



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 9B85 / pdb_00009b85
EMDB ID : EMD-44333
Title : Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1
Authors : Pawar, K.I.; Verba, K.A.
Deposited on : 2024-03-28
Resolution : 3.47 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

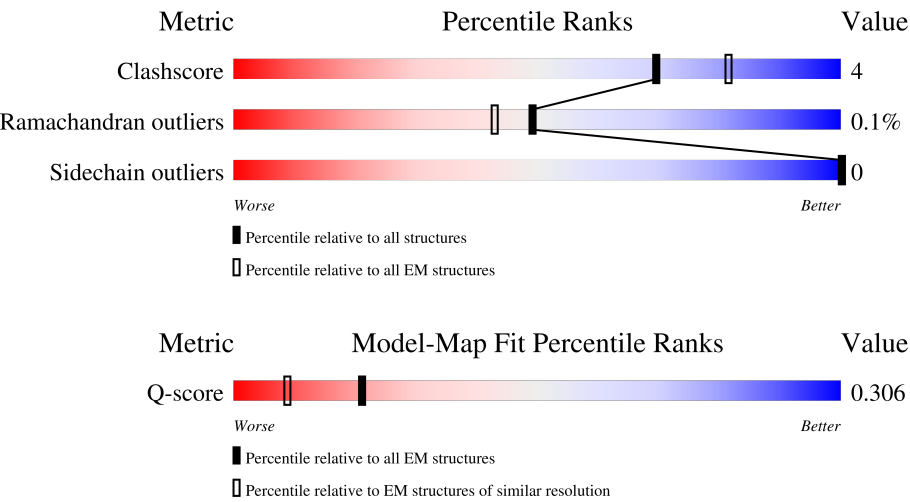
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.47 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.



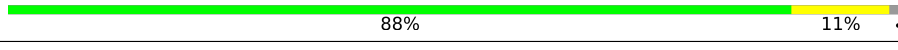
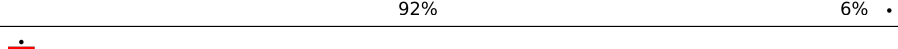
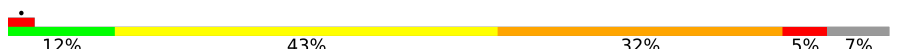
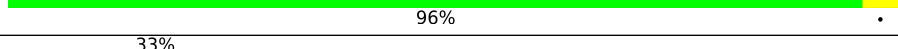
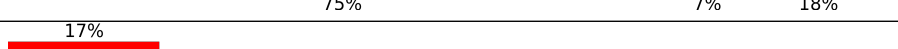
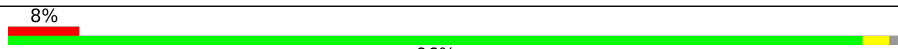
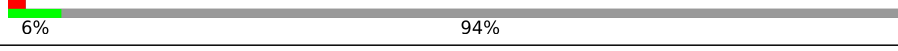
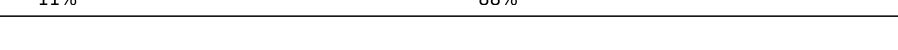
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	376	
1	B	376	
1	C	376	
1	D	376	

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Mol	Chain	Length	Quality of chain
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	460	
5	L	182	
6	M	190	
7	N	286	
8	O	272	
9	P	401	
9	Q	401	
9	p	401	
9	q	401	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 82296 atoms, of which 41052 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 Alpha-centractin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	B	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	C	375	Total	C	H	N	O	S	0	0
			5982	1918	2984	514	556	10		
1	D	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	E	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	F	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	G	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		
1	I	370	Total	C	H	N	O	S	0	0
			5907	1892	2951	509	545	10		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	370	Total	C	H	N	O	S	0	0
			5742	1827	2857	486	550	22		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	J	387	Total	C	H	N	O	S	0	0
			6140	1944	3113	514	552	17		

- Molecule 4 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	361	Total	C	H	N	O	S	0	0
			5895	1848	2982	517	525	23		

- Molecule 5 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	182	Total	C	H	N	O	S	0	0
			2846	897	1438	241	257	13		

- Molecule 6 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	M	156	Total	C	H	N	O	S	0	0
			2408	753	1217	206	222	10		

- Molecule 7 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	286	Total	C	H	N	O	S	0	0
			4559	1462	2235	404	451	7		

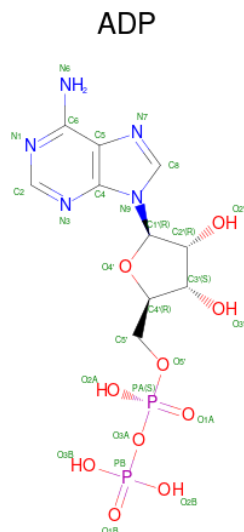
- Molecule 8 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	O	269	Total	C	H	N	O	S	0	0
			4236	1323	2114	370	418	11		

- Molecule 9 is a protein called Dynactin subunit 2.

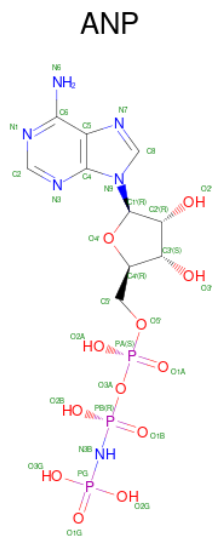
Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	74	Total	C	H	N	O		0	0
			1141	361	560	98	122			
9	Q	24	Total	C	H	N	O		0	0
			361	118	173	29	41			
9	p	37	Total	C	H	N	O	S	0	0
			543	179	257	42	63	2		
9	q	48	Total	C	H	N	O		0	0
			733	238	354	59	82			

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	G	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms						AltConf
11	H	1	Total	C	H	N	O	P	0
			46	10	15	6	12	3	

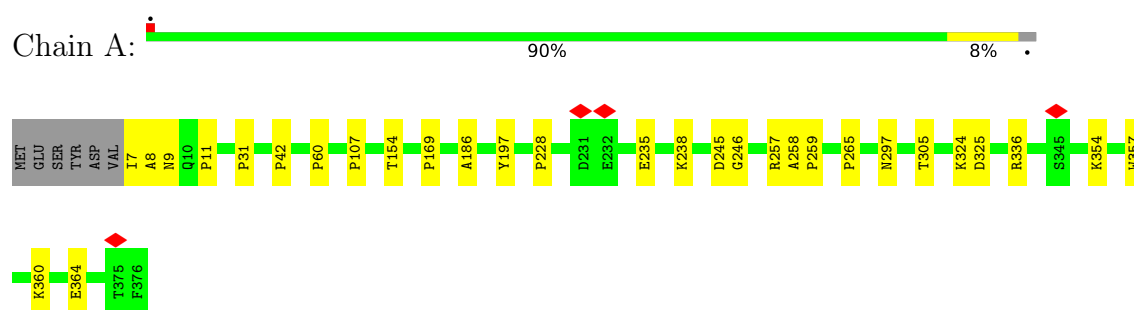
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
12	K	3	Total Zn 3 3	0

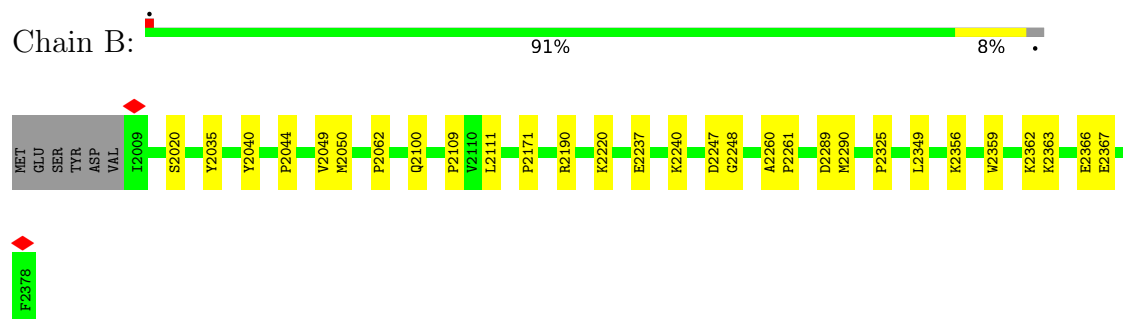
3 Residue-property plots [i](#)

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

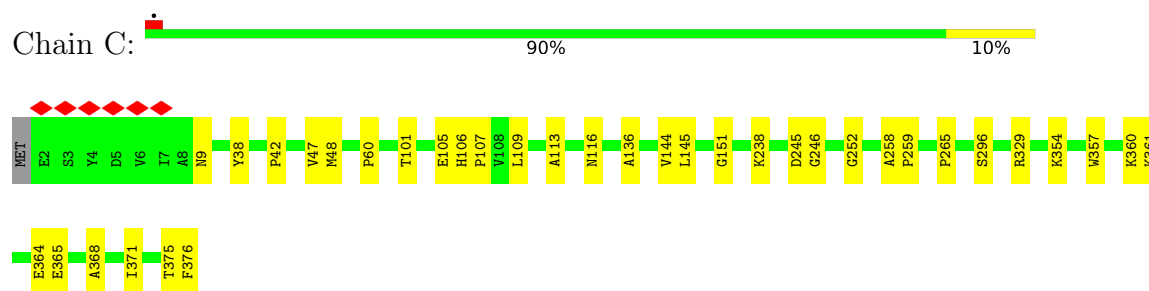
• Molecule 1: Alpha-centractin



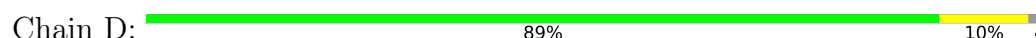
• Molecule 1: Alpha-centractin

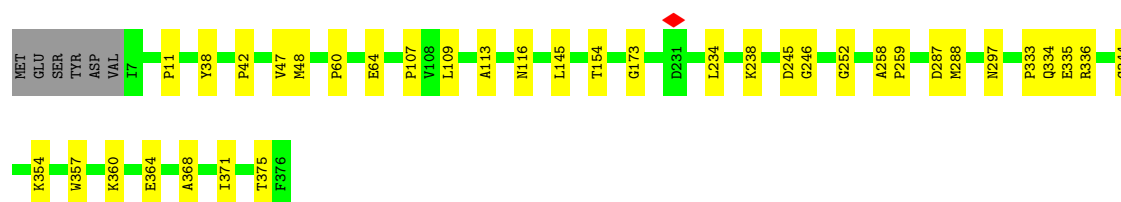


• Molecule 1: Alpha-centractin



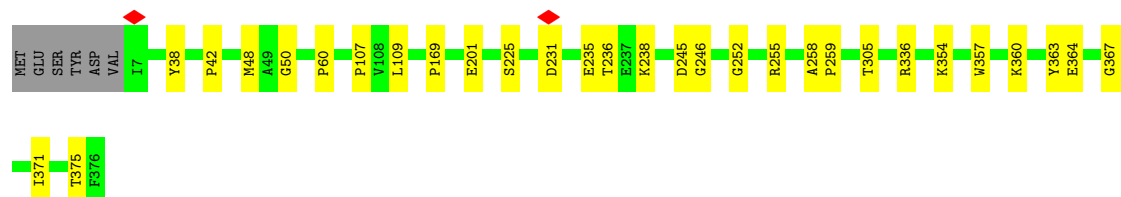
• Molecule 1: Alpha-centractin





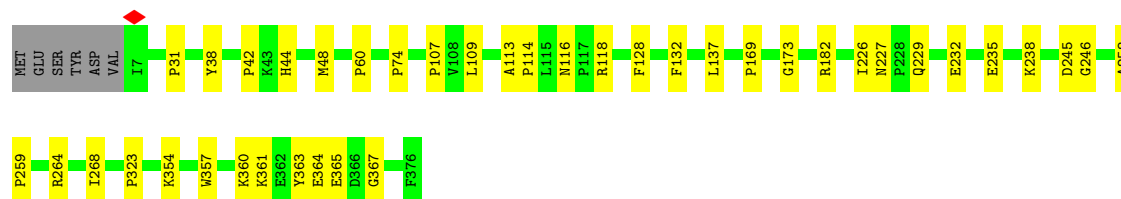
- Molecule 1: Alpha-centractin

Chain E: 90% 8% .



