



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:01 AM UTC

PDB ID : 9E2W / pdb_00009e2w
EMDB ID : EMD-47470
Title : Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 1
Authors : Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on : 2024-10-23
Resolution : 3.30 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:

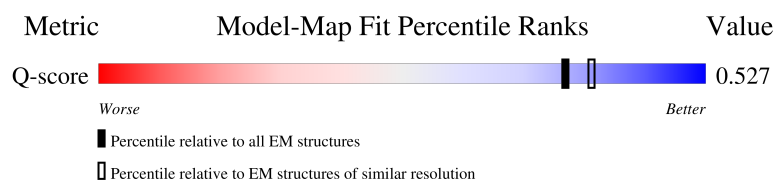
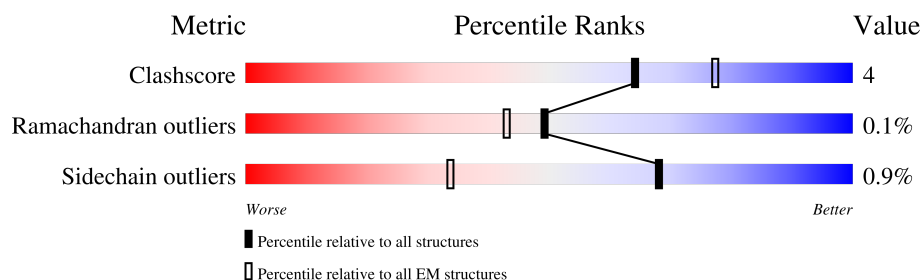
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	15087 (2.80 - 3.80)

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	868	
2	3	971	
3	4	933	
4	5	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	
7	A	208	
8	B	213	
9	C	217	
10	D	294	
11	E	650	
12	F	48	
13	G	21	
14	X	1238	
15	Y	92	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 96909 atoms, of which 48318 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	664	Total	C	H	N	O	S	0	0
			10576	3305	5309	944	999	19		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	618	Total	C	H	N	O	S	0	0
			9718	3044	4893	860	908	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	614	Total	C	H	N	O	S	0	0
			9812	3077	4933	840	934	28		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	594	Total	C	H	N	O	S	0	0
			9417	2945	4746	798	905	23		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	634	Total	C	H	N	O	S	0	0
			10040	3159	5035	873	948	25		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	615	Total	C	H	N	O	S	0	0
			9786	3075	4921	847	917	26		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	196	Total	C	H	N	O	S	0	0
			3202	1005	1602	276	310	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	189	Total	C	H	N	O	S	0	0
			3195	1014	1618	276	282	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	173	Total	C	H	N	O	S	0	0
			2805	910	1409	224	256	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
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 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	222	Total	C	H	N	O	S	0	0
			3671	1170	1843	299	347	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	566	Total	C	H	N	O	S	0	0
			9129	2922	4560	770	863	14		

- Molecule 12 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	F	48	Total	C	H	N	O	P	0	0
			1547	475	544	182	298	48		

- Molecule 13 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	G	21	Total	C	H	N	O	P	0	0
			664	204	234	84	121	21		

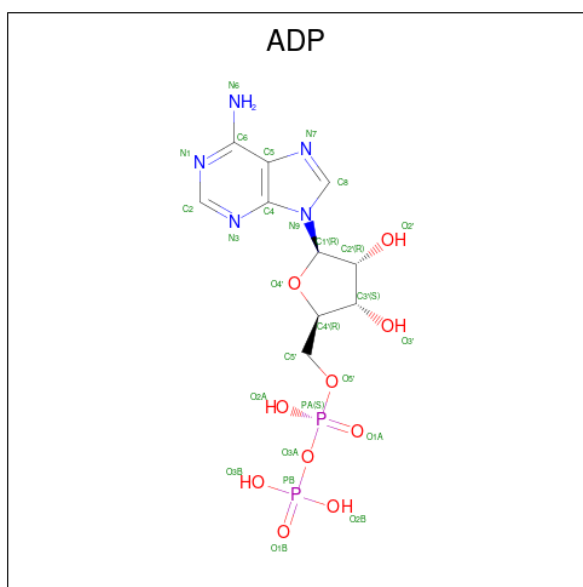
- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	X	705	Total	C	H	N	O	S	0	0
			11543	3691	5828	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
			1539	495	771	138	131	4		

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf	
16	2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total	Mg	0
			1	1	
17	3	1	Total	Mg	0
			1	1	
17	4	1	Total	Mg	0
			1	1	
17	5	1	Total	Mg	0
			1	1	
17	6	1	Total	Mg	0
			1	1	
17	7	1	Total	Mg	0
			1	1	

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

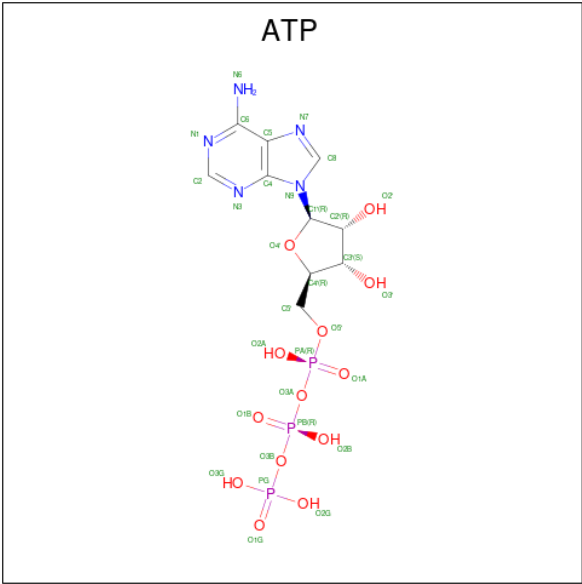
Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	Zn	0
			1	1	
18	4	1	Total	Zn	0
			1	1	

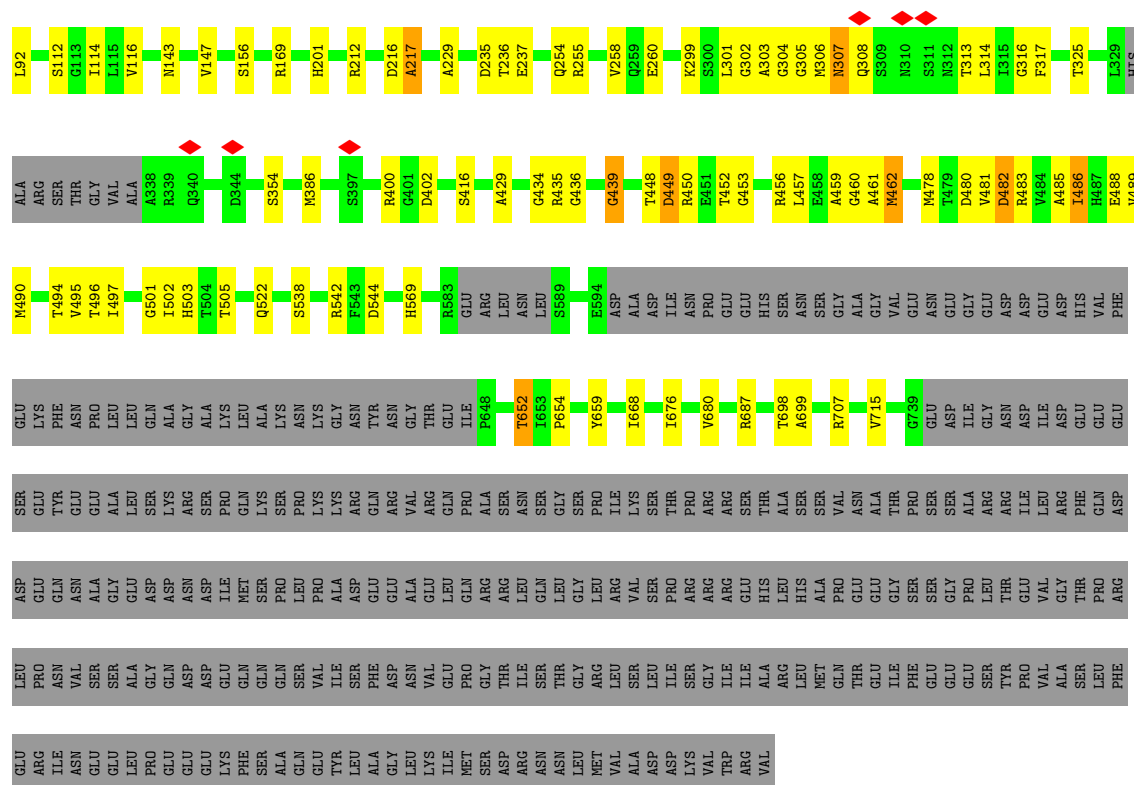
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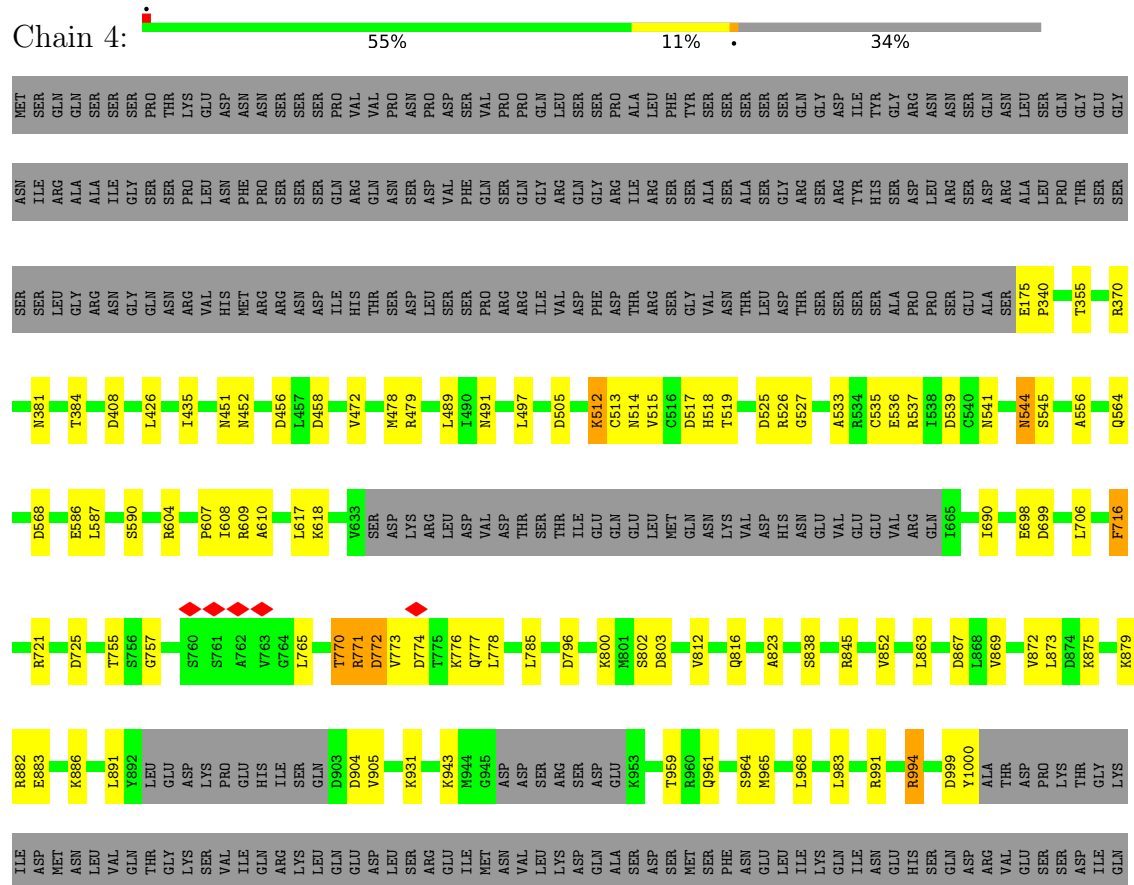
Mol	Chain	Residues	Atoms		AltConf
18	5	1	Total	Zn	0
			1	1	
18	6	1	Total	Zn	0
			1	1	
18	7	1	Total	Zn	0
			1	1	

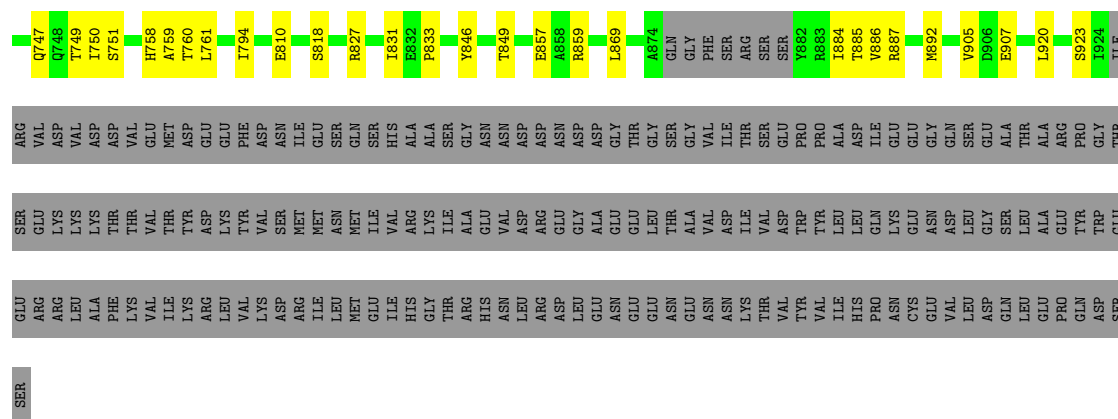
- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).





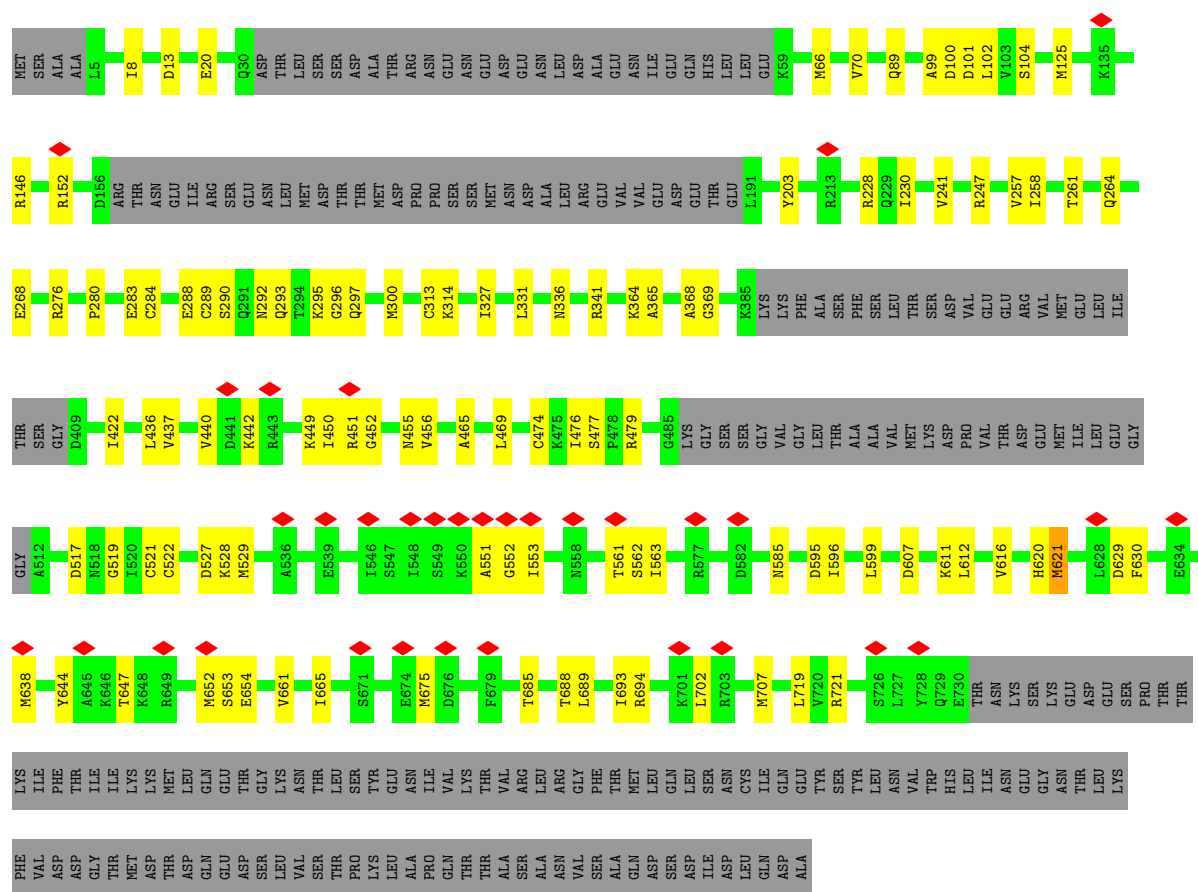
• Molecule 3: DNA replication licensing factor MCM4





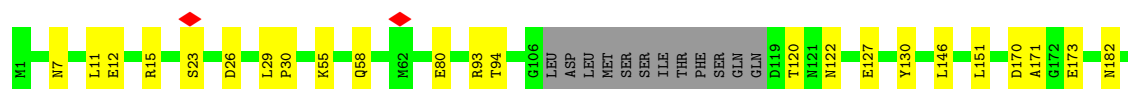
• Molecule 6: DNA replication licensing factor MCM7

Chain 7: 60% 13% 27%



• Molecule 7: DNA replication complex GINS protein PSF1

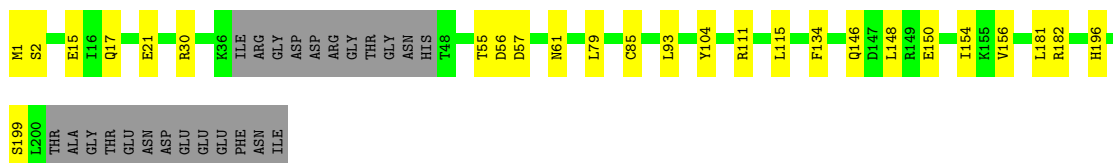
Chain A: 81% 13% 6%





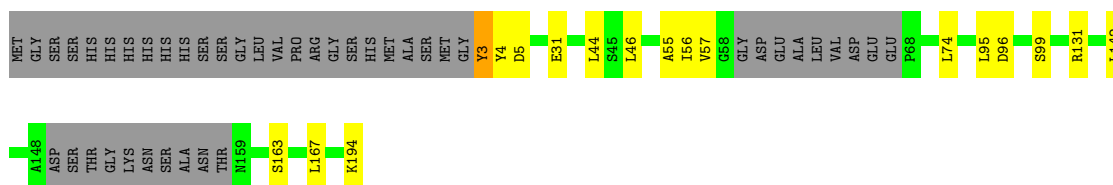
- Molecule 8: DNA replication complex GINS protein PSF2

Chain B: 77% 12% 11%



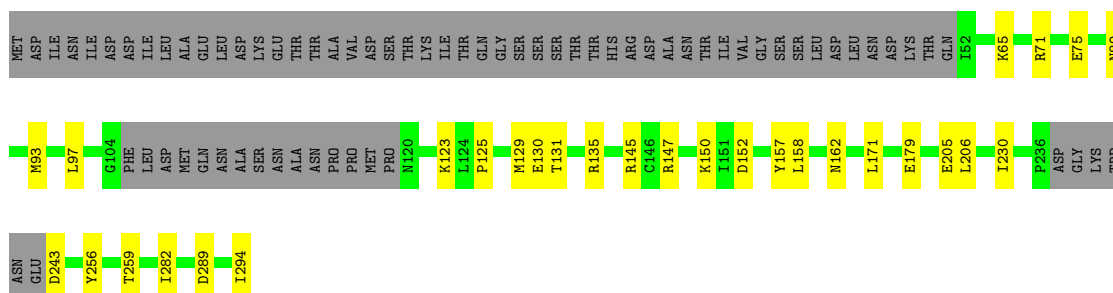
- Molecule 9: DNA replication complex GINS protein PSF3

Chain C: 71% 8% 20%



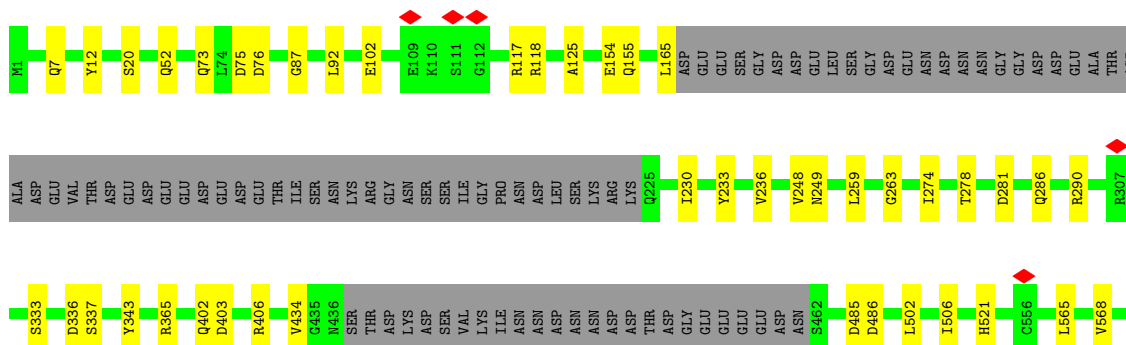
- Molecule 10: DNA replication complex GINS protein SLD5

Chain D: 65% 10% 24%



- Molecule 11: Cell division control protein 45

Chain E: 78% 9% 13%



GLU	VAL	LYS	ASP	ASP
GLU	ASN	PHE	GLU	ASP
ALA	ASN	ALA	GLN	GLN
ILE	ASN	ALA	PRO	ILE
LEU	ASN	GLU	GLN	SER
PHE	ASN	MET	THR	LYS
GLY	GLN	ASN	VAL	SER
LYS	LEU	ASN	ARG	SER
LYS	SER	GLY	GLU	ALA
SER	ASP	VAL	HIS	ALA
ARG	ASP	GLY	GLY	TYR
VAL	ASP	VAL	VAL	PHE
VAL	VAL	THR	PHE	LYS
LEU	ASN	GLY	SER	ASP
GLN	ASP	LYS	LYS	LEU
SER	GLU	TYR	GLU	ASP
GLY	SER	THR	PHE	ASN
ASP	ARG	SER	ILE	ASN
SER	ASN	LEU	SER	ALA
ASP	SER	PHE	ASP	SER
ASP	LEU	GLY	SER	ASP
ASP	GLY	SER	GLU	LYS
	SER	ILE	ASP	LEU
	GLN	PRO	GLU	LYS
	PRO	SER	ASP	THR
	SER	ILE	LEU	LYS
	ASN	GLU	MET	PHE
	GLN	ILE	ASN	SER
	ASN	ARG	LYS	GLY
	GLN	ARG	ILE	GLY
	MET	ALA	PHE	ALA
	PHE	THR	PHE	ALA
	GLN	GLU	GLU	ARG
	SER	SER	ASN	SER
	GLU	SER	GLU	LYS
	VAL	SER	THR	LYS
	TYR	PHE	TYR	LYS
	SER	ALA	MET	ASP
	ARG	PRO	ARG	LYS
	LYS	ASP	TRP	ARG
	GLU	LYS	LEU	LYS
	SER	SER	LEU	ARG
	THR	LEU	ASP	ARG
	LYS	ILE	LYS	GLY
	ARG	SER	ASN	GLY
	SER	LEU	ASN	GLU
	LEU	ALA	GLY	ALA
	GLU	SER	GLN	LYS
	ALA	HIS	LEU	THR
	SER	VAL	THR	ASN
	ALA	ALA	GLU	LEU
	ALA	SER	ASP	PRO
	ASP	GLU	ARG	MET
	GLU	MET	TYR	PHE
	SER	ILE	ILE	GLY
	ASP	ILE	GLN	ASP
	GLU	PHE	PHE	GLN
	ASP	ALA	ALA	ASP

