	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: ATP, MG, ZN, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.11	0/1608	0.26	0/2163
2	B	0.24	0/1609	0.41	0/2177
3	C	0.50	1/1434 (0.1%)	0.26	0/1938
4	D	0.10	0/1861	0.24	0/2514
5	E	0.12	0/4654	0.27	1/6303 (0.0%)
6	F	0.21	0/1125	0.53	0/1741
7	G	0.22	0/459	0.50	0/705
8	2	0.15	0/5292	0.29	0/7145
9	3	0.18	0/5112	0.34	4/6930 (0.1%)
10	4	0.18	0/4931	0.35	1/6666 (0.0%)
11	5	0.09	0/5155	0.24	0/6956
12	6	0.15	0/5143	0.31	0/6938
13	7	0.37	1/5120 (0.0%)	0.43	2/6921 (0.0%)
14	X	0.10	0/5828	0.26	0/7868
15	Y	0.38	0/784	0.72	2/1049 (0.2%)
All	All	0.20	2/50115 (0.0%)	0.33	10/68014 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	2	0	3
10	4	0	3
12	6	0	3
13	7	0	3
14	X	0	1
15	Y	0	4
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	37	PRO	N-CD	18.64	1.73	1.47
13	7	501	PRO	N-CD	18.41	1.73	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	571	TYR	N-CA-CB	6.11	119.02	110.04
9	3	570	ARG	N-CA-C	-6.06	105.38	112.89
15	Y	128	TYR	N-CA-CB	-5.93	101.40	110.12
15	Y	137	MET	N-CA-C	-5.57	105.21	111.28
5	E	397	ASP	CA-CB-CG	5.56	118.16	112.60
13	7	727	LEU	N-CA-CB	-5.26	102.76	111.49
9	3	571	TYR	N-CA-C	-5.19	103.29	110.35
13	7	728	TYR	N-CA-C	-5.14	106.34	113.18
10	4	833	ILE	N-CA-C	-5.13	104.09	111.17
9	3	573	PRO	N-CA-C	-5.13	104.44	110.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	2	581	ARG	Sidechain
8	2	795	ARG	Sidechain
8	2	808	ARG	Sidechain
10	4	246	ARG	Sidechain
10	4	827	ARG	Sidechain
10	4	830	ARG	Sidechain
12	6	446	ARG	Sidechain
12	6	614	ARG	Sidechain
12	6	752	ARG	Sidechain
13	7	479	ARG	Sidechain
13	7	718	ARG	Sidechain
13	7	721	ARG	Sidechain
5	E	398	ARG	Sidechain
14	X	41	ASP	Peptide
15	Y	129	ARG	Sidechain
15	Y	134	ARG	Sidechain
15	Y	48	ARG	Sidechain
15	Y	49	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1588	1592	1593	27	0
2	B	1577	1614	1625	38	0
3	C	1401	1412	1415	27	0
4	D	1827	1844	1844	37	0
5	E	4567	4552	4555	53	0
6	F	1003	545	545	11	0
7	G	409	224	224	2	0
8	2	5204	5250	5261	101	0
9	3	5024	5073	5087	114	0
10	4	4858	4914	4924	88	0
11	5	5085	5164	5177	117	0
12	6	5062	5068	5078	66	0
13	7	5040	5101	5101	120	0
14	X	5715	5821	5833	85	0
15	Y	768	769	801	14	0
16	2	31	12	12	2	0
16	3	31	12	12	1	0
16	5	31	10	11	1	0
16	7	31	12	12	1	0
17	2	1	0	0	0	0
17	3	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	7	1	0	0	0	0
18	2	1	0	0	1	0
18	4	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
19	4	54	24	24	2	0
All	All	49316	49013	49134	797	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 8.