- Molecule 1: Alpha-centractin

Chain F: 88% 11% .



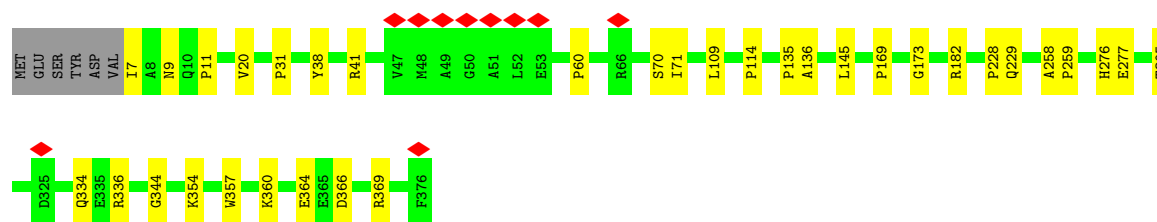
- Molecule 1: Alpha-centractin

Chain G: 92% 6% .



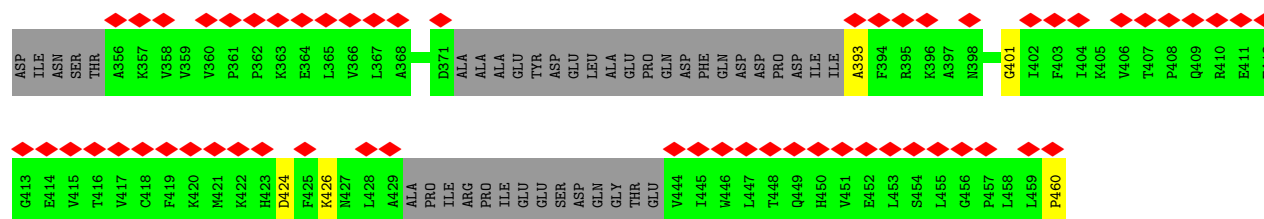
- Molecule 1: Alpha-centractin

Chain I: 89% 9% .

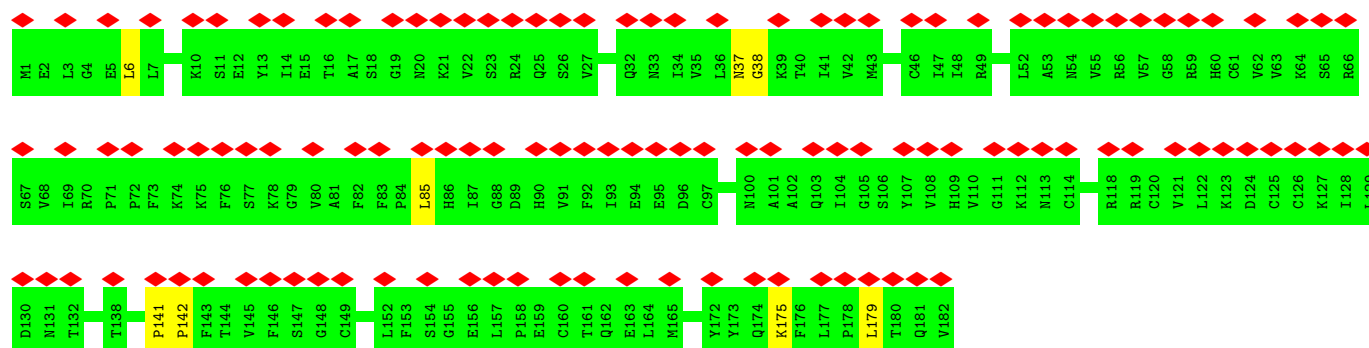


- Molecule 2: Actin, cytoplasmic 1

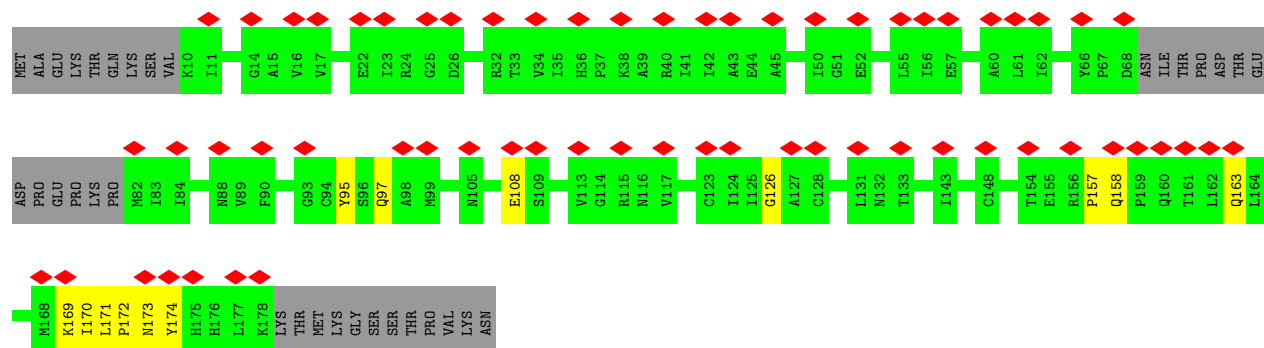
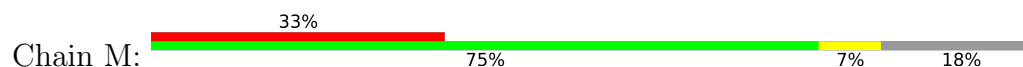
Chain H: 93% 6% .



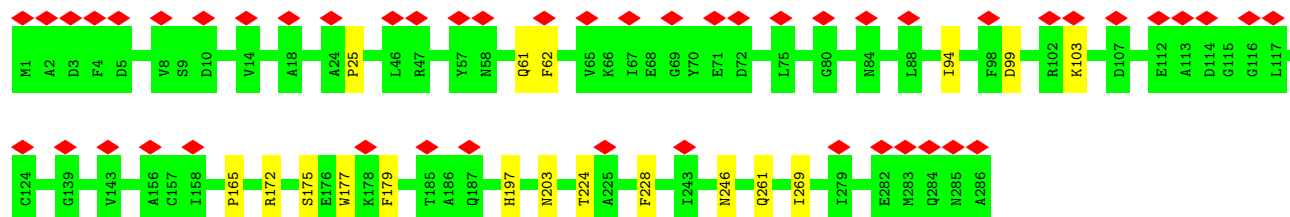
• Molecule 5: Dynactin subunit 5



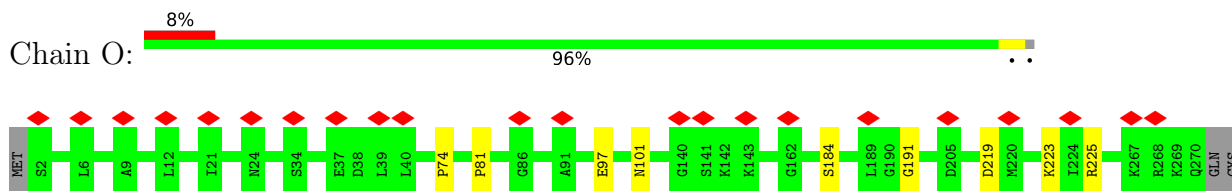
• Molecule 6: Dynactin subunit 6



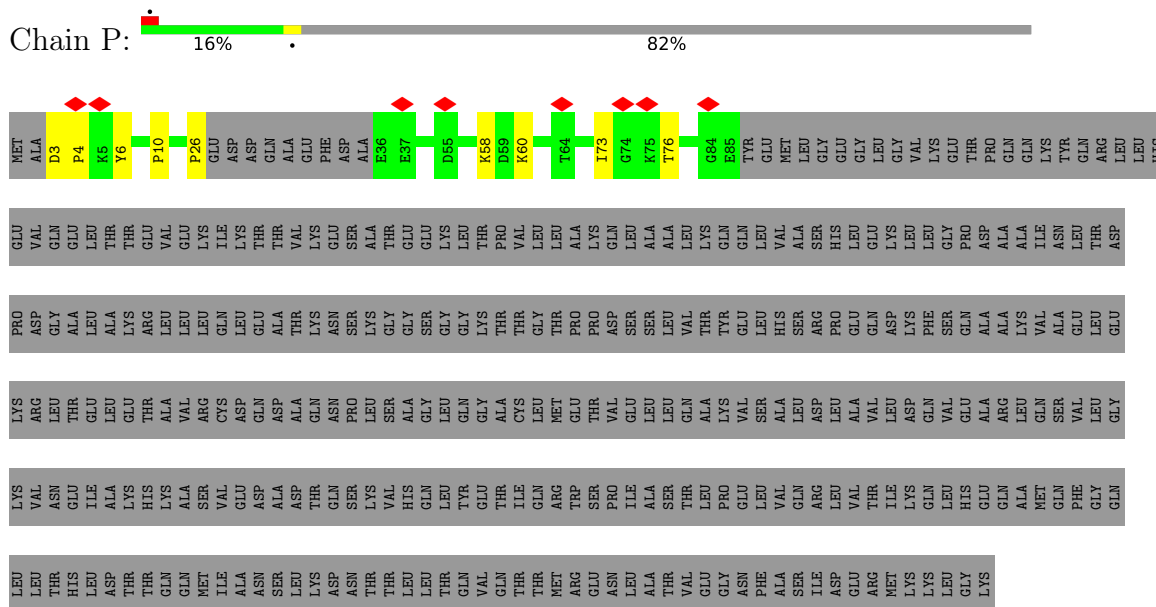
• Molecule 7: F-actin-capping protein subunit alpha-1