- 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	66410	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	1.140	Depositor
Minimum map value	-0.548	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	2	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.29	34/5356 (0.6%)	1.38	157/7233 (2.2%)
2	3	1.07	35/4909 (0.7%)	1.08	77/6657 (1.2%)
3	4	0.82	16/4952 (0.3%)	0.92	56/6693 (0.8%)
4	5	1.12	37/4737 (0.8%)	1.13	70/6403 (1.1%)
5	6	1.14	34/5086 (0.7%)	1.15	90/6860 (1.3%)
6	7	0.79	14/4943 (0.3%)	0.85	30/6682 (0.4%)
7	A	0.11	0/1620	0.33	0/2179
8	B	0.14	0/1609	0.38	0/2177
9	C	0.37	2/1429 (0.1%)	0.45	2/1932 (0.1%)
10	D	0.12	0/1861	0.33	0/2512
11	E	0.14	0/4656	0.36	0/6306
12	F	0.68	0/1125	1.31	2/1741 (0.1%)
13	G	0.65	0/483	1.30	2/742 (0.3%)
14	X	1.06	18/5828 (0.3%)	1.12	101/7868 (1.3%)
15	Y	1.93	12/784 (1.5%)	1.98	42/1049 (4.0%)
All	All	0.94	202/49378 (0.4%)	1.02	629/67034 (0.9%)

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
1	2	0	3
2	3	0	1
3	4	0	4
4	5	0	2
8	B	0	1
11	E	0	1
12	F	0	11
13	G	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	Y	0	2
All	All	0	30

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	518	HIS	ND1-CE1	-8.76	1.23	1.32
5	6	758	HIS	CE1-NE2	-8.76	1.23	1.32
1	2	405	HIS	ND1-CE1	-8.74	1.23	1.32
4	5	239	ASP	CA-CB	-8.72	1.46	1.52
14	X	406	HIS	CE1-NE2	-8.71	1.23	1.32
2	3	503	HIS	ND1-CE1	-8.63	1.24	1.32
4	5	245	HIS	CE1-NE2	-8.63	1.24	1.32
5	6	715	GLY	N-CA	-8.38	1.37	1.44
1	2	406	ARG	CZ-NH2	-8.35	1.22	1.33
1	2	383	ARG	CZ-NH2	-8.33	1.22	1.33
4	5	272	ARG	CZ-NH2	-8.33	1.22	1.33
3	4	609	ARG	CZ-NH2	-8.32	1.22	1.33
5	6	184	ARG	CZ-NH2	-8.30	1.22	1.33
14	X	712	ARG	CZ-NH2	-8.30	1.22	1.33
4	5	324	ARG	CZ-NH2	-8.29	1.22	1.33
3	4	537	ARG	CZ-NH2	-8.29	1.22	1.33
4	5	149	ARG	CZ-NH2	-8.29	1.22	1.33
14	X	681	ARG	CZ-NH2	-8.28	1.22	1.33
1	2	360	ARG	CZ-NH2	-8.27	1.22	1.33
2	3	255	ARG	CZ-NH2	-8.27	1.22	1.33
4	5	175	ARG	CZ-NH2	-8.27	1.22	1.33
4	5	490	ARG	CZ-NH2	-8.26	1.22	1.33
1	2	617	ARG	CZ-NH2	-8.26	1.22	1.33
15	Y	129	ARG	CZ-NH2	-8.26	1.22	1.33
5	6	530	ARG	CZ-NH2	-8.25	1.22	1.33
3	4	771	ARG	CZ-NH2	-8.25	1.22	1.33
15	Y	134	ARG	CZ-NH2	-8.25	1.22	1.33
2	3	450	ARG	CZ-NH2	-8.24	1.22	1.33
5	6	385	ARG	CZ-NH2	-8.24	1.22	1.33
5	6	390	ARG	CZ-NH2	-8.23	1.22	1.33
5	6	703	ARG	CZ-NH2	-8.23	1.22	1.33
2	3	435	ARG	CZ-NH2	-8.22	1.22	1.33
4	5	209	ARG	CZ-NH2	-8.22	1.22	1.33
1	2	327	ARG	CZ-NH2	-8.22	1.22	1.33
6	7	276	ARG	CZ-NH2	-8.22	1.22	1.33
6	7	247	ARG	CZ-NH2	-8.22	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	778	ARG	CZ-NH2	-8.21	1.22	1.33
2	3	483	ARG	CZ-NH2	-8.20	1.22	1.33
5	6	449	ARG	CZ-NH2	-8.18	1.22	1.33
2	3	456	ARG	CZ-NH2	-8.18	1.22	1.33
14	X	406	HIS	CD2-NE2	-8.05	1.28	1.37
5	6	758	HIS	CD2-NE2	-7.97	1.29	1.37
4	5	245	HIS	CD2-NE2	-7.91	1.29	1.37
5	6	431	ALA	CA-CB	-7.64	1.42	1.53
1	2	571	ALA	CA-CB	-7.23	1.42	1.53
3	4	823	ALA	CA-CB	-7.21	1.42	1.53
1	2	623	ALA	CA-CB	-7.21	1.42	1.53
5	6	695	ALA	CA-CB	-7.20	1.42	1.53
5	6	185	ALA	CA-CB	-7.19	1.42	1.53
1	2	595	ALA	CA-CB	-7.18	1.42	1.53
15	Y	100	HIS	CE1-NE2	-7.16	1.25	1.32
4	5	446	ALA	CA-CB	-7.14	1.42	1.53
9	C	4	TYR	CA-C	-7.13	1.44	1.52
2	3	461	ALA	CA-CB	-7.12	1.42	1.53
4	5	496	ALA	CA-CB	-7.10	1.42	1.53
5	6	716	ALA	CA-CB	-7.10	1.42	1.53
5	6	740	ALA	CA-CB	-7.08	1.42	1.53
6	7	365	ALA	CA-CB	-7.07	1.42	1.53
1	2	440	ALA	CA-CB	-7.07	1.42	1.53
2	3	485	ALA	CA-CB	-7.06	1.42	1.53
3	4	610	ALA	CA-CB	-7.05	1.42	1.53
2	3	201	HIS	CE1-NE2	-7.03	1.25	1.32
1	2	279	THR	C-O	-7.02	1.16	1.24
2	3	460	GLY	N-CA	-7.02	1.37	1.45
14	X	664	ALA	CA-CB	-7.02	1.42	1.53
2	3	229	ALA	CA-CB	-6.96	1.42	1.53
6	7	551	ALA	CA-CB	-6.95	1.42	1.53
3	4	533	ALA	CA-CB	-6.88	1.42	1.53
1	2	412	ALA	CA-CB	-6.86	1.42	1.53
6	7	368	ALA	CA-CB	-6.83	1.42	1.53
5	6	691	ALA	CA-CB	-6.79	1.42	1.53
5	6	759	ALA	CA-CB	-6.78	1.42	1.53
1	2	406	ARG	CZ-NH1	-6.76	1.23	1.32
14	X	712	ARG	CZ-NH1	-6.76	1.23	1.32
1	2	453	ALA	CA-CB	-6.75	1.42	1.53
1	2	383	ARG	CZ-NH1	-6.75	1.23	1.32
15	Y	129	ARG	CZ-NH1	-6.75	1.23	1.32
1	2	428	GLY	N-CA	-6.75	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	324	ARG	CZ-NH1	-6.75	1.23	1.32
5	6	385	ARG	CZ-NH1	-6.74	1.23	1.32
1	2	360	ARG	CZ-NH1	-6.73	1.23	1.32
1	2	617	ARG	CZ-NH1	-6.72	1.23	1.32
6	7	247	ARG	CZ-NH1	-6.72	1.23	1.32
3	4	537	ARG	CZ-NH1	-6.72	1.23	1.32
14	X	681	ARG	CZ-NH1	-6.72	1.23	1.32
14	X	708	ALA	CA-CB	-6.72	1.42	1.53
4	5	149	ARG	CZ-NH1	-6.71	1.23	1.32
5	6	390	ARG	CZ-NH1	-6.71	1.23	1.32
5	6	699	ALA	CA-CB	-6.71	1.42	1.53
5	6	184	ARG	CZ-NH1	-6.71	1.23	1.32
2	3	483	ARG	CZ-NH1	-6.70	1.23	1.32
15	Y	134	ARG	CZ-NH1	-6.69	1.23	1.32
9	C	5	ASP	C-O	-6.69	1.15	1.24
2	3	217	ALA	CA-CB	-6.68	1.42	1.53
2	3	435	ARG	CZ-NH1	-6.68	1.23	1.32
4	5	272	ARG	CZ-NH1	-6.68	1.23	1.32
6	7	276	ARG	CZ-NH1	-6.68	1.23	1.32
2	3	456	ARG	CZ-NH1	-6.67	1.23	1.32
14	X	758	ALA	CA-CB	-6.67	1.42	1.53
4	5	175	ARG	CZ-NH1	-6.66	1.23	1.32
4	5	490	ARG	CZ-NH1	-6.66	1.23	1.32
2	3	255	ARG	CZ-NH1	-6.66	1.23	1.32
4	5	209	ARG	CZ-NH1	-6.66	1.23	1.32
1	2	327	ARG	CZ-NH1	-6.65	1.23	1.32
14	X	778	ARG	CZ-NH1	-6.65	1.23	1.32
3	4	609	ARG	CZ-NH1	-6.64	1.23	1.32
5	6	449	ARG	CZ-NH1	-6.63	1.23	1.32
2	3	450	ARG	CZ-NH1	-6.63	1.23	1.32
5	6	530	ARG	CZ-NH1	-6.63	1.23	1.32
5	6	703	ARG	CZ-NH1	-6.62	1.23	1.32
4	5	239	ASP	N-CA	-6.59	1.41	1.46
3	4	771	ARG	CZ-NH1	-6.59	1.23	1.32
2	3	459	ALA	CA-CB	-6.58	1.42	1.53
15	Y	106	ALA	CA-CB	-6.58	1.42	1.53
2	3	201	HIS	CD2-NE2	-6.52	1.30	1.37
5	6	714	ALA	CA-CB	-6.49	1.42	1.53
15	Y	100	HIS	CD2-NE2	-6.49	1.30	1.37
2	3	303	ALA	CA-CB	-6.48	1.42	1.53
15	Y	56	ALA	CA-CB	-6.48	1.42	1.53
1	2	448	ALA	CA-CB	-6.39	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	434	GLY	N-CA	-6.29	1.38	1.45
14	X	774	GLY	N-CA	-6.27	1.38	1.45
2	3	439	GLY	N-CA	-6.24	1.38	1.45
4	5	448	GLY	N-CA	-6.23	1.38	1.45
1	2	436	GLY	N-CA	-6.22	1.38	1.45
4	5	492	ALA	CA-CB	-6.17	1.42	1.53
15	Y	119	GLY	N-CA	-6.10	1.38	1.45
4	5	441	GLY	N-CA	-6.03	1.38	1.45
6	7	296	GLY	CA-C	-6.03	1.48	1.52
6	7	552	GLY	N-CA	-5.92	1.38	1.45
14	X	762	GLY	N-CA	-5.91	1.38	1.45
1	2	593	GLY	N-CA	-5.87	1.37	1.45
1	2	332	PRO	CA-CB	-5.83	1.46	1.53
5	6	525	GLY	N-CA	-5.80	1.37	1.45
4	5	470	VAL	C-O	-5.61	1.17	1.24
5	6	530	ARG	CD-NE	-5.61	1.38	1.46
14	X	569	ARG	CZ-NH2	-5.60	1.26	1.33
14	X	580	GLY	N-CA	-5.59	1.38	1.45
2	3	316	GLY	N-CA	-5.58	1.37	1.45
4	5	452	SER	CA-CB	-5.57	1.43	1.53
2	3	212	ARG	CZ-NH2	-5.57	1.26	1.33
14	X	681	ARG	CD-NE	-5.56	1.38	1.46
1	2	329	GLY	N-CA	-5.54	1.37	1.45
2	3	450	ARG	CD-NE	-5.53	1.38	1.46
1	2	406	ARG	CD-NE	-5.52	1.38	1.46
2	3	302	GLY	N-CA	-5.50	1.37	1.45
5	6	390	ARG	CD-NE	-5.50	1.38	1.46
4	5	209	ARG	CD-NE	-5.46	1.38	1.46
2	3	483	ARG	CD-NE	-5.46	1.38	1.46
4	5	237	GLY	N-CA	-5.45	1.37	1.44
6	7	247	ARG	CD-NE	-5.43	1.38	1.46
2	3	456	ARG	CD-NE	-5.43	1.38	1.46
1	2	371	GLY	N-CA	-5.43	1.37	1.44
1	2	617	ARG	CD-NE	-5.41	1.38	1.46
2	3	501	GLY	N-CA	-5.40	1.38	1.45
4	5	324	ARG	CD-NE	-5.39	1.38	1.46
14	X	712	ARG	CD-NE	-5.36	1.38	1.46
1	2	566	ALA	CA-CB	-5.36	1.42	1.54
5	6	184	ARG	CD-NE	-5.35	1.38	1.46
4	5	149	ARG	CD-NE	-5.33	1.38	1.46
2	3	255	ARG	CD-NE	-5.33	1.38	1.46
2	3	436	GLY	N-CA	-5.32	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	490	ARG	CD-NE	-5.30	1.38	1.46
15	Y	129	ARG	CD-NE	-5.30	1.38	1.46
3	4	771	ARG	CD-NE	-5.30	1.38	1.46
4	5	175	ARG	CD-NE	-5.30	1.38	1.46
3	4	537	ARG	CD-NE	-5.29	1.38	1.46
1	2	327	ARG	CD-NE	-5.29	1.38	1.46
5	6	449	ARG	CD-NE	-5.27	1.38	1.46
6	7	276	ARG	CD-NE	-5.27	1.38	1.46
6	7	296	GLY	N-CA	-5.27	1.38	1.45
4	5	508	GLY	N-CA	-5.26	1.37	1.45
1	2	383	ARG	CD-NE	-5.25	1.38	1.46
15	Y	134	ARG	CD-NE	-5.23	1.39	1.46
2	3	304	GLY	N-CA	-5.22	1.38	1.45
5	6	385	ARG	CD-NE	-5.22	1.39	1.46
2	3	453	GLY	N-CA	-5.22	1.38	1.45
3	4	609	ARG	CD-NE	-5.22	1.39	1.46
4	5	272	ARG	CD-NE	-5.21	1.39	1.46
4	5	326	PRO	CA-CB	-5.20	1.46	1.53
1	2	360	ARG	CD-NE	-5.19	1.39	1.46
2	3	435	ARG	CD-NE	-5.19	1.39	1.46
4	5	472	ALA	C-O	-5.18	1.17	1.24
5	6	703	ARG	CD-NE	-5.16	1.39	1.46
14	X	778	ARG	CD-NE	-5.14	1.39	1.46
5	6	500	GLY	N-CA	-5.12	1.38	1.45
4	5	451	ALA	CA-CB	-5.12	1.44	1.53
5	6	708	GLY	N-CA	-5.12	1.38	1.45
3	4	527	GLY	N-CA	-5.11	1.38	1.45
4	5	453	VAL	C-O	-5.08	1.19	1.24
6	7	280	PRO	CA-CB	-5.08	1.46	1.53
15	Y	65	LEU	CA-CB	-5.07	1.48	1.53
1	2	568	GLY	N-CA	-5.06	1.38	1.45
4	5	443	GLY	N-CA	-5.06	1.38	1.45
1	2	594	GLY	N-CA	-5.05	1.38	1.45
3	4	544	ASN	CG-ND2	-5.05	1.22	1.33
2	3	456	ARG	CA-CB	-5.04	1.47	1.53
6	7	369	GLY	N-CA	-5.04	1.38	1.45
3	4	772	ASP	CA-CB	-5.04	1.46	1.52
4	5	238	PRO	CA-CB	-5.03	1.47	1.53
5	6	528	GLY	N-CA	-5.02	1.38	1.45
1	2	413	ASP	CA-CB	-5.02	1.48	1.54