All (797) 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)
11:5:755:LEU:HD13	11:5:761:ILE:CD1	1.48	1.40
8:2:854:ARG:NH2	8:2:858:ARG:HH22	1.20	1.39
2:B:99:ASP:OD1	2:B:144:LYS:CE	1.75	1.33
3:C:37:PRO:N	3:C:37:PRO:CD	1.73	1.32
2:B:146:GLN:CG	11:5:47:ARG:HH11	1.41	1.32
8:2:854:ARG:NH2	8:2:858:ARG:NH2	1.76	1.29
13:7:501:PRO:N	13:7:501:PRO:CD	1.73	1.27
9:3:456:ARG:NH2	13:7:327:ILE:HG21	1.47	1.26
9:3:456:ARG:NH2	13:7:327:ILE:CG2	1.99	1.23
8:2:344:CYS:SG	8:2:367:CYS:SG	2.44	1.16
10:4:709:LEU:CD1	10:4:711:LYS:HG2	1.78	1.13
5:E:577:ASP:OD1	5:E:634:ARG:CB	1.97	1.13
2:B:146:GLN:HG2	11:5:47:ARG:HH11	1.01	1.12
8:2:670:THR:HG22	8:2:672:PRO:HD2	1.22	1.12
8:2:364:CYS:SG	8:2:369:SER:N	2.21	1.11
14:X:291:PHE:CD2	14:X:474:GLU:HG2	1.86	1.10
8:2:854:ARG:HH21	8:2:858:ARG:NH2	1.38	1.10
11:5:755:LEU:HD13	11:5:761:ILE:HD12	1.09	1.08
11:5:755:LEU:CD1	11:5:761:ILE:HD12	1.82	1.08
2:B:146:GLN:HG2	11:5:47:ARG:NH1	1.69	1.08
9:3:456:ARG:NH2	13:7:327:ILE:CB	2.17	1.07
9:3:462:MET:HG2	9:3:489:VAL:HG11	1.17	1.07
4:D:255:CYS:SG	4:D:269:LEU:C	2.38	1.06
2:B:1:MET:HG2	2:B:2:SER:H	1.19	1.05
2:B:146:GLN:CG	11:5:47:ARG:NH1	2.20	1.05
11:5:755:LEU:HD13	11:5:761:ILE:HD11	1.36	1.05
2:B:99:ASP:OD1	2:B:144:LYS:HE2	1.48	1.05
9:3:456:ARG:HH22	13:7:327:ILE:CG2	1.63	1.05
11:5:755:LEU:CD1	11:5:761:ILE:CD1	2.34	1.04
3:C:105:PHE:CD2	3:C:170:GLU:OE1	2.11	1.04
5:E:577:ASP:OD1	5:E:634:ARG:HB3	1.57	1.03
8:2:854:ARG:HH21	8:2:858:ARG:CZ	1.72	1.03
10:4:709:LEU:HD11	10:4:711:LYS:HG2	1.39	1.03
4:D:255:CYS:HG	4:D:269:LEU:C	1.69	1.00
9:3:456:ARG:HH22	13:7:327:ILE:HG21	0.98	0.99
2:B:99:ASP:OD1	2:B:144:LYS:HE3	1.60	0.99
12:6:523:GLU:OE2	12:6:524:HIS:CD2	2.16	0.99
5:E:577:ASP:OD1	5:E:634:ARG:HB2	1.62	0.96
9:3:456:ARG:NH2	13:7:327:ILE:HB	1.80	0.95
14:X:291:PHE:CG	14:X:474:GLU:HG2	2.00	0.95
8:2:854:ARG:CZ	8:2:858:ARG:NH2	2.31	0.93
8:2:839:LYS:HE3	8:2:843:ASP:OD2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:PHE:HB3	3:C:170:GLU:OE2	1.69	0.93
5:E:292:TYR:CZ	5:E:296:GLN:NE2	2.35	0.93
2:B:146:GLN:HG3	11:5:47:ARG:HH11	1.36	0.91
8:2:591:LEU:HD22	11:5:270:MET:HE1	1.50	0.91
8:2:670:THR:HG22	8:2:672:PRO:CD	2.01	0.90
2:B:105:GLU:OE1	2:B:113:SER:OG	1.90	0.89
12:6:569:ILE:HG23	12:6:710:ASP:OD2	1.73	0.89
9:3:451:GLU:HB2	11:5:460:ARG:HH22	1.39	0.89
19:4:1004:ADP:O3B	12:6:581:LYS:NZ	2.06	0.89
13:7:469:LEU:O	13:7:473:ILE:HG22	1.74	0.88
9:3:462:MET:HG2	9:3:489:VAL:CG1	2.03	0.88
14:X:593:GLU:OE1	14:X:692:LYS:NZ	2.06	0.87
10:4:529:SER:OG	13:7:448:MET:SD	2.33	0.87
4:D:255:CYS:SG	4:D:269:LEU:O	2.31	0.86
9:3:456:ARG:HH21	13:7:327:ILE:HB	1.42	0.84
8:2:670:THR:CG2	8:2:672:PRO:HD2	2.05	0.84
9:3:391:LYS:NZ	13:7:620:HIS:O	2.10	0.84
9:3:456:ARG:HH21	13:7:327:ILE:CG2	1.87	0.84
9:3:456:ARG:HH22	13:7:327:ILE:CD1	1.91	0.84
14:X:45:TYR:OH	14:X:87:ASP:OD1	1.96	0.83
8:2:591:LEU:HD11	8:2:631:ILE:HD12	1.60	0.83
8:2:364:CYS:SG	8:2:368:LYS:N	2.51	0.83
9:3:544:ASP:OD1	9:3:704:THR:OG1	1.95	0.83
12:6:509:SER:OG	12:6:511:ASP:OD1	1.96	0.83
13:7:246:THR:O	13:7:247:ARG:HG3	1.78	0.83
8:2:241:SER:OG	8:2:413:ASP:OD2	1.96	0.82
13:7:558:ASN:OD1	13:7:560:ARG:NH1	2.12	0.82
2:B:79:LEU:HB3	2:B:85:CYS:SG	2.19	0.82
8:2:839:LYS:CE	8:2:843:ASP:OD2	2.28	0.82
4:D:209:ILE:O	4:D:218:MET:HE2	1.80	0.81
2:B:174:SER:OG	2:B:177:GLU:OE1	1.98	0.81
9:3:527:ARG:NH2	11:5:715:GLU:OE1	2.13	0.81
12:6:523:GLU:OE2	12:6:524:HIS:NE2	2.13	0.81
13:7:459:MET:HE2	13:7:597:LEU:HD21	1.61	0.81
3:C:97:LEU:HD13	3:C:170:GLU:OE2	1.81	0.80
2:B:182:ARG:NH2	4:D:294:ILE:O	2.14	0.80
12:6:161:ARG:HG2	12:6:162:GLU:HG3	1.62	0.80
14:X:144:GLN:N	14:X:144:GLN:OE1	2.14	0.80
14:X:291:PHE:CD2	14:X:474:GLU:CG	2.65	0.79
12:6:584:PHE:O	12:6:588:VAL:HG23	1.83	0.79
14:X:87:ASP:O	14:X:91:ILE:HD12	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:420:PRO:O	13:7:625:GLN:NE2	2.17	0.78
12:6:406:ASP:OD1	12:6:408:THR:OG1	1.99	0.78
8:2:752:GLU:O	8:2:756:SER:OG	2.01	0.78
8:2:591:LEU:CD1	8:2:631:ILE:HD12	2.13	0.78
10:4:531:TYR:OH	10:4:719:GLU:OE1	2.01	0.78
16:2:1001:ATP:O1B	12:6:798:ARG:NH2	2.16	0.77
10:4:274:GLN:NE2	10:4:278:ASP:OD1	2.18	0.76
5:E:624:ASN:OD1	5:E:626:GLU:N	2.18	0.76
13:7:290:SER:O	13:7:293:GLN:NE2	2.18	0.76
5:E:292:TYR:CE2	5:E:296:GLN:NE2	2.54	0.76
2:B:190:ASP:OD1	2:B:193:ARG:NH2	2.18	0.76
8:2:190:LYS:NZ	14:X:87:ASP:OD2	2.13	0.75
8:2:794:ARG:NH2	11:5:558:ASP:OD2	2.19	0.75
11:5:659:ILE:O	11:5:662:SER:OG	2.03	0.75
9:3:39:ARG:HG3	9:3:136:MET:HE1	1.68	0.75
11:5:375:ALA:HB1	11:5:378:ILE:HD12	1.69	0.75
11:5:374:ILE:HD12	11:5:428:PHE:HE1	1.49	0.75
9:3:451:GLU:OE2	11:5:460:ARG:NH1	2.20	0.75
12:6:711:LEU:HD21	12:6:806:LEU:HD11	1.67	0.75
13:7:101:ASP:OD2	13:7:104:SER:OG	2.01	0.74
2:B:1:MET:HG2	2:B:2:SER:N	1.98	0.74
4:D:98:ILE:HD12	4:D:133:LEU:HD12	1.69	0.74
11:5:449:LEU:HD22	11:5:493:ILE:HD11	1.68	0.74
9:3:462:MET:CG	9:3:489:VAL:HG11	2.10	0.74
5:E:232:GLU:O	5:E:236:VAL:HG23	1.88	0.74
5:E:630:ILE:HD11	5:E:632:ILE:HD11	1.70	0.74
8:2:485:ARG:NH2	8:2:769:TYR:OH	2.21	0.73
8:2:591:LEU:CD2	11:5:270:MET:HE1	2.16	0.73
11:5:729:SER:HG	11:5:732:THR:HG1	0.74	0.73
5:E:76:ASP:OD1	5:E:117:ARG:NH1	2.22	0.73
6:F:47:DG:OP1	9:3:193:ARG:NH1	2.21	0.73
8:2:591:LEU:HD23	8:2:592:GLU:O	1.89	0.73
8:2:549:LYS:NZ	16:2:1001:ATP:O1G	2.15	0.73
9:3:244:GLU:OE1	13:7:14:TYR:OH	2.06	0.73
11:5:755:LEU:CD1	11:5:761:ILE:HD11	2.09	0.73
10:4:574:LYS:NZ	19:4:1001:ADP:O3B	2.22	0.73
2:B:1:MET:CG	2:B:2:SER:H	1.99	0.72
5:E:79:ASN:ND2	5:E:117:ARG:O	2.22	0.72
8:2:785:LYS:O	8:2:789:VAL:HG23	1.90	0.72
8:2:839:LYS:HD2	8:2:843:ASP:OD2	1.90	0.71
11:5:370:LEU:HD11	11:5:602:TYR:CE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:320:GLN:OE1	13:7:320:GLN:N	2.23	0.71
11:5:384:ILE:HD11	11:5:556:VAL:HG22	1.72	0.71
9:3:456:ARG:HH22	13:7:327:ILE:CB	1.93	0.71
13:7:420:PRO:C	13:7:625:GLN:HE22	1.98	0.71
4:D:270:THR:O	4:D:273:SER:OG	2.08	0.71
8:2:854:ARG:HH21	8:2:858:ARG:NH1	1.88	0.71
13:7:585:ASN:OD1	13:7:585:ASN:O	2.08	0.71
11:5:263:GLU:N	11:5:263:GLU:OE2	2.24	0.70
13:7:122:ASP:OD2	13:7:198:ARG:NH1	2.25	0.70
8:2:656:ARG:NH2	12:6:792:SER:O	2.25	0.70
11:5:209:ARG:NH1	11:5:239:ASP:OD1	2.24	0.70
8:2:510:ASP:OD1	8:2:511:ILE:N	2.25	0.70
8:2:425:GLU:OE2	8:2:459:ARG:NE	2.25	0.69
9:3:365:GLN:NE2	9:3:636:ALA:HB1	2.07	0.69
5:E:249:ASN:OD1	5:E:250:SER:N	2.23	0.69
13:7:605:SER:OG	13:7:607:ASP:OD1	2.09	0.69
4:D:205:GLU:OE2	4:D:205:GLU:N	2.25	0.69
9:3:343:THR:OG1	9:3:346:ASP:OD2	2.06	0.69
9:3:688:ASN:HD22	13:7:606:ARG:HE	1.39	0.69
12:6:364:ASN:CG	12:6:394:ARG:HE	2.00	0.69
1:A:6:GLY:O	1:A:10:VAL:HG23	1.93	0.69
8:2:364:CYS:SG	8:2:368:LYS:CA	2.81	0.68
2:B:99:ASP:OD1	2:B:144:LYS:NZ	2.25	0.68
6:F:25:DT:H2"	6:F:26:DG:C8	2.29	0.68
13:7:599:LEU:H	13:7:727:LEU:HD13	1.58	0.68
9:3:366:SER:OG	9:3:651:VAL:O	2.12	0.68
13:7:258:ILE:HG21	13:7:300:MET:HE2	1.74	0.68
13:7:709:ASP:OD1	13:7:710:ILE:HG22	1.93	0.68
12:6:642:ASP:OD2	12:6:683:ASN:N	2.26	0.68
14:X:194:ARG:NH1	14:X:276:GLU:O	2.26	0.68
5:E:75:ASP:OD1	5:E:76:ASP:N	2.27	0.67
8:2:839:LYS:CD	8:2:843:ASP:OD2	2.43	0.67
14:X:300:GLU:OE1	14:X:300:GLU:N	2.27	0.67
13:7:598:PHE:HA	13:7:727:LEU:HD13	1.76	0.67
5:E:124:ASP:OD1	5:E:125:ALA:N	2.28	0.67
10:4:683:ASN:HD22	10:4:686:LEU:CD1	2.07	0.67
13:7:420:PRO:C	13:7:625:GLN:NE2	2.52	0.67
12:6:765:LEU:HD11	12:6:804:ILE:HD12	1.77	0.67
9:3:456:ARG:NH2	13:7:327:ILE:CD1	2.57	0.67
14:X:207:ASN:O	14:X:211:ASN:ND2	2.27	0.66
9:3:572:LEU:HD11	11:5:613:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:723:SER:O	13:7:727:LEU:HD12	1.96	0.66
11:5:682:ARG:NH1	11:5:685:GLN:OE1	2.28	0.66
9:3:712:HIS:ND1	9:3:725:ASP:OD1	2.26	0.66
9:3:570:ARG:NE	11:5:614:LEU:HD11	2.11	0.66
8:2:344:CYS:SG	8:2:367:CYS:CB	2.85	0.65
12:6:607:GLY:O	12:6:627:ALA:N	2.29	0.65
13:7:428:VAL:O	13:7:432:LEU:HD22	1.97	0.65
8:2:781:MET:SD	8:2:782:ASP:N	2.70	0.65
9:3:456:ARG:HH21	13:7:327:ILE:CB	1.94	0.65
9:3:318:LYS:HE2	9:3:320:LEU:HD11	1.78	0.65
8:2:360:ARG:NH2	12:6:345:THR:OG1	2.30	0.65
9:3:410:ASP:O	9:3:415:LYS:NZ	2.30	0.65
9:3:476:ASP:OD1	11:5:757:LYS:NZ	2.29	0.65
12:6:366:ASN:OD1	12:6:367:GLU:N	2.29	0.64
4:D:255:CYS:SG	4:D:269:LEU:N	2.70	0.64
8:2:367:CYS:SG	18:2:1003:ZN:ZN	1.86	0.64
9:3:341:MET:N	9:3:341:MET:HE2	2.12	0.64
9:3:623:GLU:OE1	9:3:624:LYS:N	2.31	0.64
13:7:89:GLN:OE1	13:7:102:LEU:N	2.28	0.64
13:7:455:ASN:N	13:7:595:ASP:OD2	2.31	0.64
2:B:187:GLU:OE2	3:C:179:LYS:NZ	2.24	0.64
8:2:344:CYS:SG	8:2:367:CYS:HB3	2.36	0.64
14:X:351:LYS:O	14:X:351:LYS:NZ	2.24	0.64
13:7:596:ILE:HD11	13:7:695:LEU:HD11	1.79	0.63
14:X:302:LEU:HD12	14:X:438:LYS:HG2	1.81	0.63
8:2:578:ALA:O	8:2:633:LYS:NZ	2.31	0.63
8:2:761:GLU:OE1	8:2:761:GLU:N	2.32	0.63
11:5:374:ILE:HD12	11:5:428:PHE:CE1	2.32	0.63
11:5:667:GLU:OE2	11:5:675:ARG:NH2	2.32	0.63
15:Y:71:ASN:ND2	15:Y:71:ASN:O	2.31	0.63
8:2:786:VAL:CG2	11:5:573:ILE:HD11	2.29	0.63
8:2:856:GLN:OE1	8:2:856:GLN:N	2.31	0.63
13:7:246:THR:O	13:7:247:ARG:CG	2.45	0.63
4:D:190:TRP:CZ3	4:D:209:ILE:HD11	2.34	0.63
4:D:190:TRP:HZ3	4:D:209:ILE:HD11	1.64	0.62
8:2:626:GLN:OE1	8:2:626:GLN:N	2.30	0.62
14:X:656:GLU:O	14:X:661:LYS:NZ	2.32	0.62
5:E:345:ASN:O	5:E:349:SER:N	2.32	0.62
11:5:448:GLY:O	11:5:468:ALA:N	2.32	0.62
4:D:147:ARG:NE	4:D:179:GLU:OE2	2.29	0.62
11:5:658:ARG:NH1	11:5:661:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:O	1:A:44:VAL:HG23	2.00	0.62
9:3:703:GLU:OE1	16:7:1001:ATP:O3'	2.17	0.62
1:A:154:SER:OG	1:A:197:GLU:OE2	2.17	0.62
11:5:353:GLU:OE1	11:5:353:GLU:N	2.33	0.62
2:B:180:GLU:OE1	3:C:187:THR:HG21	1.99	0.61
10:4:378:GLU:OE1	12:6:95:ARG:NH2	2.33	0.61
5:E:105:ILE:HD11	5:E:117:ARG:HB3	1.82	0.61
4:D:98:ILE:HD11	4:D:129:MET:HB3	1.82	0.61
11:5:276:MET:HE3	11:5:330:ILE:HD11	1.83	0.61
1:A:36:ILE:HD12	1:A:36:ILE:H	1.66	0.61
8:2:552:ILE:O	8:2:556:VAL:HG13	2.00	0.61
9:3:671:LEU:HD21	9:3:706:ILE:HG23	1.82	0.61
14:X:533:MET:HE1	14:X:591:CYS:SG	2.41	0.60
13:7:634:GLU:OE1	13:7:634:GLU:N	2.32	0.60
8:2:511:ILE:O	8:2:515:VAL:HG12	2.02	0.60
10:4:632:ASP:O	10:4:674:SER:OG	2.19	0.60
14:X:465:ASP:OD1	14:X:466:ARG:N	2.34	0.60
8:2:631:ILE:HD11	8:2:640:LEU:HD13	1.84	0.59
9:3:456:ARG:NH2	13:7:327:ILE:HD12	2.16	0.59
3:C:105:PHE:CE2	3:C:170:GLU:OE1	2.54	0.59
8:2:358:GLU:OE1	8:2:358:GLU:N	2.35	0.59
9:3:688:ASN:HD22	13:7:606:ARG:HH21	1.49	0.59
10:4:206:ARG:NH1	10:4:247:ASN:OD1	2.36	0.59
12:6:585:LEU:CD1	12:6:679:LEU:HD21	2.33	0.59
9:3:318:LYS:HE2	9:3:320:LEU:HD21	1.85	0.59
10:4:820:GLU:N	10:4:820:GLU:OE1	2.35	0.59
13:7:336:ASN:ND2	13:7:377:GLU:OE2	2.35	0.59
13:7:615:HIS:CE1	13:7:625:GLN:OE1	2.55	0.59
8:2:824:ARG:NH1	8:2:833:ASP:OD2	2.36	0.59
5:E:71:TYR:CD2	5:E:96:LEU:HD22	2.38	0.58
9:3:449:ASP:OD1	9:3:450:ARG:N	2.37	0.58
12:6:570:ASN:O	12:6:710:ASP:HB3	2.02	0.58
10:4:274:GLN:NE2	10:4:274:GLN:O	2.36	0.58
13:7:508:LEU:HD21	13:7:557:LEU:HD11	1.84	0.58
4:D:261:PRO:O	4:D:264:LYS:NZ	2.32	0.58
13:7:595:ASP:C	13:7:596:ILE:HD12	2.28	0.58
8:2:854:ARG:NE	8:2:858:ARG:NH2	2.51	0.58
10:4:374:ILE:N	10:4:374:ILE:HD12	2.18	0.58
11:5:350:THR:N	11:5:353:GLU:OE2	2.37	0.58
3:C:108:ALA:O	3:C:112:ILE:HG13	2.03	0.58
9:3:358:ASP:OD1	9:3:358:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:234:GLU:N	9:3:234:GLU:OE1	2.36	0.58
10:4:709:LEU:HD13	10:4:711:LYS:HG2	1.79	0.58
12:6:574:VAL:HG21	12:6:699:LEU:HD21	1.85	0.58
4:D:204:GLU:OE2	4:D:207:GLN:NE2	2.37	0.57
8:2:778:LEU:HD11	8:2:814:LEU:HD12	1.85	0.57
14:X:729:ASP:O	14:X:732:SER:OG	2.20	0.57
11:5:552:MET:CE	11:5:687:SER:OG	2.52	0.57
12:6:523:GLU:N	12:6:523:GLU:OE1	2.37	0.57
9:3:98:ILE:HD11	9:3:157:PHE:CE1	2.40	0.57
3:C:23:ASP:OD1	3:C:23:ASP:N	2.36	0.57
8:2:399:PRO:O	8:2:401:ARG:NH1	2.38	0.57
12:6:742:ILE:HG22	12:6:744:PRO:HD3	1.87	0.57
4:D:188:LEU:HD23	4:D:188:LEU:C	2.29	0.56
10:4:562:ILE:HA	10:4:703:ASP:OD2	2.05	0.56
14:X:84:LEU:HA	14:X:88:LEU:HD23	1.87	0.56
6:F:24:DG:O3'	14:X:401:ARG:NH2	2.39	0.56
9:3:688:ASN:ND2	13:7:606:ARG:HH21	2.03	0.56
12:6:609:THR:HG22	12:6:610:ALA:H	1.70	0.56
9:3:716:ARG:NH2	9:3:718:SER:OG	2.39	0.56
2:B:53:ILE:N	4:D:132:GLU:OE2	2.36	0.56
1:A:44:VAL:HG11	4:D:202:MET:HE2	1.86	0.56
10:4:262:LEU:HD21	10:4:308:VAL:HG22	1.86	0.56
13:7:607:ASP:OD1	13:7:607:ASP:N	2.39	0.56
14:X:291:PHE:HB2	14:X:474:GLU:OE2	2.06	0.56
10:4:709:LEU:CD1	10:4:711:LYS:CG	2.70	0.56
12:6:525:ILE:O	12:6:529:LEU:HD12	2.05	0.56
10:4:308:VAL:HG21	10:4:325:LEU:HD23	1.88	0.56
11:5:396:SER:OG	11:5:398:LYS:NZ	2.38	0.56
13:7:709:ASP:OD1	13:7:710:ILE:N	2.39	0.56
12:6:262:VAL:HG13	12:6:262:VAL:O	2.06	0.55
11:5:602:TYR:OH	11:5:666:LEU:O	2.24	0.55
13:7:203:TYR:OH	13:7:336:ASN:O	2.22	0.55
10:4:583:LYS:NZ	13:7:447:GLY:O	2.39	0.55
11:5:552:MET:HE3	11:5:687:SER:OG	2.06	0.55
12:6:576:ASP:OD1	12:6:689:TYR:N	2.40	0.55
14:X:517:LEU:HD23	14:X:572:LEU:HD21	1.88	0.55
3:C:104:PHE:HB3	3:C:170:GLU:CD	2.30	0.55
10:4:705:VAL:O	10:4:705:VAL:HG13	2.06	0.55
13:7:599:LEU:O	13:7:727:LEU:HD22	2.06	0.55
2:B:146:GLN:CB	11:5:47:ARG:NH1	2.70	0.55
3:C:112:ILE:O	3:C:116:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:282:ILE:C	4:D:282:ILE:HD12	2.31	0.55
10:4:516:GLU:OE1	10:4:516:GLU:N	2.37	0.55
10:4:547:GLY:N	10:4:560:GLY:O	2.37	0.55
9:3:235:ASP:OD1	9:3:236:THR:N	2.37	0.55
10:4:234:ARG:NE	10:4:284:ILE:HD11	2.22	0.55
4:D:151:ILE:HD11	4:D:175:LEU:HD22	1.88	0.55
8:2:636:ILE:O	8:2:638:THR:HG22	2.07	0.54
9:3:456:ARG:HH22	13:7:327:ILE:HD13	1.70	0.54
8:2:781:MET:HE3	8:2:782:ASP:O	2.07	0.54
12:6:144:LYS:HA	12:6:196:LEU:HD13	1.90	0.54
9:3:451:GLU:CD	11:5:460:ARG:HH12	2.13	0.54
13:7:612:LEU:C	13:7:612:LEU:HD23	2.33	0.54
14:X:119:ALA:O	14:X:123:LYS:HE3	2.08	0.54
14:X:497:ASP:OD1	14:X:498:ILE:N	2.39	0.54
2:B:132:ASP:OD1	2:B:132:ASP:C	2.50	0.54
9:3:570:ARG:CZ	11:5:614:LEU:HD11	2.38	0.54
10:4:183:THR:OG1	10:4:185:VAL:HG22	2.07	0.54
8:2:789:VAL:HG22	8:2:864:TYR:CE1	2.42	0.54
10:4:713:ASP:OD1	10:4:714:GLU:N	2.40	0.54
11:5:162:LEU:HD21	11:5:328:ILE:CD1	2.38	0.54
5:E:411:ARG:NH2	5:E:486:ASP:OD1	2.40	0.54
9:3:416:SER:O	9:3:420:ARG:HG2	2.08	0.54
12:6:147:ASP:OD1	12:6:147:ASP:O	2.25	0.54
14:X:200:MET:N	14:X:200:MET:HE2	2.24	0.53
8:2:808:ARG:HG2	8:2:808:ARG:HH11	1.72	0.53
9:3:212:ARG:HH11	9:3:232:PRO:HG3	1.73	0.53
13:7:247:ARG:HD3	13:7:314:LYS:HD2	1.90	0.53
15:Y:62:ASP:OD1	15:Y:63:LYS:N	2.42	0.53
12:6:150:THR:OG1	12:6:384:ASP:OD2	2.26	0.53
14:X:96:GLU:O	14:X:96:GLU:OE1	2.27	0.53
9:3:676:ILE:HD11	13:7:617:THR:HG23	1.91	0.53
10:4:508:LYS:NZ	10:4:512:VAL:HG23	2.24	0.53
13:7:453:ASP:OD2	13:7:562:SER:N	2.42	0.53
9:3:582:VAL:HG11	11:5:399:ILE:HG13	1.91	0.53
2:B:79:LEU:CB	2:B:85:CYS:SG	2.95	0.53
8:2:311:GLU:OE1	8:2:312:SER:N	2.42	0.53
10:4:375:ASP:OD1	14:X:681:ARG:NH1	2.41	0.53
14:X:187:ILE:HD13	14:X:277:PHE:CE2	2.44	0.53
9:3:216:ASP:OD1	9:3:217:ALA:N	2.42	0.53
10:4:740:ASP:OD1	10:4:740:ASP:C	2.52	0.53
11:5:633:LEU:HD13	11:5:647:PRO:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:393:ASP:OD1	12:6:393:ASP:C	2.52	0.53
12:6:523:GLU:CD	12:6:524:HIS:CD2	2.86	0.53
11:5:708:LEU:HA	11:5:711:ILE:HD12	1.91	0.52
10:4:532:GLU:O	10:4:533:LEU:HD12	2.10	0.52
5:E:294:LEU:O	5:E:298:GLU:HG3	2.09	0.52
5:E:609:PHE:CD2	5:E:630:ILE:HD13	2.44	0.52
9:3:412:SER:N	16:3:1001:ATP:O2B	2.42	0.52
11:5:719:LYS:HE3	11:5:755:LEU:HD21	1.90	0.52
11:5:648:ILE:HD11	11:5:689:MET:HE2	1.91	0.52
13:7:615:HIS:HE1	13:7:625:GLN:OE1	1.92	0.52
5:E:259:LEU:HD22	5:E:264:GLU:O	2.09	0.52
15:Y:94:PHE:CD1	15:Y:94:PHE:C	2.88	0.52
12:6:765:LEU:HD11	12:6:804:ILE:CD1	2.40	0.52
14:X:47:LEU:HD12	14:X:47:LEU:N	2.25	0.52
5:E:345:ASN:OD1	5:E:345:ASN:C	2.52	0.52
8:2:670:THR:HG22	8:2:671:GLU:N	2.24	0.52
10:4:199:MET:HE3	10:4:199:MET:HA	1.92	0.52
14:X:206:LEU:HD13	14:X:285:PRO:HB2	1.90	0.52
4:D:281:VAL:HG23	4:D:282:ILE:HG23	1.90	0.52
8:2:319:ARG:NH2	8:2:425:GLU:OE1	2.43	0.52
13:7:464:VAL:HG23	13:7:466:LYS:HG3	1.92	0.52
13:7:517:ASP:C	13:7:517:ASP:OD1	2.53	0.52
13:7:726:SER:C	13:7:727:LEU:HD23	2.35	0.52
3:C:104:PHE:CB	3:C:170:GLU:OE2	2.50	0.52
8:2:591:LEU:HD13	8:2:631:ILE:HD12	1.92	0.52
11:5:463:TYR:HA	11:5:509:ILE:HD13	1.92	0.52
10:4:758:ILE:O	10:4:759:HIS:ND1	2.43	0.51
13:7:598:PHE:HA	13:7:727:LEU:CD1	2.39	0.51
1:A:84:ARG:NH1	4:D:216:VAL:HG21	2.25	0.51
3:C:175:GLU:OE2	3:C:178:LYS:NZ	2.43	0.51
5:E:71:TYR:HH	5:E:103:TYR:HH	1.57	0.51
11:5:162:LEU:C	11:5:162:LEU:HD12	2.35	0.51
11:5:690:ASP:OD1	11:5:691:ALA:N	2.43	0.51
13:7:214:ARG:HG2	13:7:215:TYR:CD1	2.45	0.51
14:X:463:GLU:CD	14:X:463:GLU:O	2.54	0.51
12:6:447:ASP:OD1	12:6:447:ASP:O	2.28	0.51
13:7:246:THR:C	13:7:247:ARG:HG3	2.34	0.51
13:7:726:SER:O	13:7:727:LEU:HD23	2.10	0.51
9:3:225:ILE:HD12	9:3:225:ILE:H	1.75	0.51
5:E:92:LEU:HD13	5:E:140:ILE:HD11	1.92	0.51
9:3:386:MET:O	9:3:714:LYS:NZ	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:450:ARG:NH1	9:3:450:ARG:O	2.43	0.51
9:3:648:PRO:HG2	9:3:650:LEU:HD13	1.93	0.51
9:3:688:ASN:ND2	13:7:606:ARG:HE	2.06	0.51
10:4:234:ARG:CD	10:4:284:ILE:HD11	2.41	0.51
1:A:7:ASN:O	1:A:11:LEU:HD23	2.11	0.51
12:6:668:ILE:O	12:6:668:ILE:HG23	2.10	0.51
8:2:364:CYS:SG	8:2:368:LYS:C	2.93	0.51
10:4:709:LEU:HD12	10:4:709:LEU:O	2.10	0.51
11:5:371:THR:O	11:5:374:ILE:HG22	2.10	0.51
14:X:486:GLN:NE2	14:X:497:ASP:O	2.44	0.51
9:3:576:TYR:O	9:3:577:LEU:C	2.52	0.51
14:X:422:GLN:N	14:X:422:GLN:OE1	2.44	0.51
5:E:16:LEU:O	5:E:20:SER:OG	2.18	0.50
9:3:39:ARG:NH1	9:3:136:MET:CE	2.74	0.50
10:4:534:GLU:OE1	10:4:534:GLU:N	2.40	0.50
10:4:709:LEU:HD12	10:4:709:LEU:C	2.35	0.50
12:6:613:VAL:HG21	12:6:624:GLU:OE1	2.11	0.50
9:3:688:ASN:HD22	13:7:606:ARG:NE	2.08	0.50
13:7:258:ILE:CG2	13:7:300:MET:HE2	2.41	0.50
14:X:180:ILE:O	14:X:184:LEU:HG	2.10	0.50
14:X:768:LEU:HD23	15:Y:130:VAL:HG22	1.92	0.50
8:2:328:THR:O	8:2:386:GLN:NE2	2.43	0.50
10:4:718:ARG:HB2	13:7:665:ILE:HD11	1.92	0.50
14:X:743:ASP:OD1	14:X:743:ASP:C	2.55	0.50
8:2:184:GLU:O	8:2:187:SER:OG	2.29	0.50
12:6:679:LEU:C	12:6:679:LEU:HD23	2.37	0.50
14:X:132:LEU:HD11	14:X:167:ILE:HD11	1.93	0.50
14:X:301:LEU:HD21	14:X:426:ALA:HB1	1.93	0.50
8:2:755:ILE:HD11	12:6:560:VAL:CG2	2.42	0.50
10:4:199:MET:HE3	10:4:227:ILE:HD11	1.94	0.50
10:4:769:GLU:OE2	10:4:822:VAL:HG21	2.12	0.50
12:6:516:LEU:HD21	12:6:757:TYR:CG	2.46	0.50
13:7:26:VAL:HG12	13:7:26:VAL:O	2.12	0.50
9:3:449:ASP:OD2	9:3:452:THR:OG1	2.30	0.50
11:5:393:MET:CE	11:5:602:TYR:CE2	2.95	0.50
9:3:676:ILE:CG1	13:7:617:THR:HG21	2.42	0.50
12:6:577:PRO:O	12:6:578:SER:OG	2.21	0.50
9:3:308:GLN:OE1	11:5:209:ARG:NE	2.40	0.50
10:4:241:LEU:HD23	10:4:276:ILE:HD11	1.94	0.50
8:2:234:LEU:C	8:2:234:LEU:HD23	2.37	0.49
10:4:502:THR:OG1	10:4:505:ASP:OD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:406:LEU:HD12	9:3:407:MET:N	2.27	0.49
10:4:608:ASP:O	10:4:612:LYS:N	2.44	0.49
8:2:488:SER:OG	8:2:824:ARG:O	2.24	0.49
13:7:508:LEU:C	13:7:508:LEU:HD23	2.37	0.49