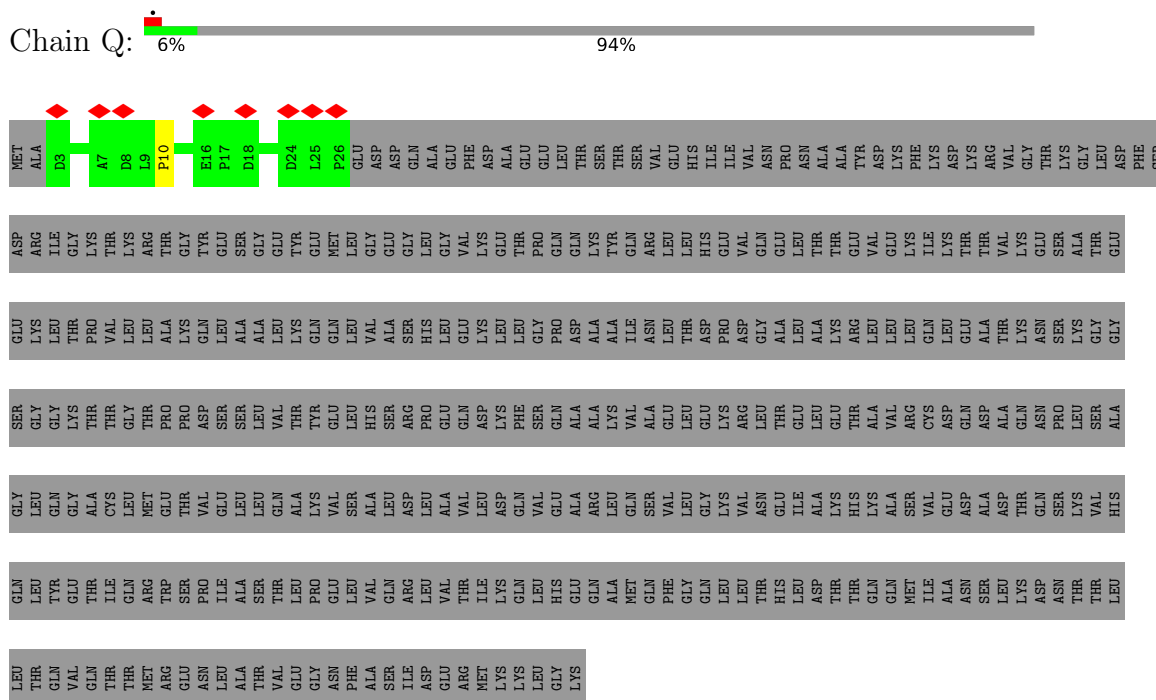
• Molecule 8: F-actin-capping protein subunit beta



- Molecule 9: Dynactin subunit 2



- Molecule 9: Dynactin subunit 2



- Molecule 9: Dynactin subunit 2

[illegible]

Chain q:

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	26.658	Depositor
Minimum map value	-12.272	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	1.217	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.835, 0.835, 0.835	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, ANP, 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	1.18	8/3025 (0.3%)	1.48	4/4085 (0.1%)
1	B	1.16	5/3025 (0.2%)	1.47	0/4085
1	C	1.16	4/3068 (0.1%)	1.47	0/4144
1	D	1.15	4/3025 (0.1%)	1.46	2/4085 (0.0%)
1	E	1.15	4/3025 (0.1%)	1.45	0/4085
1	F	1.18	7/3025 (0.2%)	1.49	0/4085
1	G	1.18	8/3025 (0.3%)	1.50	0/4085
1	I	1.17	6/3025 (0.2%)	1.47	0/4085
2	H	1.16	4/2948 (0.1%)	1.53	2/3991 (0.1%)
3	J	3.17	354/3088 (11.5%)	3.91	608/4188 (14.5%)
4	K	0.72	4/2970 (0.1%)	0.85	0/4005
5	L	0.70	2/1435 (0.1%)	0.86	0/1941
6	M	0.68	0/1209	0.89	0/1641
7	N	0.72	2/2376 (0.1%)	0.90	0/3214
8	O	1.18	2/2156 (0.1%)	1.54	0/2906
9	P	0.93	1/591 (0.2%)	1.22	2/797 (0.3%)
9	Q	1.03	1/193 (0.5%)	1.24	0/265
9	p	1.13	2/292 (0.7%)	1.23	3/395 (0.8%)
9	q	0.93	1/387 (0.3%)	1.26	0/528
All	All	1.35	419/41888 (1.0%)	1.69	621/56610 (1.1%)