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	279	THR	N-CA-C	-7.92	102.59	111.14
3	4	541	ASN	CA-CB-CG	7.82	120.42	112.60
5	6	492	VAL	CA-C-N	7.79	131.12	123.02
5	6	492	VAL	C-N-CA	7.79	131.12	123.02
14	X	665	ASN	CA-CB-CG	7.63	120.23	112.60
4	5	463	TYR	CA-C-O	-7.54	112.48	121.60
5	6	467	ASP	CA-CB-CG	7.53	120.13	112.60
14	X	770	ASN	CA-CB-CG	7.46	120.06	112.60
14	X	394	ASP	CA-CB-CG	7.41	120.01	112.60
1	2	447	PHE	CA-CB-CG	7.34	121.14	113.80
1	2	384	ASN	CA-CB-CG	7.26	119.86	112.60
4	5	482	PHE	CA-CB-CG	7.26	121.06	113.80
3	4	544	ASN	CA-CB-CG	7.24	119.84	112.60
2	3	503	HIS	CA-CB-CG	7.23	121.03	113.80
5	6	421	PHE	CA-CB-CG	7.21	121.00	113.80
5	6	432	PHE	CA-CB-CG	7.17	120.97	113.80
14	X	587	PHE	CA-CB-CG	7.14	120.94	113.80
1	2	614	ASP	CA-CB-CG	7.14	119.74	112.60
15	Y	103	PHE	CA-CB-CG	7.12	120.92	113.80
2	3	216	ASP	CA-CB-CG	7.11	119.71	112.60
1	2	444	PHE	CA-CB-CG	7.10	120.90	113.80
15	Y	133	PHE	CA-CB-CG	7.07	120.86	113.80
15	Y	102	LEU	CA-C-N	7.06	130.22	122.74
15	Y	102	LEU	C-N-CA	7.06	130.22	122.74
4	5	302	ASN	CA-CB-CG	7.05	119.65	112.60
2	3	317	PHE	CA-CB-CG	7.04	120.84	113.80
3	4	514	ASN	CA-CB-CG	6.99	119.59	112.60
5	6	734	ASP	CA-CB-CG	6.99	119.59	112.60
5	6	737	ASP	CA-CB-CG	6.96	119.56	112.60
14	X	677	ASN	CA-CB-CG	6.95	119.55	112.60
4	5	514	ASN	CA-CB-CG	6.93	119.53	112.60
4	5	478	CYS	CA-C-N	6.91	130.17	122.22
4	5	478	CYS	C-N-CA	6.91	130.17	122.22
3	4	514	ASN	CA-C-N	6.90	129.64	121.84
3	4	514	ASN	C-N-CA	6.90	129.64	121.84
1	2	416	ASP	CA-CB-CG	6.89	119.49	112.60
5	6	495	ASP	CA-CB-CG	6.88	119.48	112.60
1	2	435	ASP	CA-CB-CG	6.88	119.48	112.60
15	Y	110	ASP	CA-CB-CG	6.87	119.47	112.60
1	2	439	ASN	CA-CB-CG	6.84	119.44	112.60
14	X	393	ASP	CA-CB-CG	6.83	119.43	112.60
15	Y	111	PHE	CA-CB-CG	6.82	120.62	113.80
4	5	245	HIS	CA-CB-CG	6.81	120.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	352	PHE	CA-CB-CG	6.80	120.60	113.80
3	4	772	ASP	CA-CB-CG	6.76	119.36	112.60
3	4	803	ASP	CA-CB-CG	6.76	119.36	112.60
14	X	775	PHE	CA-CB-CG	6.76	120.56	113.80
6	7	292	ASN	CA-CB-CG	6.69	119.29	112.60
4	5	511	THR	CA-C-N	6.68	131.02	122.93
4	5	511	THR	C-N-CA	6.68	131.02	122.93
15	Y	108	PHE	CA-CB-CG	6.67	120.47	113.80
3	4	518	HIS	CA-CB-CG	6.66	120.45	113.80
4	5	542	PHE	CA-CB-CG	6.64	120.44	113.80
2	3	459	ALA	CA-C-N	6.57	128.78	122.27
2	3	459	ALA	C-N-CA	6.57	128.78	122.27
1	2	339	PHE	CA-CB-CG	6.57	120.37	113.80
1	2	413	ASP	CA-CB-CG	6.55	119.15	112.60
1	2	380	THR	CA-C-N	6.51	130.51	122.37
1	2	380	THR	C-N-CA	6.51	130.51	122.37
14	X	765	PHE	CA-CB-CG	6.49	120.29	113.80
1	2	322	GLY	CA-C-N	6.48	131.23	123.19
1	2	322	GLY	C-N-CA	6.48	131.23	123.19
14	X	696	PHE	CA-CB-CG	6.46	120.26	113.80
1	2	358	GLU	CA-C-N	6.46	131.07	122.93
1	2	358	GLU	C-N-CA	6.46	131.07	122.93
14	X	406	HIS	CA-CB-CG	6.46	120.25	113.80
1	2	613	ASN	CA-CB-CG	6.45	119.05	112.60
9	C	3	TYR	CB-CA-C	-6.45	97.84	110.10
1	2	442	ASN	CA-CB-CG	6.44	119.04	112.60
4	5	487	ASP	CA-CB-CG	6.44	119.04	112.60
1	2	583	ASP	CA-CB-CG	6.44	119.04	112.60
2	3	307	ASN	CA-CB-CG	6.43	119.03	112.60
4	5	255	PHE	CA-CB-CG	6.41	120.21	113.80
15	Y	122	ASP	CA-CB-CG	6.40	119.00	112.60
5	6	429	ASN	CA-CB-CG	6.39	118.99	112.60
5	6	401	ASP	CA-CB-CG	6.36	118.95	112.60
1	2	407	GLU	CA-C-N	6.35	130.93	122.93
1	2	407	GLU	C-N-CA	6.35	130.93	122.93
4	5	273	ASN	CA-CB-CG	6.34	118.94	112.60
4	5	239	ASP	CA-CB-CG	6.32	118.92	112.60
1	2	454	ASN	CA-CB-CG	6.30	118.90	112.60
1	2	351	PHE	CA-CB-CG	6.29	120.09	113.80
2	3	314	LEU	CA-C-N	6.27	130.97	123.19
2	3	314	LEU	C-N-CA	6.27	130.97	123.19
3	4	774	ASP	CA-CB-CG	6.25	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	336	TYR	CA-C-N	6.19	130.87	123.19
1	2	336	TYR	C-N-CA	6.19	130.87	123.19
2	3	449	ASP	CA-CB-CG	6.17	118.77	112.60
1	2	445	PRO	CA-C-N	6.16	130.83	123.19
1	2	445	PRO	C-N-CA	6.16	130.83	123.19
3	4	609	ARG	CD-NE-CZ	6.15	133.01	124.40
4	5	489	ASP	CA-CB-CG	6.15	118.75	112.60
14	X	778	ARG	CD-NE-CZ	6.15	133.01	124.40
1	2	616	ASP	CA-CB-CG	6.14	118.74	112.60
1	2	328	THR	CA-C-N	6.14	126.17	120.34
1	2	328	THR	C-N-CA	6.14	126.17	120.34
4	5	235	ASN	CA-CB-CG	6.14	118.74	112.60
1	2	360	ARG	CD-NE-CZ	6.13	132.99	124.40
1	2	383	ARG	CD-NE-CZ	6.13	132.99	124.40
12	F	35	DT	C4'-C3'-O3'	6.13	119.19	110.00
2	3	435	ARG	CD-NE-CZ	6.12	132.97	124.40
4	5	508	GLY	CA-C-N	6.12	130.95	122.93
4	5	508	GLY	C-N-CA	6.12	130.95	122.93
6	7	276	ARG	CD-NE-CZ	6.11	132.95	124.40
1	2	360	ARG	CA-C-N	6.11	131.06	123.12
1	2	360	ARG	C-N-CA	6.11	131.06	123.12
14	X	712	ARG	CD-NE-CZ	6.11	132.95	124.40
4	5	175	ARG	CD-NE-CZ	6.10	132.94	124.40
1	2	428	GLY	CA-C-N	6.10	130.71	122.90
1	2	428	GLY	C-N-CA	6.10	130.71	122.90
14	X	232	GLY	CA-C-N	6.10	129.28	120.98
14	X	232	GLY	C-N-CA	6.10	129.28	120.98
4	5	492	ALA	CA-C-N	6.10	130.23	121.02
4	5	492	ALA	C-N-CA	6.10	130.23	121.02
14	X	497	ASP	N-CA-C	6.10	118.97	109.52
1	2	628	SER	CA-C-N	6.09	131.21	123.10
1	2	628	SER	C-N-CA	6.09	131.21	123.10
2	3	501	GLY	CA-C-N	6.09	131.03	123.12
2	3	501	GLY	C-N-CA	6.09	131.03	123.12
5	6	449	ARG	CD-NE-CZ	6.09	132.92	124.40
1	2	590	THR	CA-C-N	6.08	131.11	122.72
1	2	590	THR	C-N-CA	6.08	131.11	122.72
5	6	466	LEU	CA-C-N	6.08	130.85	122.77
5	6	466	LEU	C-N-CA	6.08	130.85	122.77
4	5	272	ARG	CD-NE-CZ	6.07	132.90	124.40
4	5	490	ARG	CD-NE-CZ	6.07	132.90	124.40
15	Y	129	ARG	CD-NE-CZ	6.06	132.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	327	ARG	CD-NE-CZ	6.06	132.88	124.40
15	Y	134	ARG	CD-NE-CZ	6.05	132.88	124.40
1	2	363	PHE	CA-CB-CG	6.05	119.85	113.80
14	X	223	ASN	CA-CB-CG	6.05	118.65	112.60
5	6	703	ARG	CD-NE-CZ	6.05	132.87	124.40
3	4	527	GLY	CA-C-N	6.02	130.94	123.12
3	4	527	GLY	C-N-CA	6.02	130.94	123.12
1	2	629	ILE	CA-C-N	6.01	130.77	122.77
1	2	629	ILE	C-N-CA	6.01	130.77	122.77
2	3	255	ARG	CD-NE-CZ	6.01	132.81	124.40
6	7	261	THR	CA-C-N	6.01	130.76	122.77
6	7	261	THR	C-N-CA	6.01	130.76	122.77
3	4	537	ARG	CD-NE-CZ	6.00	132.81	124.40
3	4	607	PRO	CA-C-N	6.00	130.92	123.12
3	4	607	PRO	C-N-CA	6.00	130.92	123.12
5	6	711	THR	CA-C-N	5.99	130.09	122.37
5	6	711	THR	C-N-CA	5.99	130.09	122.37
4	5	198	ASN	CA-CB-CG	5.98	118.58	112.60
6	7	295	LYS	CA-C-N	5.97	128.29	122.73
6	7	295	LYS	C-N-CA	5.97	128.29	122.73
2	3	482	ASP	CA-CB-CG	5.96	118.56	112.60
5	6	503	GLY	CA-C-N	5.95	130.86	123.12
5	6	503	GLY	C-N-CA	5.95	130.86	123.12
2	3	494	THR	CA-C-N	5.95	131.01	123.10
2	3	494	THR	C-N-CA	5.95	131.01	123.10
1	2	278	ALA	N-CA-C	-5.94	105.69	113.12
6	7	313	CYS	CA-C-N	5.93	131.19	123.00
6	7	313	CYS	C-N-CA	5.93	131.19	123.00
5	6	385	ARG	CD-NE-CZ	5.91	132.68	124.40
1	2	635	GLY	CA-C-N	5.91	130.67	122.93
1	2	635	GLY	C-N-CA	5.91	130.67	122.93
14	X	772	GLU	CA-C-N	5.90	129.60	122.16
14	X	772	GLU	C-N-CA	5.90	129.60	122.16
4	5	501	THR	CA-C-N	5.88	131.01	123.13
4	5	501	THR	C-N-CA	5.88	131.01	123.13
5	6	750	ILE	CA-C-N	5.88	130.59	122.77
5	6	750	ILE	C-N-CA	5.88	130.59	122.77
2	3	453	GLY	CA-C-N	5.87	131.10	123.00
2	3	453	GLY	C-N-CA	5.87	131.10	123.00
2	3	496	THR	CA-C-N	5.86	130.82	123.14
2	3	496	THR	C-N-CA	5.86	130.82	123.14
1	2	426	VAL	CA-C-N	5.86	130.57	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	426	VAL	C-N-CA	5.86	130.57	122.77
14	X	399	ASN	CA-CB-CG	5.85	118.45	112.60
5	6	448	VAL	CA-C-N	5.84	130.53	122.77
5	6	448	VAL	C-N-CA	5.84	130.53	122.77
5	6	749	THR	CA-C-N	5.82	130.93	123.13
5	6	749	THR	C-N-CA	5.82	130.93	123.13
1	2	570	GLY	CA-C-N	5.82	131.03	123.00
1	2	570	GLY	C-N-CA	5.82	131.03	123.00
1	2	630	SER	CA-C-N	5.82	130.83	123.10
1	2	630	SER	C-N-CA	5.82	130.83	123.10
9	C	3	TYR	N-CA-CB	5.81	120.38	110.50
1	2	406	ARG	CA-C-N	5.81	130.14	122.30
1	2	406	ARG	C-N-CA	5.81	130.14	122.30
1	2	337	VAL	CA-C-N	5.79	131.00	123.00
1	2	337	VAL	C-N-CA	5.79	131.00	123.00
4	5	503	SER	CA-C-N	5.79	130.80	123.10
4	5	503	SER	C-N-CA	5.79	130.80	123.10
1	2	368	LYS	CA-C-N	5.77	130.97	123.00
1	2	368	LYS	C-N-CA	5.77	130.97	123.00
2	3	429	ALA	CA-C-N	5.77	131.01	122.99
2	3	429	ALA	C-N-CA	5.77	131.01	122.99
5	6	760	THR	CA-C-N	5.75	130.66	122.72
5	6	760	THR	C-N-CA	5.75	130.66	122.72
1	2	414	LEU	CA-C-N	5.75	128.90	120.91
1	2	414	LEU	C-N-CA	5.75	128.90	120.91
1	2	425	GLU	CA-C-N	5.75	130.59	123.12
1	2	425	GLU	C-N-CA	5.75	130.59	123.12
3	4	770	THR	CA-C-N	5.74	131.08	123.05
3	4	770	THR	C-N-CA	5.74	131.08	123.05
4	5	439	THR	CA-C-N	5.73	130.63	122.72
4	5	439	THR	C-N-CA	5.73	130.63	122.72
4	5	502	ILE	CA-C-N	5.73	130.39	122.77
4	5	502	ILE	C-N-CA	5.73	130.39	122.77
12	F	45	DT	O4'-C1'-N1	5.72	116.98	108.40
1	2	563	ALA	CA-C-N	5.72	130.94	122.99
1	2	563	ALA	C-N-CA	5.72	130.94	122.99
15	Y	123	PRO	CA-C-N	5.70	128.51	120.42
15	Y	123	PRO	C-N-CA	5.70	128.51	120.42
14	X	406	HIS	CA-C-N	5.69	131.03	123.00
14	X	406	HIS	C-N-CA	5.69	131.03	123.00
4	5	254	GLN	CA-C-N	5.69	130.85	123.00
4	5	254	GLN	C-N-CA	5.69	130.85	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	446	VAL	CA-C-N	5.68	130.56	122.72
1	2	446	VAL	C-N-CA	5.68	130.56	122.72
1	2	636	ILE	CA-C-N	5.68	131.06	123.10
1	2	636	ILE	C-N-CA	5.68	131.06	123.10
14	X	584	SER	CA-C-N	5.68	127.83	120.44
14	X	584	SER	C-N-CA	5.68	127.83	120.44
1	2	362	SER	CA-C-N	5.68	131.00	123.05
1	2	362	SER	C-N-CA	5.68	131.00	123.05
3	4	771	ARG	CD-NE-CZ	5.67	132.34	124.40
4	5	256	LEU	CA-C-N	5.67	130.99	123.05
4	5	256	LEU	C-N-CA	5.67	130.99	123.05
3	4	545	SER	CA-C-N	5.66	130.53	122.72
3	4	545	SER	C-N-CA	5.66	130.53	122.72
1	2	450	ILE	CA-C-N	5.66	130.62	123.10
1	2	450	ILE	C-N-CA	5.66	130.62	123.10
5	6	714	ALA	CA-C-N	5.65	129.60	122.77
5	6	714	ALA	C-N-CA	5.65	129.60	122.77
2	3	495	VAL	CA-C-N	5.63	130.93	123.05
2	3	495	VAL	C-N-CA	5.63	130.93	123.05
5	6	446	GLN	CA-C-N	5.63	130.93	123.05
5	6	446	GLN	C-N-CA	5.63	130.93	123.05
5	6	712	ILE	CA-C-N	5.62	130.92	123.05
5	6	712	ILE	C-N-CA	5.62	130.92	123.05
2	3	254	GLN	CA-C-N	5.62	130.92	123.00
2	3	254	GLN	C-N-CA	5.62	130.92	123.00
4	5	197	PHE	CA-C-N	5.62	130.47	122.72
4	5	197	PHE	C-N-CA	5.62	130.47	122.72
15	Y	126	ARG	CA-C-N	5.60	127.72	120.44
15	Y	126	ARG	C-N-CA	5.60	127.72	120.44
2	3	448	THR	CA-C-N	5.60	129.86	122.30
2	3	448	THR	C-N-CA	5.60	129.86	122.30
14	X	221	THR	CA-C-N	5.58	130.75	122.99
14	X	221	THR	C-N-CA	5.58	130.75	122.99
4	5	513	LEU	CA-C-N	5.57	130.85	123.05
4	5	513	LEU	C-N-CA	5.57	130.85	123.05
1	2	342	LEU	CA-C-N	5.56	129.44	121.71
1	2	342	LEU	C-N-CA	5.56	129.44	121.71
2	3	457	LEU	CA-C-N	5.56	130.83	123.05
2	3	457	LEU	C-N-CA	5.56	130.83	123.05
3	4	778	LEU	CA-C-N	5.56	130.72	122.99
3	4	778	LEU	C-N-CA	5.56	130.72	122.99
5	6	751	SER	CA-C-N	5.56	130.73	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	751	SER	C-N-CA	5.56	130.73	123.06
1	2	640	LEU	CA-C-N	5.55	130.82	123.05
1	2	640	LEU	C-N-CA	5.55	130.82	123.05
14	X	497	ASP	CB-CA-C	-5.55	98.41	109.79
5	6	184	ARG	CA-C-N	5.54	130.65	123.00
5	6	184	ARG	C-N-CA	5.54	130.65	123.00
14	X	699	ARG	CA-C-N	5.54	127.63	120.70
14	X	699	ARG	C-N-CA	5.54	127.63	120.70
1	2	638	THR	CA-C-N	5.54	130.81	123.00
1	2	638	THR	C-N-CA	5.54	130.81	123.00
5	6	185	ALA	CA-C-N	5.53	131.23	122.94
5	6	185	ALA	C-N-CA	5.53	131.23	122.94
4	5	274	LEU	CA-C-N	5.52	129.39	121.50
4	5	274	LEU	C-N-CA	5.52	129.39	121.50
1	2	603	VAL	CA-C-N	5.51	130.76	123.05
1	2	603	VAL	C-N-CA	5.51	130.76	123.05
14	X	220	PHE	CA-C-N	5.50	129.94	122.19
14	X	220	PHE	C-N-CA	5.50	129.94	122.19
5	6	536	ASP	CA-C-N	5.49	130.74	123.05
5	6	536	ASP	C-N-CA	5.49	130.74	123.05
6	7	297	GLN	CA-C-N	5.48	129.92	122.19
6	7	297	GLN	C-N-CA	5.48	129.92	122.19
3	4	517	ASP	CA-C-N	5.47	129.91	122.19
3	4	517	ASP	C-N-CA	5.47	129.91	122.19
2	3	486	ILE	N-CA-CB	5.47	116.95	110.55
2	3	505	THR	CA-C-N	5.47	130.27	122.72
2	3	505	THR	C-N-CA	5.47	130.27	122.72
14	X	521	TYR	N-CA-CB	5.46	117.93	110.01
14	X	570	ILE	N-CA-CB	5.46	116.58	110.51
1	2	388	VAL	CA-C-N	5.45	130.84	122.77
1	2	388	VAL	C-N-CA	5.45	130.84	122.77
2	3	456	ARG	CA-C-N	5.45	131.12	122.94
2	3	456	ARG	C-N-CA	5.45	131.12	122.94
14	X	771	SER	CA-C-N	5.45	127.52	120.44
14	X	771	SER	C-N-CA	5.45	127.52	120.44
5	6	420	THR	CA-C-N	5.45	130.45	122.77
5	6	420	THR	C-N-CA	5.45	130.45	122.77
14	X	591	CYS	CA-C-N	5.44	127.41	120.56
14	X	591	CYS	C-N-CA	5.44	127.41	120.56
5	6	690	LYS	CA-C-N	5.43	128.48	120.82
5	6	690	LYS	C-N-CA	5.43	128.48	120.82
14	X	696	PHE	N-CA-CB	5.43	118.11	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	405	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
2	3	299	LYS	CA-C-N	5.43	131.09	122.74
2	3	299	LYS	C-N-CA	5.43	131.09	122.74
2	3	478	MET	CA-C-N	5.42	131.60	122.87
2	3	478	MET	C-N-CA	5.42	131.60	122.87
13	G	11	DC	O5'-C5'-C4'	5.42	118.93	110.80
1	2	357	GLU	CA-C-N	5.42	129.44	120.94
1	2	357	GLU	C-N-CA	5.42	129.44	120.94
3	4	518	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
2	3	307	ASN	N-CA-CB	5.41	118.00	109.83
5	6	529	LEU	CA-C-N	5.41	127.53	120.28
5	6	529	LEU	C-N-CA	5.41	127.53	120.28
14	X	592	ILE	N-CA-CB	5.41	116.88	110.55
14	X	670	PRO	CA-C-N	5.41	127.37	120.56
14	X	670	PRO	C-N-CA	5.41	127.37	120.56
14	X	675	TYR	CA-C-N	5.41	127.37	120.56
14	X	675	TYR	C-N-CA	5.41	127.37	120.56
3	4	537	ARG	CA-C-N	5.40	127.36	120.56
3	4	537	ARG	C-N-CA	5.40	127.36	120.56
1	2	455	SER	CA-C-N	5.38	130.47	122.99
1	2	455	SER	C-N-CA	5.38	130.47	122.99
2	3	502	ILE	CA-C-N	5.38	130.70	122.95
2	3	502	ILE	C-N-CA	5.38	130.70	122.95
14	X	705	LYS	CA-C-N	5.38	130.01	122.05
14	X	705	LYS	C-N-CA	5.38	130.01	122.05
1	2	612	MET	CA-CB-CG	5.38	124.85	114.10
2	3	258	VAL	CA-C-N	5.38	130.73	122.93
2	3	258	VAL	C-N-CA	5.38	130.73	122.93
14	X	661	LYS	CA-C-N	5.37	127.33	120.56
14	X	661	LYS	C-N-CA	5.37	127.33	120.56
13	G	19	DG	C4'-C3'-O3'	5.37	118.05	110.00
5	6	464	ARG	CA-C-N	5.37	131.24	122.81
5	6	464	ARG	C-N-CA	5.37	131.24	122.81
4	5	323	ILE	CA-C-N	5.37	131.00	122.74
4	5	323	ILE	C-N-CA	5.37	131.00	122.74
14	X	673	GLU	CA-C-N	5.37	127.42	120.44
14	X	673	GLU	C-N-CA	5.37	127.42	120.44
2	3	489	VAL	N-CA-CB	5.36	116.47	110.62
14	X	225	LYS	CA-C-N	5.36	130.64	122.65
14	X	225	LYS	C-N-CA	5.36	130.64	122.65
15	Y	133	PHE	CA-C-N	5.36	127.41	120.44
15	Y	133	PHE	C-N-CA	5.36	127.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	539	ASP	CA-C-N	5.36	130.69	122.77
3	4	539	ASP	C-N-CA	5.36	130.69	122.77
2	3	462	MET	CA-C-N	5.35	127.41	120.56
2	3	462	MET	C-N-CA	5.35	127.41	120.56
1	2	591	LEU	CA-C-N	5.35	130.97	122.94
1	2	591	LEU	C-N-CA	5.35	130.97	122.94
1	2	379	LYS	CA-C-N	5.35	130.53	122.99
1	2	379	LYS	C-N-CA	5.35	130.53	122.99
2	3	456	ARG	CD-NE-CZ	5.34	131.88	124.40
2	3	503	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	2	338	LYS	CA-C-N	5.34	130.67	122.93
1	2	338	LYS	C-N-CA	5.34	130.67	122.93
2	3	305	GLY	CA-C-N	5.34	127.43	120.28
2	3	305	GLY	C-N-CA	5.34	127.43	120.28
15	Y	127	GLU	CA-C-N	5.33	127.38	120.44
15	Y	127	GLU	C-N-CA	5.33	127.38	120.44
3	4	999	ASP	N-CA-C	-5.33	105.47	111.28
15	Y	57	GLU	CA-C-N	5.33	127.37	120.44
15	Y	57	GLU	C-N-CA	5.33	127.37	120.44
4	5	299	SER	CA-C-N	5.33	130.38	122.71
4	5	299	SER	C-N-CA	5.33	130.38	122.71
15	Y	58	LYS	CA-CB-CG	5.33	124.75	114.10
14	X	700	VAL	N-CA-CB	5.33	116.43	110.62
14	X	233	ILE	N-CA-CB	5.32	116.86	110.31
4	5	489	ASP	CA-C-N	5.32	127.36	120.44
4	5	489	ASP	C-N-CA	5.32	127.36	120.44
14	X	572	LEU	CA-C-N	5.32	127.41	120.28
14	X	572	LEU	C-N-CA	5.32	127.41	120.28
15	Y	124	VAL	CA-C-N	5.32	127.41	120.28
15	Y	124	VAL	C-N-CA	5.32	127.41	120.28
4	5	40	LEU	N-CA-C	-5.32	107.16	113.97
5	6	694	ALA	CA-C-N	5.31	127.35	120.44
5	6	694	ALA	C-N-CA	5.31	127.35	120.44
1	2	341	CYS	CA-C-N	5.31	127.34	120.44
1	2	341	CYS	C-N-CA	5.31	127.34	120.44
14	X	571	GLN	CA-C-N	5.31	127.34	120.44
14	X	571	GLN	C-N-CA	5.31	127.34	120.44
14	X	776	TYR	N-CA-CB	5.31	117.70	110.01
15	Y	114	ILE	CA-C-N	5.31	127.34	120.44
15	Y	114	ILE	C-N-CA	5.31	127.34	120.44
6	7	290	SER	CA-C-N	5.29	127.32	120.44
6	7	290	SER	C-N-CA	5.29	127.32	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	739	VAL	CA-C-N	5.29	127.36	120.28
5	6	739	VAL	C-N-CA	5.29	127.36	120.28
2	3	481	VAL	CA-C-N	5.28	127.79	120.29
2	3	481	VAL	C-N-CA	5.28	127.79	120.29
6	7	296	GLY	CA-C-N	5.28	128.97	121.42
6	7	296	GLY	C-N-CA	5.28	128.97	121.42
14	X	708	ALA	CA-C-N	5.28	127.35	120.28
14	X	708	ALA	C-N-CA	5.28	127.35	120.28
1	2	334	LEU	CA-C-N	5.27	127.61	120.44
1	2	334	LEU	C-N-CA	5.27	127.61	120.44
6	7	284	CYS	CA-C-N	5.26	130.48	122.37
6	7	284	CYS	C-N-CA	5.26	130.48	122.37
14	X	587	PHE	CA-C-N	5.26	127.28	120.44
14	X	587	PHE	C-N-CA	5.26	127.28	120.44
1	2	324	VAL	CA-C-N	5.26	127.76	120.29
1	2	324	VAL	C-N-CA	5.26	127.76	120.29
1	2	434	TYR	CA-C-N	5.26	130.75	123.07
1	2	434	TYR	C-N-CA	5.26	130.75	123.07
1	2	618	THR	CA-C-N	5.26	127.27	120.44
1	2	618	THR	C-N-CA	5.26	127.27	120.44
5	6	421	PHE	CA-C-N	5.25	127.69	120.39
5	6	421	PHE	C-N-CA	5.25	127.69	120.39
14	X	398	TRP	CA-C-N	5.25	130.40	122.99
14	X	398	TRP	C-N-CA	5.25	130.40	122.99
4	5	487	ASP	CA-C-N	5.25	127.26	120.44
4	5	487	ASP	C-N-CA	5.25	127.26	120.44
5	6	734	ASP	CA-C-N	5.25	127.17	120.56
5	6	734	ASP	C-N-CA	5.25	127.17	120.56
15	Y	128	TYR	CA-C-N	5.25	127.26	120.44
15	Y	128	TYR	C-N-CA	5.25	127.26	120.44
4	5	271	PRO	CA-C-N	5.25	130.47	122.65
4	5	271	PRO	C-N-CA	5.25	130.47	122.65
14	X	774	GLY	CA-C-N	5.24	127.26	120.44
14	X	774	GLY	C-N-CA	5.24	127.26	120.44
1	2	405	HIS	ND1-CG-CD2	-5.24	100.86	106.10
5	6	184	ARG	CD-NE-CZ	5.24	131.73	124.40
1	2	405	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	2	409	ILE	CA-C-N	5.23	129.64	122.84
1	2	409	ILE	C-N-CA	5.23	129.64	122.84
1	2	596	LEU	CA-C-N	5.23	127.15	120.56
1	2	596	LEU	C-N-CA	5.23	127.15	120.56
1	2	631	ILE	CA-C-N	5.23	131.30	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	631	ILE	C-N-CA	5.23	131.30	123.24
5	6	400	CYS	CA-C-N	5.23	127.29	120.28
5	6	400	CYS	C-N-CA	5.23	127.29	120.28
5	6	427	CYS	N-CA-CB	5.23	117.66	109.97
1	2	439	ASN	CA-C-N	5.23	127.24	120.44
1	2	439	ASN	C-N-CA	5.23	127.24	120.44
6	7	289	CYS	CA-C-N	5.23	127.23	120.44
6	7	289	CYS	C-N-CA	5.23	127.23	120.44
5	6	429	ASN	N-CA-CB	5.22	117.67	109.69
4	5	481	GLU	CA-C-N	5.22	127.27	120.28
4	5	481	GLU	C-N-CA	5.22	127.27	120.28
1	2	434	TYR	N-CA-CB	5.21	117.62	109.85
14	X	393	ASP	CA-C-N	5.21	127.79	120.28
14	X	393	ASP	C-N-CA	5.21	127.79	120.28
15	Y	127	GLU	N-CA-CB	5.21	117.57	110.01
2	3	313	THR	CA-C-N	5.21	130.37	122.08
2	3	313	THR	C-N-CA	5.21	130.37	122.08
14	X	590	SER	CA-C-N	5.21	127.21	120.44
14	X	590	SER	C-N-CA	5.21	127.21	120.44
3	4	518	HIS	CG-CD2-NE2	5.21	112.41	107.20
14	X	777	GLN	N-CA-CB	5.20	117.50	109.91
3	4	518	HIS	ND1-CG-CD2	-5.20	100.90	106.10
4	5	44	PHE	CB-CA-C	5.20	120.14	111.30
5	6	400	CYS	N-CA-CB	5.20	117.59	109.85
4	5	509	ILE	CA-C-N	5.20	130.98	123.13
4	5	509	ILE	C-N-CA	5.20	130.98	123.13
2	3	488	GLU	CA-C-N	5.19	127.19	120.70
2	3	488	GLU	C-N-CA	5.19	127.19	120.70
3	4	609	ARG	CA-C-N	5.19	127.19	120.44
3	4	609	ARG	C-N-CA	5.19	127.19	120.44
5	6	494	PRO	CA-C-N	5.18	130.63	122.34
5	6	494	PRO	C-N-CA	5.18	130.63	122.34
15	Y	111	PHE	CA-C-N	5.18	127.18	120.44
15	Y	111	PHE	C-N-CA	5.18	127.18	120.44
2	3	503	HIS	CG-CD2-NE2	5.18	112.38	107.20
5	6	424	ASN	CA-CB-CG	5.18	117.78	112.60
5	6	691	ALA	CA-C-N	5.18	127.49	120.44
5	6	691	ALA	C-N-CA	5.18	127.49	120.44
5	6	734	ASP	N-CA-CB	5.18	117.63	110.17
2	3	503	HIS	ND1-CG-CD2	-5.18	100.92	106.10
6	7	264	GLN	CA-C-N	5.18	127.48	120.44
6	7	264	GLN	C-N-CA	5.18	127.48	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	405	HIS	CA-C-N	5.17	130.83	122.29
1	2	405	HIS	C-N-CA	5.17	130.83	122.29
5	6	703	ARG	CG-CD-NE	5.17	123.38	112.00
2	3	449	ASP	CA-C-N	5.17	127.16	120.44
2	3	449	ASP	C-N-CA	5.17	127.16	120.44
5	6	702	VAL	CA-C-N	5.17	130.29	123.05
5	6	702	VAL	C-N-CA	5.17	130.29	123.05
2	3	483	ARG	CA-CB-CG	5.17	124.43	114.10
5	6	427	CYS	CA-C-N	5.17	130.50	122.49
5	6	427	CYS	C-N-CA	5.17	130.50	122.49
1	2	335	LYS	CA-C-N	5.16	130.69	122.74
1	2	335	LYS	C-N-CA	5.16	130.69	122.74
4	5	488	GLU	CA-C-N	5.16	127.15	120.44
4	5	488	GLU	C-N-CA	5.16	127.15	120.44
15	Y	58	LYS	CA-C-N	5.16	127.19	120.28
15	Y	58	LYS	C-N-CA	5.16	127.19	120.28
15	Y	111	PHE	N-CA-CB	5.16	117.49	110.01
5	6	497	THR	CA-C-N	5.16	127.14	120.44
5	6	497	THR	C-N-CA	5.16	127.14	120.44
1	2	366	ASN	CA-C-N	5.15	127.19	120.28
1	2	366	ASN	C-N-CA	5.15	127.19	120.28
1	2	438	LEU	CA-C-N	5.15	127.13	120.44
1	2	438	LEU	C-N-CA	5.15	127.13	120.44
6	7	300	MET	N-CA-CB	5.15	117.60	109.83
1	2	622	GLU	CA-C-N	5.14	127.17	120.28
1	2	622	GLU	C-N-CA	5.14	127.17	120.28
14	X	663	GLN	CA-C-N	5.14	127.17	120.28
14	X	663	GLN	C-N-CA	5.14	127.17	120.28
15	Y	101	GLU	CA-C-N	5.14	127.63	120.63
15	Y	101	GLU	C-N-CA	5.14	127.63	120.63
1	2	358	GLU	N-CA-CB	5.14	117.58	110.17
1	2	641	GLN	CA-CB-CG	5.14	124.38	114.10
5	6	539	TYR	CA-C-N	5.14	130.96	122.33
5	6	539	TYR	C-N-CA	5.14	130.96	122.33
6	7	364	LYS	N-CA-CB	5.14	117.67	110.12
1	2	364	CYS	N-CA-CB	5.14	117.91	109.95
14	X	230	LYS	CA-C-N	5.13	127.42	120.44
14	X	230	LYS	C-N-CA	5.13	127.42	120.44
14	X	760	PHE	CA-C-N	5.13	127.71	120.42
14	X	760	PHE	C-N-CA	5.13	127.71	120.42
15	Y	130	VAL	CA-C-N	5.13	127.11	120.44
15	Y	130	VAL	C-N-CA	5.13	127.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	497	ILE	CA-C-N	5.13	131.15	123.24
2	3	497	ILE	C-N-CA	5.13	131.15	123.24
4	5	257	LYS	CA-CB-CG	5.13	124.36	114.10
5	6	419	PRO	CA-C-N	5.13	129.93	122.08
5	6	419	PRO	C-N-CA	5.13	129.93	122.08
14	X	775	PHE	N-CA-CB	5.13	117.44	110.01
15	Y	110	ASP	CA-C-N	5.13	127.11	120.44
15	Y	110	ASP	C-N-CA	5.13	127.11	120.44
3	4	618	LYS	CA-C-N	5.12	127.10	120.44
3	4	618	LYS	C-N-CA	5.12	127.10	120.44
6	7	283	GLU	CA-C-N	5.12	127.99	120.71
6	7	283	GLU	C-N-CA	5.12	127.99	120.71
2	3	480	ASP	CA-C-N	5.12	127.20	120.60
2	3	480	ASP	C-N-CA	5.12	127.20	120.60
1	2	413	ASP	CA-C-N	5.12	130.40	122.26
1	2	413	ASP	C-N-CA	5.12	130.40	122.26
3	4	535	CYS	N-CA-CB	5.11	117.41	109.48
6	7	314	LYS	CA-CB-CG	5.11	124.32	114.10
14	X	663	GLN	CA-CB-CG	5.11	124.32	114.10
5	6	530	ARG	CA-C-N	5.11	127.08	120.44
5	6	530	ARG	C-N-CA	5.11	127.08	120.44
5	6	425	PRO	CA-C-N	5.11	127.54	120.29
5	6	425	PRO	C-N-CA	5.11	127.54	120.29
1	2	352	PHE	N-CA-CB	5.10	117.50	109.69
6	7	257	VAL	CA-C-N	5.10	129.52	123.19
6	7	257	VAL	C-N-CA	5.10	129.52	123.19
3	4	774	ASP	N-CA-CB	5.10	117.41	110.01
3	4	802	SER	CA-C-N	5.10	127.07	120.44
3	4	802	SER	C-N-CA	5.10	127.07	120.44
4	5	209	ARG	CA-CB-CG	5.10	124.30	114.10
14	X	220	PHE	CA-CB-CG	5.10	118.90	113.80
14	X	671	VAL	CA-C-N	5.10	127.44	120.46
14	X	671	VAL	C-N-CA	5.10	127.44	120.46
14	X	233	ILE	CA-C-N	5.10	129.14	120.88
14	X	233	ILE	C-N-CA	5.10	129.14	120.88
1	2	429	ILE	CA-C-N	5.09	129.58	121.99
1	2	429	ILE	C-N-CA	5.09	129.58	121.99
1	2	617	ARG	CA-CB-CG	5.09	124.28	114.10
2	3	450	ARG	CA-C-N	5.09	127.06	120.44
2	3	450	ARG	C-N-CA	5.09	127.06	120.44
4	5	485	MET	N-CA-CB	5.09	117.48	109.69
15	Y	134	ARG	CA-CB-CG	5.09	124.28	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	616	ASP	CA-C-N	5.09	127.06	120.44
1	2	616	ASP	C-N-CA	5.09	127.06	120.44
1	2	587	LYS	CA-C-N	5.09	130.56	122.62
1	2	587	LYS	C-N-CA	5.09	130.56	122.62
6	7	288	GLU	CA-C-N	5.09	127.06	120.44
6	7	288	GLU	C-N-CA	5.09	127.06	120.44
3	4	513	CYS	N-CA-CB	5.09	117.83	109.95
14	X	672	ILE	CA-C-N	5.08	127.05	120.44
14	X	672	ILE	C-N-CA	5.08	127.05	120.44
1	2	433	ASN	CA-C-N	5.08	128.06	120.95
1	2	433	ASN	C-N-CA	5.08	128.06	120.95
2	3	317	PHE	CA-C-N	5.08	129.82	121.39
2	3	317	PHE	C-N-CA	5.08	129.82	121.39
4	5	155	HIS	CA-C-N	5.08	127.89	120.98
4	5	155	HIS	C-N-CA	5.08	127.89	120.98
14	X	588	MET	CA-CB-CG	5.08	124.26	114.10
3	4	772	ASP	N-CA-CB	5.08	117.90	109.88
3	4	773	VAL	CA-C-N	5.08	127.04	120.44
3	4	773	VAL	C-N-CA	5.08	127.04	120.44
1	2	431	LYS	CA-C-N	5.07	130.53	122.62
1	2	431	LYS	C-N-CA	5.07	130.53	122.62
1	2	614	ASP	CA-C-N	5.07	127.03	120.44
1	2	614	ASP	C-N-CA	5.07	127.03	120.44
4	5	482	PHE	CA-C-N	5.07	128.02	120.31
4	5	482	PHE	C-N-CA	5.07	128.02	120.31
5	6	525	GLY	CA-C-N	5.07	129.31	121.71
5	6	525	GLY	C-N-CA	5.07	129.31	121.71
3	4	617	LEU	CA-C-N	5.07	128.67	121.42
3	4	617	LEU	C-N-CA	5.07	128.67	121.42
1	2	595	ALA	CA-C-N	5.07	127.03	120.44
1	2	595	ALA	C-N-CA	5.07	127.03	120.44
15	Y	56	ALA	CA-C-N	5.07	127.02	120.44
15	Y	56	ALA	C-N-CA	5.07	127.02	120.44
3	4	777	GLN	CA-C-N	5.06	129.06	121.72
3	4	777	GLN	C-N-CA	5.06	129.06	121.72
4	5	441	GLY	CA-C-N	5.06	127.02	120.44
4	5	441	GLY	C-N-CA	5.06	127.02	120.44
4	5	442	LYS	N-CA-CB	5.06	117.35	110.01
6	7	293	GLN	CA-CB-CG	5.06	124.22	114.10
1	2	360	ARG	CG-CD-NE	5.06	123.13	112.00
14	X	225	LYS	N-CA-CB	5.06	117.34	110.01
14	X	676	ILE	N-CA-CB	5.05	116.46	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	302	GLY	CA-C-N	5.05	127.98	120.31
2	3	302	GLY	C-N-CA	5.05	127.98	120.31
2	3	478	MET	CA-CB-CG	5.05	124.20	114.10
14	X	223	ASN	CA-C-N	5.05	130.47	122.60
14	X	223	ASN	C-N-CA	5.05	130.47	122.60
14	X	396	LYS	CB-CG-CD	5.04	122.90	111.30
5	6	406	ILE	CA-C-N	5.04	129.81	123.10
5	6	406	ILE	C-N-CA	5.04	129.81	123.10
3	4	774	ASP	CA-C-N	5.04	130.30	122.49
3	4	774	ASP	C-N-CA	5.04	130.30	122.49
5	6	718	MET	CA-CB-CG	5.04	124.18	114.10
14	X	223	ASN	N-CA-CB	5.04	117.44	109.83
3	4	512	LYS	CA-C-N	5.03	128.69	121.50
3	4	512	LYS	C-N-CA	5.03	128.69	121.50
1	2	401	ARG	CA-C-N	5.03	127.38	120.39
1	2	401	ARG	C-N-CA	5.03	127.38	120.39
1	2	367	CYS	N-CA-CB	5.03	117.51	110.12
3	4	608	ILE	CA-C-N	5.02	127.84	120.71
3	4	608	ILE	C-N-CA	5.02	127.84	120.71
5	6	540	LYS	CA-CB-CG	5.02	124.14	114.10
1	2	327	ARG	CA-CB-CG	5.02	124.13	114.10
2	3	460	GLY	CA-C-N	5.01	126.96	120.44
2	3	460	GLY	C-N-CA	5.01	126.96	120.44
2	3	461	ALA	CA-C-N	5.01	127.26	120.44
2	3	461	ALA	C-N-CA	5.01	127.26	120.44
14	X	224	THR	CA-C-N	5.01	126.96	120.44
14	X	224	THR	C-N-CA	5.01	126.96	120.44
1	2	641	GLN	CA-C-N	5.01	130.96	123.24
1	2	641	GLN	C-N-CA	5.01	130.96	123.24
14	X	777	GLN	CA-C-N	5.01	126.95	120.44
14	X	777	GLN	C-N-CA	5.01	126.95	120.44
3	4	536	GLU	CA-C-N	5.01	127.96	120.95
3	4	536	GLU	C-N-CA	5.01	127.96	120.95
14	X	673	GLU	N-CA-CB	5.01	117.27	110.01
14	X	222	ILE	CA-C-N	5.01	127.82	120.71
14	X	222	ILE	C-N-CA	5.01	127.82	120.71
1	2	335	LYS	CA-CB-CG	5.01	124.11	114.10
1	2	338	LYS	CA-CB-CG	5.00	124.11	114.10
14	X	776	TYR	CA-C-N	5.00	127.26	120.65
14	X	776	TYR	C-N-CA	5.00	127.26	120.65