7:G:4:DG:OP2	10:4:451:ARG:NH1	2.45	0.49
8:2:707:HIS:NE2	12:6:763:PRO:O	2.44	0.49
11:5:350:THR:OG1	11:5:353:GLU:OE1	2.23	0.49
11:5:719:LYS:CE	11:5:755:LEU:HD21	2.43	0.49
14:X:540:LEU:HA	14:X:543:VAL:HG12	1.93	0.49
5:E:393:ASP:OD1	5:E:393:ASP:C	2.55	0.49
5:E:624:ASN:OD1	5:E:625:PHE:N	2.45	0.49
9:3:441:GLY:O	9:3:461:ALA:N	2.42	0.49
9:3:570:ARG:HE	11:5:614:LEU:HD11	1.77	0.49
10:4:656:ILE:HD11	10:4:665:LEU:HD11	1.94	0.49
1:A:130:TYR:HB2	4:D:193:LEU:HD12	1.93	0.49
11:5:420:THR:O	11:5:420:THR:HG22	2.13	0.49
13:7:312:GLU:OE1	13:7:334:HIS:NE2	2.46	0.49
13:7:526:PHE:O	13:7:529:MET:HE2	2.12	0.49
10:4:629:CYS:N	10:4:670:SER:O	2.43	0.49
10:4:652:GLN:HA	10:4:652:GLN:OE1	2.13	0.49
10:4:683:ASN:HD22	10:4:686:LEU:HD13	1.78	0.49
13:7:544:GLN:O	13:7:545:THR:OG1	2.26	0.49
10:4:678:ILE:HD11	10:4:693:ASP:HB2	1.94	0.49
13:7:510:GLY:HA3	13:7:514:VAL:HG21	1.93	0.49
8:2:591:LEU:O	11:5:270:MET:HE2	2.12	0.49
9:3:456:ARG:CZ	13:7:327:ILE:HD12	2.42	0.49
14:X:400:LYS:HG3	14:X:401:ARG:N	2.28	0.49
14:X:517:LEU:CD2	14:X:572:LEU:HD21	2.43	0.49
11:5:276:MET:HE1	11:5:294:ILE:HG13	1.94	0.48
14:X:28:ALA:HB2	14:X:83:ILE:HD11	1.95	0.48
9:3:456:ARG:HH22	13:7:327:ILE:CG1	2.26	0.48
14:X:592:ILE:HD12	14:X:675:TYR:CE1	2.48	0.48
14:X:768:LEU:CD2	15:Y:130:VAL:HG22	2.43	0.48
12:6:781:ARG:NH1	12:6:792:SER:OG	2.46	0.48
14:X:731:MET:HE2	14:X:731:MET:HA	1.93	0.48
9:3:580:GLU:HB2	9:3:581:PRO:HD2	1.96	0.48
10:4:744:VAL:O	10:4:748:THR:HG23	2.14	0.48
11:5:393:MET:HE2	11:5:602:TYR:CE2	2.49	0.48
13:7:685:THR:O	13:7:688:THR:N	2.45	0.48
10:4:696:PRO:N	10:4:697:PRO:HD2	2.28	0.48
12:6:652:ILE:HG13	12:6:652:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:291:PHE:CB	14:X:474:GLU:OE2	2.62	0.48
10:4:234:ARG:HD3	10:4:284:ILE:HD11	1.95	0.48
13:7:517:ASP:OD1	13:7:518:ASN:N	2.47	0.48
2:B:105:GLU:OE2	2:B:155:LYS:NZ	2.46	0.48
2:B:164:ASN:OD1	2:B:164:ASN:N	2.46	0.48
10:4:331:LEU:HD23	10:4:332:VAL:O	2.13	0.48
13:7:258:ILE:HD13	13:7:300:MET:HE2	1.95	0.48
2:B:51:GLN:H	4:D:129:MET:HE1	1.78	0.48
8:2:562:ARG:NH1	8:2:600:ASP:O	2.47	0.48
14:X:89:LEU:HD22	14:X:175:VAL:HG21	1.95	0.48
9:3:673:GLN:OE1	9:3:677:ASN:ND2	2.39	0.48
14:X:742:SER:O	14:X:743:ASP:C	2.57	0.48
2:B:10:THR:OG1	2:B:11:PHE:N	2.47	0.48
10:4:565:LEU:HD23	10:4:566:LEU:N	2.29	0.48
11:5:708:LEU:H	11:5:708:LEU:HD22	1.76	0.48
13:7:605:SER:OG	13:7:608:ASP:OD1	2.32	0.48
4:D:255:CYS:SG	4:D:270:THR:N	2.85	0.47
8:2:486:LYS:O	8:2:486:LYS:NZ	2.44	0.47
9:3:485:ALA:O	9:3:489:VAL:HG23	2.14	0.47
12:6:807:SER:CB	12:6:824:ILE:HD13	2.44	0.47
13:7:482:TYR:HA	13:7:522:CYS:HB2	1.94	0.47
14:X:291:PHE:CB	14:X:474:GLU:HG2	2.43	0.47
5:E:71:TYR:OH	5:E:98:ILE:HD11	2.14	0.47
14:X:493:ASP:OD1	14:X:494:ASN:N	2.46	0.47
2:B:150:GLU:OE2	11:5:47:ARG:HD3	2.13	0.47
3:C:131:ARG:NH2	3:C:168:LYS:O	2.47	0.47
5:E:466:LEU:HD11	5:E:470:ARG:NE	2.29	0.47
9:3:192:VAL:HG21	9:3:284:ASP:OD1	2.15	0.47
10:4:541:LEU:HD23	10:4:541:LEU:C	2.39	0.47
10:4:683:ASN:ND2	10:4:686:LEU:CD1	2.77	0.47
10:4:692:ILE:HG22	10:4:692:ILE:O	2.14	0.47
11:5:648:ILE:HG21	11:5:653:LEU:HD23	1.96	0.47
14:X:476:LEU:HD12	14:X:535:ALA:CB	2.44	0.47
1:A:38:ARG:HA	1:A:41:LEU:HD12	1.96	0.47
2:B:146:GLN:HB3	11:5:47:ARG:NH1	2.29	0.47
5:E:292:TYR:OH	5:E:296:GLN:NE2	2.28	0.47
8:2:515:VAL:HG21	8:2:556:VAL:HG11	1.94	0.47
9:3:470:VAL:CG1	9:3:512:VAL:HG22	2.44	0.47
1:A:40:ILE:HG21	1:A:86:LEU:HD21	1.97	0.47
4:D:98:ILE:HD12	4:D:133:LEU:CD1	2.43	0.47
8:2:790:TYR:OH	8:2:794:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:318:LYS:CE	9:3:320:LEU:HD21	2.45	0.47
10:4:606:THR:OG1	10:4:607:ARG:N	2.46	0.47
13:7:409:ASP:O	13:7:410:VAL:C	2.57	0.47
5:E:426:GLU:OE2	5:E:547:ARG:NH1	2.47	0.47
9:3:442:LEU:CD1	9:3:486:ILE:HD11	2.45	0.47
11:5:648:ILE:HG21	11:5:653:LEU:CD2	2.45	0.47
12:6:629:MET:HE1	12:6:672:LEU:HD13	1.97	0.47
15:Y:70:LYS:HD2	15:Y:70:LYS:C	2.39	0.47
3:C:96:ASP:OD2	3:C:99:SER:OG	2.31	0.47
5:E:622:ILE:O	5:E:622:ILE:HG22	2.13	0.47
8:2:234:LEU:HD23	8:2:235:GLY:N	2.29	0.47
8:2:695:LEU:O	8:2:699:VAL:HG23	2.14	0.47
11:5:490:ARG:NH2	11:5:541:ASP:O	2.48	0.47
11:5:755:LEU:HB3	11:5:761:ILE:HD12	1.97	0.47
2:B:97:GLU:OE2	2:B:97:GLU:HA	2.15	0.47
5:E:572:ILE:HD12	5:E:579:TYR:OH	2.15	0.47
11:5:657:ILE:HG22	11:5:658:ARG:N	2.30	0.47
7:G:11:DC:H2''	7:G:12:DT:H72	1.97	0.47
8:2:472:ASP:O	8:2:475:SER:OG	2.32	0.47
12:6:574:VAL:CG2	12:6:699:LEU:HD21	2.45	0.47
13:7:414:LEU:HD12	13:7:638:MET:HG3	1.97	0.47
13:7:546:ILE:O	13:7:557:LEU:N	2.44	0.47
14:X:418:LEU:HD12	14:X:418:LEU:O	2.14	0.47
6:F:25:DT:C4'	14:X:401:ARG:HH12	2.27	0.46
11:5:361:SER:HA	11:5:366:LEU:HD22	1.96	0.46
13:7:67:LEU:HD22	13:7:121:ILE:HG23	1.97	0.46
1:A:77:LEU:HD11	3:C:53:ILE:HG21	1.97	0.46
1:A:79:MET:HE1	4:D:203:PRO:HG3	1.98	0.46
5:E:635:GLU:OE2	5:E:635:GLU:N	2.45	0.46
10:4:320:ASN:OD1	10:4:320:ASN:C	2.58	0.46
12:6:743:GLU:N	12:6:743:GLU:OE1	2.49	0.46
14:X:463:GLU:OE2	14:X:466:ARG:HB3	2.16	0.46
11:5:266:PRO:HG2	11:5:269:GLU:HG3	1.98	0.46
16:5:1001:ATP:N3	16:5:1001:ATP:C2'	2.79	0.46
13:7:459:MET:CE	13:7:597:LEU:HD21	2.40	0.46
14:X:58:LEU:HD23	14:X:131:LEU:HD21	1.97	0.46
5:E:624:ASN:OD1	5:E:624:ASN:C	2.58	0.46
11:5:392:LEU:HD11	11:5:432:VAL:HG11	1.97	0.46
11:5:568:ILE:O	11:5:572:VAL:HG23	2.15	0.46
13:7:263:ASP:OD1	13:7:263:ASP:N	2.41	0.46
1:A:165:VAL:HG11	1:A:200:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:PRO:O	4:D:129:MET:HG2	2.15	0.46
14:X:507:GLU:O	14:X:511:ILE:HG12	2.15	0.46
9:3:698:THR:HG22	9:3:699:ALA:N	2.31	0.46
10:4:422:GLU:HG2	10:4:423:LEU:N	2.29	0.46
14:X:92:LEU:HD22	14:X:175:VAL:HG13	1.97	0.46
5:E:18:ASN:ND2	5:E:79:ASN:OD1	2.46	0.46
8:2:615:GLN:O	8:2:618:THR:OG1	2.29	0.46
9:3:283:VAL:HG13	9:3:284:ASP:N	2.30	0.46
13:7:440:VAL:HG11	13:7:452:GLY:O	2.15	0.46
14:X:97:ASN:O	14:X:101:LEU:HD22	2.15	0.46
14:X:520:ALA:HB1	14:X:528:VAL:HG13	1.97	0.46
8:2:797:SER:O	8:2:802:SER:OG	2.34	0.46
11:5:648:ILE:HG22	11:5:649:THR:N	2.31	0.46
12:6:323:GLN:OE1	12:6:323:GLN:N	2.48	0.46
5:E:45:LEU:HD21	5:E:255:ILE:HD12	1.97	0.46
9:3:377:ILE:HG21	9:3:407:MET:HE1	1.98	0.46
10:4:835:ASP:O	10:4:836:TYR:C	2.59	0.46
11:5:374:ILE:HG23	11:5:385:LYS:HD3	1.98	0.46
13:7:455:ASN:ND2	13:7:541:MET:SD	2.89	0.46
14:X:251:ASN:OD1	14:X:433:ASN:ND2	2.45	0.46
3:C:33:ASN:OD1	3:C:33:ASN:C	2.59	0.46
8:2:597:VAL:HG21	8:2:640:LEU:HD23	1.98	0.46
1:A:41:LEU:HD22	4:D:201:TYR:CD2	2.50	0.45
8:2:255:ILE:HD11	8:2:259:PHE:CE1	2.51	0.45
9:3:456:ARG:NH1	13:7:327:ILE:HD12	2.31	0.45
12:6:96:ALA:HB2	14:X:221:THR:HG22	1.97	0.45
1:A:204:TYR:C	1:A:205:LEU:HD12	2.42	0.45
8:2:591:LEU:CD2	11:5:270:MET:CE	2.92	0.45
8:2:783:MET:HG2	11:5:573:ILE:HG21	1.97	0.45
12:6:710:ASP:O	12:6:711:LEU:HD23	2.16	0.45
14:X:184:LEU:HA	14:X:187:ILE:HG22	1.99	0.45
14:X:753:LEU:HD21	14:X:760:PHE:CE1	2.51	0.45
8:2:778:LEU:CD1	8:2:814:LEU:HD12	2.46	0.45
10:4:635:ASP:OD1	10:4:636:LYS:N	2.49	0.45
13:7:441:ASP:O	13:7:442:LYS:C	2.58	0.45
13:7:492:GLY:O	13:7:494:THR:N	2.49	0.45
2:B:74:TRP:CD1	2:B:74:TRP:C	2.94	0.45
3:C:135:LEU:HD21	3:C:177:TYR:HB2	1.98	0.45
9:3:638:ASN:ND2	9:3:644:GLY:O	2.50	0.45
10:4:772:ARG:C	10:4:772:ARG:HD2	2.42	0.45
11:5:377:SER:OG	11:5:575:ILE:HD11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:ASP:OD1	5:E:146:GLY:N	2.49	0.45
9:3:688:ASN:HD22	13:7:606:ARG:NH2	2.13	0.45
1:A:104:ASN:OD1	1:A:104:ASN:C	2.59	0.45
5:E:229:GLN:O	5:E:232:GLU:HG2	2.17	0.45
6:F:21:DT:H2"	6:F:22:DG:C8	2.51	0.45
11:5:450:THR:OG1	11:5:451:ALA:N	2.49	0.45
11:5:749:ASP:N	11:5:749:ASP:OD1	2.49	0.45
9:3:705:LEU:HD21	9:3:733:LEU:HD23	1.98	0.45
13:7:347:ASP:OD1	13:7:348:ILE:N	2.49	0.45
1:A:93:ARG:NH1	1:A:127:GLU:OE2	2.50	0.45
8:2:536:ASP:OD2	8:2:627:GLN:NE2	2.44	0.45
2:B:118:ASN:OD1	2:B:118:ASN:O	2.34	0.45
4:D:248:GLU:OE2	4:D:252:GLY:HA2	2.17	0.45
8:2:814:LEU:O	8:2:818:GLU:HG3	2.17	0.45
5:E:124:ASP:OD1	5:E:126:HIS:N	2.44	0.44
10:4:421:ASP:O	10:4:424:VAL:HG12	2.18	0.44
11:5:541:ASP:OD1	11:5:541:ASP:N	2.50	0.44
12:6:373:MET:SD	12:6:373:MET:N	2.90	0.44
8:2:578:ALA:CB	8:2:591:LEU:HD21	2.47	0.44
11:5:403:GLY:O	11:5:405:ARG:NH1	2.50	0.44
13:7:419:ALA:O	13:7:420:PRO:C	2.58	0.44
5:E:27:LEU:HD11	5:E:82:LEU:HD23	2.00	0.44
5:E:319:ASN:N	5:E:319:ASN:OD1	2.50	0.44
9:3:347:ILE:O	9:3:350:ILE:HG22	2.18	0.44
14:X:554:SER:HA	14:X:557:ILE:HD12	1.99	0.44
9:3:39:ARG:NH1	9:3:136:MET:HE2	2.33	0.44
10:4:401:GLU:OE2	10:4:413:HIS:N	2.45	0.44
11:5:393:MET:HE2	11:5:602:TYR:HE2	1.83	0.44
11:5:761:ILE:HG22	11:5:762:GLN:N	2.33	0.44
14:X:450:ASN:OD1	14:X:451:ILE:N	2.50	0.44
3:C:97:LEU:HD13	3:C:170:GLU:CD	2.40	0.44
8:2:397:VAL:HG12	8:2:398:PRO:O	2.18	0.44
8:2:547:THR:HG21	8:2:683:VAL:CG1	2.46	0.44
12:6:366:ASN:OD1	12:6:366:ASN:C	2.60	0.44
14:X:92:LEU:HD21	14:X:178:ALA:HB3	1.99	0.44
3:C:33:ASN:OD1	3:C:33:ASN:O	2.36	0.44
3:C:96:ASP:OD1	3:C:96:ASP:C	2.61	0.44
5:E:579:TYR:CE2	5:E:637:LEU:HD22	2.51	0.44
9:3:570:ARG:HG3	11:5:614:LEU:HD21	1.98	0.44
10:4:686:LEU:HD12	10:4:686:LEU:H	1.83	0.44
11:5:455:ARG:HD3	11:5:460:ARG:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:402:ILE:HG21	12:6:455:LEU:HD12	1.99	0.44
5:E:570:ALA:HB2	5:E:581:VAL:HG22	1.99	0.44
9:3:702:LEU:O	9:3:702:LEU:HD23	2.17	0.44
10:4:199:MET:CE	10:4:227:ILE:HD11	2.48	0.44
12:6:585:LEU:HD11	12:6:679:LEU:HD21	1.99	0.44
15:Y:119:GLY:HA2	15:Y:125:LEU:HD23	1.98	0.44
2:B:146:GLN:HB3	11:5:47:ARG:HH12	1.82	0.44
9:3:436:GLY:O	9:3:438:SER:N	2.51	0.44
11:5:472:ALA:O	11:5:517:THR:HG22	2.18	0.44
13:7:293:GLN:HB2	15:Y:105:LYS:HZ3	1.83	0.44
1:A:52:GLU:OE1	1:A:52:GLU:HA	2.18	0.44
5:E:151:THR:O	5:E:151:THR:OG1	2.27	0.44
9:3:572:LEU:CD1	9:3:578:GLU:HB3	2.48	0.44
10:4:686:LEU:HD12	10:4:686:LEU:N	2.33	0.44
11:5:760:THR:HG22	11:5:761:ILE:HG13	1.99	0.44
1:A:141:LEU:HD11	4:D:182:TYR:CD1	2.53	0.43
5:E:71:TYR:CZ	5:E:98:ILE:HD11	2.53	0.43
9:3:672:THR:OG1	9:3:720:THR:OG1	2.34	0.43
12:6:124:VAL:HG12	12:6:135:VAL:CG2	2.48	0.43
14:X:282:ILE:CG2	14:X:286:LEU:HD11	2.48	0.43
4:D:205:GLU:C	4:D:206:LEU:HD12	2.42	0.43
10:4:374:ILE:HD12	10:4:374:ILE:H	1.80	0.43
15:Y:126:ARG:O	15:Y:130:VAL:HG23	2.18	0.43
8:2:247:ARG:HB3	8:2:247:ARG:NH1	2.34	0.43
8:2:786:VAL:HG21	11:5:573:ILE:HD11	1.98	0.43
13:7:596:ILE:HD12	13:7:596:ILE:N	2.33	0.43
14:X:734:SER:O	14:X:738:VAL:HG23	2.19	0.43
11:5:374:ILE:O	11:5:374:ILE:CG2	2.65	0.43
15:Y:78:ILE:HD11	15:Y:91:ILE:HD11	2.00	0.43
6:F:31:DC:H2'	6:F:32:DT:H72	2.00	0.43
14:X:540:LEU:HD11	14:X:598:VAL:HG22	1.99	0.43
14:X:344:GLN:OE1	14:X:344:GLN:HA	2.17	0.43
2:B:22:ASN:OD1	4:D:135:ARG:NH1	2.47	0.43
9:3:451:GLU:HB2	11:5:460:ARG:NH2	2.21	0.43
11:5:626:PHE:CD1	11:5:653:LEU:HD21	2.54	0.43
12:6:364:ASN:CG	12:6:394:ARG:NE	2.74	0.43
12:6:511:ASP:OD1	12:6:512:GLU:N	2.51	0.43
14:X:180:ILE:HD11	14:X:262:VAL:HA	2.00	0.43
14:X:739:SER:O	14:X:742:SER:OG	2.36	0.43
9:3:580:GLU:C	11:5:611:ALA:HB3	2.44	0.43
11:5:740:THR:HG22	11:5:742:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:263:ASN:ND2	13:7:136:ASP:OD2	2.52	0.43
10:4:774:TYR:HD2	12:6:728:ALA:HB2	1.84	0.43
11:5:400:LEU:HD12	11:5:404:MET:O	2.19	0.43
11:5:402:ASP:OD1	11:5:403:GLY:N	2.52	0.43
13:7:513:LEU:HD13	13:7:540:VAL:HG21	2.01	0.43
3:C:39:THR:OG1	3:C:40:LYS:N	2.52	0.43
5:E:609:PHE:CE2	5:E:630:ILE:HD13	2.54	0.43
10:4:592:SER:OG	10:4:593:GLY:N	2.51	0.43
11:5:162:LEU:HD11	11:5:258:LEU:CD2	2.49	0.43
11:5:393:MET:HE1	11:5:602:TYR:CE2	2.54	0.43
4:D:248:GLU:OE1	4:D:249:ASN:O	2.36	0.42
6:F:26:DG:H2''	6:F:27:DA:C8	2.54	0.42
9:3:562:SER:O	9:3:566:LEU:HG	2.19	0.42
12:6:143:MET:O	12:6:147:ASP:N	2.52	0.42
13:7:146:ARG:NH1	13:7:268:GLU:O	2.51	0.42
13:7:629:ASP:OD1	13:7:630:PHE:N	2.52	0.42
14:X:546:THR:HG23	14:X:557:ILE:HD13	2.01	0.42
2:B:15:GLU:OE1	4:D:71:ARG:NH1	2.51	0.42
9:3:185:ILE:HD11	9:3:291:ARG:NH1	2.34	0.42
10:4:432:ARG:HH11	10:4:432:ARG:HG3	1.84	0.42
13:7:711:ASP:O	13:7:715:GLU:HG3	2.18	0.42
8:2:653:ASN:N	8:2:666:ASN:O	2.49	0.42
14:X:540:LEU:O	14:X:543:VAL:HG12	2.19	0.42
14:X:542:LEU:O	14:X:542:LEU:HD12	2.19	0.42
6:F:31:DC:H2'	6:F:32:DT:C7	2.49	0.42
8:2:264:PRO:HB3	8:2:317:LEU:HD13	2.01	0.42
9:3:479:THR:HG22	9:3:480:ASP:N	2.34	0.42
11:5:483:ASP:OD1	11:5:484:LYS:N	2.51	0.42
13:7:440:VAL:HG22	13:7:441:ASP:N	2.34	0.42
1:A:5:LEU:N	1:A:5:LEU:HD22	2.35	0.42
1:A:74:VAL:O	1:A:78:CYS:SG	2.74	0.42
5:E:312:THR:O	5:E:315:THR:HG22	2.20	0.42
13:7:481:VAL:O	13:7:522:CYS:HB2	2.20	0.42
5:E:256:TYR:HE2	5:E:298:GLU:OE1	2.02	0.42
6:F:29:DA:C8	6:F:30:DT:H72	2.55	0.42
9:3:572:LEU:HD11	9:3:578:GLU:HB3	2.01	0.42
10:4:616:LEU:O	10:4:616:LEU:HD23	2.20	0.42
11:5:711:ILE:HG23	11:5:751:ALA:HB2	2.01	0.42
13:7:414:LEU:HD13	13:7:414:LEU:HA	1.94	0.42
14:X:484:LYS:HD2	14:X:538:GLU:OE2	2.20	0.42
1:A:67:VAL:HG12	1:A:71:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:599:LEU:N	13:7:727:LEU:HD13	2.31	0.42
1:A:92:LEU:O	1:A:96:ILE:HG12	2.19	0.42
1:A:136:ASP:OD1	1:A:136:ASP:C	2.62	0.42
9:3:456:ARG:NH2	13:7:327:ILE:CG1	2.80	0.42
9:3:673:GLN:O	9:3:676:ILE:HG22	2.20	0.42
10:4:833:ILE:O	10:4:834:LYS:CB	2.68	0.42
8:2:311:GLU:OE1	8:2:311:GLU:N	2.53	0.42
9:3:170:THR:O	9:3:170:THR:HG22	2.20	0.42
12:6:101:LYS:HA	14:X:422:GLN:HE22	1.85	0.42
1:A:94:THR:HG23	1:A:130:TYR:CE2	2.55	0.42
2:B:146:GLN:HG3	11:5:47:ARG:NH1	2.13	0.42
3:C:135:LEU:HD23	3:C:135:LEU:O	2.20	0.42
4:D:193:LEU:C	4:D:193:LEU:HD23	2.45	0.42
9:3:312:ASN:O	9:3:313:THR:OG1	2.31	0.42
9:3:687:ARG:NH2	13:7:602:ASP:OD1	2.53	0.42
10:4:549:ASN:OD1	10:4:559:ARG:NH2	2.53	0.42
10:4:577:ILE:O	10:4:581:VAL:HG13	2.19	0.42
10:4:746:PHE:CD1	10:4:746:PHE:C	2.98	0.42
11:5:383:ASP:OD1	11:5:383:ASP:N	2.50	0.42
14:X:42:PRO:O	14:X:43:PRO:C	2.62	0.42
2:B:150:GLU:CD	11:5:47:ARG:HD3	2.45	0.41
3:C:21:GLN:OE1	3:C:69:VAL:HG13	2.20	0.41
8:2:578:ALA:HB1	8:2:591:LEU:HD21	2.02	0.41
9:3:281:ASP:OD1	9:3:281:ASP:N	2.52	0.41
10:4:832:ALA:C	10:4:834:LYS:N	2.77	0.41
11:5:450:THR:O	11:5:467:GLY:N	2.43	0.41
11:5:486:ARG:NE	11:5:488:GLU:OE2	2.47	0.41
12:6:406:ASP:OD1	12:6:406:ASP:C	2.63	0.41
9:3:107:ASP:OD1	9:3:109:SER:OG	2.37	0.41
12:6:147:ASP:OD1	12:6:147:ASP:C	2.63	0.41
2:B:50:TRP:HD1	2:B:52:LEU:HD21	1.86	0.41
8:2:344:CYS:SG	8:2:346:SER:OG	2.79	0.41
8:2:812:SER:O	8:2:816:ILE:HG12	2.19	0.41
10:4:508:LYS:HZ2	10:4:512:VAL:HG23	1.83	0.41
11:5:755:LEU:HD23	11:5:755:LEU:HA	1.95	0.41
12:6:551:MET:HE1	12:6:591:PHE:CD1	2.55	0.41
3:C:163:SER:O	3:C:167:LEU:HD23	2.20	0.41
5:E:259:LEU:O	5:E:263:GLY:N	2.53	0.41
8:2:612:MET:O	8:2:617:ARG:NH2	2.53	0.41
9:3:48:TYR:CD1	9:3:92:LEU:HD23	2.56	0.41
11:5:485:MET:SD	11:5:493:ILE:HD12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:139:LEU:O	14:X:140:ILE:HD13	2.20	0.41
6:F:27:DA:C8	6:F:28:DT:H72	2.56	0.41
9:3:676:ILE:CG1	13:7:617:THR:CG2	2.98	0.41
11:5:162:LEU:CD1	11:5:258:LEU:HD21	2.50	0.41
11:5:690:ASP:O	11:5:694:GLN:N	2.52	0.41
14:X:348:ASN:ND2	14:X:725:PRO:O	2.53	0.41
15:Y:93:GLN:O	15:Y:97:LEU:HD23	2.21	0.41
3:C:105:PHE:HD2	3:C:170:GLU:OE1	1.89	0.41
9:3:712:HIS:CD2	9:3:728:VAL:HG11	2.56	0.41
10:4:709:LEU:HD13	10:4:711:LYS:CD	2.50	0.41
14:X:554:SER:O	14:X:558:GLU:N	2.48	0.41
5:E:572:ILE:HD12	5:E:579:TYR:CZ	2.55	0.41
9:3:568:THR:CG2	11:5:400:LEU:HD11	2.50	0.41
10:4:444:ILE:HD11	10:4:458:LYS:HB2	2.01	0.41
10:4:579:GLN:O	10:4:583:LYS:HG3	2.20	0.41
10:4:756:GLU:OE1	10:4:756:GLU:HA	2.20	0.41
4:D:194:VAL:HG21	4:D:209:ILE:HD12	2.03	0.41
8:2:502:ALA:N	8:2:503:PRO:CD	2.84	0.41
8:2:580:VAL:HG23	8:2:590:THR:O	2.21	0.41
8:2:670:THR:CG2	8:2:671:GLU:N	2.83	0.41
13:7:710:ILE:HD12	13:7:713:VAL:CG2	2.51	0.41
1:A:37:ILE:HG22	1:A:41:LEU:HD11	2.02	0.41
1:A:92:LEU:HD22	3:C:6:ILE:HD11	2.02	0.41
6:F:27:DA:H2''	6:F:28:DT:C7	2.51	0.41
8:2:684:ARG:HG2	8:2:686:LEU:CD2	2.51	0.41
9:3:389:VAL:H	9:3:710:THR:HG21	1.86	0.41
9:3:470:VAL:HG13	9:3:470:VAL:O	2.20	0.41
9:3:676:ILE:HG12	13:7:617:THR:CG2	2.51	0.41
10:4:742:LEU:HD13	10:4:746:PHE:HE1	1.86	0.41
11:5:646:ILE:O	11:5:646:ILE:HG13	2.20	0.41
12:6:527:ASP:OD1	12:6:527:ASP:N	2.54	0.41
13:7:13:ASP:OD1	13:7:13:ASP:C	2.64	0.41
14:X:282:ILE:O	14:X:286:LEU:HG	2.21	0.41
14:X:453:LEU:HD21	14:X:479:PHE:HE2	1.86	0.41
14:X:765:PHE:CE1	15:Y:125:LEU:HD21	2.56	0.41
15:Y:129:ARG:HA	15:Y:132:LEU:HD12	2.01	0.41
10:4:632:ASP:OD2	10:4:633:GLU:HG2	2.21	0.41
10:4:709:LEU:HD13	10:4:711:LYS:CG	2.47	0.41
13:7:728:TYR:CG	13:7:729:GLN:N	2.86	0.41
8:2:431:LYS:NZ	8:2:452:GLU:OE1	2.43	0.40
10:4:239:SER:O	10:4:239:SER:OG	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:591:LEU:HD22	11:5:270:MET:CE	2.35	0.40
12:6:646:ILE:HD13	12:6:646:ILE:HA	2.00	0.40
13:7:77:SER:OG	13:7:338:THR:HG21	2.21	0.40
14:X:510:PHE:CD2	14:X:511:ILE:HD13	2.55	0.40
5:E:539:TYR:CE1	5:E:548:LEU:HD22	2.56	0.40
8:2:651:ASN:O	8:2:651:ASN:OD1	2.39	0.40
10:4:832:ALA:O	10:4:833:ILE:C	2.64	0.40
14:X:370:ASP:OD1	14:X:370:ASP:O	2.38	0.40
5:E:30:PHE:CD2	5:E:81:LEU:HD21	2.57	0.40
5:E:84:VAL:O	5:E:84:VAL:HG23	2.21	0.40
12:6:629:MET:CE	12:6:672:LEU:HD13	2.52	0.40
13:7:139:LEU:HD22	13:7:196:LEU:HD21	2.04	0.40
9:3:467:ARG:N	9:3:509:ARG:O	2.45	0.40
10:4:273:ASP:OD1	10:4:303:VAL:HG12	2.22	0.40
11:5:564:ARG:O	11:5:568:ILE:HG13	2.20	0.40
13:7:214:ARG:HG2	13:7:215:TYR:CE1	2.57	0.40
13:7:293:GLN:HB2	15:Y:105:LYS:NZ	2.37	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	A	190/208 (91%)	186 (98%)	4 (2%)	0	100	100
2	B	185/213 (87%)	176 (95%)	8 (4%)	1 (0%)	24	57
3	C	168/217 (77%)	163 (97%)	5 (3%)	0	100	100
4	D	216/294 (74%)	211 (98%)	5 (2%)	0	100	100
5	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
8	2	649/868 (75%)	625 (96%)	24 (4%)	0	100	100
9	3	632/971 (65%)	613 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	4	603/933 (65%)	582 (96%)	19 (3%)	2 (0%)	36	67
11	5	623/775 (80%)	597 (96%)	26 (4%)	0	100	100
12	6	630/1017 (62%)	610 (97%)	20 (3%)	0	100	100
13	7	633/845 (75%)	603 (95%)	29 (5%)	1 (0%)	43	74
14	X	699/1238 (56%)	683 (98%)	16 (2%)	0	100	100
15	Y	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	5878/8321 (71%)	5683 (97%)	191 (3%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	4	834	LYS
2	B	94	THR
13	7	493	LEU
10	4	694	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/193 (93%)	178 (99%)	1 (1%)	78	79
2	B	178/198 (90%)	171 (96%)	7 (4%)	28	54
3	C	156/192 (81%)	155 (99%)	1 (1%)	78	79
4	D	213/279 (76%)	212 (100%)	1 (0%)	81	80
5	E	504/586 (86%)	499 (99%)	5 (1%)	68	75
8	2	576/770 (75%)	571 (99%)	5 (1%)	70	76
9	3	551/835 (66%)	549 (100%)	2 (0%)	84	81
10	4	551/848 (65%)	541 (98%)	10 (2%)	51	69
11	5	577/688 (84%)	574 (100%)	3 (0%)	81	80
12	6	559/886 (63%)	549 (98%)	10 (2%)	51	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	7	560/753 (74%)	554 (99%)	6 (1%)	65	74
14	X	639/1125 (57%)	630 (99%)	9 (1%)	59	71
15	Y	85/85 (100%)	83 (98%)	2 (2%)	43	64
All	All	5328/7438 (72%)	5266 (99%)	62 (1%)	61	73