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
3	J	0	29

All (419) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	83	ASN	CA-C	-20.17	1.38	1.53
3	J	206	VAL	CA-C	-18.29	1.27	1.52
3	J	102	ARG	N-CA	-17.75	1.23	1.46
3	J	318	ARG	CA-C	-17.66	1.28	1.52
3	J	346	PRO	CA-C	-14.87	1.38	1.52
3	J	144	ARG	CA-C	-14.72	1.34	1.52
3	J	184	THR	C-O	14.45	1.40	1.23
3	J	230	LYS	CA-C	-14.33	1.34	1.53
3	J	319	LEU	CA-C	-14.01	1.34	1.52
3	J	330	PRO	N-CA	-14.01	1.29	1.47
3	J	316	LEU	CA-C	-13.51	1.34	1.52
3	J	331	LYS	N-CA	-13.11	1.28	1.46
3	J	377	TYR	CA-C	-12.97	1.35	1.52
3	J	82	VAL	CA-C	12.75	1.66	1.52
3	J	322	GLU	CA-C	-12.69	1.35	1.52
3	J	164	LEU	CA-C	-12.47	1.39	1.52
3	J	155	ILE	CA-C	-12.45	1.39	1.52
3	J	109	LEU	CA-C	-12.35	1.36	1.52
3	J	186	ASP	N-CA	-12.27	1.30	1.46
3	J	319	LEU	N-CA	-12.24	1.31	1.46
3	J	329	LYS	CA-C	-12.16	1.39	1.52
3	J	183	CYS	N-CA	-12.08	1.30	1.46
3	J	65	TYR	CA-C	-11.95	1.37	1.52
3	J	162	GLY	CA-C	11.66	1.61	1.51
3	J	82	VAL	C-N	11.65	1.46	1.33
3	J	112	TYR	CA-C	-11.60	1.38	1.53
3	J	322	GLU	C-N	-11.56	1.19	1.33
3	J	329	LYS	C-N	-11.47	1.20	1.33
3	J	71	PHE	CA-C	-11.36	1.38	1.52
3	J	276	GLU	N-CA	-11.24	1.32	1.45
3	J	77	PHE	N-CA	-11.22	1.32	1.46
3	J	352	CYS	C-N	-11.21	1.21	1.33
3	J	209	ASP	CA-C	-10.98	1.37	1.52
3	J	83	ASN	C-O	-10.97	1.18	1.23
3	J	109	LEU	C-N	-10.94	1.21	1.33
3	J	381	THR	CA-C	-10.94	1.39	1.52
3	J	89	VAL	C-N	-10.76	1.20	1.33
3	J	360	ILE	CA-C	-10.74	1.39	1.52
3	J	152	TYR	CA-C	-10.60	1.39	1.53
3	J	25	THR	CA-C	10.57	1.67	1.52
3	J	91	ILE	CA-C	-10.53	1.39	1.52
3	J	182	GLN	C-O	10.46	1.35	1.23
3	J	38	ILE	C-N	-10.39	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	172	HIS	N-CA	-10.38	1.33	1.46
3	J	368	LEU	CA-C	-10.25	1.38	1.52
3	J	198	VAL	N-CA	-10.22	1.36	1.46
3	J	317	HIS	CA-C	-10.14	1.40	1.52
3	J	364	LEU	N-CA	-10.12	1.32	1.46
3	J	39	ILE	CA-C	-10.06	1.41	1.52
3	J	82	VAL	N-CA	10.05	1.55	1.46
3	J	321	ALA	N-CA	-10.01	1.34	1.46
3	J	313	PRO	CA-C	-10.00	1.39	1.52
3	J	209	ASP	C-N	-10.00	1.21	1.33
3	J	313	PRO	N-CA	-9.95	1.35	1.47
3	J	101	PHE	C-N	-9.92	1.19	1.33
3	J	343	ILE	CA-C	-9.88	1.40	1.52
3	J	185	VAL	CA-C	-9.86	1.40	1.52
3	J	156	PRO	CA-C	-9.86	1.40	1.52
3	J	288	LEU	C-N	-9.81	1.23	1.34
3	J	102	ARG	CA-C	-9.79	1.39	1.52
3	J	164	LEU	N-CA	9.79	1.53	1.45
3	J	37	CYS	N-CA	-9.70	1.34	1.46
3	J	324	ARG	C-N	-9.70	1.21	1.33
3	J	356	LEU	C-N	-9.71	1.18	1.33
3	J	300	ALA	CA-C	-9.64	1.39	1.53
3	J	153	GLU	CA-C	-9.62	1.40	1.52
3	J	276	GLU	CA-C	9.57	1.64	1.52
3	J	248	TYR	CA-C	-9.46	1.41	1.52
3	J	242	PRO	CA-C	-9.29	1.43	1.52
3	J	236	ASN	N-CA	-9.29	1.34	1.46
3	J	269	ILE	CA-C	-9.28	1.41	1.52
3	J	393	PRO	CA-C	-9.28	1.46	1.52
3	J	237	ASN	CA-C	-9.27	1.42	1.52
3	J	340	THR	CA-C	-9.23	1.41	1.53
3	J	318	ARG	N-CA	-9.20	1.34	1.46
3	J	93	GLU	CA-C	-9.17	1.40	1.53
3	J	158	LEU	CA-C	-9.17	1.40	1.52
3	J	83	ASN	N-CA	-9.16	1.39	1.46
3	J	74	ILE	C-N	-9.16	1.20	1.33
3	J	388	CYS	N-CA	-9.14	1.33	1.46
3	J	266	VAL	CA-C	-9.11	1.39	1.52
3	J	93	GLU	N-CA	-9.11	1.34	1.46
3	J	320	LEU	N-CA	-9.04	1.34	1.46
3	J	24	PHE	C-N	-9.03	1.21	1.33
3	J	177	THR	CA-C	-8.98	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	268	GLU	CA-C	-8.88	1.41	1.53
3	J	290	GLN	N-CA	-8.87	1.34	1.46
3	J	198	VAL	CA-C	-8.83	1.41	1.52
3	J	154	GLY	N-CA	-8.81	1.37	1.46
3	J	92	ILE	CA-C	-8.80	1.41	1.52
3	J	212	ALA	CA-C	-8.80	1.40	1.52
3	J	100	HIS	CA-C	-8.78	1.41	1.52
3	J	231	PHE	N-CA	-8.77	1.34	1.46
3	J	66	SER	N-CA	-8.76	1.34	1.46
3	J	61	THR	CA-C	-8.73	1.40	1.52
3	J	120	LEU	N-CA	-8.72	1.35	1.46
3	J	29	PHE	CA-C	-8.72	1.41	1.52
3	J	36	ARG	C-N	-8.65	1.21	1.33
3	J	367	ILE	CA-C	-8.64	1.43	1.52
3	J	208	GLU	N-CA	-8.62	1.35	1.46
3	J	266	VAL	N-CA	-8.59	1.35	1.46
3	J	102	ARG	C-N	-8.56	1.22	1.33
3	J	376	GLU	CA-C	-8.49	1.41	1.52
3	J	19	ASP	CA-C	-8.48	1.41	1.52
3	J	372	SER	N-CA	-8.46	1.34	1.45
3	J	311	MET	N-CA	-8.45	1.33	1.45
3	J	230	LYS	C-O	-8.42	1.13	1.23
3	J	382	GLY	CA-C	-8.42	1.41	1.51
3	J	173	LYS	CA-C	-8.41	1.41	1.52
3	J	387	TRP	CA-C	-8.40	1.41	1.52
3	J	185	VAL	C-N	-8.40	1.19	1.33
3	J	346	PRO	C-N	-8.35	1.23	1.34
3	J	363	ALA	C-N	-8.34	1.22	1.33
3	J	326	LEU	C-N	-8.28	1.24	1.34
3	J	296	ARG	C-N	-8.23	1.22	1.33
3	J	151	ILE	CA-C	8.22	1.63	1.52
3	J	256	LEU	N-CA	-8.20	1.35	1.46
3	J	153	GLU	N-CA	-8.18	1.36	1.46
3	J	210	ILE	N-CA	-8.17	1.36	1.46
3	J	60	ASN	CA-C	-8.13	1.42	1.52
3	J	248	TYR	C-N	-8.12	1.22	1.33
3	J	371	ARG	C-N	-8.04	1.22	1.33
3	J	123	SER	CA-C	-7.99	1.41	1.52
3	J	93	GLU	C-N	-7.97	1.22	1.33
3	J	110	PHE	N-CA	-7.93	1.33	1.47
3	J	277	GLU	N-CA	7.92	1.56	1.45
3	J	323	ILE	CA-C	-7.89	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	152	TYR	N-CA	7.87	1.55	1.45
3	J	110	PHE	CA-C	-7.86	1.44	1.53
3	J	130	THR	CA-C	-7.83	1.42	1.52
3	J	122	PRO	C-O	-7.83	1.14	1.23
3	J	365	GLN	CA-C	7.82	1.63	1.52
3	J	282	THR	CA-C	-7.82	1.42	1.52
3	J	88	ARG	C-N	7.77	1.43	1.33
3	J	177	THR	N-CA	-7.76	1.37	1.46
3	J	92	ILE	C-N	-7.74	1.23	1.33
3	J	375	LYS	N-CA	-7.68	1.36	1.46
3	J	365	GLN	N-CA	7.68	1.56	1.46
3	J	356	LEU	CA-C	-7.66	1.42	1.52
3	J	357	GLY	CA-C	7.66	1.65	1.51
3	J	359	ALA	N-CA	-7.61	1.36	1.46
3	J	76	TYR	C-N	-7.60	1.24	1.33
3	J	316	LEU	N-CA	-7.60	1.35	1.46
3	J	91	ILE	N-CA	-7.57	1.37	1.46
3	J	70	GLU	N-CA	-7.55	1.36	1.46
3	J	101	PHE	CA-C	-7.54	1.37	1.52
3	J	307	GLY	C-O	-7.54	1.16	1.24
3	J	307	GLY	CA-C	-7.51	1.43	1.52
1	G	228	PRO	N-CD	-7.51	1.37	1.47
3	J	25	THR	N-CA	-7.50	1.36	1.46
3	J	331	LYS	C-O	-7.49	1.14	1.24
3	J	178	GLN	CA-C	-7.49	1.42	1.52
3	J	46	ALA	CA-C	-7.47	1.42	1.52
3	J	155	ILE	N-CA	7.47	1.55	1.46
3	J	306	ILE	N-CA	7.46	1.54	1.46
3	J	130	THR	C-N	-7.43	1.22	1.33
3	J	39	ILE	C-N	-7.41	1.24	1.33
3	J	166	LEU	N-CA	-7.41	1.32	1.46
3	J	94	SER	CA-C	-7.40	1.37	1.52
3	J	280	VAL	CA-C	-7.39	1.42	1.52
3	J	32	GLU	CA-C	-7.38	1.42	1.52
3	J	62	GLU	CA-C	-7.35	1.42	1.52
3	J	222	ARG	N-CA	-7.33	1.36	1.46
3	J	78	ARG	CA-C	-7.31	1.43	1.52
3	J	308	GLY	C-N	-7.28	1.23	1.33
3	J	378	TYR	C-N	-7.28	1.24	1.34
3	J	301	GLU	C-O	-7.27	1.14	1.24
3	J	350	ALA	C-N	-7.27	1.24	1.33
3	J	19	ASP	C-N	-7.26	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	347	PRO	N-CA	-7.26	1.37	1.47
3	J	301	GLU	N-CA	-7.25	1.36	1.46
3	J	283	LEU	C-N	-7.25	1.24	1.33
3	J	212	ALA	N-CA	-7.25	1.37	1.46
3	J	23	ALA	N-CA	-7.22	1.36	1.46
1	I	135	PRO	N-CD	-7.20	1.37	1.47
3	J	78	ARG	N-CA	-7.20	1.36	1.46
3	J	237	ASN	N-CA	-7.18	1.38	1.46
3	J	159	ASN	N-CA	-7.16	1.36	1.46
3	J	267	VAL	N-CA	-7.12	1.37	1.46
3	J	75	LEU	N-CA	-7.10	1.37	1.46
3	J	330	PRO	C-N	-7.08	1.23	1.33
3	J	361	PHE	N-CA	-7.08	1.36	1.46
3	J	167	GLY	N-CA	-7.04	1.34	1.45
8	O	81	PRO	N-CD	-7.02	1.38	1.47
3	J	381	THR	C-N	-7.01	1.25	1.33
3	J	92	ILE	N-CA	-7.00	1.37	1.46
3	J	71	PHE	C-N	-7.00	1.25	1.33
3	J	156	PRO	N-CA	-6.99	1.38	1.46
3	J	65	TYR	N-CA	-6.98	1.38	1.46
3	J	20	LEU	N-CA	-6.97	1.38	1.46
3	J	233	ILE	C-N	-6.95	1.24	1.33
3	J	77	PHE	CA-C	-6.94	1.43	1.52
3	J	72	ILE	CA-C	-6.92	1.42	1.52
3	J	43	ILE	C-O	-6.92	1.17	1.24
3	J	323	ILE	C-N	-6.91	1.24	1.33
4	K	256	PRO	N-CD	-6.87	1.38	1.47
3	J	158	LEU	C-N	-6.85	1.23	1.33
3	J	248	TYR	N-CA	-6.85	1.37	1.46
3	J	203	PRO	N-CA	-6.82	1.38	1.47
3	J	21	GLY	C-N	6.82	1.44	1.33
3	J	368	LEU	C-N	-6.79	1.22	1.33
3	J	315	PHE	CA-C	-6.77	1.43	1.52
3	J	131	LEU	N-CA	-6.75	1.36	1.46
3	J	69	LYS	C-N	-6.73	1.24	1.33
3	J	165	PRO	N-CA	-6.72	1.39	1.47
3	J	199	MET	CA-C	-6.71	1.44	1.52
3	J	166	LEU	C-N	-6.70	1.24	1.33
3	J	355	TRP	CA-C	-6.69	1.43	1.52