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	274	VAL	Mainchain
1	2	374	ARG	Sidechain
1	2	509	ARG	Sidechain
2	3	687	ARG	Sidechain
3	4	526	ARG	Sidechain
3	4	721	ARG	Sidechain
3	4	991	ARG	Sidechain
3	4	994	ARG	Sidechain
4	5	39	ARG	Sidechain
4	5	460	ARG	Sidechain
8	B	30	ARG	Sidechain
11	E	365	ARG	Sidechain
12	F	16	DC	Sidechain
12	F	17	DG	Sidechain
12	F	18	DT	Sidechain
12	F	24	DG	Sidechain
12	F	26	DG	Sidechain
12	F	32	DT	Sidechain
12	F	34	DC	Sidechain
12	F	36	DT	Sidechain
12	F	38	DG	Sidechain
12	F	39	DG	Sidechain
12	F	52	DG	Sidechain
13	G	1	DG	Sidechain
13	G	11	DC	Sidechain
13	G	14	DA	Sidechain
13	G	15	DG	Sidechain
13	G	9	DC	Sidechain
15	Y	48	ARG	Sidechain
15	Y	49	ARG	Sidechain

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	5267	5309	5311	33	0
2	3	4825	4893	4897	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	4879	4933	4949	60	0
4	5	4671	4746	4742	39	0
5	6	5005	5035	5035	51	0
6	7	4865	4921	4919	47	0
7	A	1600	1602	1602	16	0
8	B	1577	1618	1625	19	0
9	C	1396	1409	1410	14	0
10	D	1828	1843	1842	22	0
11	E	4569	4560	4562	39	0
12	F	1003	544	545	2	0
13	G	430	234	235	1	0
14	X	5715	5828	5833	71	0
15	Y	768	771	801	16	0
16	2	27	12	12	2	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	6	1	0	0	0	0
17	7	1	0	0	0	0
18	2	1	0	0	0	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	3	31	12	12	1	0
19	4	31	12	12	0	0
19	5	31	12	12	0	0
19	6	31	12	12	0	0
19	7	31	12	12	0	0
All	All	48591	48318	48380	401	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 4.