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	SER
2	B	27	ILE
2	B	51	GLN
2	B	74	TRP
2	B	93	LEU
2	B	107	THR
2	B	128	ASN
2	B	154	ILE
3	C	23	ASP
4	D	102	SER
5	E	151	THR
5	E	397	ASP
5	E	434	VAL
5	E	607	MET
5	E	638	SER
8	2	234	LEU
8	2	590	THR
8	2	621	HIS
8	2	630	SER
8	2	680	LEU
9	3	393	LEU
9	3	686	LEU
10	4	279	CYS
10	4	389	CYS
10	4	599	VAL
10	4	624	SER
10	4	638	SER
10	4	644	VAL
10	4	670	SER
10	4	712	VAL
10	4	802	ILE
10	4	827	ARG
11	5	196	ASN

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Mol	Chain	Res	Type
11	5	239	ASP
11	5	325	THR
12	6	119	LEU
12	6	170	ILE
12	6	286	SER
12	6	317	ILE
12	6	552	LEU
12	6	614	ARG
12	6	617	GLU
12	6	648	ASP
12	6	676	THR
12	6	679	LEU
13	7	8	ILE
13	7	410	VAL
13	7	432	LEU
13	7	547	SER
13	7	631	THR
13	7	677	SER
14	X	20	LEU
14	X	76	MET
14	X	101	LEU
14	X	151	THR
14	X	195	THR
14	X	237	ASP
14	X	238	THR
14	X	293	PHE
14	X	584	SER
15	Y	60	LEU
15	Y	137	MET