3	J	209	ASP	C-O	-6.67	1.15	1.24
3	J	249	PRO	N-CA	-6.66	1.39	1.47
3	J	231	PHE	CA-C	-6.66	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	166	LEU	CA-C	-6.63	1.39	1.52
3	J	230	LYS	N-CA	-6.62	1.37	1.46
3	J	326	LEU	CA-C	-6.60	1.43	1.52
3	J	160	CYS	N-CA	-6.59	1.37	1.46
3	J	228	ALA	N-CA	6.56	1.55	1.46
3	J	121	ALA	C-O	-6.54	1.16	1.24
3	J	213	ARG	N-CA	-6.54	1.36	1.45
3	J	182	GLN	CA-C	-6.53	1.44	1.52
3	J	183	CYS	CA-C	-6.53	1.46	1.53
3	J	317	HIS	N-CA	-6.53	1.38	1.46
3	J	364	LEU	C-O	-6.53	1.15	1.24
3	J	143	TYR	CA-C	-6.51	1.44	1.52
3	J	103	GLU	CA-C	-6.50	1.44	1.52
8	O	74	PRO	N-CD	-6.50	1.38	1.47
3	J	75	LEU	C-N	-6.48	1.24	1.33
3	J	204	GLU	C-N	-6.47	1.26	1.33
3	J	83	ASN	C-N	6.47	1.41	1.33
3	J	103	GLU	N-CA	-6.44	1.38	1.46
3	J	76	TYR	N-CA	-6.43	1.38	1.46
3	J	333	LYS	C-N	-6.43	1.24	1.33
3	J	275	ASN	C-N	-6.42	1.24	1.33
9	p	26	PRO	N-CD	-6.42	1.38	1.47
3	J	334	LYS	CA-C	-6.41	1.44	1.52
3	J	219	ASP	CA-C	-6.40	1.44	1.52
3	J	367	ILE	C-O	-6.35	1.17	1.23
1	A	265	PRO	N-CD	-6.34	1.38	1.47
3	J	40	PRO	N-CA	-6.33	1.39	1.46
3	J	269	ILE	C-N	-6.31	1.25	1.33
3	J	176	GLU	CA-C	-6.31	1.44	1.52
3	J	73	HIS	N-CA	-6.29	1.38	1.46
3	J	275	ASN	CA-C	-6.28	1.45	1.53
3	J	100	HIS	C-N	-6.27	1.24	1.33
3	J	137	MET	N-CA	6.27	1.58	1.46
1	D	107	PRO	N-CD	-6.25	1.39	1.47
1	I	60	PRO	N-CD	-6.24	1.39	1.47
1	I	11	PRO	N-CD	-6.23	1.39	1.47
3	J	61	THR	N-CA	-6.23	1.38	1.46
3	J	297	LYS	N-CA	-6.21	1.38	1.46
3	J	122	PRO	N-CD	-6.17	1.39	1.47
3	J	53	ARG	CA-C	-6.17	1.45	1.52
1	C	265	PRO	N-CD	-6.16	1.39	1.47
3	J	98	PRO	N-CD	-6.14	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	17	VAL	CA-C	6.14	1.60	1.52
3	J	375	LYS	CA-C	-6.12	1.44	1.52
3	J	227	GLN	CA-C	-6.11	1.44	1.52
1	F	107	PRO	N-CD	-6.10	1.39	1.47
3	J	197	SER	CA-C	-6.10	1.43	1.53
4	K	460	PRO	N-CD	-6.09	1.39	1.47
1	A	228	PRO	N-CD	-6.09	1.39	1.47
1	B	2109	PRO	N-CD	-6.07	1.39	1.47
3	J	298	GLN	N-CA	-6.07	1.38	1.46
3	J	278	GLN	CA-C	-6.04	1.44	1.52
3	J	40	PRO	CA-C	-6.04	1.45	1.52
3	J	120	LEU	CA-C	-6.04	1.45	1.52
3	J	207	LEU	C-N	-6.00	1.25	1.33
3	J	179	LEU	CA-C	-5.99	1.44	1.52
3	J	124	HIS	N-CA	-5.98	1.38	1.46
1	A	107	PRO	N-CD	-5.97	1.39	1.47
1	C	107	PRO	N-CD	-5.97	1.39	1.47
3	J	270	LEU	N-CA	-5.96	1.39	1.46
3	J	199	MET	N-CA	-5.96	1.39	1.46
3	J	193	GLN	N-CA	-5.95	1.38	1.45
3	J	242	PRO	C-N	-5.95	1.26	1.33
3	J	315	PHE	C-N	-5.92	1.24	1.33
1	A	60	PRO	N-CD	-5.87	1.39	1.47
3	J	192	GLU	CA-C	-5.87	1.45	1.52
3	J	104	THR	CA-C	-5.87	1.44	1.52
3	J	343	ILE	C-N	-5.85	1.25	1.33
1	G	169	PRO	N-CD	-5.85	1.39	1.47
3	J	241	SER	C-N	-5.85	1.26	1.33
1	B	2044	PRO	N-CD	-5.84	1.39	1.47
3	J	144	ARG	C-N	-5.82	1.41	1.33
3	J	63	GLU	N-CA	-5.82	1.39	1.46
3	J	333	LYS	CA-C	-5.81	1.45	1.52
1	D	42	PRO	N-CD	-5.81	1.39	1.47
3	J	68	LEU	C-N	-5.81	1.26	1.33
3	J	332	TYR	C-N	-5.81	1.26	1.33
1	G	60	PRO	N-CD	-5.80	1.39	1.47
3	J	222	ARG	CA-C	-5.80	1.45	1.52
1	F	169	PRO	N-CD	-5.80	1.39	1.47
3	J	184	THR	CA-C	-5.79	1.59	1.52
3	J	216	PHE	CA-C	-5.79	1.45	1.52
3	J	282	THR	C-N	-5.78	1.25	1.33
3	J	98	PRO	CA-C	-5.76	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	139	PRO	N-CD	-5.76	1.39	1.47
3	J	383	ARG	N-CA	-5.73	1.39	1.46
1	E	42	PRO	N-CD	-5.73	1.39	1.47
3	J	127	ALA	CA-C	-5.73	1.45	1.52
9	p	17	PRO	N-CD	-5.72	1.39	1.47
3	J	173	LYS	C-N	-5.72	1.25	1.33
1	E	60	PRO	N-CD	-5.71	1.39	1.47
9	Q	10	PRO	N-CD	-5.71	1.39	1.47
1	C	42	PRO	N-CD	-5.69	1.39	1.47
3	J	206	VAL	C-O	-5.69	1.17	1.24
1	F	60	PRO	N-CD	-5.69	1.39	1.47
3	J	123	SER	C-N	-5.68	1.25	1.33
3	J	378	TYR	N-CA	-5.68	1.38	1.46
3	J	145	GLU	N-CA	-5.67	1.53	1.46
3	J	27	CYS	C-N	-5.65	1.26	1.33
1	F	42	PRO	N-CD	-5.65	1.39	1.47
1	A	42	PRO	N-CD	-5.64	1.39	1.47
3	J	84	PRO	C-N	-5.64	1.26	1.33
3	J	105	LEU	C-N	-5.64	1.25	1.33
3	J	143	TYR	C-N	-5.64	1.25	1.33
3	J	282	THR	C-O	-5.63	1.16	1.24
3	J	107	ARG	N-CA	-5.62	1.39	1.46
3	J	43	ILE	CA-C	-5.62	1.45	1.52
1	G	42	PRO	N-CD	-5.61	1.39	1.47
3	J	327	VAL	N-CA	-5.60	1.38	1.46
1	E	169	PRO	N-CD	-5.58	1.40	1.47
3	J	289	ILE	CA-C	-5.58	1.45	1.52
9	q	10	PRO	N-CD	-5.56	1.40	1.47
1	D	60	PRO	N-CD	-5.54	1.40	1.47
1	I	169	PRO	N-CD	-5.54	1.40	1.47
1	E	107	PRO	N-CD	-5.53	1.40	1.47
1	A	11	PRO	N-CD	-5.53	1.40	1.47
3	J	263	ARG	C-O	-5.52	1.31	1.24
3	J	318	ARG	C-N	-5.52	1.26	1.33
3	J	202	VAL	C-N	-5.52	1.26	1.33
3	J	149	LEU	C-N	-5.51	1.26	1.33
3	J	330	PRO	C-O	-5.50	1.17	1.24
3	J	139	LEU	CA-C	-5.48	1.46	1.52
3	J	197	SER	C-N	-5.47	1.27	1.33
3	J	158	LEU	N-CA	-5.47	1.39	1.46
1	B	2062	PRO	N-CD	-5.46	1.40	1.47
3	J	320	LEU	CA-C	-5.45	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	363	ALA	CA-C	-5.45	1.45	1.52
2	H	130	PRO	N-CD	-5.44	1.40	1.47
5	L	141	PRO	N-CD	-5.44	1.40	1.47
3	J	226	ILE	N-CA	-5.44	1.39	1.46
3	J	202	VAL	N-CA	-5.43	1.42	1.46
3	J	163	ALA	N-CA	5.43	1.52	1.46
1	A	169	PRO	N-CD	-5.42	1.40	1.47
1	C	60	PRO	N-CD	-5.42	1.40	1.47
3	J	114	GLU	CA-C	-5.38	1.46	1.52
3	J	293	ILE	C-N	-5.38	1.26	1.33
7	N	25	PRO	CA-C	5.36	1.54	1.51
3	J	67	TYR	CA-C	-5.36	1.45	1.52
3	J	28	GLY	N-CA	-5.34	1.39	1.45
3	J	166	LEU	C-O	-5.33	1.12	1.23
3	J	391	ASN	CA-C	-5.31	1.46	1.53
3	J	321	ALA	CA-C	-5.31	1.46	1.52
3	J	289	ILE	C-N	-5.30	1.25	1.33
3	J	361	PHE	C-N	-5.29	1.25	1.33
3	J	136	ALA	N-CA	5.29	1.53	1.45
3	J	356	LEU	C-O	-5.29	1.17	1.24
3	J	389	SER	N-CA	5.29	1.52	1.46
3	J	388	CYS	C-N	5.29	1.41	1.33
1	G	323	PRO	N-CD	-5.28	1.40	1.47
3	J	358	GLY	C-N	-5.28	1.25	1.33
3	J	64	LEU	CA-C	-5.28	1.45	1.52
3	J	317	HIS	C-N	-5.27	1.26	1.34
1	G	31	PRO	N-CD	-5.27	1.40	1.47
3	J	62	GLU	N-CA	-5.27	1.39	1.46
2	H	32	PRO	N-CD	-5.27	1.40	1.47
3	J	241	SER	CA-C	-5.26	1.47	1.53
3	J	219	ASP	C-N	-5.26	1.26	1.33
3	J	328	GLU	N-CA	-5.26	1.39	1.46
3	J	159	ASN	C-N	-5.25	1.27	1.33
1	F	31	PRO	N-CD	-5.24	1.40	1.47
3	J	69	LYS	CA-C	-5.23	1.46	1.52
1	G	107	PRO	N-CD	-5.23	1.40	1.47
1	I	31	PRO	N-CD	-5.23	1.40	1.47
3	J	280	VAL	C-N	-5.22	1.26	1.33
1	D	11	PRO	N-CD	-5.22	1.40	1.47
4	K	291	PRO	N-CD	-5.22	1.40	1.47
3	J	284	ILE	N-CA	-5.21	1.40	1.46
1	A	31	PRO	N-CD	-5.21	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	128	LEU	N-CA	-5.21	1.39	1.46
3	J	173	LYS	N-CA	5.21	1.53	1.46
3	J	341	PHE	N-CA	-5.20	1.39	1.45
2	H	70	PRO	N-CD	-5.20	1.40	1.47
5	L	142	PRO	N-CD	-5.19	1.40	1.47
3	J	140	ASP	CA-C	5.19	1.59	1.52
1	B	2171	PRO	N-CD	-5.18	1.40	1.47
1	B	2325	PRO	N-CD	-5.18	1.40	1.47
3	J	337	GLY	N-CA	5.17	1.52	1.45
3	J	23	ALA	C-O	-5.16	1.17	1.24
3	J	208	GLU	CA-C	-5.16	1.46	1.52
7	N	165	PRO	N-CD	-5.15	1.40	1.47
2	H	27	PRO	N-CD	-5.15	1.40	1.47
3	J	385	PRO	N-CD	-5.14	1.40	1.47
3	J	378	TYR	CA-C	-5.13	1.45	1.52
3	J	195	LEU	C-O	-5.13	1.17	1.24
3	J	124	HIS	C-N	-5.12	1.26	1.33
3	J	180	LEU	N-CA	-5.12	1.39	1.46
3	J	326	LEU	N-CA	-5.10	1.39	1.46
3	J	271	PHE	CA-C	5.09	1.60	1.52
3	J	111	LYS	N-CA	-5.08	1.39	1.46
3	J	236	ASN	C-N	-5.08	1.26	1.33
3	J	377	TYR	N-CA	-5.08	1.39	1.46
3	J	79	HIS	N-CA	-5.07	1.40	1.46
3	J	387	TRP	C-N	-5.07	1.26	1.33
3	J	325	TYR	N-CA	-5.07	1.40	1.46
1	G	74	PRO	N-CD	-5.07	1.40	1.47
3	J	344	HIS	N-CA	-5.06	1.39	1.46
3	J	147	LEU	CA-C	5.05	1.58	1.52
9	P	26	PRO	N-CD	-5.05	1.40	1.47
3	J	73	HIS	C-O	-5.05	1.18	1.24
1	F	323	PRO	N-CD	-5.05	1.40	1.47
1	F	74	PRO	N-CD	-5.04	1.40	1.47
1	I	228	PRO	N-CD	-5.04	1.40	1.47
3	J	271	PHE	N-CA	-5.04	1.40	1.46
3	J	310	SER	C-N	-5.04	1.25	1.33
3	J	316	LEU	C-N	-5.03	1.27	1.33
3	J	371	ARG	CA-C	-5.02	1.46	1.52
3	J	45	ARG	C-N	-5.00	1.27	1.34
3	J	293	ILE	CA-C	-5.00	1.45	1.52