All (401) 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)
14:X:720:ARG:NH2	15:Y:92:ILE:HG21	1.32	1.41
14:X:720:ARG:HH22	15:Y:92:ILE:CG2	1.51	1.20
14:X:720:ARG:NH2	15:Y:92:ILE:CG2	2.06	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:66:ASP:OD1	14:X:74:VAL:HB	1.47	1.13
1:2:589:TRP:CD1	4:5:454:GLN:HE22	1.69	1.10
14:X:511:ILE:HG21	14:X:563:ARG:NH1	1.72	1.05
10:D:157:TYR:C	10:D:158:LEU:CA	2.43	0.92
14:X:393:ASP:OD2	15:Y:96:GLN:NE2	2.05	0.90
15:Y:79:SER:OG	15:Y:82:LYS:HB2	1.72	0.90
2:3:217:ALA:HB1	2:3:301:LEU:HD22	1.55	0.89
14:X:190:ASP:O	14:X:194:ARG:HG3	1.73	0.88
1:2:589:TRP:HD1	4:5:454:GLN:HE22	1.22	0.85
4:5:348:MET:HE1	9:C:163:SER:OG	1.77	0.84
14:X:720:ARG:HH22	15:Y:92:ILE:HG21	0.94	0.83
5:6:857:GLU:OE1	5:6:857:GLU:N	2.12	0.83
2:3:217:ALA:HB1	2:3:301:LEU:CD2	2.09	0.82
11:E:521:HIS:HE1	11:E:565:LEU:HD12	1.44	0.82
3:4:698:GLU:N	3:4:698:GLU:OE1	2.12	0.82
3:4:515:VAL:CG1	5:6:186:LEU:HD23	2.11	0.80
14:X:511:ILE:CG2	14:X:563:ARG:NH1	2.44	0.80
8:B:79:LEU:CB	8:B:85:CYS:SG	2.70	0.80
6:7:685:THR:O	6:7:688:THR:OG1	1.99	0.80
1:2:190:LYS:NZ	14:X:87:ASP:OD1	2.15	0.79
14:X:251:ASN:OD1	14:X:433:ASN:ND2	2.16	0.79
14:X:720:ARG:CZ	15:Y:92:ILE:HG21	2.13	0.78
8:B:2:SER:O	10:D:145:ARG:NH2	2.18	0.77
3:4:497:LEU:HD23	6:7:553:ILE:HD11	1.66	0.77
14:X:15:PHE:O	14:X:19:VAL:HG23	1.85	0.77
8:B:182:ARG:NH1	10:D:294:ILE:O	2.18	0.76
14:X:197:ARG:O	14:X:201:VAL:HG23	1.86	0.76
10:D:65:LYS:NZ	10:D:289:ASP:OD2	2.18	0.76
1:2:488:SER:OG	1:2:824:ARG:O	2.02	0.76
8:B:79:LEU:HB2	8:B:85:CYS:SG	2.26	0.76
1:2:589:TRP:CD1	4:5:454:GLN:NE2	2.52	0.75
2:3:538:SER:O	2:3:542:ARG:NH2	2.19	0.75
6:7:465:ALA:O	6:7:469:LEU:HD22	1.86	0.75
11:E:154:GLU:N	11:E:154:GLU:OE1	2.20	0.75
4:5:563:GLU:N	4:5:563:GLU:OE1	2.20	0.75
5:6:222:GLU:OE1	5:6:222:GLU:N	2.20	0.74
4:5:350:THR:OG1	4:5:353:GLU:HG3	1.88	0.73
15:Y:79:SER:OG	15:Y:82:LYS:CB	2.36	0.73
14:X:489:ARG:NH1	14:X:496:ALA:HB1	2.03	0.73
2:3:236:THR:OG1	2:3:237:GLU:OE1	2.06	0.73
1:2:504:SER:OG	5:6:650:GLU:OE2	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:12:TYR:OH	11:E:52:GLN:OE1	2.07	0.73
8:B:1:MET:SD	10:D:152:ASP:HB3	2.30	0.71
8:B:79:LEU:HB3	8:B:85:CYS:SG	2.29	0.71
4:5:535:SER:OG	4:5:538:ASP:OD2	2.07	0.71
14:X:442:ASN:OD1	14:X:485:TYR:OH	2.07	0.71
2:3:449:ASP:OD2	2:3:452:THR:OG1	2.07	0.71
1:2:356:ASN:OD1	1:2:450:ILE:HD11	1.91	0.70
5:6:279:ARG:NH2	14:X:246:ASP:OD1	2.24	0.70
2:3:416:SER:OG	19:3:1001:ATP:O1B	2.09	0.70
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.25	0.69
11:E:521:HIS:HE1	11:E:565:LEU:CD1	2.04	0.69
1:2:576:LEU:O	1:2:577:THR:OG1	2.05	0.69
6:7:101:ASP:OD2	6:7:104:SER:OG	2.06	0.68
7:A:30:PRO:O	7:A:93:ARG:NH1	2.26	0.68
14:X:66:ASP:CG	14:X:74:VAL:HB	2.19	0.68
14:X:720:ARG:HH22	15:Y:92:ILE:HG22	1.54	0.67
2:3:354:SER:OG	2:3:659:TYR:OH	2.13	0.67
8:B:57:ASP:O	8:B:61:ASN:ND2	2.27	0.67
4:5:346:VAL:CG1	4:5:348:MET:HE3	2.25	0.67
2:3:462:MET:HE3	2:3:486:ILE:HG12	1.77	0.67
5:6:733:MET:O	5:6:738:GLN:NE2	2.28	0.66
6:7:146:ARG:NH1	6:7:268:GLU:O	2.28	0.66
5:6:650:GLU:N	5:6:650:GLU:OE1	2.27	0.66
6:7:527:ASP:OD1	6:7:528:LYS:N	2.29	0.66
15:Y:71:ASN:OD1	15:Y:75:ARG:NH1	2.28	0.66
1:2:589:TRP:HD1	4:5:454:GLN:NE2	1.89	0.66
10:D:123:LYS:NZ	11:E:20:SER:OG	2.29	0.65
11:E:521:HIS:CE1	11:E:565:LEU:HD12	2.30	0.65
7:A:192:ARG:NH2	10:D:130:GLU:OE1	2.29	0.65
9:C:95:LEU:O	9:C:131:ARG:NH1	2.30	0.65
1:2:544:ASP:OD2	1:2:685:ASP:N	2.29	0.65
14:X:84:LEU:HD11	14:X:132:LEU:HD21	1.79	0.65
5:6:532:LEU:HD11	5:6:537:LEU:HB2	1.79	0.65
6:7:451:ARG:O	6:7:694:ARG:NE	2.29	0.65
9:C:96:ASP:OD2	9:C:99:SER:OG	2.02	0.65
2:3:676:ILE:O	2:3:680:VAL:HG13	1.97	0.64
3:4:904:ASP:OD1	3:4:905:VAL:N	2.31	0.63
6:7:689:LEU:O	6:7:693:ILE:HD12	1.99	0.63
11:E:485:ASP:OD1	11:E:486:ASP:N	2.32	0.63
3:4:943:LYS:NZ	5:6:810:GLU:OE2	2.29	0.63
14:X:180:ILE:HD11	14:X:262:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:7:GLN:N	11:E:7:GLN:OE1	2.32	0.63
4:5:211:CYS:SG	4:5:212:LEU:N	2.72	0.62
2:3:439:GLY:N	2:3:482:ASP:OD1	2.33	0.62
3:4:725:ASP:OD2	3:4:816:GLN:NE2	2.32	0.62
5:6:198:GLU:OE1	5:6:201:ARG:NH2	2.32	0.62
10:D:75:GLU:O	10:D:150:LYS:NZ	2.28	0.62
3:4:515:VAL:HG11	5:6:186:LEU:HD23	1.82	0.62
5:6:520:GLU:N	5:6:520:GLU:OE1	2.32	0.62
5:6:668:THR:O	5:6:669:SER:OG	2.15	0.61
1:2:184:GLU:OE1	1:2:184:GLU:N	2.33	0.61
3:4:515:VAL:HG11	5:6:186:LEU:CD2	2.31	0.61
6:7:228:ARG:NH1	6:7:327:ILE:O	2.34	0.61
11:E:521:HIS:CE1	11:E:565:LEU:CD1	2.84	0.61
8:B:104:TYR:OH	8:B:111:ARG:NH2	2.33	0.60
2:3:112:SER:O	2:3:116:VAL:HG12	2.01	0.60
10:D:230:ILE:HG21	10:D:282:ILE:HD13	1.83	0.60
1:2:705:ARG:NH2	1:2:754:GLU:OE1	2.34	0.60
1:2:573:ALA:N	1:2:616:ASP:OD1	2.35	0.60
6:7:437:VAL:HG21	6:7:702:LEU:HD21	1.83	0.60
14:X:71:ARG:NH1	14:X:73:ASP:OD2	2.34	0.59
4:5:617:GLN:OE1	4:5:617:GLN:N	2.34	0.59
3:4:515:VAL:HG13	5:6:186:LEU:HD23	1.85	0.59
11:E:612:ILE:O	11:E:616:THR:OG1	2.17	0.59
2:3:668:ILE:HG22	2:3:668:ILE:O	2.03	0.59
14:X:597:SER:O	14:X:601:VAL:HG23	2.02	0.58
3:4:604:ARG:NH1	14:X:359:ARG:O	2.36	0.58
7:A:173:GLU:HG2	7:A:182:ASN:HB2	1.85	0.58
11:E:281:ASP:OD2	11:E:406:ARG:NH2	2.36	0.58
11:E:155:GLN:OE1	11:E:155:GLN:N	2.37	0.58
10:D:125:PRO:O	10:D:129:MET:HG2	2.04	0.58
14:X:603:GLU:OE1	14:X:699:ARG:NH1	2.37	0.58
2:3:676:ILE:CD1	6:7:621:MET:HE2	2.34	0.58
14:X:511:ILE:HG21	14:X:563:ARG:HH12	1.64	0.58
11:E:579:TYR:CE2	11:E:637:LEU:HD22	2.39	0.58
3:4:755:THR:HG21	3:4:765:LEU:HD21	1.86	0.57
14:X:62:PHE:CD1	14:X:66:ASP:OD2	2.57	0.57
2:3:544:ASP:OD2	2:3:707:ARG:NH2	2.37	0.57
4:5:370:LEU:HD12	4:5:666:LEU:HD11	1.85	0.57
3:4:873:LEU:HD12	3:4:873:LEU:O	2.05	0.56
5:6:703:ARG:NE	5:6:708:GLY:O	2.38	0.56
4:5:346:VAL:HG13	4:5:348:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:102:GLU:N	11:E:102:GLU:OE1	2.39	0.56
5:6:192:VAL:HG22	14:X:422:GLN:HE22	1.71	0.56
4:5:541:ASP:OD1	4:5:541:ASP:C	2.49	0.56
2:3:486:ILE:O	2:3:490:MET:HG3	2.06	0.56
4:5:354:GLU:O	4:5:358:LEU:HD23	2.05	0.56
5:6:831:ILE:HG22	5:6:833:PRO:HD3	1.88	0.56
6:7:152:ARG:NH2	14:X:372:THR:OG1	2.38	0.56
1:2:670:THR:HG22	1:2:671:GLU:H	1.70	0.55
11:E:286:GLN:NE2	11:E:597:THR:O	2.39	0.55
2:3:169:ARG:NH2	2:3:260:GLU:OE1	2.39	0.55
3:4:872:VAL:O	3:4:872:VAL:HG13	2.07	0.55
1:2:795:ARG:O	1:2:798:ILE:HG22	2.07	0.55
10:D:243:ASP:OD2	10:D:256:TYR:OH	2.20	0.55
3:4:796:ASP:O	3:4:838:SER:OG	2.19	0.55
3:4:983:LEU:HD12	3:4:983:LEU:H	1.72	0.54
14:X:380:GLN:HA	14:X:383:VAL:HG22	1.89	0.54
6:7:456:VAL:HG22	6:7:596:ILE:CG2	2.37	0.54
11:E:75:ASP:O	11:E:118:ARG:NH1	2.39	0.54
6:7:652:MET:SD	6:7:652:MET:N	2.80	0.54
3:4:852:VAL:HG11	3:4:1000:TYR:CZ	2.43	0.54
4:5:348:MET:CE	9:C:163:SER:OG	2.51	0.54
5:6:846:TYR:O	5:6:849:THR:OG1	2.24	0.54
4:5:348:MET:HE1	9:C:163:SER:CB	2.38	0.54
14:X:542:LEU:O	14:X:546:THR:HG23	2.08	0.53
1:2:589:TRP:NE1	4:5:454:GLN:HE22	2.03	0.53
11:E:611:GLN:OE1	11:E:612:ILE:N	2.41	0.53
6:7:479:ARG:NE	6:7:517:ASP:O	2.42	0.53
14:X:171:GLU:O	14:X:172:SER:OG	2.23	0.53
6:7:693:ILE:HD12	6:7:693:ILE:H	1.72	0.53
3:4:381:ASN:ND2	3:4:384:THR:OG1	2.41	0.53
9:C:3:TYR:CG	9:C:3:TYR:O	2.59	0.53
14:X:238:THR:HG22	14:X:238:THR:O	2.09	0.52
2:3:217:ALA:CB	2:3:301:LEU:HD22	2.33	0.52
4:5:458:MET:HB3	12:F:40:DG:H2'	1.91	0.52
8:B:1:MET:SD	10:D:152:ASP:CB	2.98	0.52
1:2:241:SER:OG	1:2:413:ASP:OD2	2.23	0.52
14:X:729:ASP:OD1	14:X:730:ARG:N	2.42	0.52
2:3:462:MET:CE	2:3:486:ILE:HG12	2.40	0.52
3:4:370:ARG:NH2	3:4:408:ASP:OD2	2.40	0.52
11:E:622:ILE:O	11:E:622:ILE:HG22	2.10	0.52
3:4:568:ASP:OD1	3:4:568:ASP:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:276:MET:HE3	4:5:330:ILE:HD11	1.93	0.51
9:C:56:ILE:HG13	9:C:57:VAL:HG23	1.92	0.51
6:7:455:ASN:N	6:7:595:ASP:OD2	2.39	0.51
2:3:306:MET:HE3	2:3:306:MET:HA	1.91	0.51
4:5:52:ASN:ND2	9:C:142:LEU:O	2.43	0.51
5:6:348:THR:OG1	5:6:441:ARG:NH1	2.44	0.51
14:X:384:ASP:OD1	14:X:385:GLU:N	2.42	0.51
10:D:158:LEU:HB3	10:D:171:LEU:HD21	1.93	0.51
2:3:676:ILE:HD12	6:7:621:MET:HE2	1.92	0.51
11:E:577:ASP:OD1	11:E:634:ARG:NE	2.44	0.51
3:4:175:GLU:HG2	3:4:340:PRO:HD2	1.93	0.51
2:3:92:LEU:N	2:3:92:LEU:HD12	2.26	0.50
5:6:347:GLN:O	5:6:347:GLN:NE2	2.44	0.50
6:7:89:GLN:OE1	6:7:102:LEU:N	2.41	0.50
4:5:40:LEU:HD12	4:5:45:ILE:HD11	1.92	0.50
5:6:624:PRO:HB2	5:6:831:ILE:HG23	1.93	0.50
3:4:472:VAL:H	3:4:491:ASN:HD21	1.57	0.50
6:7:20:GLU:OE2	6:7:99:ALA:HB1	2.12	0.50
11:E:76:ASP:OD2	11:E:117:ARG:NH2	2.44	0.50
7:A:55:LYS:NZ	7:A:58:GLN:OE1	2.41	0.50
8:B:115:LEU:HD11	8:B:148:LEU:HD21	1.94	0.49
4:5:346:VAL:HG13	4:5:348:MET:CE	2.42	0.49
14:X:540:LEU:O	14:X:543:VAL:HG12	2.13	0.49
14:X:547:LYS:NZ	14:X:608:ASP:OD2	2.42	0.49
4:5:353:GLU:O	4:5:354:GLU:C	2.54	0.49
11:E:402:GLN:OE1	11:E:402:GLN:HA	2.12	0.49
8:B:55:THR:OG1	8:B:56:ASP:N	2.46	0.49
6:7:436:LEU:HD11	6:7:477:SER:HB2	1.95	0.49
11:E:248:VAL:O	11:E:290:ARG:NH1	2.46	0.49
3:4:716:PHE:CE1	5:6:827:ARG:HA	2.47	0.49
3:4:505:ASP:O	3:4:556:ALA:N	2.43	0.49
14:X:66:ASP:OD1	14:X:74:VAL:CB	2.39	0.49
5:6:869:LEU:HD22	5:6:884:ILE:HD11	1.95	0.49
3:4:959:THR:OG1	5:6:667:SER:OG	2.15	0.48
5:6:920:LEU:O	5:6:923:SER:OG	2.22	0.48
16:2:1001:ADP:O3A	5:6:887:ARG:NH1	2.46	0.48
1:2:534:ARG:NH1	1:2:625:GLU:OE1	2.45	0.48
3:4:845:ARG:HH11	6:7:675:MET:HE3	1.78	0.48
6:7:203:TYR:OH	6:7:336:ASN:O	2.28	0.48
6:7:707:MET:HE3	6:7:707:MET:HA	1.95	0.48
7:A:93:ARG:NH2	7:A:127:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:90:ASN:OD1	2:3:90:ASN:N	2.44	0.48
14:X:677:ASN:O	14:X:681:ARG:NH2	2.46	0.48
7:A:94:THR:HG23	7:A:130:TYR:CZ	2.48	0.48
14:X:511:ILE:CG2	14:X:563:ARG:CZ	2.92	0.48
3:4:852:VAL:HG11	3:4:1000:TYR:CE2	2.49	0.48
3:4:867:ASP:OD1	3:4:964:SER:OG	2.17	0.48
5:6:885:THR:OG1	5:6:886:VAL:N	2.47	0.48
7:A:12:GLU:OE2	7:A:15:ARG:NH2	2.47	0.48
1:2:511:ILE:HD11	1:2:683:VAL:HG22	1.96	0.47
14:X:186:VAL:HG13	14:X:198:ASP:HB3	1.96	0.47
2:3:143:ASN:O	2:3:147:VAL:HG23	2.14	0.47
5:6:731:ASP:N	5:6:731:ASP:OD1	2.42	0.47
3:4:479:ARG:O	6:7:341:ARG:NH1	2.47	0.47
3:4:882:ARG:O	3:4:886:LYS:HG3	2.13	0.47
5:6:892:MET:HG3	5:6:920:LEU:HD12	1.96	0.47
6:7:689:LEU:CD1	6:7:693:ILE:HD11	2.43	0.47
3:4:515:VAL:CG1	5:6:186:LEU:CD2	2.85	0.47
7:A:29:LEU:O	7:A:122:ASN:ND2	2.47	0.47
3:4:706:LEU:HD12	3:4:968:LEU:HD12	1.95	0.47
5:6:734:ASP:OD1	5:6:735:ILE:N	2.47	0.47
11:E:572:ILE:HD11	11:E:634:ARG:NH1	2.29	0.47
5:6:687:THR:OG1	5:6:688:SER:N	2.47	0.47
11:E:343:TYR:CE2	11:E:403:ASP:HB2	2.49	0.47
11:E:165:LEU:HD22	11:E:230:ILE:HD11	1.97	0.47
14:X:497:ASP:OD1	14:X:497:ASP:O	2.33	0.47
5:6:532:LEU:HD22	5:6:535:ARG:HB2	1.96	0.47
3:4:869:VAL:HG11	3:4:1000:TYR:OH	2.15	0.46
1:2:783:MET:SD	4:5:570:ASN:ND2	2.88	0.46
14:X:96:GLU:OE1	14:X:181:ARG:NE	2.36	0.46
2:3:386:MET:HE3	2:3:715:VAL:HG22	1.96	0.46
3:4:451:ASN:O	3:4:452:ASN:OD1	2.33	0.46
2:3:522:GLN:HG3	4:5:544:THR:HG21	1.97	0.46
6:7:519:GLY:O	6:7:561:THR:OG1	2.33	0.46
8:B:196:HIS:O	8:B:199:SER:OG	2.27	0.46
11:E:125:ALA:HB1	11:E:249:ASN:O	2.16	0.46
1:2:319:ARG:NH1	1:2:425:GLU:OE1	2.46	0.46
3:4:525:ASP:OD2	14:X:391:LYS:CE	2.64	0.46
14:X:505:LEU:HD11	14:X:546:THR:HG21	1.98	0.46
1:2:339:PHE:O	1:2:348:LEU:N	2.46	0.46
4:5:453:VAL:HB	12:F:56:DA:H4'	1.98	0.46
8:B:146:GLN:O	8:B:150:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:757:GLY:O	3:4:800:LYS:NZ	2.43	0.46
6:7:644:TYR:O	6:7:647:THR:OG1	2.31	0.46
6:7:653:SER:OG	6:7:654:GLU:N	2.49	0.46
1:2:307:ARG:NH1	1:2:402:LEU:O	2.49	0.46
3:4:544:ASN:OD1	5:6:530:ARG:NE	2.48	0.46
11:E:274:ILE:O	11:E:278:THR:HG22	2.16	0.46
6:7:442:LYS:HG3	6:7:449:LYS:HB3	1.98	0.45
14:X:720:ARG:NH2	15:Y:92:ILE:CB	2.74	0.45
1:2:781:MET:HE1	4:5:573:ILE:HG23	1.98	0.45
3:4:770:THR:OG1	3:4:771:ARG:N	2.48	0.45
4:5:156:VAL:O	4:5:157:SER:OG	2.31	0.45
1:2:624:MET:HE1	1:2:673:ILE:HD12	1.99	0.45
2:3:217:ALA:HB1	2:3:301:LEU:HD21	1.93	0.45
3:4:699:ASP:OD1	3:4:699:ASP:N	2.50	0.45
3:4:873:LEU:HD12	3:4:873:LEU:C	2.42	0.45
6:7:721:ARG:HB3	6:7:721:ARG:NH2	2.31	0.45
14:X:729:ASP:OD1	14:X:731:MET:N	2.45	0.45
14:X:720:ARG:CZ	15:Y:92:ILE:HD13	2.46	0.45
7:A:7:ASN:O	7:A:11:LEU:HD23	2.17	0.45
8:B:15:GLU:OE2	10:D:71:ARG:NH1	2.48	0.45
10:D:97:LEU:C	10:D:97:LEU:HD23	2.42	0.45
3:4:755:THR:HG21	3:4:765:LEU:CD2	2.47	0.45
4:5:472:ALA:O	4:5:517:THR:HG22	2.16	0.45
1:2:781:MET:HG3	1:2:834:LEU:HD22	1.98	0.45
1:2:785:LYS:NZ	1:2:835:ASP:OD1	2.48	0.45
4:5:101:ILE:O	8:B:154:ILE:HD11	2.16	0.45
7:A:191:VAL:HG21	7:A:196:VAL:HG11	1.99	0.45
15:Y:126:ARG:O	15:Y:130:VAL:HG23	2.17	0.45
14:X:718:LEU:O	14:X:722:MET:HG3	2.17	0.44
10:D:97:LEU:HD23	10:D:97:LEU:O	2.16	0.44
4:5:346:VAL:HG23	9:C:167:LEU:CD1	2.46	0.44
2:3:156:SER:OG	2:3:325:THR:CG2	2.66	0.44
10:D:147:ARG:NE	10:D:179:GLU:OE2	2.44	0.44
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.51	0.44
14:X:89:LEU:HB2	14:X:90:PRO:HD3	1.98	0.44
15:Y:61:SER:OG	15:Y:62:ASP:N	2.49	0.44
6:7:230:ILE:HD11	6:7:241:VAL:HG22	1.98	0.44
7:A:170:ASP:OD1	7:A:171:ALA:N	2.51	0.44
1:2:670:THR:HG22	1:2:671:GLU:N	2.32	0.44
6:7:476:ILE:HD12	6:7:638:MET:SD	2.58	0.44
7:A:173:GLU:OE2	11:E:73:GLN:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:57:ASP:OD1	8:B:57:ASP:N	2.39	0.44
3:4:772:ASP:O	3:4:776:LYS:N	2.51	0.44
4:5:687:SER:OG	4:5:688:THR:N	2.50	0.44
5:6:278:VAL:HG13	5:6:285:LEU:HD23	2.00	0.44
10:D:162:ASN:CG	10:D:171:LEU:HD12	2.43	0.44
11:E:333:SER:OG	11:E:336:ASP:OD1	2.30	0.44
14:X:287:LEU:HD11	14:X:474:GLU:OE1	2.18	0.44
14:X:729:ASP:OD1	14:X:729:ASP:C	2.60	0.43
14:X:605:TYR:HB3	14:X:611:LEU:HD11	2.00	0.43
14:X:667:MET:SD	14:X:700:VAL:HG22	2.58	0.43
4:5:417:ASP:OD1	4:5:417:ASP:N	2.49	0.43
6:7:450:ILE:HD12	6:7:450:ILE:H	1.82	0.43
14:X:67:ASP:OD1	14:X:67:ASP:N	2.50	0.43
5:6:401:ASP:O	5:6:404:ARG:NH1	2.51	0.43
6:7:440:VAL:HG11	6:7:452:GLY:CA	2.48	0.43
3:4:931:LYS:NZ	5:6:818:SER:OG	2.50	0.43
6:7:422:ILE:CD1	6:7:469:LEU:HD11	2.48	0.43
10:D:205:GLU:C	10:D:206:LEU:HD22	2.43	0.43
14:X:540:LEU:HD12	14:X:601:VAL:HG21	2.01	0.43
3:4:456:ASP:OD1	3:4:458:ASP:N	2.52	0.43
6:7:629:ASP:OD1	6:7:630:PHE:N	2.51	0.43
2:3:235:ASP:OD1	2:3:236:THR:N	2.45	0.43
11:E:624:ASN:OD1	11:E:626:GLU:N	2.49	0.43
14:X:380:GLN:HB3	14:X:387:ILE:HG21	2.00	0.43
14:X:489:ARG:CZ	14:X:496:ALA:HB1	2.47	0.43
5:6:495:ASP:OD1	5:6:497:THR:OG1	2.30	0.43
1:2:356:ASN:OD1	1:2:450:ILE:CD1	2.63	0.43
16:2:1001:ADP:O2A	5:6:747:GLN:NE2	2.49	0.43
2:3:652:THR:HG22	2:3:654:PRO:HD2	2.00	0.43
5:6:721:ASP:C	5:6:721:ASP:OD1	2.62	0.43
5:6:721:ASP:OD1	5:6:722:ASN:N	2.51	0.43
6:7:13:ASP:OD1	6:7:13:ASP:N	2.47	0.43
9:C:55:ALA:HB2	9:C:74:LEU:HD13	2.01	0.43
14:X:723:LEU:O	14:X:735:ARG:NH1	2.51	0.43
8:B:17:GLN:O	8:B:21:GLU:HG3	2.18	0.42
14:X:368:THR:OG1	14:X:370:ASP:O	2.37	0.42
2:3:698:THR:HG22	2:3:699:ALA:N	2.34	0.42
5:6:905:VAL:HG12	5:6:907:GLU:H	1.85	0.42
14:X:84:LEU:CD1	14:X:132:LEU:HD21	2.48	0.42
3:4:964:SER:O	3:4:968:LEU:HD23	2.20	0.42
1:2:296:ARG:NH2	1:2:454:ASN:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:434:VAL:O	11:E:434:VAL:HG13	2.19	0.42
3:4:863:LEU:HD21	3:4:1000:TYR:OH	2.19	0.42
3:4:873:LEU:CD1	3:4:875:LYS:HB3	2.50	0.42
6:7:455:ASN:OD1	6:7:563:ILE:N	2.43	0.42
11:E:87:GLY:O	11:E:92:LEU:HD21	2.20	0.42
3:4:785:LEU:HD13	3:4:812:VAL:HG21	2.02	0.42
5:6:242:ILE:HD12	5:6:354:ILE:HG23	2.02	0.42
6:7:20:GLU:OE2	6:7:100:ASP:N	2.53	0.42
8:B:93:LEU:HD13	8:B:134:PHE:HE1	1.85	0.42
4:5:420:THR:O	4:5:421:ALA:HB3	2.20	0.42
14:X:734:SER:O	14:X:738:VAL:HG23	2.20	0.42
3:4:587:LEU:O	3:4:590:SER:OG	2.21	0.42
4:5:41:ASP:OD2	9:C:194:LYS:HG2	2.20	0.42
5:6:518:THR:OG1	5:6:519:THR:N	2.49	0.42
7:A:23:SER:OG	7:A:26:ASP:O	2.36	0.42
3:4:852:VAL:HG21	3:4:1000:TYR:OH	2.20	0.41
5:6:252:ASN:O	5:6:252:ASN:CG	2.63	0.41
8:B:156:VAL:HG11	8:B:181:LEU:HD11	2.01	0.41
11:E:568:VAL:HG22	11:E:605:PHE:HE2	1.85	0.41
2:3:400:ARG:NH2	2:3:402:ASP:O	2.52	0.41
11:E:632:ILE:HD11	11:E:640:PHE:CD2	2.55	0.41
3:4:512:LYS:HG3	3:4:519:THR:HG22	2.03	0.41
14:X:720:ARG:HD3	15:Y:92:ILE:HD12	2.02	0.41
2:3:307:ASN:OD1	2:3:308:GLN:N	2.54	0.41
3:4:852:VAL:HG21	3:4:1000:TYR:CZ	2.55	0.41
6:7:661:VAL:O	6:7:665:ILE:HG12	2.21	0.41
7:A:80:GLU:HG2	10:D:206:LEU:HD11	2.02	0.41
10:D:131:THR:O	10:D:135:ARG:HG3	2.20	0.41
11:E:579:TYR:CD2	11:E:637:LEU:HD22	2.55	0.41
1:2:247:ARG:O	1:2:251:GLU:HG2	2.21	0.41
1:2:547:THR:HB	1:2:683:VAL:HG11	2.02	0.41
2:3:354:SER:OG	2:3:659:TYR:CZ	2.72	0.41
3:4:525:ASP:OD2	14:X:391:LYS:HE3	2.21	0.41
3:4:872:VAL:O	3:4:872:VAL:CG1	2.68	0.41
5:6:742:HIS:ND1	5:6:794:ILE:HD11	2.35	0.41
7:A:146:LEU:HD12	7:A:151:LEU:HD11	2.03	0.41
3:4:961:GLN:O	3:4:965:MET:HG3	2.20	0.41
6:7:66:MET:O	6:7:70:VAL:HG23	2.20	0.41
10:D:89:ASN:O	10:D:93:MET:HG2	2.21	0.41
15:Y:57:GLU:OE1	15:Y:58:LYS:N	2.54	0.41
6:7:521:CYS:N	6:7:562:SER:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:607:ASP:O	6:7:611:LYS:HG2	2.20	0.41
1:2:704:VAL:HG21	5:6:859:ARG:HD3	2.03	0.41
3:4:497:LEU:CD1	3:4:564:GLN:HB2	2.51	0.41
3:4:879:LYS:O	3:4:883:GLU:HG2	2.21	0.41
4:5:346:VAL:HG23	9:C:167:LEU:HD12	2.03	0.41
9:C:44:LEU:CD1	9:C:46:LEU:HD21	2.51	0.41
14:X:536:PHE:O	14:X:540:LEU:HD23	2.21	0.41
5:6:471:ARG:O	5:6:474:SER:OG	2.39	0.41
6:7:612:LEU:O	6:7:616:VAL:HG23	2.21	0.41
11:E:611:GLN:OE1	11:E:611:GLN:C	2.64	0.41
13:G:10:DA:H2"	13:G:11:DC:C6	2.56	0.41
11:E:233:TYR:O	11:E:236:VAL:HG12	2.21	0.40
11:E:502:LEU:O	11:E:506:ILE:HD13	2.21	0.40
3:4:355:THR:HG22	3:4:435:ILE:HG23	2.03	0.40
3:4:586:GLU:OE1	3:4:586:GLU:N	2.46	0.40
6:7:125:MET:HE2	6:7:125:MET:HB2	2.01	0.40
6:7:585:ASN:OD1	6:7:585:ASN:N	2.54	0.40
3:4:175:GLU:HG2	3:4:340:PRO:CD	2.51	0.40
14:X:129:LEU:HD22	14:X:182:LEU:HD13	2.04	0.40
14:X:156:LEU:HD12	14:X:156:LEU:HA	1.97	0.40
5:6:190:LYS:O	14:X:422:GLN:OE1	2.38	0.40
7:A:198:ARG:O	7:A:202:GLN:HG3	2.22	0.40
11:E:259:LEU:O	11:E:263:GLY:N	2.54	0.40
14:X:487:LEU:HD22	14:X:545:ARG:HD2	2.04	0.40
3:4:472:VAL:HG11	3:4:489:LEU:HD23	2.03	0.40
5:6:869:LEU:HD22	5:6:884:ILE:CD1	2.51	0.40
9:C:3:TYR:O	9:C:3:TYR:CD2	2.75	0.40
14:X:378:GLY:O	14:X:382:LEU:HD12	2.21	0.40
14:X:409:VAL:HG21	14:X:420:ASN:ND2	2.35	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	660/868 (76%)	645 (98%)	15 (2%)	0	100	100
2	3	608/971 (63%)	594 (98%)	14 (2%)	0	100	100
3	4	606/933 (65%)	598 (99%)	8 (1%)	0	100	100
4	5	582/775 (75%)	562 (97%)	20 (3%)	0	100	100
5	6	622/1017 (61%)	609 (98%)	12 (2%)	1 (0%)	43	71
6	7	605/845 (72%)	594 (98%)	11 (2%)	0	100	100
7	A	192/208 (92%)	190 (99%)	2 (1%)	0	100	100
8	B	185/213 (87%)	183 (99%)	2 (1%)	0	100	100
9	C	167/217 (77%)	166 (99%)	1 (1%)	0	100	100
10	D	214/294 (73%)	210 (98%)	4 (2%)	0	100	100
11	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
14	X	699/1238 (56%)	682 (98%)	15 (2%)	2 (0%)	36	65
15	Y	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	5790/8321 (70%)	5667 (98%)	120 (2%)	3 (0%)	49	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	707	GLY
14	X	498	ILE
14	X	495	SER