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

Mol	Chain	Res	Type
1	A	182	ASN
5	E	77	ASN
5	E	296	GLN
5	E	382	HIS
5	E	493	ASN
8	2	290	HIS
8	2	391	GLN
8	2	561	HIS
9	3	177	ASN

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Mol	Chain	Res	Type
9	3	201	HIS
9	3	210	HIS
9	3	365	GLN
9	3	392	ASN
9	3	688	ASN
10	4	259	HIS
10	4	354	HIS
10	4	683	ASN
12	6	258	GLN
12	6	274	HIS
12	6	524	HIS
12	6	633	ASN
13	7	292	ASN
13	7	585	ASN
13	7	615	HIS
13	7	669	GLN
14	X	148	ASN
14	X	343	HIS
14	X	367	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 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	$\# Z > 2$
16	ATP	2	1001	17	32,33,33	0.34	0	48,52,52	0.71	0
16	ATP	7	1001	17	32,33,33	0.33	0	48,52,52	0.71	0
19	ADP	4	1004	-	28,29,29	1.36	4 (14%)	43,45,45	1.89	9 (20%)
19	ADP	4	1001	17	28,29,29	1.39	4 (14%)	43,45,45	1.91	10 (23%)
16	ATP	5	1001	17	32,33,33	0.53	0	48,52,52	1.15	2 (4%)
16	ATP	3	1001	17	32,33,33	0.31	0	48,52,52	0.74	1 (2%)

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
16	ATP	2	1001	17	-	7/22/38/38	0/3/3/3
16	ATP	7	1001	17	-	6/22/38/38	0/3/3/3
19	ADP	4	1004	-	-	5/16/32/32	0/3/3/3
19	ADP	4	1001	17	-	1/16/32/32	0/3/3/3
16	ATP	5	1001	17	-	7/22/38/38	0/3/3/3
16	ATP	3	1001	17	-	0/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	1001	ADP	C5-C4	4.53	1.47	1.39
19	4	1004	ADP	C5-C4	4.44	1.47	1.39
19	4	1001	ADP	C5-C6	2.60	1.48	1.41
19	4	1004	ADP	C5-C6	2.51	1.48	1.41
19	4	1001	ADP	C5-N7	-2.48	1.34	1.39
19	4	1004	ADP	C5-N7	-2.41	1.34	1.39
19	4	1001	ADP	C8-N7	2.28	1.36	1.31
19	4	1004	ADP	C8-N7	2.23	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	1001	ADP	C5-C4-N3	-6.00	118.46	126.72
19	4	1004	ADP	C5-C4-N3	-5.80	118.72	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	1001	ATP	O2'-C2'-C1'	5.14	127.79	110.10
19	4	1004	ADP	N3-C4-N9	4.96	135.60	127.17
19	4	1001	ADP	N3-C4-N9	4.78	135.29	127.17
19	4	1001	ADP	C2-N3-C4	3.90	121.34	111.83
19	4	1004	ADP	C2-N3-C4	3.84	121.20	111.83
16	5	1001	ATP	O2'-C2'-C3'	3.76	123.88	111.82
19	4	1004	ADP	N3-C2-N1	-3.74	122.92	128.58
19	4	1001	ADP	N3-C2-N1	-3.66	123.04	128.58
19	4	1001	ADP	C4-C5-N7	-3.43	106.67	110.58
19	4	1004	ADP	C4-N9-C8	3.18	109.08	105.74
19	4	1004	ADP	C4-C5-N7	-3.00	107.15	110.58
19	4	1001	ADP	C5-N7-C8	2.71	107.71	103.45
19	4	1001	ADP	C3'-C2'-C1'	2.70	106.56	101.46
19	4	1001	ADP	C4-N9-C8	2.68	108.55	105.74
19	4	1004	ADP	C5-N7-C8	2.56	107.47	103.45
19	4	1004	ADP	C3'-C2'-C1'	2.51	106.22	101.46
19	4	1004	ADP	N9-C8-N7	-2.34	110.62	113.94
19	4	1001	ADP	N9-C8-N7	-2.19	110.83	113.94
16	3	1001	ATP	O3'-C3'-C4'	-2.02	105.28	111.08
19	4	1001	ADP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	2	1001	ATP	PB-O3B-PG-O2G
16	5	1001	ATP	PB-O3B-PG-O3G
16	5	1001	ATP	C4'-C5'-O5'-PA
16	7	1001	ATP	PB-O3B-PG-O2G
16	7	1001	ATP	PB-O3B-PG-O3G
19	4	1001	ADP	PA-O3A-PB-O3B
19	4	1004	ADP	C5'-O5'-PA-O3A
16	5	1001	ATP	C2'-C1'-N9-C4
16	2	1001	ATP	O4'-C4'-C5'-O5'
16	7	1001	ATP	O4'-C4'-C5'-O5'
19	4	1004	ADP	O4'-C4'-C5'-O5'
16	5	1001	ATP	C2'-C1'-N9-C8
16	2	1001	ATP	PB-O3A-PA-O1A
16	5	1001	ATP	PB-O3B-PG-O1G
16	7	1001	ATP	PA-O3A-PB-O2B
16	7	1001	ATP	PB-O3A-PA-O2A
19	4	1004	ADP	C3'-C4'-C5'-O5'

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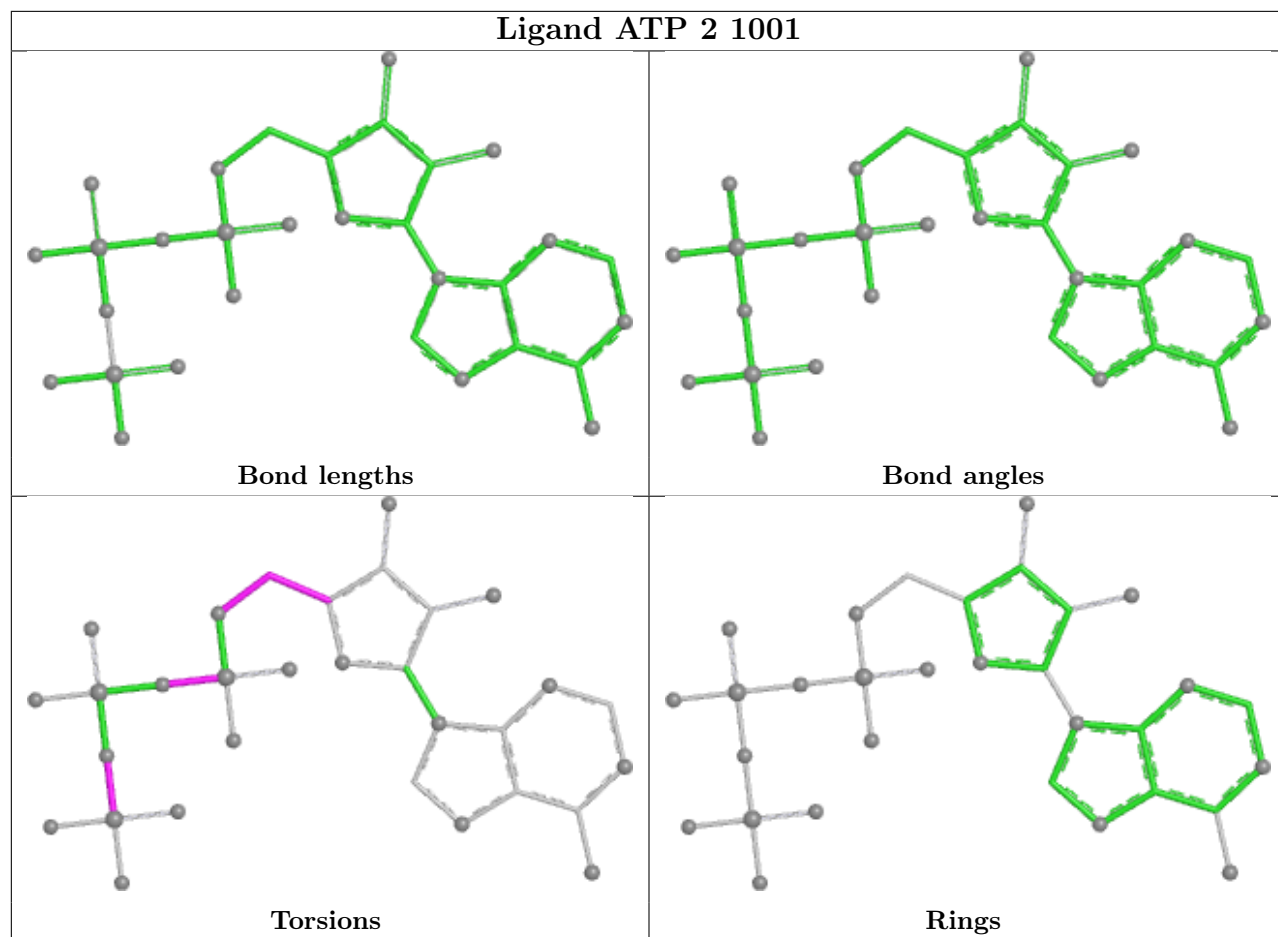
Mol	Chain	Res	Type	Atoms
16	5	1001	ATP	C5'-O5'-PA-O1A
19	4	1004	ADP	C5'-O5'-PA-O1A
16	5	1001	ATP	PA-O3A-PB-O1B
16	2	1001	ATP	PB-O3A-PA-O5'
16	2	1001	ATP	C4'-C5'-O5'-PA
16	2	1001	ATP	C3'-C4'-C5'-O5'
16	7	1001	ATP	PA-O3A-PB-O1B
19	4	1004	ADP	C4'-C5'-O5'-PA
16	2	1001	ATP	PB-O3B-PG-O1G