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	196	PRO	CA-C-N	-39.51	62.40	123.24
3	J	196	PRO	C-N-CA	-39.51	62.40	123.24
3	J	144	ARG	O-C-N	35.76	166.03	123.12
3	J	195	LEU	CA-C-N	-26.55	86.66	119.84
3	J	195	LEU	C-N-CA	-26.55	86.66	119.84
3	J	144	ARG	CA-C-O	-24.66	94.44	121.07
3	J	230	LYS	CA-C-N	-20.26	93.15	123.14
3	J	230	LYS	C-N-CA	-20.26	93.15	123.14
3	J	182	GLN	CA-C-N	-19.57	93.93	121.33
3	J	182	GLN	C-N-CA	-19.57	93.93	121.33
3	J	248	TYR	CA-C-N	-18.85	100.82	119.85
3	J	248	TYR	C-N-CA	-18.85	100.82	119.85
3	J	237	ASN	CA-C-N	-18.75	93.06	122.49
3	J	237	ASN	C-N-CA	-18.75	93.06	122.49
3	J	230	LYS	N-CA-C	-18.31	85.67	112.04
3	J	198	VAL	N-CA-C	-18.26	95.64	113.53
3	J	22	GLU	N-CA-C	-17.49	91.21	112.89
3	J	308	GLY	CA-C-N	-16.78	88.85	121.58
3	J	308	GLY	C-N-CA	-16.78	88.85	121.58
3	J	34	GLY	CA-C-N	-16.50	104.37	120.21
3	J	34	GLY	C-N-CA	-16.50	104.37	120.21
3	J	39	ILE	CA-C-N	-16.42	102.74	120.14
3	J	39	ILE	C-N-CA	-16.42	102.74	120.14
3	J	115	VAL	CA-C-N	-16.41	104.22	120.31
3	J	115	VAL	C-N-CA	-16.41	104.22	120.31
3	J	300	ALA	N-CA-C	-15.86	87.60	110.59
3	J	17	VAL	CA-C-N	15.83	147.84	122.50
3	J	17	VAL	C-N-CA	15.83	147.84	122.50
3	J	352	CYS	CA-C-N	-15.72	94.87	120.64
3	J	352	CYS	C-N-CA	-15.72	94.87	120.64
3	J	40	PRO	CA-C-N	-15.56	101.06	123.00
3	J	40	PRO	C-N-CA	-15.56	101.06	123.00
3	J	165	PRO	N-CA-C	-15.18	89.97	111.22
3	J	155	ILE	CA-C-N	-15.02	104.22	120.14
3	J	155	ILE	C-N-CA	-15.02	104.22	120.14
3	J	144	ARG	N-CA-C	14.71	130.94	110.35
3	J	329	LYS	CA-C-N	14.39	134.24	119.56
3	J	329	LYS	C-N-CA	14.39	134.24	119.56
3	J	173	LYS	N-CA-C	-14.29	95.17	112.89
3	J	125	LEU	CA-C-O	13.80	134.32	119.14
3	J	152	TYR	CA-C-N	-13.42	102.16	120.95
3	J	152	TYR	C-N-CA	-13.42	102.16	120.95
3	J	169	LYS	N-CA-C	-13.33	95.44	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	248	TYR	CA-C-O	13.31	127.94	119.29
3	J	18	ILE	CA-C-N	13.26	142.34	121.66
3	J	18	ILE	C-N-CA	13.26	142.34	121.66
3	J	16	VAL	N-CA-C	13.20	127.49	108.48
3	J	225	LYS	N-CA-C	-13.11	96.97	113.23
3	J	69	LYS	CA-C-N	-13.08	98.44	120.68
3	J	69	LYS	C-N-CA	-13.08	98.44	120.68
3	J	19	ASP	CA-C-N	-13.06	100.32	122.14
3	J	19	ASP	C-N-CA	-13.06	100.32	122.14
3	J	322	GLU	CA-C-N	-13.04	97.87	120.29
3	J	322	GLU	C-N-CA	-13.04	97.87	120.29
3	J	183	CYS	N-CA-C	13.01	129.31	107.20
3	J	23	ALA	CA-C-N	-13.00	95.43	121.18
3	J	23	ALA	C-N-CA	-13.00	95.43	121.18
3	J	315	PHE	CA-C-O	-12.99	106.60	120.63
3	J	43	ILE	N-CA-C	-12.93	89.19	108.46
3	J	306	ILE	O-C-N	12.81	137.25	123.04
3	J	100	HIS	N-CA-C	-12.55	90.37	110.20
3	J	105	LEU	CA-C-N	-12.47	99.48	120.68
3	J	105	LEU	C-N-CA	-12.47	99.48	120.68
3	J	332	TYR	N-CA-C	-12.26	98.42	113.50
3	J	173	LYS	CA-C-N	-12.17	97.85	121.58
3	J	173	LYS	C-N-CA	-12.17	97.85	121.58
3	J	78	ARG	CA-C-N	-12.14	103.93	120.44
3	J	78	ARG	C-N-CA	-12.14	103.93	120.44
3	J	16	VAL	CA-C-N	-12.13	106.13	122.99
3	J	16	VAL	C-N-CA	-12.13	106.13	122.99
3	J	151	ILE	O-C-N	-12.12	108.92	123.10
3	J	391	ASN	CA-C-N	-12.03	104.28	120.65
3	J	391	ASN	C-N-CA	-12.03	104.28	120.65
3	J	76	TYR	CA-C-N	12.03	136.78	120.54
3	J	76	TYR	C-N-CA	12.03	136.78	120.54
3	J	164	LEU	CA-C-N	11.98	131.72	120.21
3	J	164	LEU	C-N-CA	11.98	131.72	120.21
3	J	112	TYR	N-CA-C	-11.95	94.84	112.04
3	J	40	PRO	N-CA-C	-11.94	91.74	111.68
3	J	296	ARG	CA-C-O	11.94	134.57	119.05
3	J	158	LEU	CA-C-N	-11.92	98.33	121.58
3	J	158	LEU	C-N-CA	-11.92	98.33	121.58
3	J	89	VAL	CA-C-N	-11.91	108.42	123.19
3	J	89	VAL	C-N-CA	-11.91	108.42	123.19
3	J	197	SER	N-CA-C	11.85	132.43	107.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	325	TYR	N-CA-C	-11.80	98.40	111.14
3	J	212	ALA	CA-C-N	-11.77	103.75	122.23
3	J	212	ALA	C-N-CA	-11.77	103.75	122.23
3	J	110	PHE	N-CA-C	-11.65	90.76	108.00
3	J	65	TYR	CA-C-N	-11.59	100.85	121.14
3	J	65	TYR	C-N-CA	-11.59	100.85	121.14
3	J	268	GLU	CA-C-N	-11.51	101.25	121.97
3	J	268	GLU	C-N-CA	-11.51	101.25	121.97
3	J	352	CYS	O-C-N	-11.44	107.21	122.43
3	J	74	ILE	CA-C-O	11.42	132.83	120.95
3	J	352	CYS	CA-C-O	11.41	133.47	119.10
3	J	127	ALA	N-CA-C	11.34	124.75	111.71
3	J	356	LEU	CA-C-N	-11.23	95.99	121.82
3	J	356	LEU	C-N-CA	-11.23	95.99	121.82
3	J	313	PRO	O-C-N	11.17	136.79	123.06
3	J	210	ILE	N-CA-C	-11.04	100.16	110.53
3	J	357	GLY	N-CA-C	-11.04	98.44	115.66
3	J	37	CYS	CA-C-O	10.99	133.45	120.81
3	J	313	PRO	CA-C-N	10.95	141.88	122.05
3	J	313	PRO	C-N-CA	10.95	141.88	122.05
3	J	219	ASP	CA-C-N	10.93	142.41	121.54
3	J	219	ASP	C-N-CA	10.93	142.41	121.54
3	J	350	ALA	O-C-N	-10.82	109.56	122.22
3	J	63	GLU	N-CA-C	-10.81	99.47	111.14
3	J	99	SER	CA-C-O	-10.80	107.89	120.10
3	J	256	LEU	CA-C-N	-10.78	106.01	121.42
3	J	256	LEU	C-N-CA	-10.78	106.01	121.42
3	J	223	GLY	N-CA-C	-10.76	98.95	113.37
3	J	23	ALA	O-C-N	-10.74	108.31	122.59
3	J	225	LYS	CA-C-N	-10.69	105.24	120.42
3	J	225	LYS	C-N-CA	-10.69	105.24	120.42
3	J	41	SER	N-CA-C	10.69	125.83	108.41
3	J	125	LEU	O-C-N	-10.55	108.35	122.49
3	J	330	PRO	CA-C-N	-10.50	102.76	121.14
3	J	330	PRO	C-N-CA	-10.50	102.76	121.14
3	J	206	VAL	CA-C-N	-10.46	105.21	120.28
3	J	206	VAL	C-N-CA	-10.46	105.21	120.28
3	J	68	LEU	CA-C-O	10.45	132.12	119.79
3	J	67	TYR	N-CA-C	10.40	123.88	111.82
3	J	184	THR	CA-C-N	-10.37	108.58	122.99
3	J	184	THR	C-N-CA	-10.37	108.58	122.99
3	J	270	LEU	N-CA-C	-10.32	100.03	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	121	ALA	CA-C-N	10.32	130.25	120.03
3	J	121	ALA	C-N-CA	10.32	130.25	120.03
3	J	195	LEU	O-C-N	-10.30	109.48	121.32
3	J	109	LEU	CA-C-N	-10.28	100.34	122.04
3	J	109	LEU	C-N-CA	-10.28	100.34	122.04
3	J	306	ILE	CA-C-O	-10.27	110.88	121.67
3	J	162	GLY	O-C-N	-10.25	115.29	123.49
3	J	81	LEU	N-CA-C	-10.22	94.63	109.96
3	J	71	PHE	O-C-N	10.22	132.95	122.12
3	J	311	MET	N-CA-C	-10.21	99.92	114.12
3	J	122	PRO	N-CA-C	10.20	126.71	111.41
3	J	355	TRP	N-CA-C	-10.16	99.59	112.90
3	J	43	ILE	CA-C-O	-10.07	109.39	120.67
3	J	105	LEU	CA-C-O	10.01	131.48	119.97
3	J	233	ILE	CA-C-N	-9.92	108.02	122.40
3	J	233	ILE	C-N-CA	-9.92	108.02	122.40
3	J	129	LEU	CA-C-O	-9.89	108.92	120.10
3	J	86	ASP	N-CA-C	9.85	125.37	113.16
3	J	318	ARG	O-C-N	9.80	134.32	122.27
3	J	111	LYS	N-CA-C	9.78	124.47	112.54
3	J	164	LEU	O-C-N	9.77	129.17	121.55
3	J	195	LEU	CA-C-O	9.77	133.55	120.16
3	J	276	GLU	N-CA-C	-9.69	95.12	110.14