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	582/770 (76%)	576 (99%)	6 (1%)	68	76
2	3	533/835 (64%)	531 (100%)	2 (0%)	84	84
3	4	553/848 (65%)	547 (99%)	6 (1%)	65	76
4	5	534/688 (78%)	527 (99%)	7 (1%)	61	74
5	6	552/886 (62%)	547 (99%)	5 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	542/753 (72%)	532 (98%)	10 (2%)	51	70
7	A	180/193 (93%)	179 (99%)	1 (1%)	78	81
8	B	178/198 (90%)	178 (100%)	0	100	100
9	C	156/192 (81%)	155 (99%)	1 (1%)	78	81
10	D	213/279 (76%)	212 (100%)	1 (0%)	81	83
11	E	505/586 (86%)	504 (100%)	1 (0%)	87	88
14	X	639/1125 (57%)	632 (99%)	7 (1%)	65	76
15	Y	85/85 (100%)	84 (99%)	1 (1%)	63	75
All	All	5252/7438 (71%)	5204 (99%)	48 (1%)	68	78

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	362	SER
1	2	388	VAL
1	2	438	LEU
1	2	538	ASN
1	2	683	VAL
1	2	857	LEU
2	3	114	ILE
2	3	652	THR
3	4	426	LEU
3	4	478	MET
3	4	690	ILE
3	4	716	PHE
3	4	891	LEU
3	4	994	ARG
4	5	170	SER
4	5	190	THR
4	5	287	ILE
4	5	346	VAL
4	5	374	ILE
4	5	477	VAL
4	5	575	ILE
5	6	183	SER
5	6	287	ASN
5	6	524	SER
5	6	618	LEU
5	6	761	LEU

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Mol	Chain	Res	Type
6	7	8	ILE
6	7	258	ILE
6	7	331	LEU
6	7	474	CYS
6	7	522	CYS
6	7	529	MET
6	7	599	LEU
6	7	620	HIS
6	7	621	MET
6	7	719	LEU
7	A	120	THR
9	C	31	GLU
10	D	259	THR
11	E	337	SER
14	X	293	PHE
14	X	498	ILE
14	X	597	SER
14	X	688	ASP
14	X	713	PHE
14	X	726	ASP
14	X	770	ASN
15	Y	80	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	313	ASN
1	2	653	ASN
2	3	46	GLN
2	3	177	ASN
2	3	673	GLN
2	3	722	ASN
3	4	611	ASN
3	4	614	GLN
3	4	707	GLN
3	4	921	HIS
3	4	923	HIS
4	5	33	ASN
4	5	254	GLN
4	5	500	GLN
4	5	560	HIS
4	5	694	GLN

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Mol	Chain	Res	Type
5	6	453	ASN
5	6	839	GLN
6	7	332	ASN
6	7	615	HIS
7	A	7	ASN
7	A	71	GLN
7	A	90	GLN
8	B	9	GLN
8	B	103	GLN
8	B	108	HIS
9	C	136	ASN
9	C	138	HIS
10	D	160	GLN
11	E	133	ASN
11	E	331	HIS
14	X	117	ASN
14	X	422	GLN
14	X	541	ASN
14	X	596	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 11 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	$\# Z > 2$
19	ATP	7	1001	17	32,33,33	0.30	0	48,52,52	0.74	0
19	ATP	6	1201	17	32,33,33	0.31	0	48,52,52	0.74	0
19	ATP	4	1101	17	32,33,33	0.28	0	48,52,52	0.70	1 (2%)
16	ADP	2	1001	17	28,29,29	1.39	4 (14%)	43,45,45	1.91	11 (25%)
19	ATP	3	1001	17	32,33,33	0.31	0	48,52,52	0.74	0
19	ATP	5	1001	17	32,33,33	0.30	0	48,52,52	0.69	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
19	ATP	7	1001	17	-	5/22/38/38	0/3/3/3
19	ATP	6	1201	17	-	8/22/38/38	0/3/3/3
19	ATP	4	1101	17	-	1/22/38/38	0/3/3/3
16	ADP	2	1001	17	-	3/16/32/32	0/3/3/3
19	ATP	3	1001	17	-	8/22/38/38	0/3/3/3
19	ATP	5	1001	17	-	3/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	1001	ADP	C5-C4	4.57	1.47	1.39
16	2	1001	ADP	C5-C6	2.64	1.48	1.41
16	2	1001	ADP	C5-N7	-2.38	1.34	1.39
16	2	1001	ADP	C8-N7	2.33	1.36	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	1001	ADP	C5-C4-N3	-5.86	118.65	126.72
16	2	1001	ADP	N3-C4-N9	4.74	135.22	127.17
16	2	1001	ADP	C2-N3-C4	3.85	121.24	111.83
16	2	1001	ADP	N3-C2-N1	-3.67	123.03	128.58
16	2	1001	ADP	C4-C5-N7	-3.42	106.67	110.58
16	2	1001	ADP	C4-N9-C8	2.91	108.79	105.74
16	2	1001	ADP	C5-N7-C8	2.70	107.70	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	1001	ADP	C3'-C2'-C1'	2.45	106.10	101.46
16	2	1001	ADP	N9-C8-N7	-2.28	110.70	113.94
19	4	1101	ATP	O2'-C2'-C3'	-2.11	105.05	111.82
16	2	1001	ADP	C2-N1-C6	2.11	122.19	118.73
16	2	1001	ADP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (28) torsion outliers are listed below:

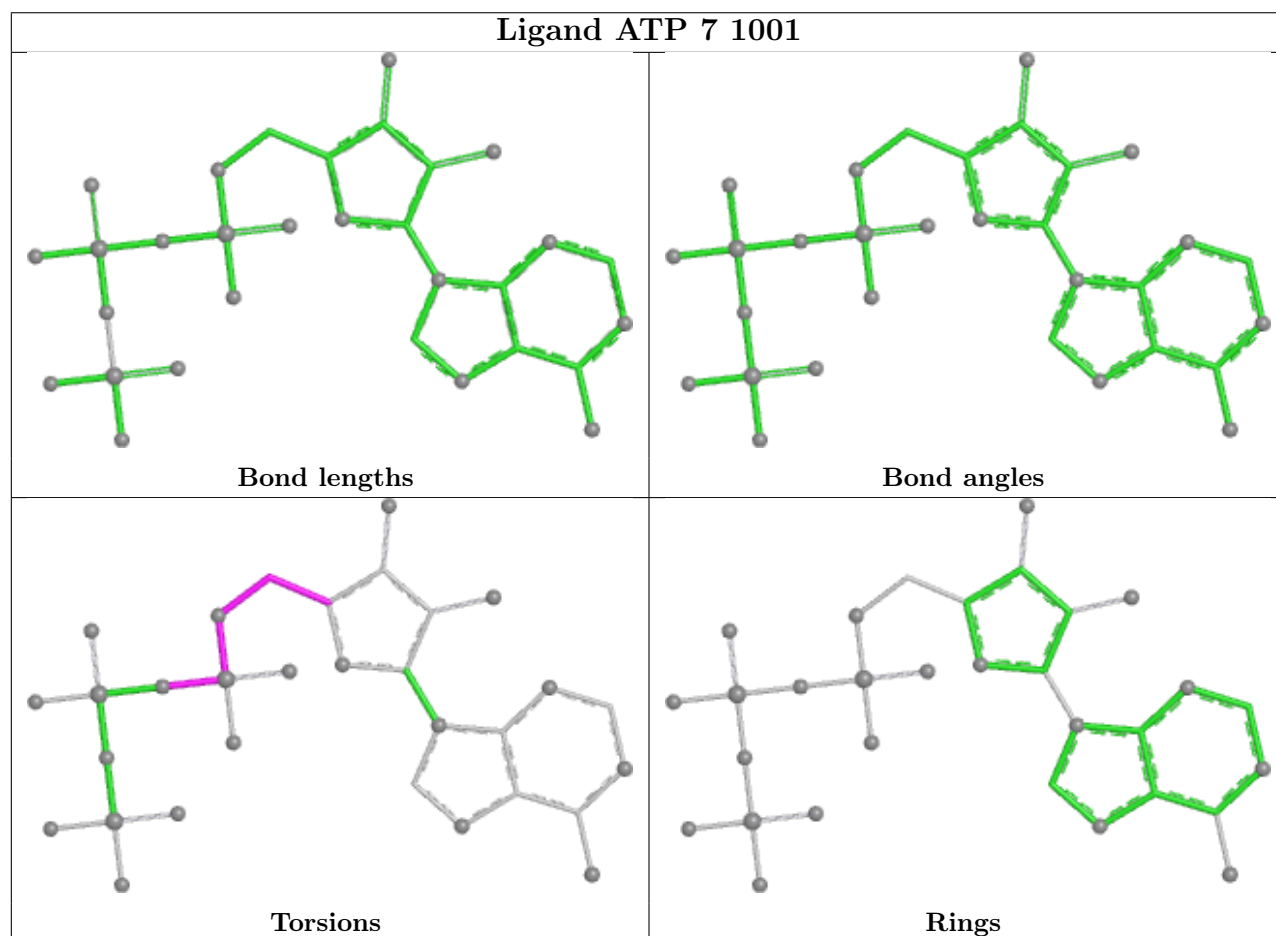
Mol	Chain	Res	Type	Atoms
16	2	1001	ADP	C5'-O5'-PA-O1A
16	2	1001	ADP	C5'-O5'-PA-O3A
19	3	1001	ATP	PB-O3B-PG-O2G
19	3	1001	ATP	C5'-O5'-PA-O3A
19	3	1001	ATP	O4'-C4'-C5'-O5'
19	6	1201	ATP	C5'-O5'-PA-O1A
19	6	1201	ATP	C5'-O5'-PA-O2A
19	6	1201	ATP	C5'-O5'-PA-O3A
19	7	1001	ATP	PB-O3A-PA-O5'
19	7	1001	ATP	C5'-O5'-PA-O2A
19	7	1001	ATP	C5'-O5'-PA-O3A
19	3	1001	ATP	C3'-C4'-C5'-O5'
19	7	1001	ATP	O4'-C4'-C5'-O5'
19	6	1201	ATP	PG-O3B-PB-O1B
19	6	1201	ATP	PB-O3A-PA-O5'
19	5	1001	ATP	O4'-C4'-C5'-O5'
19	4	1101	ATP	O4'-C4'-C5'-O5'
19	7	1001	ATP	C4'-C5'-O5'-PA
16	2	1001	ADP	C5'-O5'-PA-O2A
19	3	1001	ATP	C5'-O5'-PA-O1A
19	6	1201	ATP	C4'-C5'-O5'-PA
19	3	1001	ATP	PB-O3B-PG-O1G
19	3	1001	ATP	PG-O3B-PB-O1B
19	3	1001	ATP	PG-O3B-PB-O2B
19	6	1201	ATP	PG-O3B-PB-O2B
19	6	1201	ATP	PB-O3A-PA-O1A
19	5	1001	ATP	PG-O3B-PB-O2B
19	5	1001	ATP	PA-O3A-PB-O2B

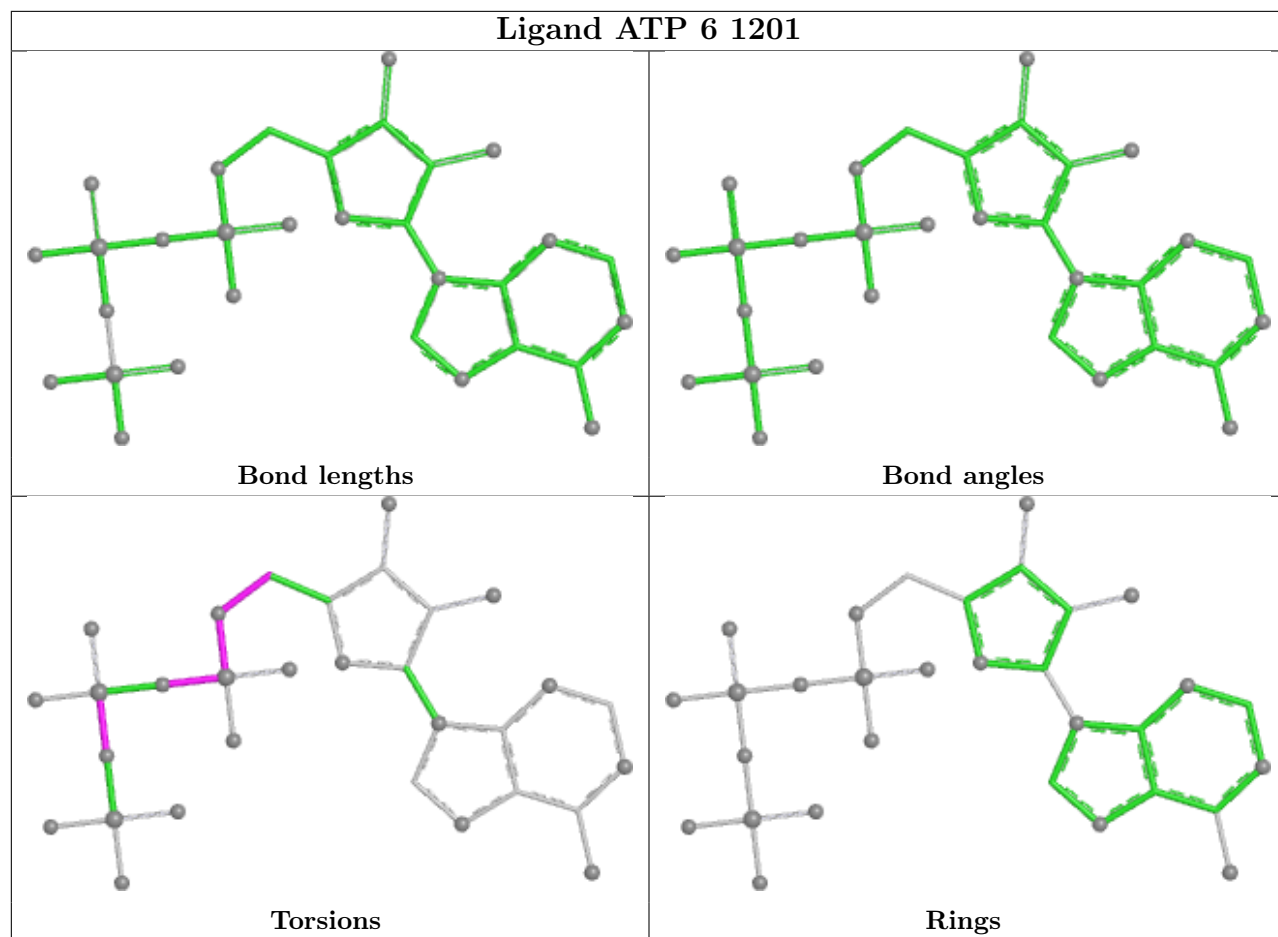
There are no ring outliers.