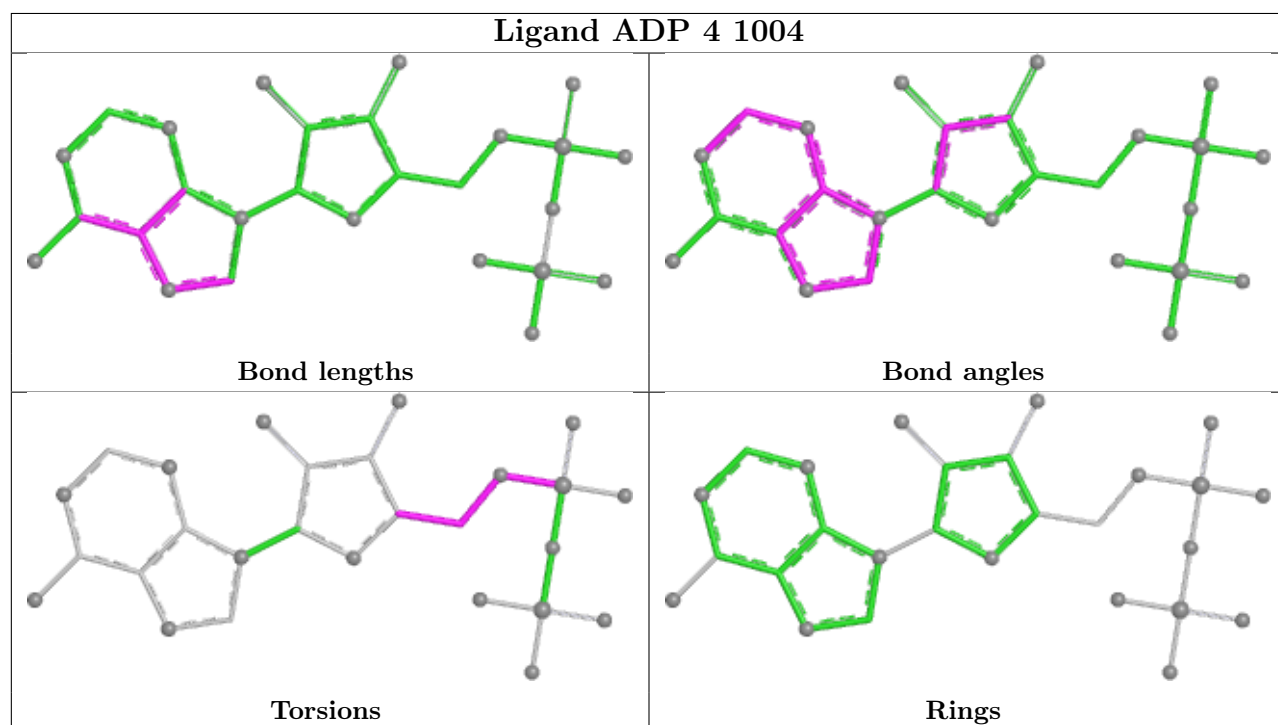
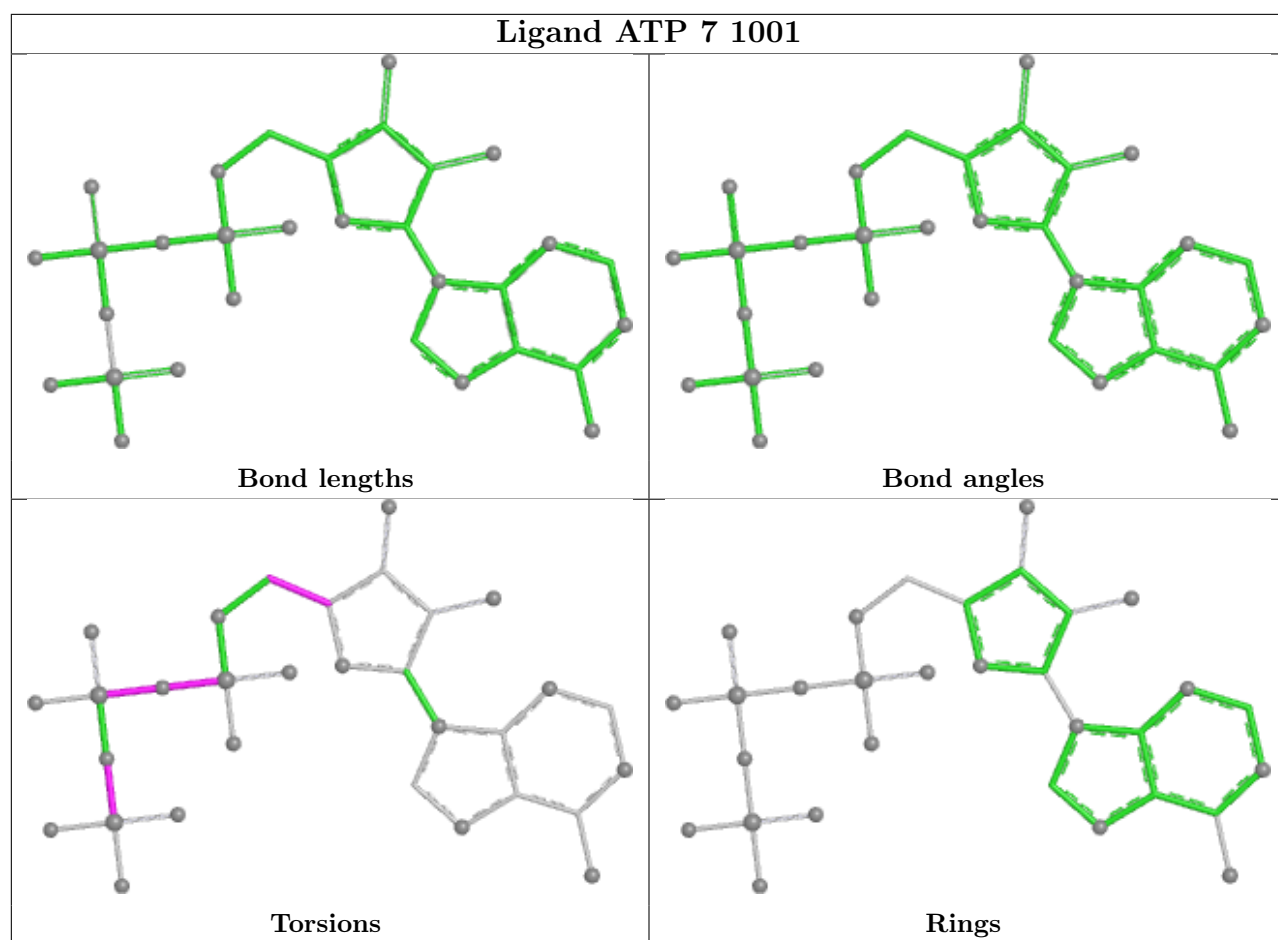
There are no ring outliers.

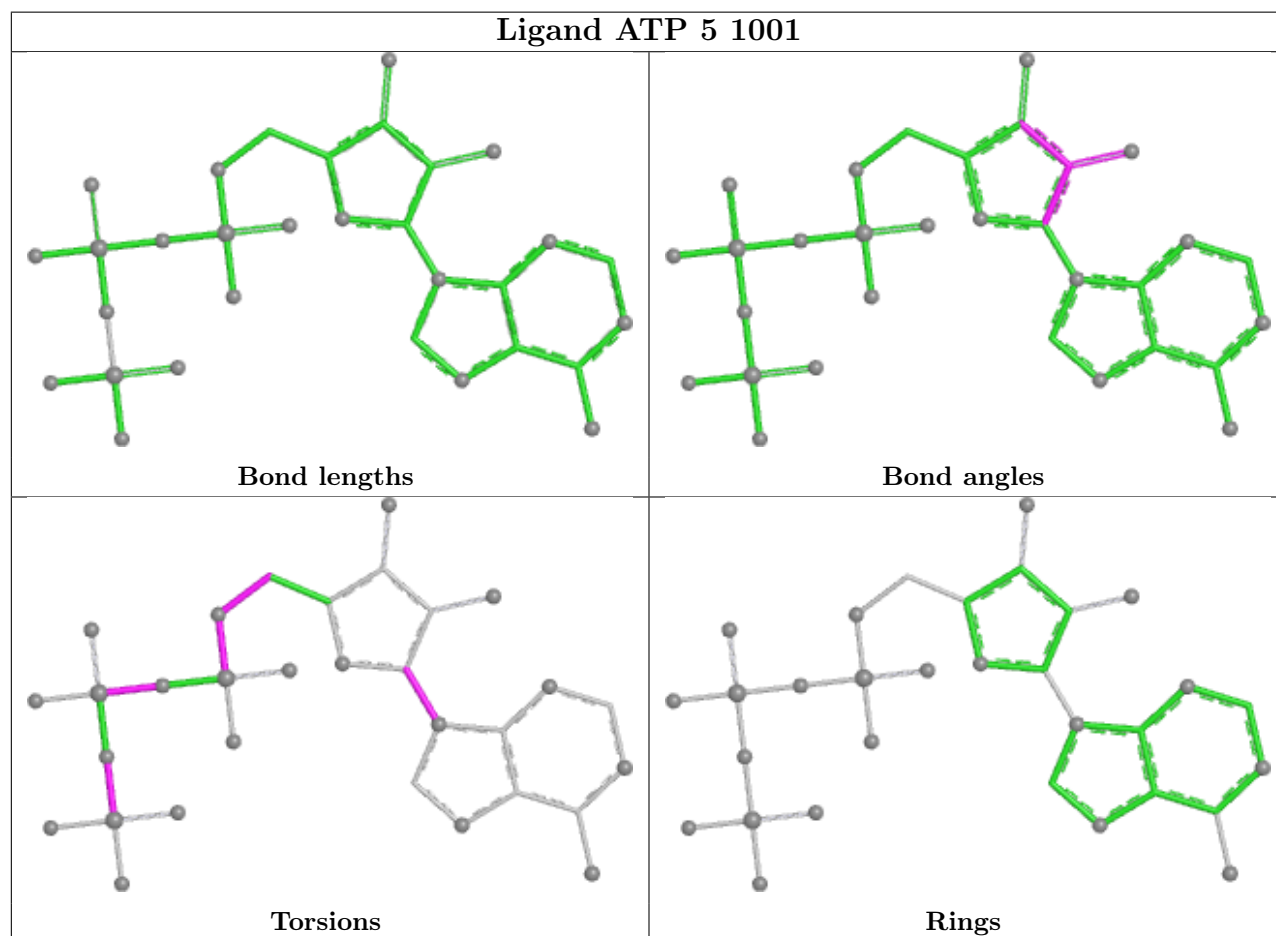
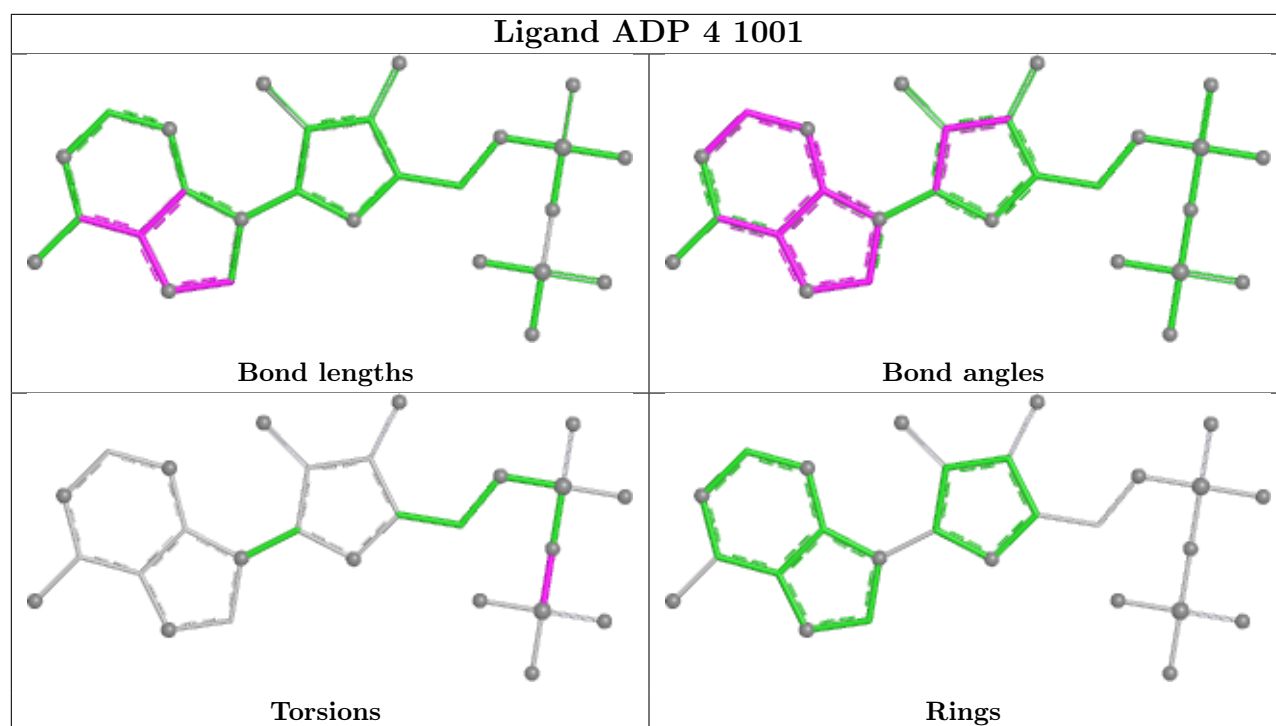
6 monomers are involved in 7 short contacts:

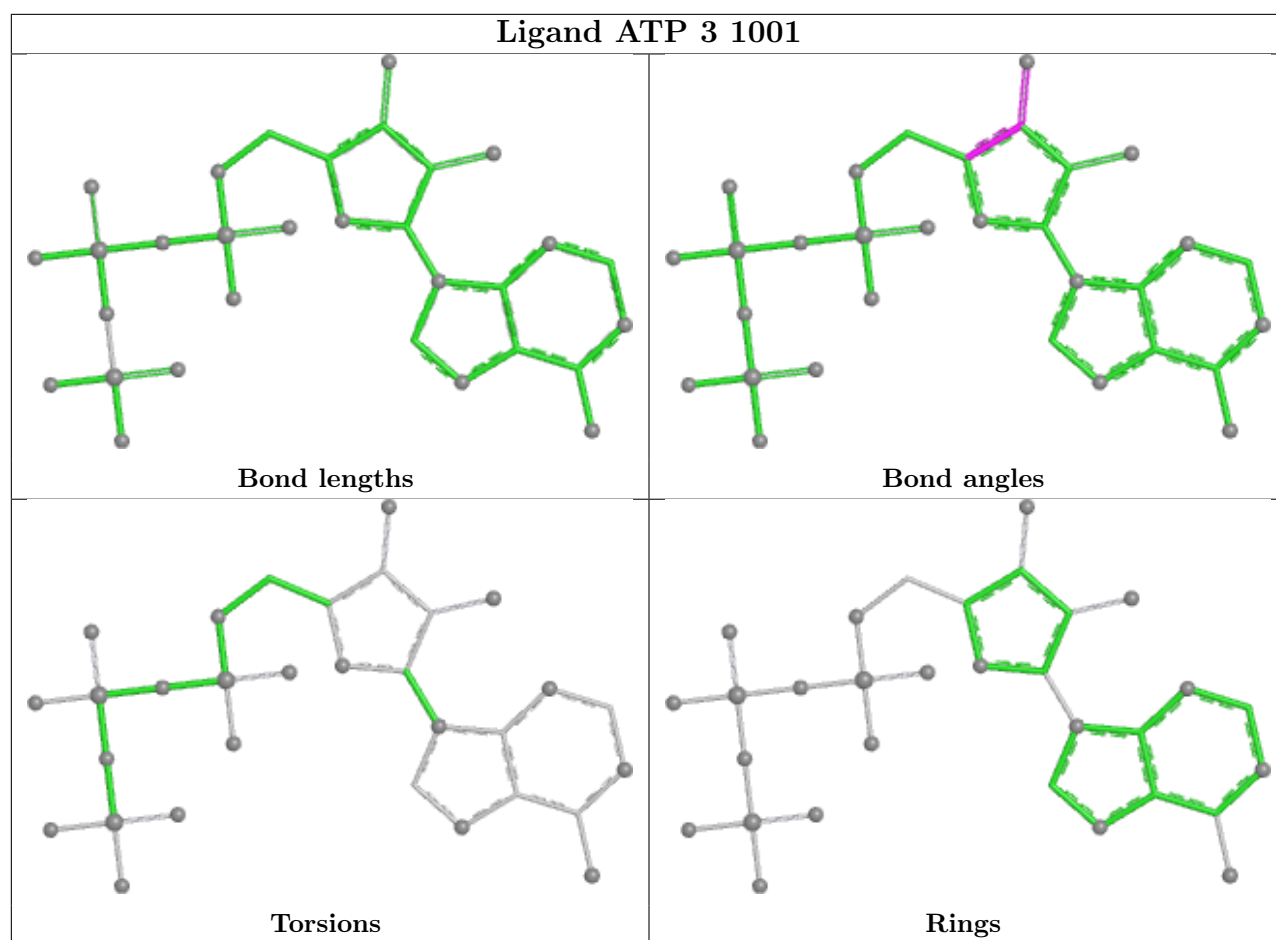
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	1001	ATP	2	0
16	7	1001	ATP	1	0
19	4	1004	ADP	1	0
19	4	1001	ADP	1	0
16	5	1001	ATP	1	0
16	3	1001	ATP	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

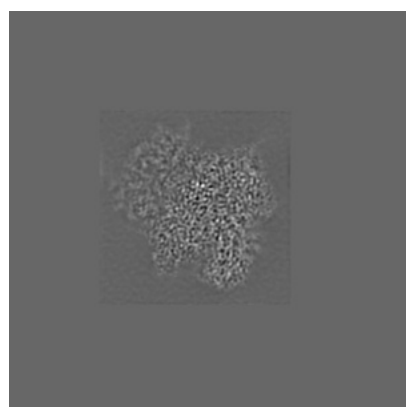
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47471. These allow visual inspection of the internal detail of the map and identification of artifacts.