3	J	204	GLU	CA-C-O	9.57	131.06	119.49
3	J	382	GLY	CA-C-N	-9.53	109.85	123.00
3	J	382	GLY	C-N-CA	-9.53	109.85	123.00
3	J	368	LEU	CA-C-N	-9.48	96.87	122.46
3	J	368	LEU	C-N-CA	-9.48	96.87	122.46
3	J	256	LEU	O-C-N	-9.46	111.80	123.05
3	J	116	PRO	N-CA-C	-9.43	97.24	111.57
3	J	349	LYS	CA-C-O	9.40	132.22	121.87
3	J	72	ILE	CA-C-N	-9.40	106.94	120.29
3	J	72	ILE	C-N-CA	-9.40	106.94	120.29
3	J	359	ALA	N-CA-C	-9.39	100.60	112.90
3	J	243	PRO	CA-C-N	9.38	129.47	119.90
3	J	243	PRO	C-N-CA	9.38	129.47	119.90
3	J	374	SER	N-CA-C	9.34	123.67	110.50
3	J	283	LEU	CA-C-N	-9.33	107.17	120.42
3	J	283	LEU	C-N-CA	-9.33	107.17	120.42
3	J	69	LYS	CA-C-O	9.28	130.25	120.42
3	J	177	THR	O-C-N	9.26	131.60	122.07
3	J	105	LEU	O-C-N	-9.25	110.89	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	178	GLN	CA-C-N	-9.24	104.97	120.68
3	J	178	GLN	C-N-CA	-9.24	104.97	120.68
3	J	259	LEU	O-C-N	-9.24	111.95	122.86
3	J	308	GLY	N-CA-C	-9.20	103.02	114.16
3	J	75	LEU	CA-C-O	9.20	130.65	119.79
3	J	73	HIS	CA-C-N	9.19	133.06	120.46
3	J	73	HIS	C-N-CA	9.19	133.06	120.46
3	J	175	LEU	CA-C-N	-9.19	104.86	120.58
3	J	175	LEU	C-N-CA	-9.19	104.86	120.58
3	J	378	TYR	CA-C-N	-9.19	106.34	120.31
3	J	378	TYR	C-N-CA	-9.19	106.34	120.31
3	J	69	LYS	O-C-N	-9.15	111.72	122.15
3	J	71	PHE	CA-C-O	-9.13	110.88	120.55
3	J	360	ILE	O-C-N	9.10	130.70	121.87
3	J	368	LEU	O-C-N	-9.09	111.59	122.22
3	J	346	PRO	CA-C-N	9.08	128.81	119.64
3	J	346	PRO	C-N-CA	9.08	128.81	119.64
3	J	191	LYS	CA-C-N	-9.03	110.11	122.30
3	J	191	LYS	C-N-CA	-9.03	110.11	122.30
3	J	318	ARG	CA-C-N	-8.99	108.24	120.28
3	J	318	ARG	C-N-CA	-8.99	108.24	120.28
3	J	128	LEU	N-CA-C	-8.98	102.33	113.38
3	J	89	VAL	O-C-N	-8.97	113.79	123.03
3	J	285	LEU	CA-C-N	-8.97	105.43	120.68
3	J	285	LEU	C-N-CA	-8.97	105.43	120.68
3	J	37	CYS	CA-C-N	-8.94	111.16	122.43
3	J	37	CYS	C-N-CA	-8.94	111.16	122.43
3	J	315	PHE	CA-C-N	-8.91	105.48	122.06
3	J	315	PHE	C-N-CA	-8.91	105.48	122.06
3	J	356	LEU	O-C-N	-8.91	109.75	122.41
3	J	333	LYS	CA-C-N	-8.90	105.56	120.68
3	J	333	LYS	C-N-CA	-8.90	105.56	120.68
3	J	125	LEU	CA-C-N	-8.88	105.59	121.14
3	J	125	LEU	C-N-CA	-8.88	105.59	121.14
3	J	348	ALA	N-CA-C	-8.88	98.56	110.55
3	J	335	ALA	N-CA-C	8.88	120.96	111.28
3	J	288	LEU	O-C-N	-8.88	111.35	122.27
3	J	103	GLU	O-C-N	8.87	132.26	122.15
3	J	371	ARG	CA-C-N	8.85	136.08	121.39
3	J	371	ARG	C-N-CA	8.85	136.08	121.39
3	J	275	ASN	CA-C-N	8.85	138.50	122.92
3	J	275	ASN	C-N-CA	8.85	138.50	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	333	LYS	CA-C-O	8.85	129.80	120.42
3	J	337	GLY	CA-C-N	-8.85	107.95	122.81
3	J	337	GLY	C-N-CA	-8.85	107.95	122.81
3	J	232	ASN	N-CA-C	-8.79	91.40	107.75
3	J	137	MET	CA-C-N	-8.78	111.43	123.10
3	J	137	MET	C-N-CA	-8.78	111.43	123.10
3	J	156	PRO	CA-C-N	-8.76	111.19	123.11
3	J	156	PRO	C-N-CA	-8.76	111.19	123.11
3	J	334	LYS	N-CA-C	-8.75	101.21	112.23
3	J	306	ILE	N-CA-C	-8.74	94.52	108.95
3	J	69	LYS	N-CA-C	-8.72	101.85	111.36
3	J	136	ALA	CA-C-N	8.70	137.36	121.70
3	J	136	ALA	C-N-CA	8.70	137.36	121.70
3	J	300	ALA	CA-C-O	-8.68	111.74	121.89
3	J	377	TYR	O-C-N	8.65	132.91	122.27
3	J	193	GLN	N-CA-C	8.62	122.88	109.52
3	J	266	VAL	CA-C-N	-8.56	106.56	121.97
3	J	266	VAL	C-N-CA	-8.56	106.56	121.97
3	J	246	VAL	O-C-N	-8.56	114.02	123.26
3	J	387	TRP	CA-C-N	-8.55	107.86	122.56
3	J	387	TRP	C-N-CA	-8.55	107.86	122.56
3	J	51	PRO	CA-C-N	8.52	133.75	123.19
3	J	51	PRO	C-N-CA	8.52	133.75	123.19
3	J	220	LEU	CA-C-N	-8.50	106.52	120.72
3	J	220	LEU	C-N-CA	-8.50	106.52	120.72
3	J	83	ASN	CA-C-N	8.50	128.23	119.56
3	J	83	ASN	C-N-CA	8.50	128.23	119.56
3	J	393	PRO	CA-C-O	-8.47	114.03	120.73
3	J	378	TYR	N-CA-C	-8.47	102.39	112.89
3	J	246	VAL	N-CA-C	8.37	119.83	108.11
3	J	145	GLU	CA-C-N	8.36	132.74	120.87
3	J	145	GLU	C-N-CA	8.36	132.74	120.87
3	J	255	ILE	CA-C-N	-8.34	112.00	122.84
3	J	255	ILE	C-N-CA	-8.34	112.00	122.84
3	J	268	GLU	N-CA-C	-8.31	101.29	112.26
3	J	82	VAL	CA-C-N	8.29	131.78	122.83
3	J	82	VAL	C-N-CA	8.29	131.78	122.83
3	J	350	ALA	CA-C-N	-8.28	108.53	120.29
3	J	350	ALA	C-N-CA	-8.28	108.53	120.29
3	J	14	THR	CA-C-N	8.28	136.60	121.70
3	J	14	THR	C-N-CA	8.28	136.60	121.70
3	J	160	CYS	N-CA-C	-8.28	92.83	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	191	LYS	O-C-N	-8.24	113.83	123.06
3	J	170	ALA	O-C-N	8.24	134.46	122.43
3	J	298	GLN	O-C-N	8.19	133.98	122.36
3	J	386	ASP	O-C-N	-8.19	112.55	123.19
3	J	60	ASN	N-CA-C	-8.18	97.92	110.10
3	J	319	LEU	CA-C-N	-8.17	106.85	121.14
3	J	319	LEU	C-N-CA	-8.17	106.85	121.14
3	J	234	ASP	N-CA-C	-8.16	101.80	112.24
3	J	319	LEU	O-C-N	8.16	130.77	122.12
3	J	72	ILE	N-CA-C	-8.09	100.98	111.09
3	J	134	ASN	N-CA-C	-8.06	103.01	113.17
3	J	381	THR	N-CA-C	-8.02	103.33	113.43
3	J	147	LEU	CA-C-N	-7.99	113.29	123.19
3	J	147	LEU	C-N-CA	-7.99	113.29	123.19
3	J	126	MET	N-CA-C	-7.97	103.00	112.89
3	J	74	ILE	O-C-N	-7.92	114.19	121.87
3	J	97	CYS	CA-C-N	-7.92	112.61	120.21
3	J	97	CYS	C-N-CA	-7.92	112.61	120.21
3	J	231	PHE	N-CA-C	7.90	123.18	107.62
3	J	280	VAL	N-CA-C	-7.88	101.23	111.09
3	J	322	GLU	CA-C-O	7.86	129.01	119.97
3	J	256	LEU	CA-C-O	7.85	128.71	120.54
3	J	374	SER	O-C-N	7.85	132.12	122.86
3	J	17	VAL	O-C-N	-7.85	114.73	123.20
3	J	337	GLY	N-CA-C	-7.82	98.50	112.58
3	J	246	VAL	CA-C-N	-7.82	112.02	122.42
3	J	246	VAL	C-N-CA	-7.82	112.02	122.42
3	J	119	LEU	CA-C-O	7.79	129.45	120.80
3	J	260	GLY	N-CA-C	-7.77	104.76	114.16
3	J	73	HIS	O-C-N	7.77	131.01	122.15
3	J	331	LYS	CA-C-N	-7.77	108.48	121.92
3	J	331	LYS	C-N-CA	-7.77	108.48	121.92
3	J	14	THR	N-CA-C	-7.73	97.63	109.85
3	J	131	LEU	N-CA-C	-7.73	103.87	113.38
3	J	181	GLU	CA-C-N	-7.72	109.35	122.33
3	J	181	GLU	C-N-CA	-7.72	109.35	122.33
3	J	252	GLY	CA-C-N	-7.70	111.43	122.36
3	J	252	GLY	C-N-CA	-7.70	111.43	122.36
3	J	293	ILE	CA-C-O	7.67	128.75	120.47
3	J	68	LEU	CA-C-N	-7.66	109.41	120.29
3	J	68	LEU	C-N-CA	-7.66	109.41	120.29
3	J	267	VAL	N-CA-C	7.66	125.28	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	65	TYR	O-C-N	-7.66	114.00	122.12
3	J	191	LYS	CA-C-O	7.64	130.53	121.36
3	J	388	CYS	N-CA-C	7.64	122.19	113.02
3	J	169	LYS	CA-C-N	-7.64	106.69	121.58
3	J	169	LYS	C-N-CA	-7.64	106.69	121.58
3	J	122	PRO	CA-C-N	-7.63	107.80	121.14
3	J	122	PRO	C-N-CA	-7.63	107.80	121.14
3	J	181	GLU	CA-C-O	-7.62	109.58	119.80