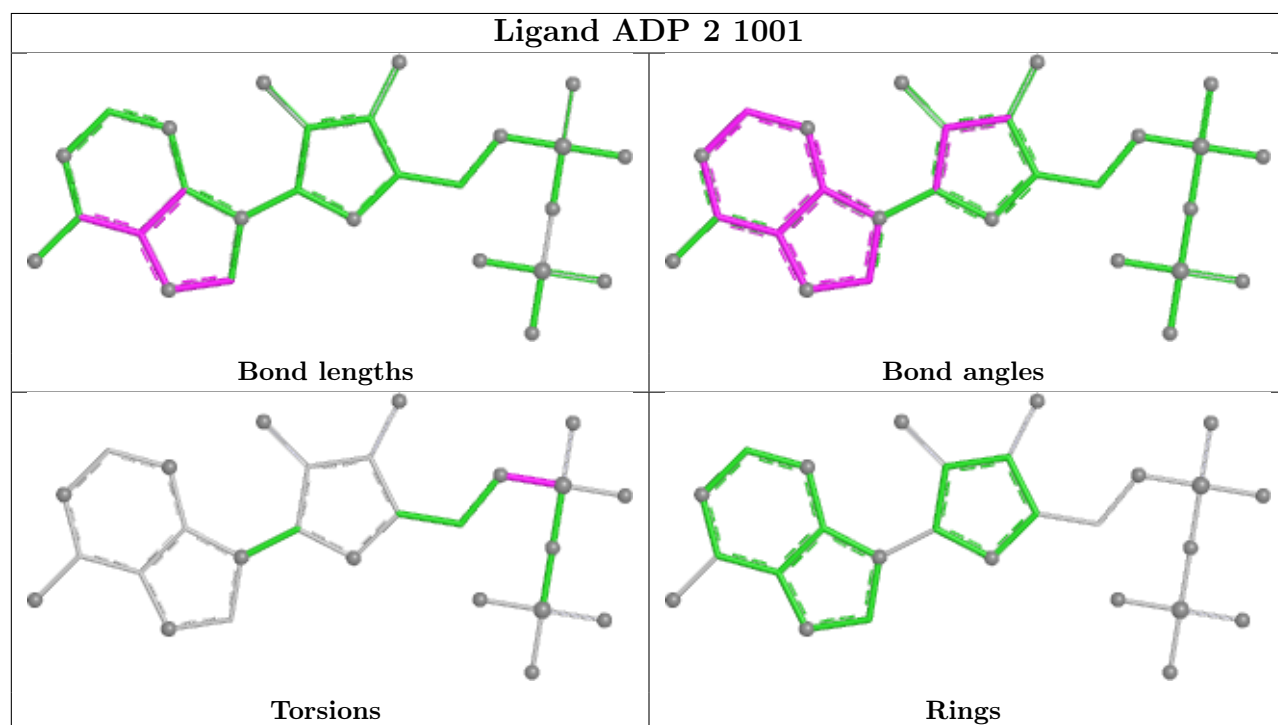
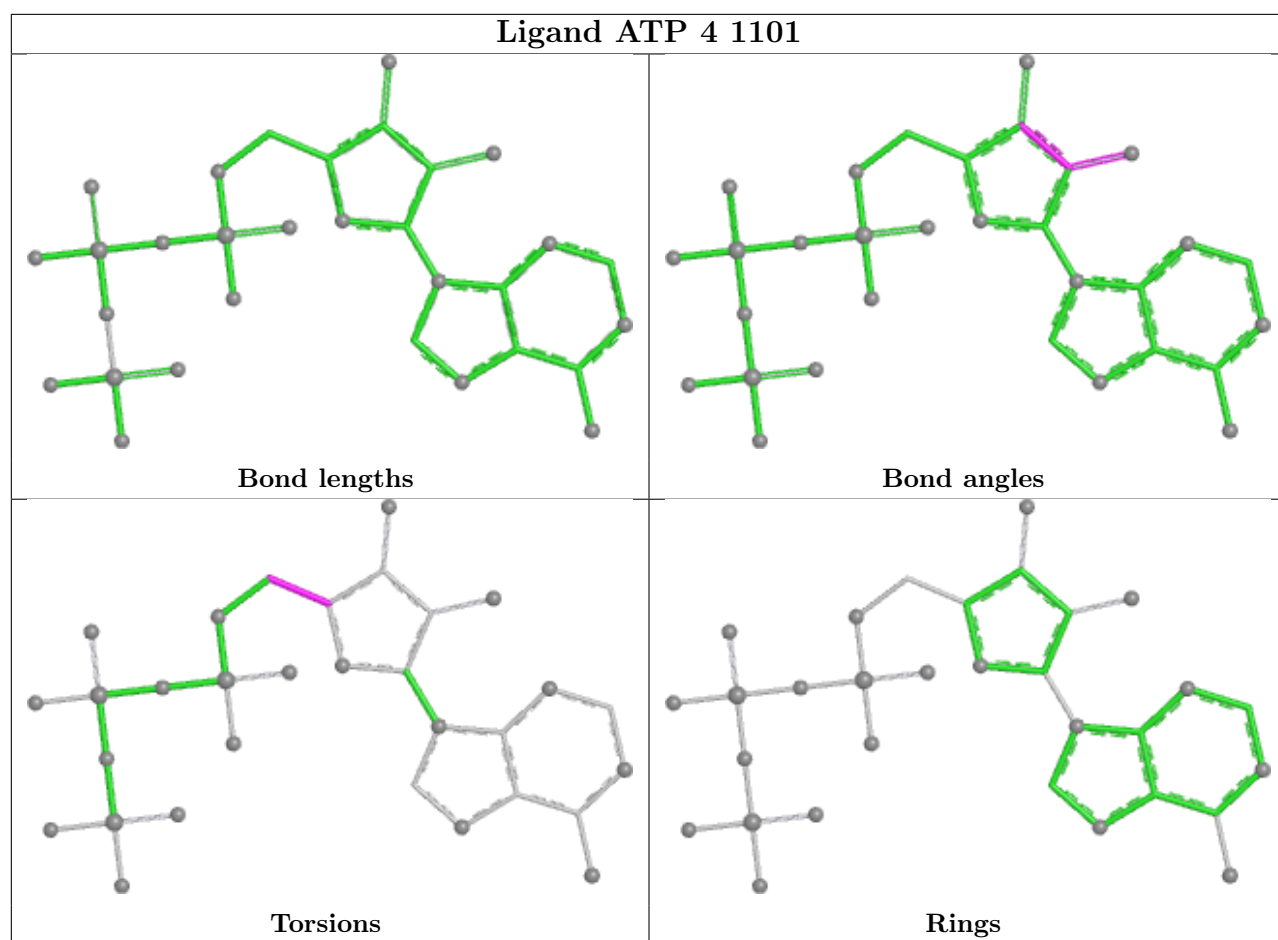
2 monomers are involved in 3 short contacts:

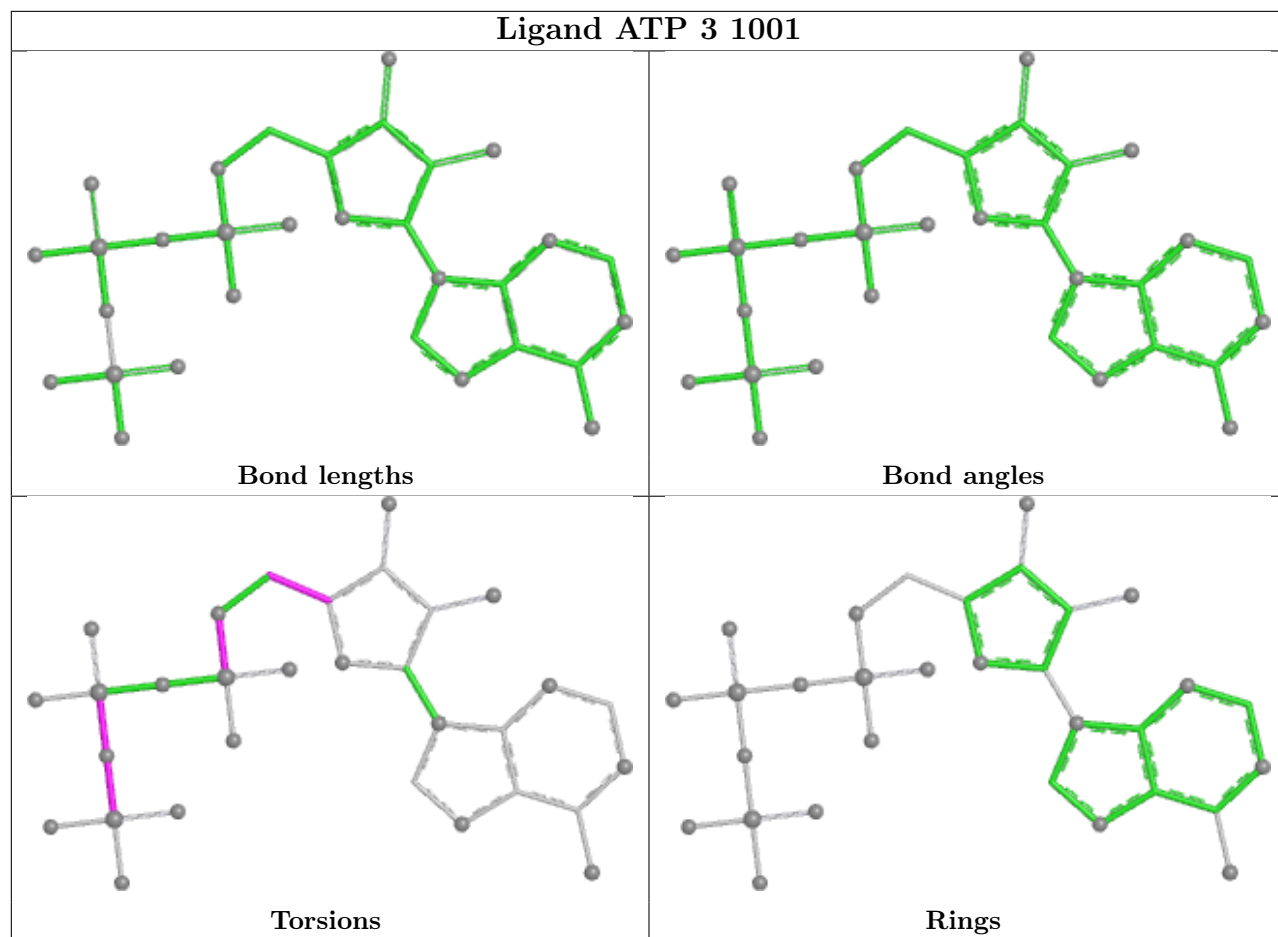
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	1001	ADP	2	0
19	3	1001	ATP	1	0

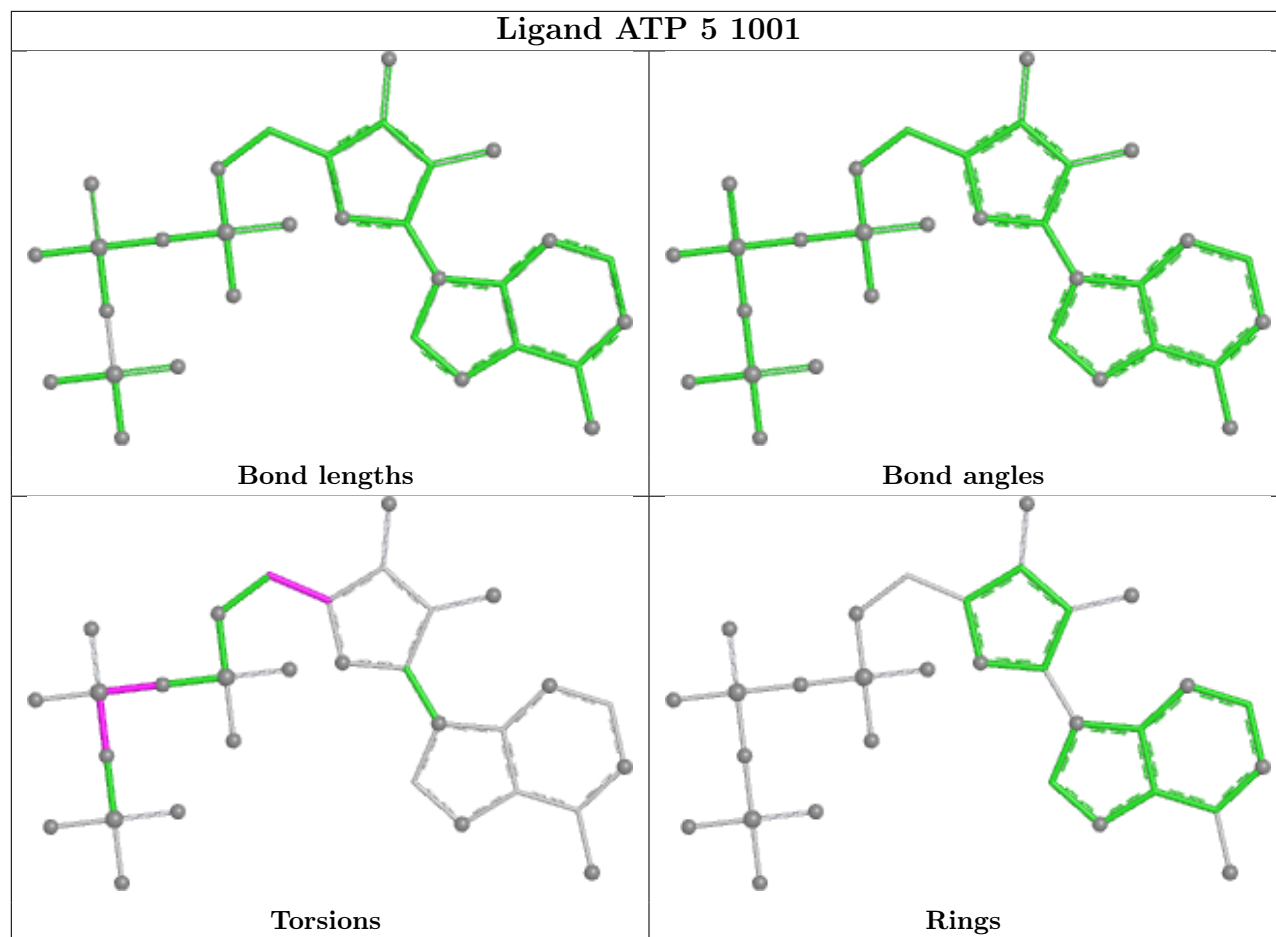
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

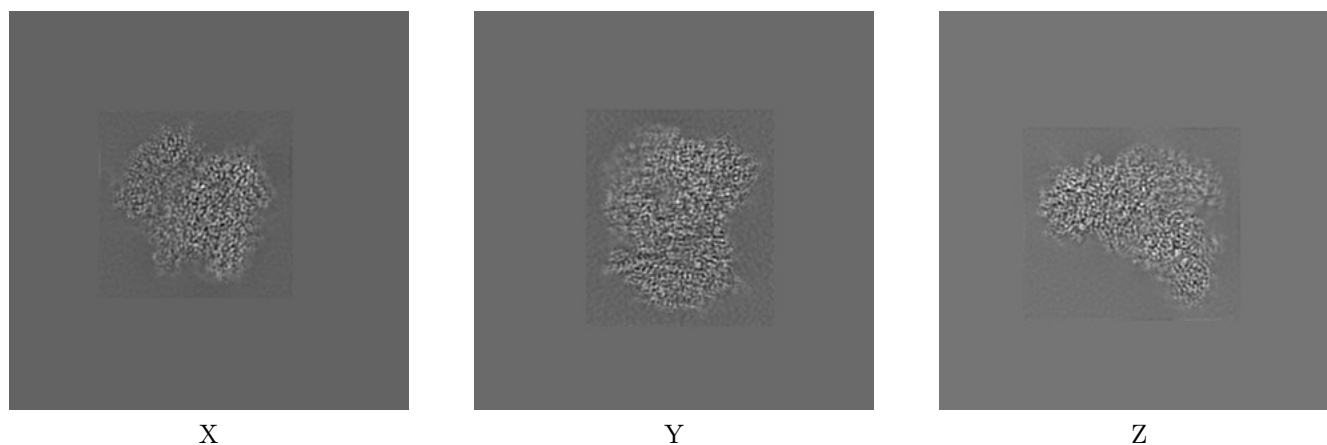
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47470. 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](#)

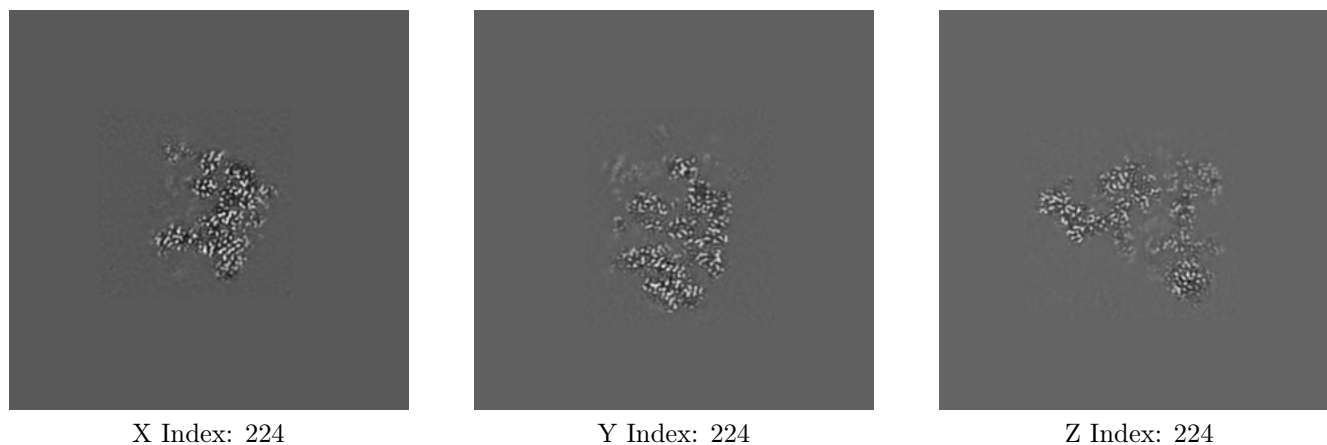
6.1.1 Primary map



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

6.2 Central slices [i](#)

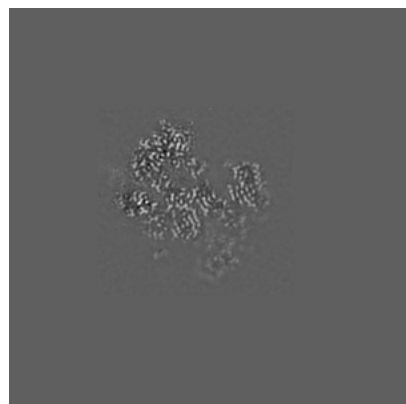
6.2.1 Primary map



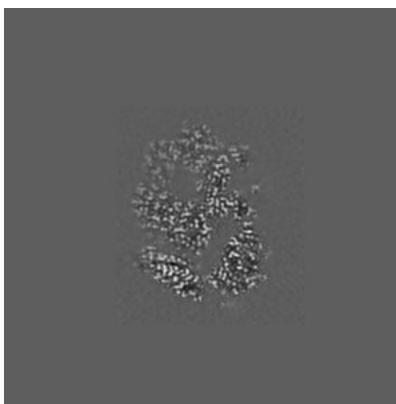
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

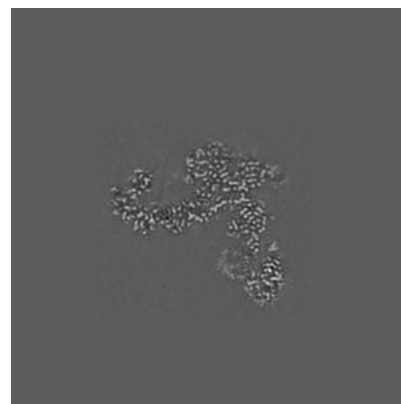
6.3.1 Primary map



X Index: 272



Y Index: 249

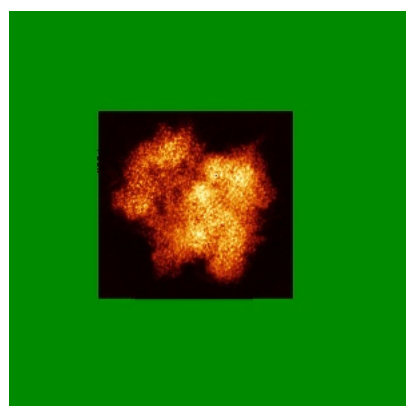


Z Index: 240

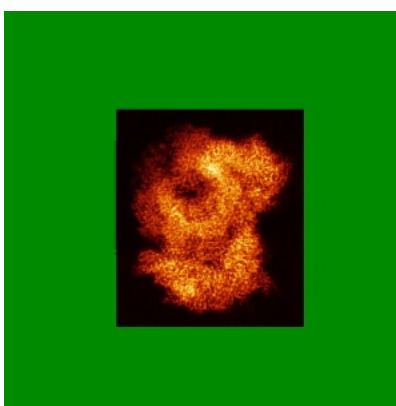
The images above show the largest variance slices of the map in three orthogonal directions.