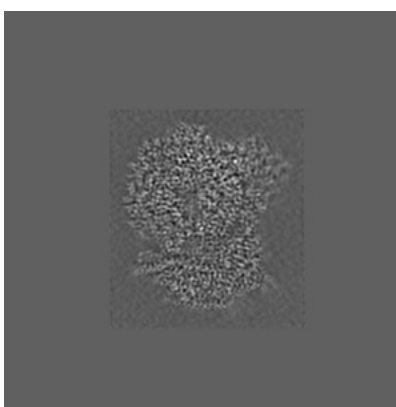
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

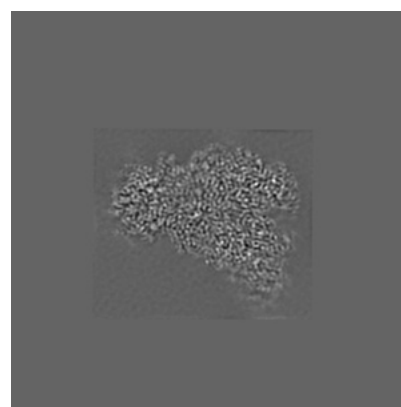
6.1.1 Primary map



X



Y

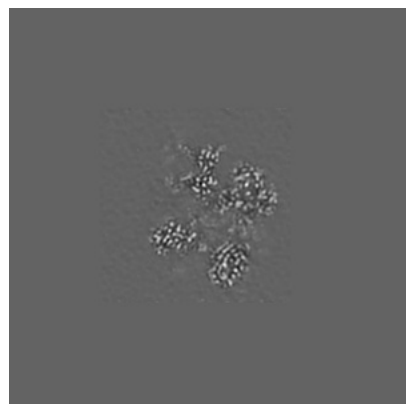


Z

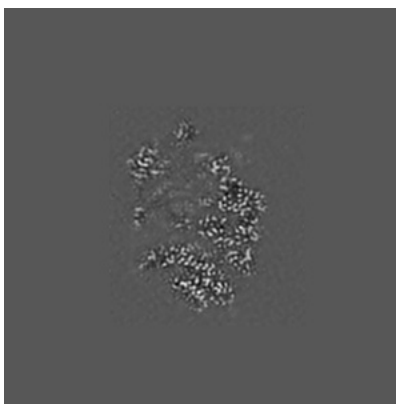
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

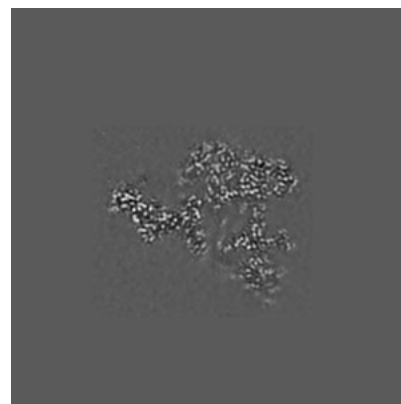
6.2.1 Primary map



X Index: 224



Y Index: 224

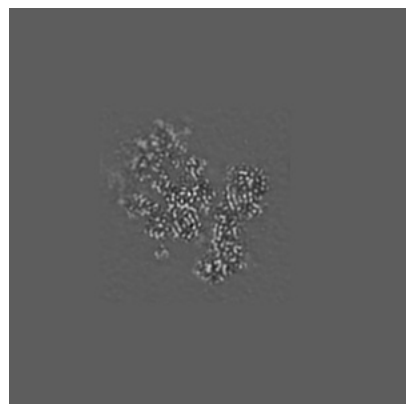


Z Index: 224

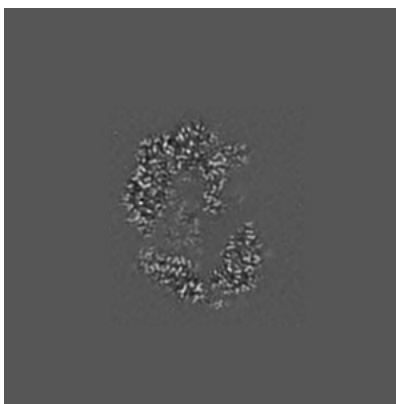
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

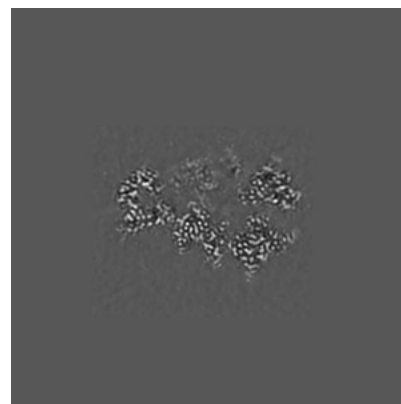
6.3.1 Primary map



X Index: 272



Y Index: 246

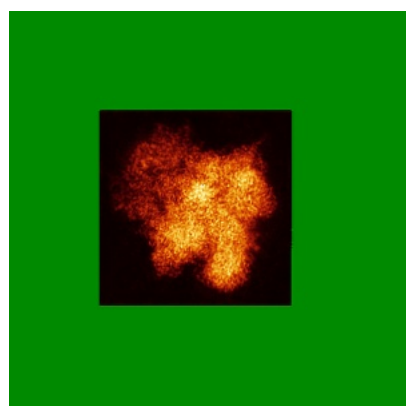


Z Index: 198

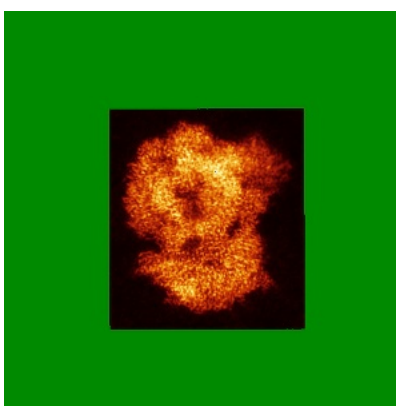
The images above show the largest variance slices of the map in three orthogonal directions.

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

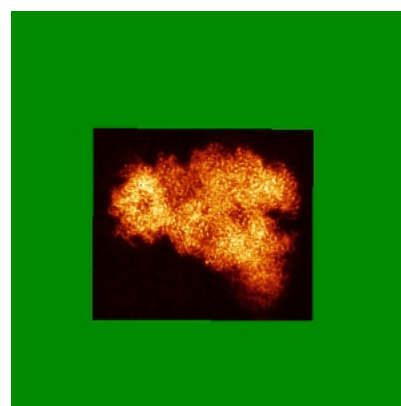
6.4.1 Primary map



X



Y

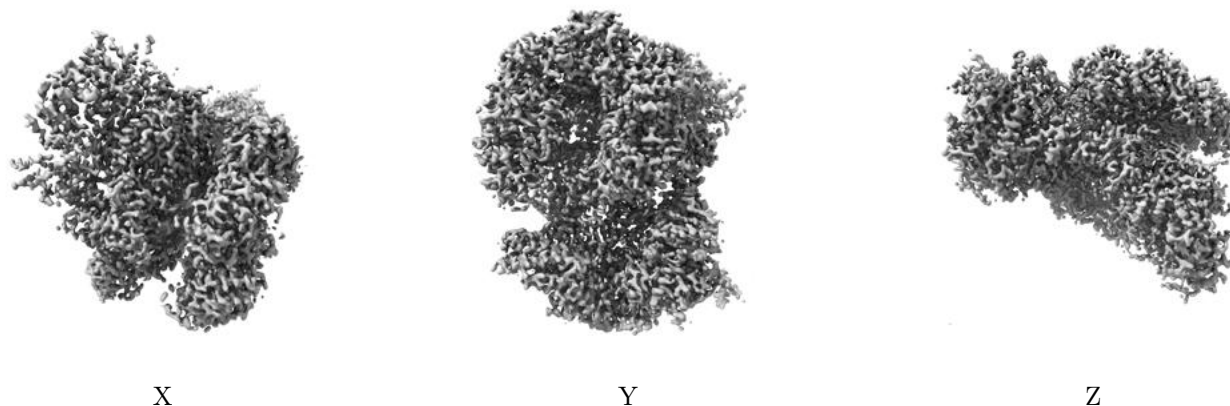


Z

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

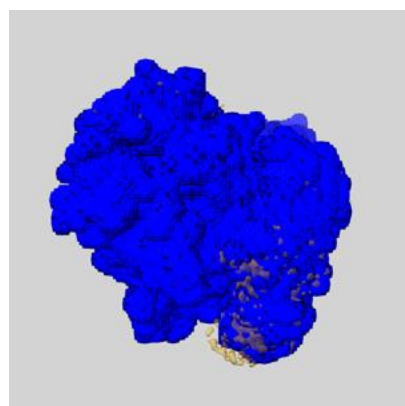
6.6 Mask visualisation [i](#)

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

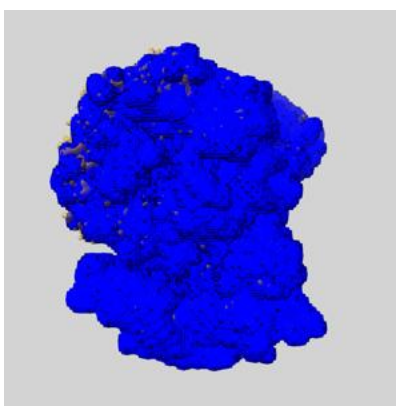
A mask typically either:

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

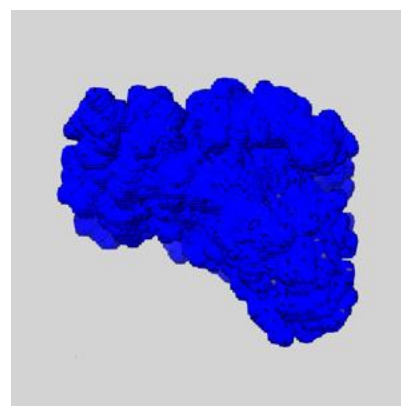
6.6.1 emd_47471_msk_1.map [i](#)



X



Y

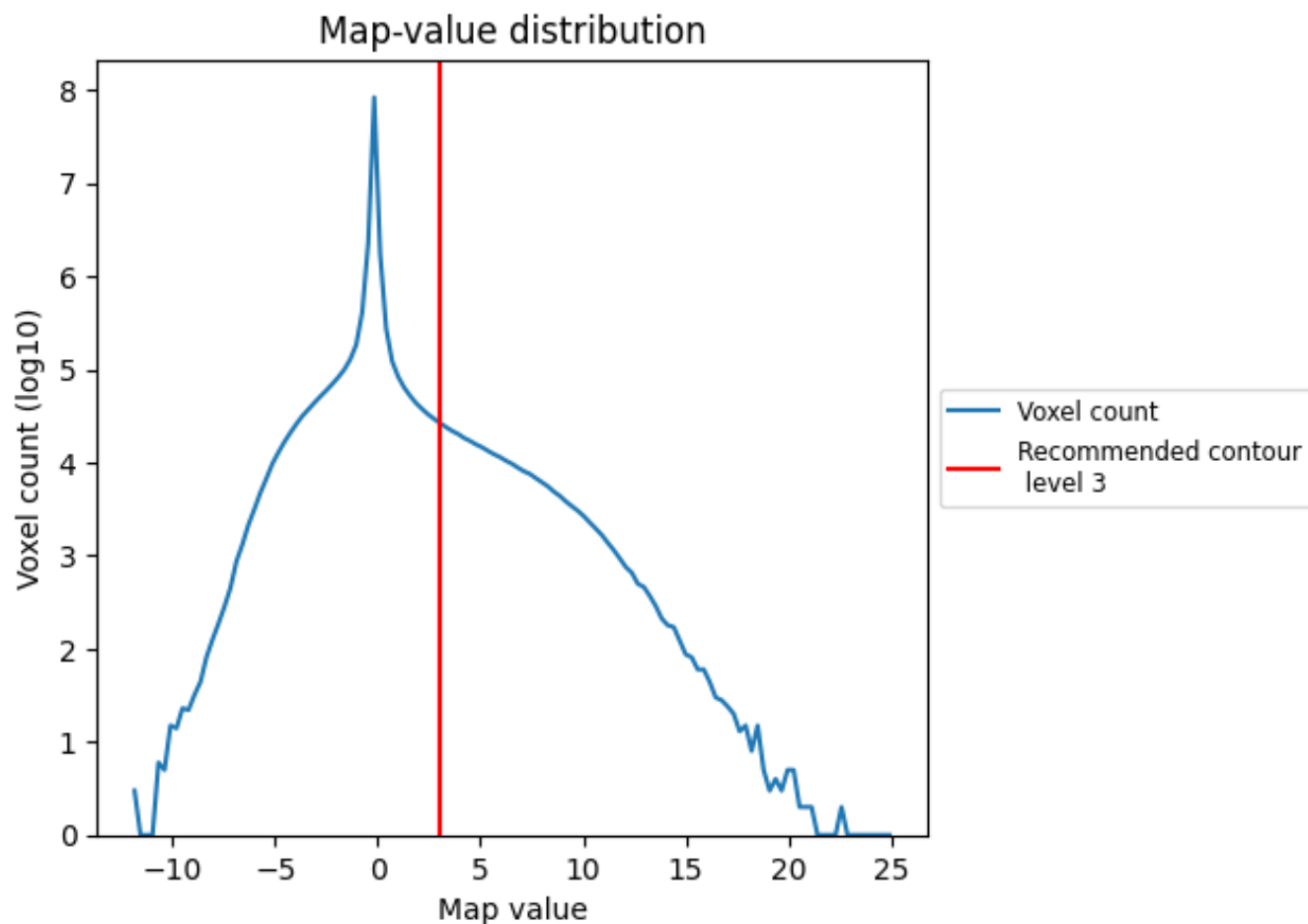


Z

7 Map analysis [i](#)

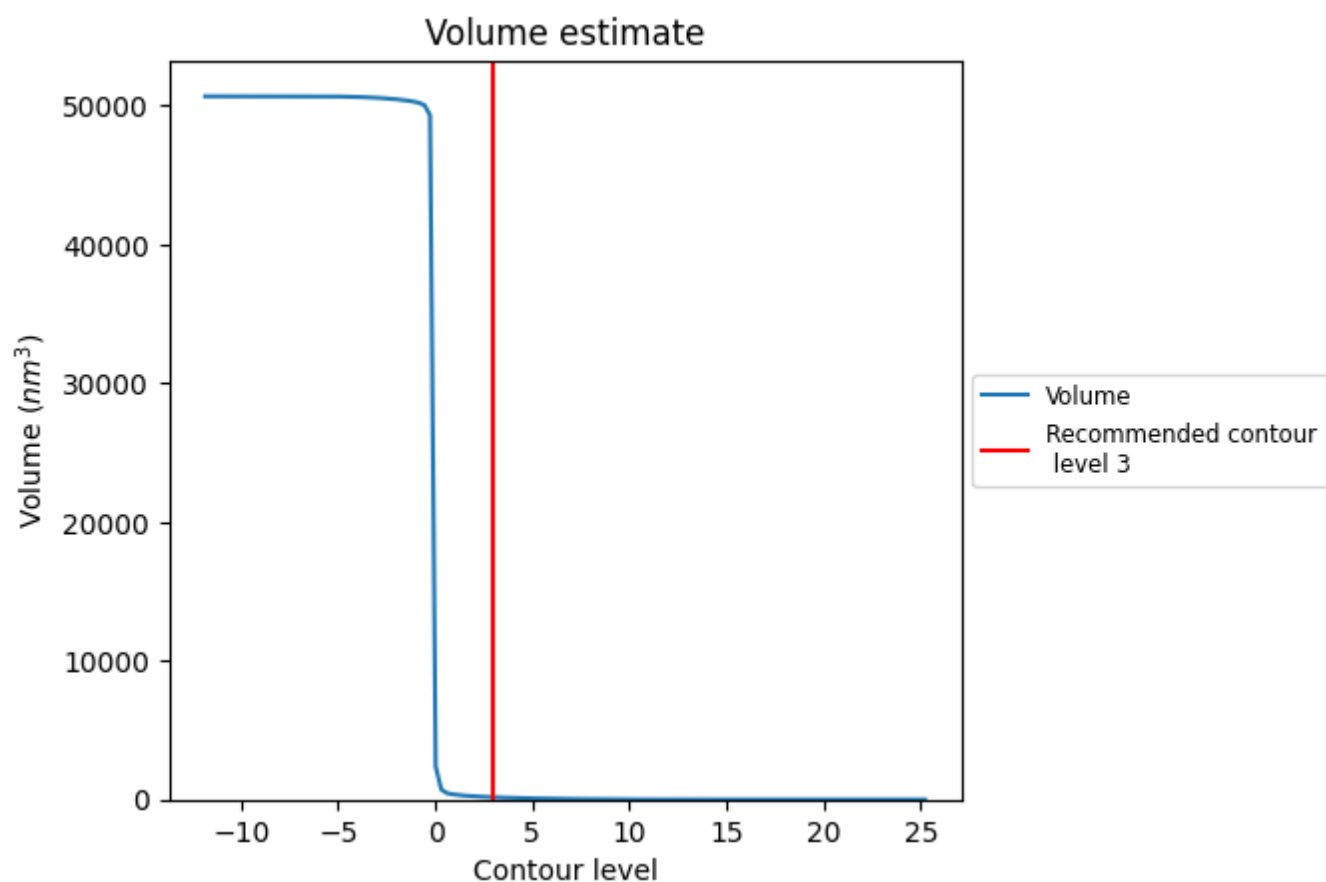
This section contains the results of statistical analysis of the map.

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.