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

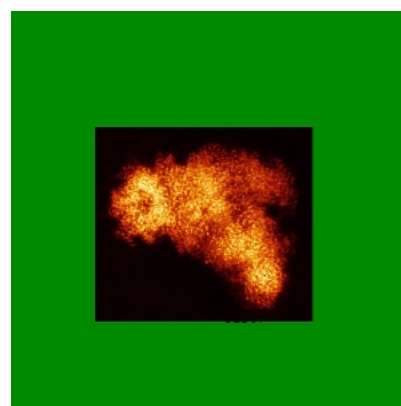
6.4.1 Primary map



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

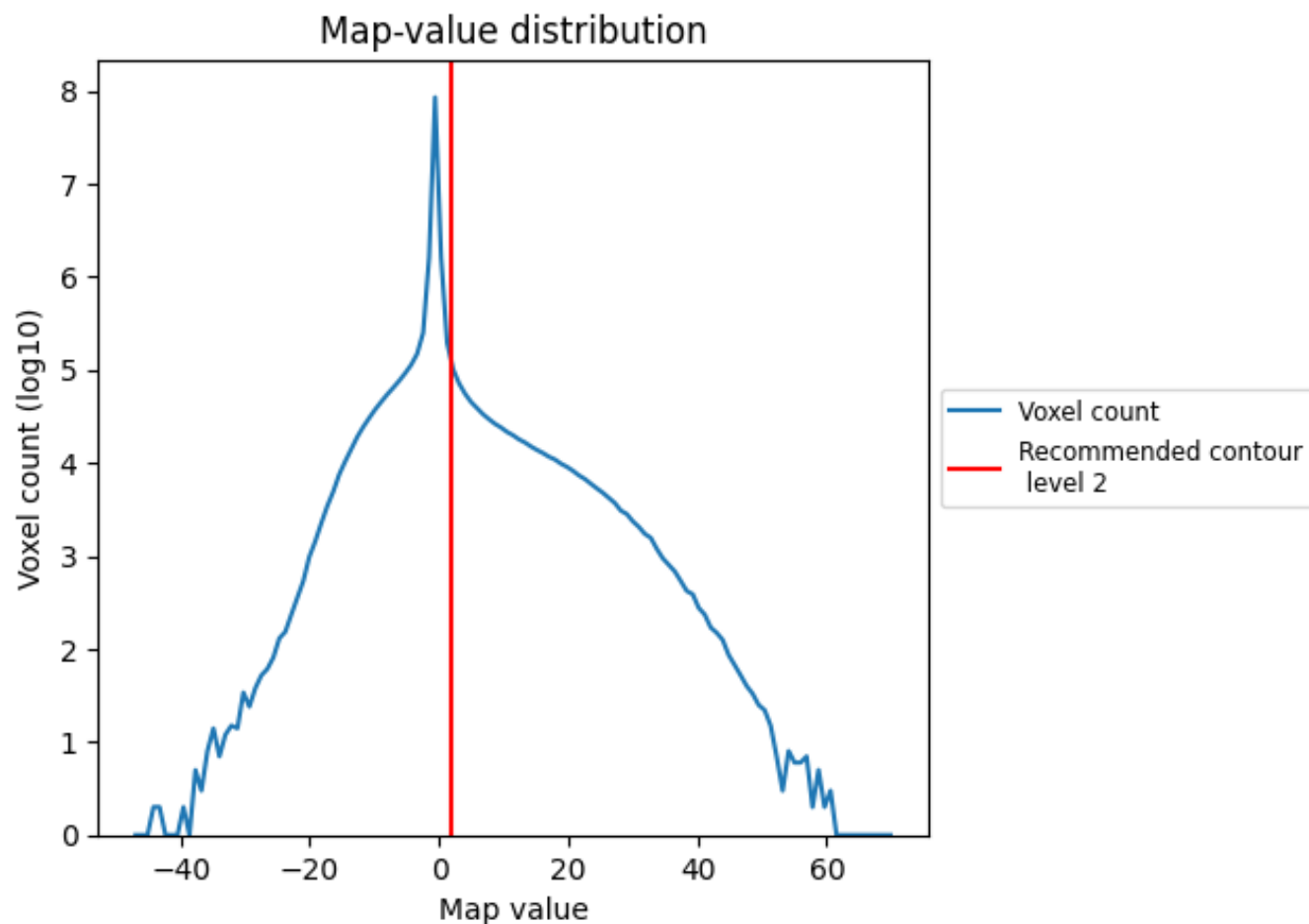
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

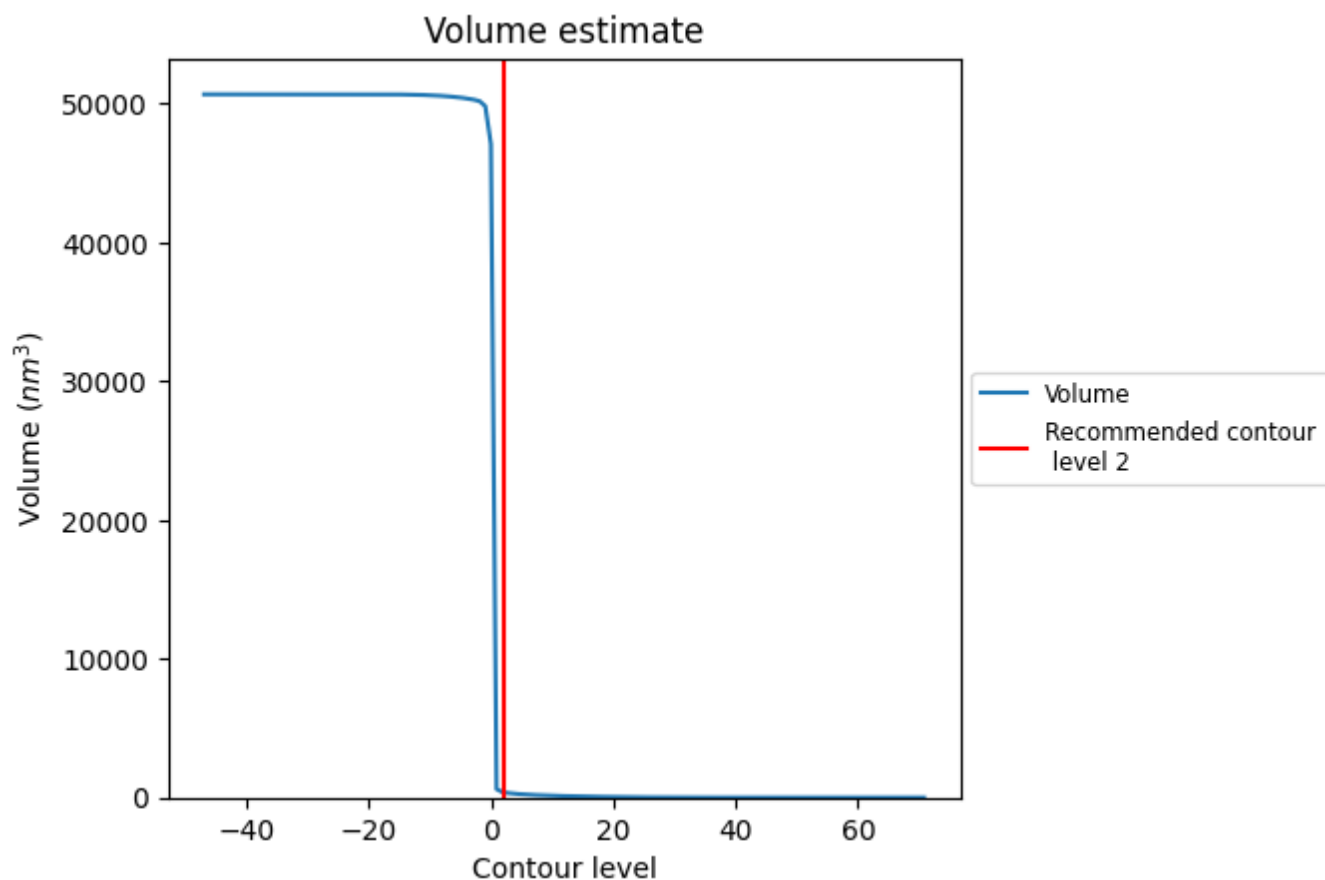
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

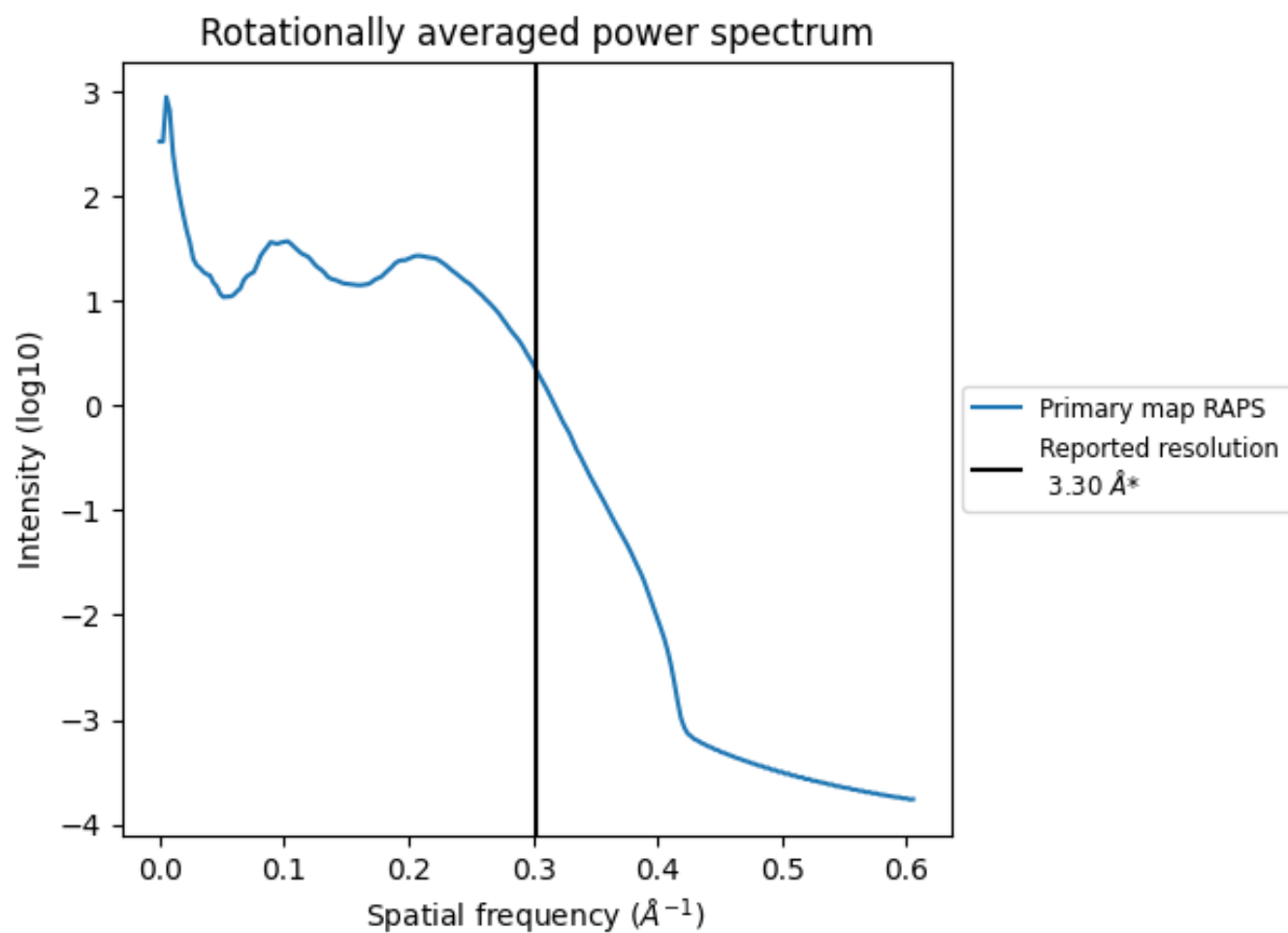
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

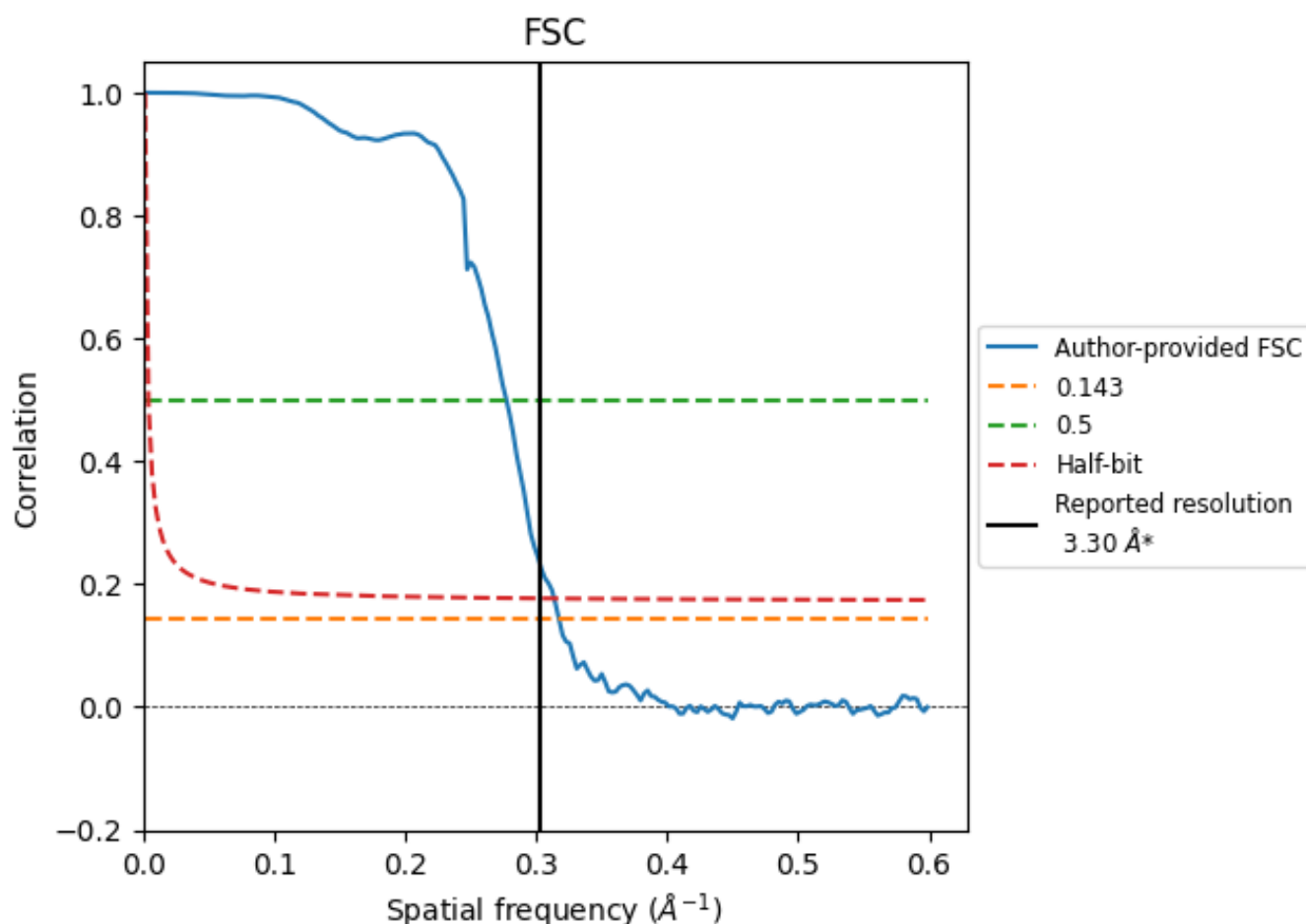


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

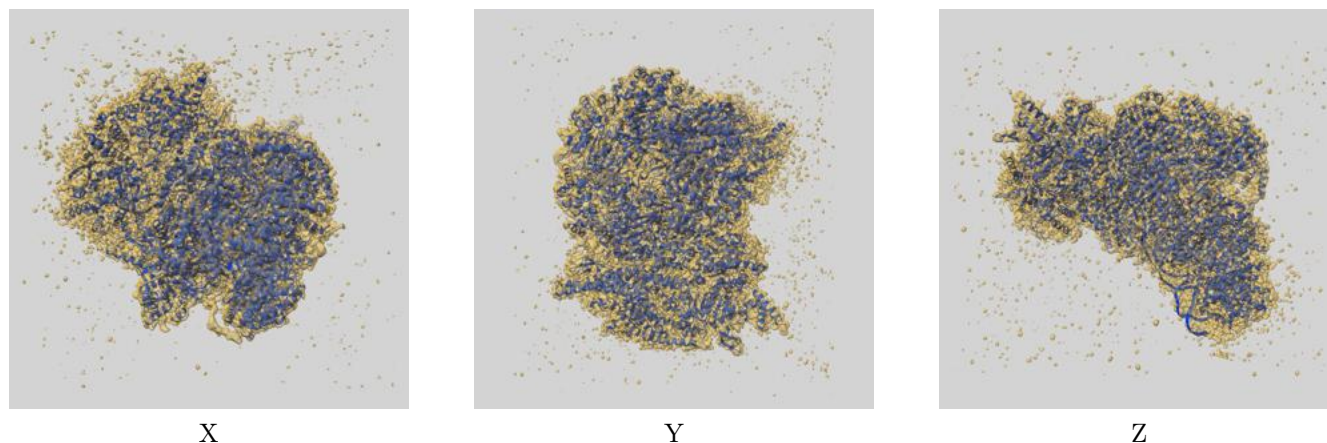
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.15	3.61	3.19
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

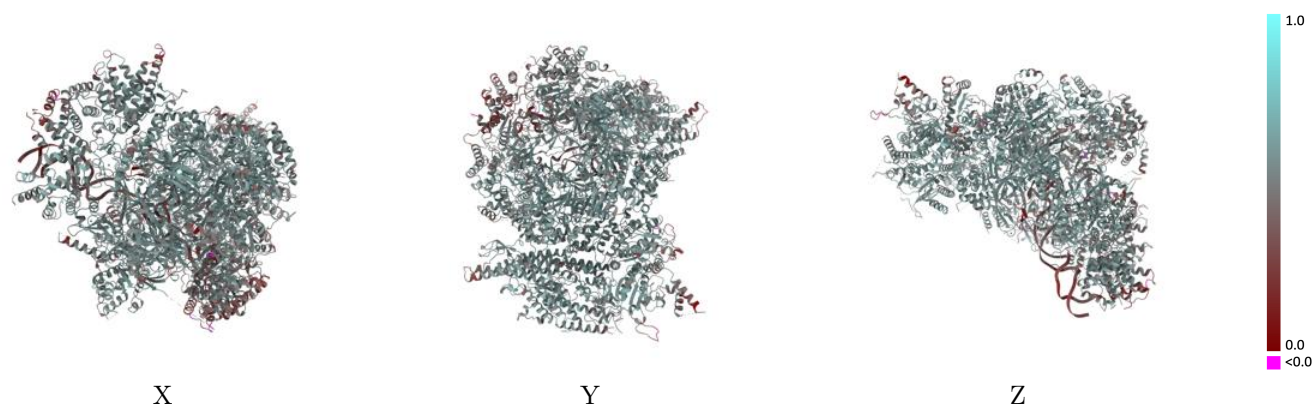
This section contains information regarding the fit between EMDB map EMD-47470 and PDB model 9E2W. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



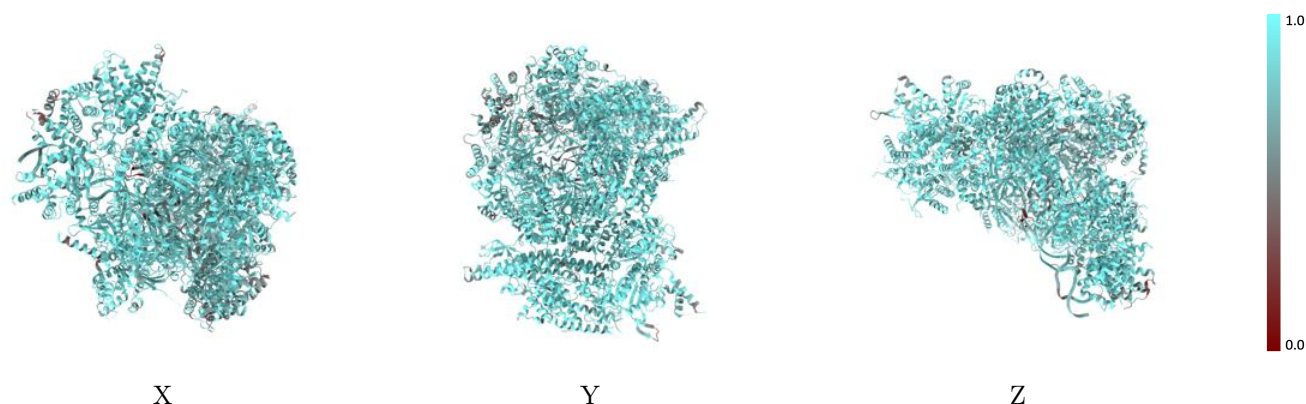
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



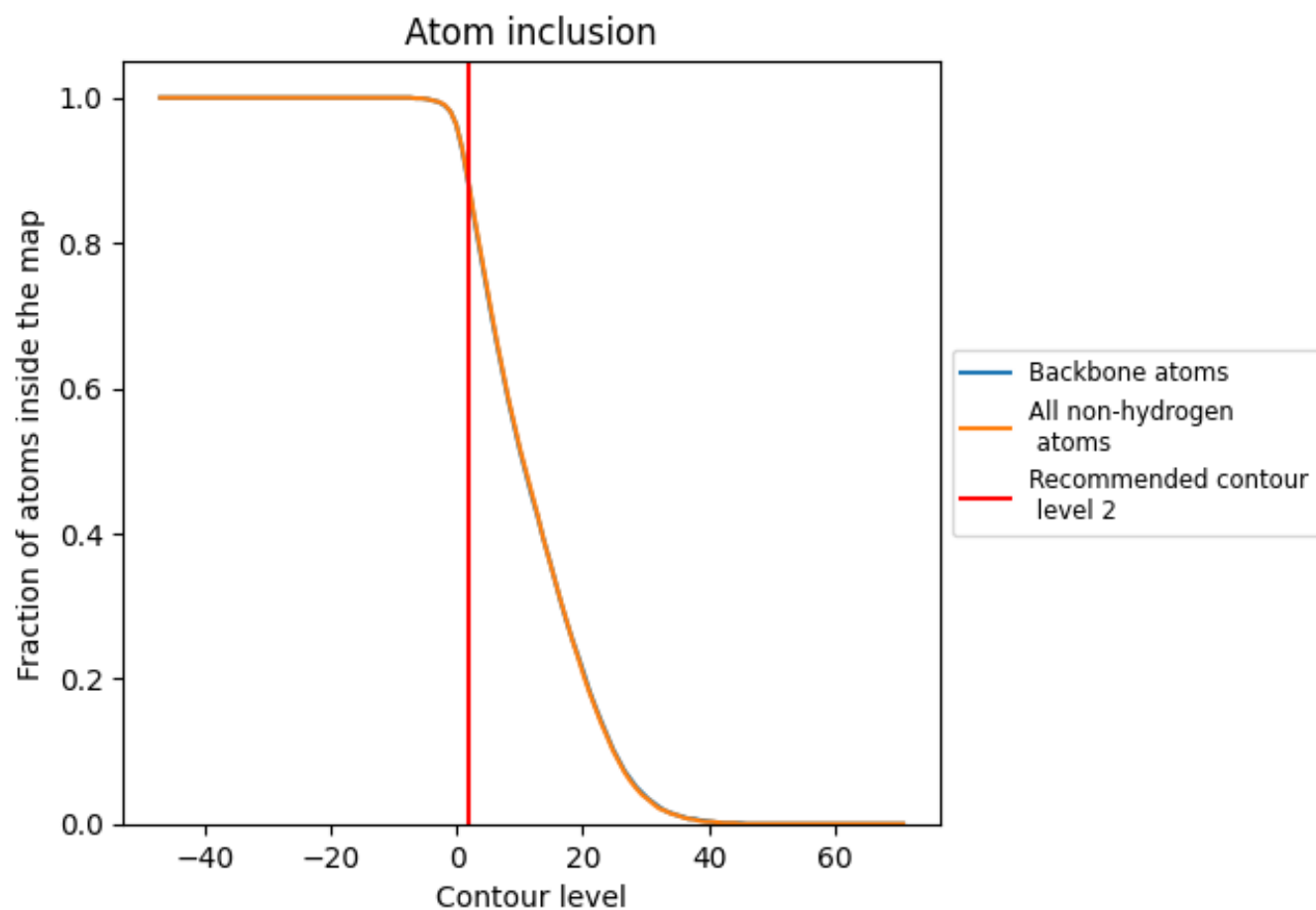
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5270
2	0.8930	0.5510
3	0.9080	0.5520
4	0.8560	0.5110
5	0.9120	0.5650
6	0.9050	0.5530
7	0.7990	0.4640
A	0.8970	0.5240
B	0.9420	0.5730
C	0.9280	0.5540
D	0.9250	0.5540
E	0.8940	0.5290
F	0.7170	0.3670
G	0.7950	0.3370
X	0.8830	0.5140
Y	0.8970	0.5150