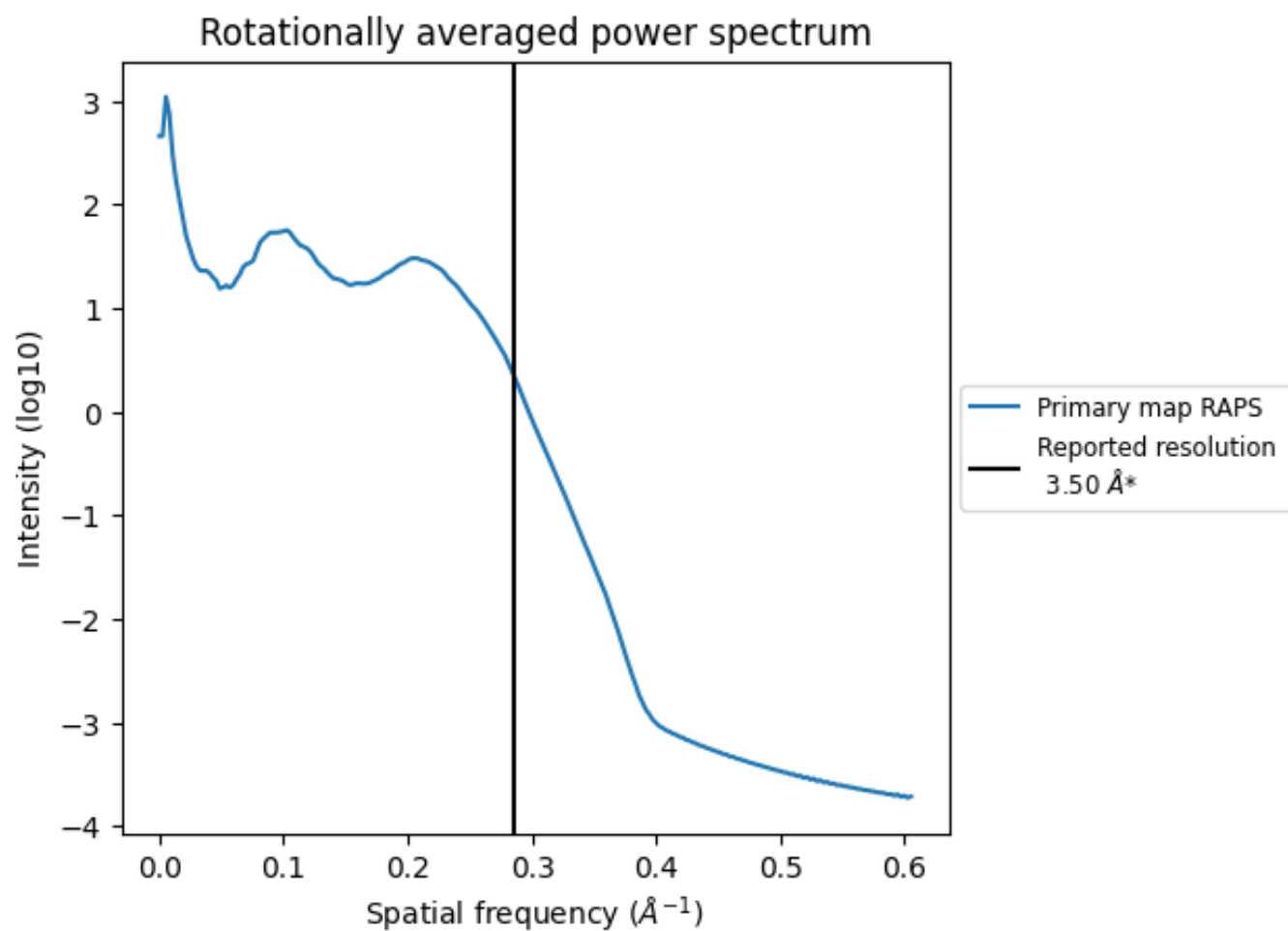
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; this corresponds to an approximate mass of 151 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 ⓘ

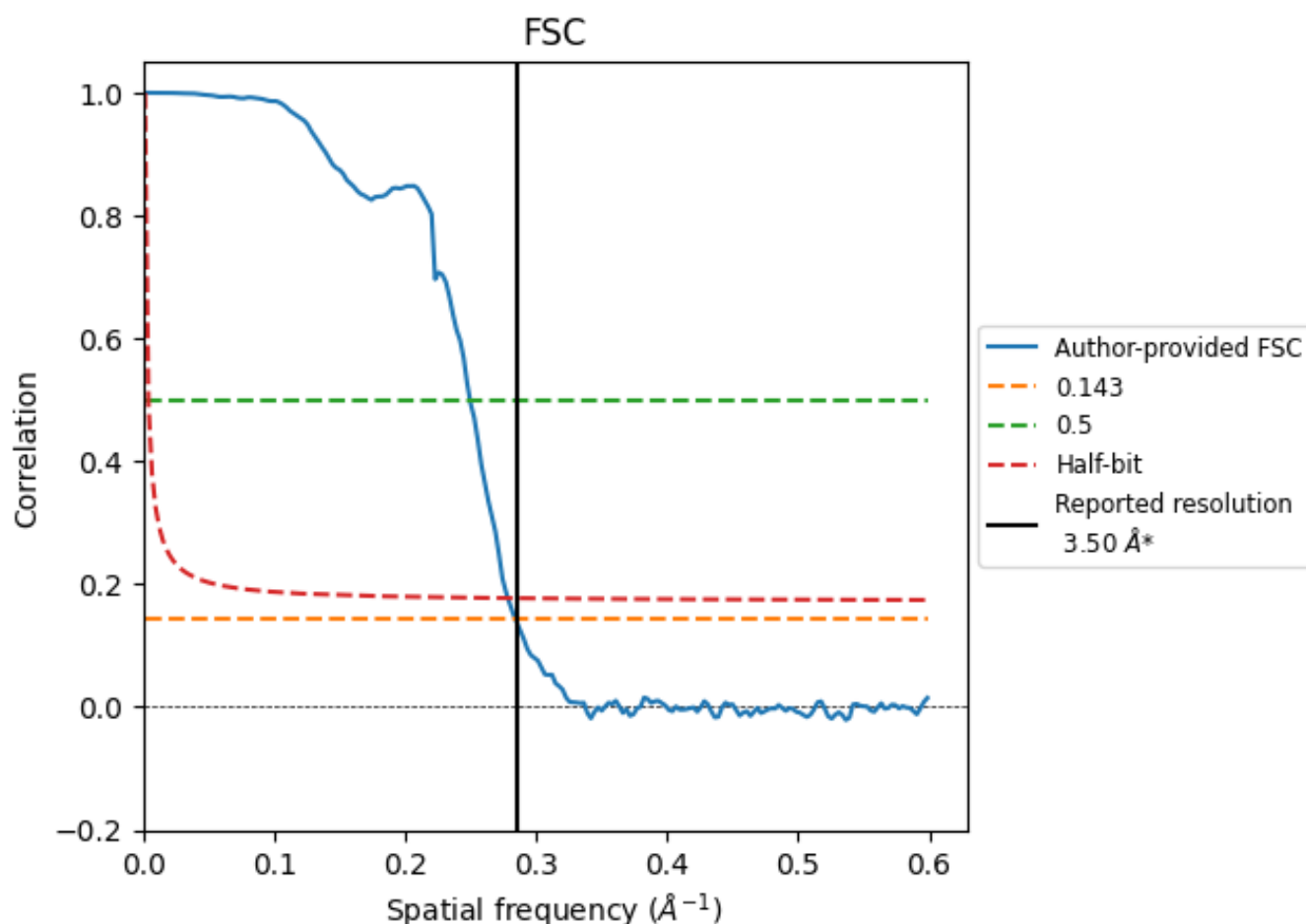


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

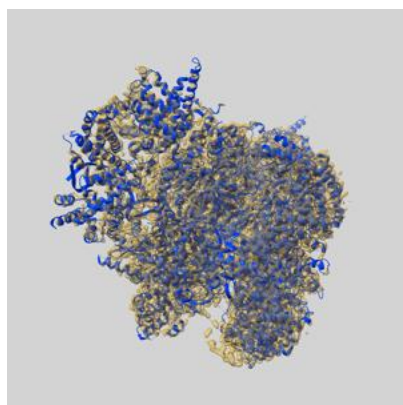
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.01	3.59
Unmasked-calculated*	-	-	-

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

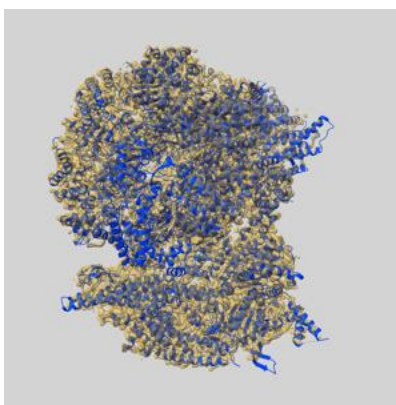
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47471 and PDB model 9E2X. Per-residue inclusion information can be found in section [3](#) on page [9](#).

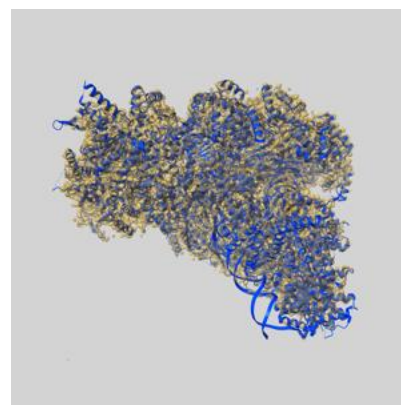
9.1 Map-model overlay [i](#)



X



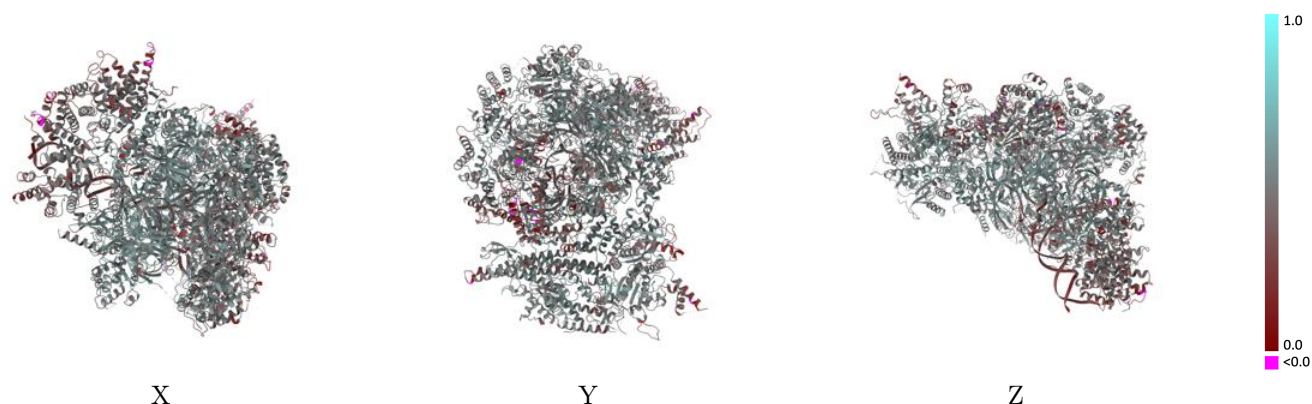
Y



Z

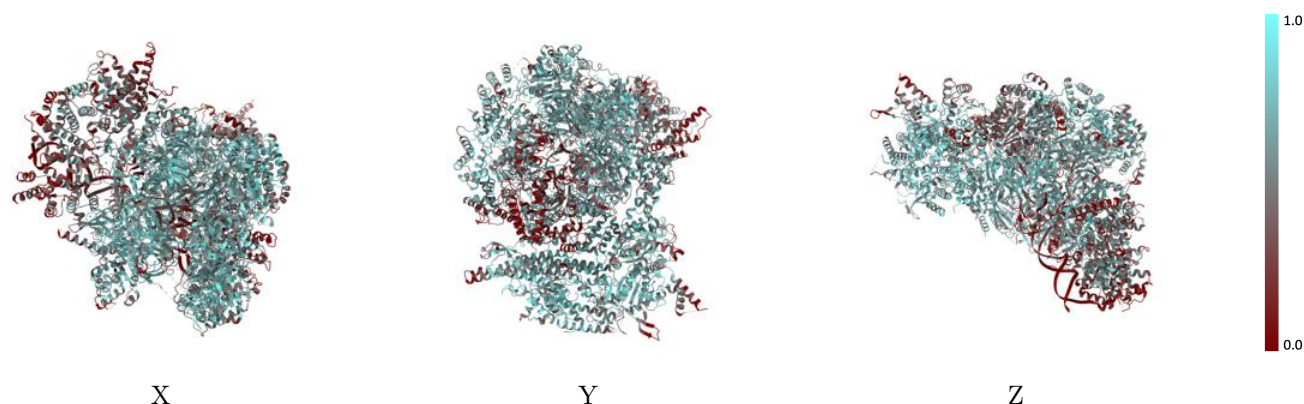
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



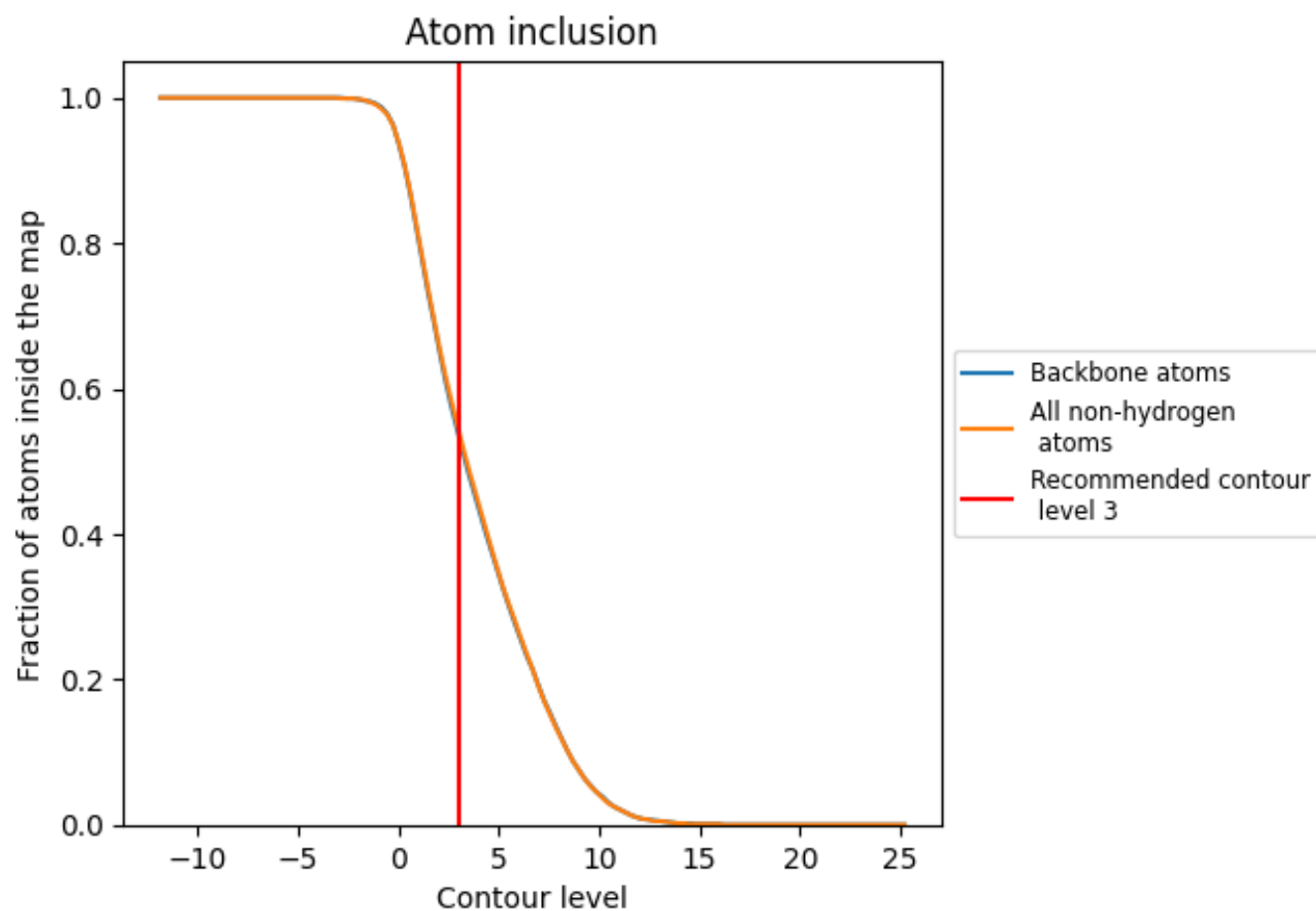
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5430	0.4730
2	0.5700	0.4870
3	0.5450	0.4670
4	0.6280	0.5060
5	0.3880	0.4210
6	0.6330	0.5090
7	0.6330	0.5010
A	0.5830	0.4700
B	0.6990	0.5260
C	0.6500	0.5150
D	0.6790	0.5030
E	0.6030	0.4770
F	0.3210	0.3810
G	0.1810	0.2750
X	0.3810	0.4270
Y	0.3360	0.4180

1.0

0.0

<0.0