3	J	373	VAL	O-C-N	-7.62	113.32	122.77
3	J	163	ALA	N-CA-C	7.61	121.75	108.75
3	J	105	LEU	N-CA-C	-7.60	103.00	111.82
3	J	368	LEU	CA-C-O	7.60	128.68	120.10
3	J	49	PRO	N-CA-C	-7.59	99.15	111.21
3	J	124	HIS	N-CA-C	-7.58	104.01	113.18
3	J	287	SER	CA-C-N	-7.57	108.81	120.31
3	J	287	SER	C-N-CA	-7.57	108.81	120.31
3	J	212	ALA	N-CA-C	-7.55	103.03	111.71
3	J	147	LEU	O-C-N	-7.54	114.33	123.30
3	J	204	GLU	CA-C-N	-7.51	107.42	120.79
3	J	204	GLU	C-N-CA	-7.51	107.42	120.79
3	J	108	VAL	O-C-N	7.50	132.24	122.26
3	J	122	PRO	O-C-N	-7.50	113.85	123.00
3	J	303	LEU	O-C-N	-7.49	113.69	123.21
3	J	338	THR	O-C-N	-7.49	113.07	123.11
3	J	52	VAL	CA-C-N	-7.47	112.48	122.42
3	J	52	VAL	C-N-CA	-7.47	112.48	122.42
3	J	109	LEU	N-CA-C	-7.47	94.89	110.80
3	J	314	GLY	N-CA-C	-7.43	105.06	115.32
3	J	82	VAL	O-C-N	-7.41	116.27	121.98
3	J	203	PRO	CA-C-N	7.41	132.46	120.60
3	J	203	PRO	C-N-CA	7.41	132.46	120.60
3	J	369	GLY	N-CA-C	-7.40	102.97	115.62
3	J	175	LEU	N-CA-C	-7.37	104.82	113.88
3	J	268	GLU	CA-C-O	-7.36	111.64	120.55
3	J	147	LEU	N-CA-C	7.35	120.89	108.90
3	J	326	LEU	CA-C-N	-7.34	108.60	120.86
3	J	326	LEU	C-N-CA	-7.34	108.60	120.86
3	J	356	LEU	CA-C-O	7.33	127.90	119.18
3	J	23	ALA	CA-C-O	7.33	130.99	120.51
3	J	319	LEU	CA-C-O	-7.32	112.79	120.55
3	J	133	ILE	CA-C-N	-7.29	110.51	122.54
3	J	133	ILE	C-N-CA	-7.29	110.51	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	252	GLY	N-CA-C	-7.28	105.17	115.30
3	J	329	LYS	N-CA-C	-7.28	100.47	109.65
3	J	176	GLU	N-CA-C	-7.28	102.73	111.69
3	J	326	LEU	CA-C-O	7.26	128.31	119.38
3	J	43	ILE	CA-C-N	7.25	134.75	121.70
3	J	43	ILE	C-N-CA	7.25	134.75	121.70
3	J	185	VAL	N-CA-C	-7.25	97.69	108.12
3	J	326	LEU	O-C-N	-7.24	112.73	122.43
3	J	288	LEU	CA-C-O	7.21	128.27	119.97
3	J	317	HIS	O-C-N	7.20	129.86	122.09
3	J	281	ALA	CA-C-N	-7.18	107.83	121.54
3	J	281	ALA	C-N-CA	-7.18	107.83	121.54
3	J	114	GLU	N-CA-C	-7.14	99.87	110.23
3	J	353	VAL	CA-C-N	-7.14	108.79	120.72
3	J	353	VAL	C-N-CA	-7.14	108.79	120.72
3	J	129	LEU	O-C-N	-7.12	113.89	122.22
3	J	111	LYS	CA-C-N	-7.10	106.46	121.80
3	J	111	LYS	C-N-CA	-7.10	106.46	121.80
3	J	14	THR	CA-C-O	-7.09	113.16	121.46
3	J	147	LEU	CA-C-O	7.09	128.02	120.36
3	J	184	THR	O-C-N	7.07	131.98	123.36
3	J	36	ARG	N-CA-C	-7.06	92.92	107.67
3	J	349	LYS	N-CA-C	7.03	119.64	110.43
3	J	84	PRO	CA-C-N	-7.00	109.02	120.72
3	J	84	PRO	C-N-CA	-7.00	109.02	120.72
3	J	37	CYS	O-C-N	-6.99	114.33	122.93
3	J	258	ILE	O-C-N	-6.99	115.71	123.26
3	J	376	GLU	CA-C-O	-6.99	113.01	120.42
3	J	220	LEU	O-C-N	-6.99	113.30	122.59
3	J	393	PRO	CA-C-N	-6.96	111.14	119.84
3	J	393	PRO	C-N-CA	-6.96	111.14	119.84
3	J	183	CYS	CA-C-O	6.96	127.12	120.09
3	J	75	LEU	O-C-N	-6.95	113.02	122.33
3	J	186	ASP	CA-C-O	6.93	128.33	120.84
3	J	303	LEU	CA-C-O	6.93	128.06	120.71
3	J	312	LEU	CA-C-O	-6.91	112.65	119.49
3	J	207	LEU	O-C-N	6.88	130.27	122.22
3	J	376	GLU	O-C-N	6.88	129.99	122.15
3	J	83	ASN	O-C-N	6.83	129.18	121.32
3	J	341	PHE	N-CA-C	-6.83	98.71	109.50
3	J	333	LYS	N-CA-C	6.80	118.78	111.36
3	J	349	LYS	O-C-N	-6.80	114.79	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	324	ARG	CA-C-O	6.80	127.74	119.38
3	J	362	GLY	N-CA-C	-6.80	106.42	115.32
3	J	330	PRO	CA-C-O	6.79	128.89	119.18
3	J	138	VAL	N-CA-C	6.78	117.65	107.75
3	J	365	GLN	O-C-N	-6.76	113.59	122.59
3	J	172	HIS	CA-C-O	-6.75	112.21	119.97
3	J	322	GLU	O-C-N	-6.72	114.00	122.27
3	J	74	ILE	N-CA-C	6.71	117.47	110.62
3	J	110	PHE	CA-C-N	-6.67	109.59	120.72
3	J	110	PHE	C-N-CA	-6.67	109.59	120.72
3	J	386	ASP	CA-C-O	6.66	128.64	121.11
9	p	80	GLY	CA-C-N	6.66	130.61	120.82
9	p	80	GLY	C-N-CA	6.66	130.61	120.82
3	J	72	ILE	CA-C-O	6.65	127.65	120.47
3	J	75	LEU	N-CA-C	-6.62	103.88	112.23
3	J	134	ASN	CA-C-O	6.62	127.09	119.35
3	J	393	PRO	O-C-N	6.60	124.25	121.15
3	J	343	ILE	CA-C-N	-6.59	112.83	122.65
3	J	343	ILE	C-N-CA	-6.59	112.83	122.65
3	J	106	THR	CA-C-N	6.57	129.74	120.28
3	J	106	THR	C-N-CA	6.57	129.74	120.28
3	J	334	LYS	CA-C-N	-6.57	111.48	120.28
3	J	334	LYS	C-N-CA	-6.57	111.48	120.28
3	J	266	VAL	O-C-N	6.56	129.22	121.80
3	J	321	ALA	N-CA-C	-6.56	104.21	111.36
3	J	364	LEU	CA-C-O	-6.54	110.56	119.05
3	J	282	THR	CA-C-O	-6.53	111.17	120.51
3	J	148	VAL	O-C-N	-6.50	116.36	123.18
3	J	208	GLU	CA-C-N	-6.49	109.78	121.14
3	J	208	GLU	C-N-CA	-6.49	109.78	121.14
3	J	61	THR	O-C-N	6.49	130.82	122.39
3	J	313	PRO	CA-C-O	-6.48	113.77	121.67
3	J	174	GLU	N-CA-C	6.47	121.01	113.18
3	J	196	PRO	O-C-N	-6.47	113.91	122.64
3	J	166	LEU	CA-C-O	-6.46	109.81	120.80
3	J	124	HIS	CA-C-N	-6.44	110.78	121.92
3	J	124	HIS	C-N-CA	-6.44	110.78	121.92
3	J	84	PRO	O-C-N	-6.44	113.61	122.24
3	J	144	ARG	CB-CA-C	-6.40	99.50	109.61
3	J	263	ARG	CA-C-O	6.36	127.29	119.97
3	J	177	THR	CA-C-O	-6.34	114.16	120.82
3	J	298	GLN	N-CA-C	-6.33	105.69	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	103	GLU	N-CA-C	-6.31	104.48	111.36
3	J	389	SER	N-CA-C	6.31	120.11	109.76
3	J	46	ALA	N-CA-C	6.31	118.96	111.71
3	J	351	ASN	CA-C-N	6.30	132.71	120.99
3	J	351	ASN	C-N-CA	6.30	132.71	120.99
3	J	113	PHE	N-CA-C	6.30	119.08	107.99
3	J	148	VAL	CA-C-O	6.28	127.13	120.48
3	J	283	LEU	O-C-N	-6.27	114.25	122.59
3	J	304	VAL	CA-C-O	-6.26	113.81	120.39
3	J	277	GLU	CA-C-N	-6.23	111.36	122.32
3	J	277	GLU	C-N-CA	-6.23	111.36	122.32
3	J	156	PRO	CA-C-O	-6.21	114.28	121.86
3	J	64	LEU	CA-C-O	-6.21	112.83	119.97
3	J	31	GLY	N-CA-C	-6.18	95.37	113.30
3	J	204	GLU	O-C-N	-6.18	114.36	122.39
3	J	210	ILE	CA-C-N	6.17	128.55	120.28
3	J	210	ILE	C-N-CA	6.17	128.55	120.28
3	J	98	PRO	CA-C-N	-6.16	111.41	120.28
3	J	98	PRO	C-N-CA	-6.16	111.41	120.28
3	J	214	THR	N-CA-C	6.16	121.86	113.97
3	J	242	PRO	CA-C-N	-6.15	114.04	120.38
3	J	242	PRO	C-N-CA	-6.15	114.04	120.38
3	J	258	ILE	CA-C-O	6.14	126.84	120.39
3	J	61	THR	CA-C-O	-6.14	112.06	119.49
3	J	293	ILE	O-C-N	-6.14	114.86	121.80
3	J	346	PRO	O-C-N	6.11	128.67	121.46
3	J	164	LEU	N-CA-C	-6.07	98.53	109.09
3	J	197	SER	CB-CA-C	-6.07	103.42	112.09
3	J	209	ASP	O-C-N	-6.06	114.09	122.46
3	J	350	ALA	CA-C-O	6.06	126.95	120.10
3	J	60	ASN	CA-C-O	-6.06	114.02	120.92
3	J	46	ALA	CA-C-N	-6.04	106.15	122.46
3	J	46	ALA	C-N-CA	-6.04	106.15	122.46
3	J	63	GLU	CA-C-N	-6.01	111.18	120.31
3	J	63	GLU	C-N-CA	-6.01	111.18	120.31
3	J	332	TYR	O-C-N	6.01	130.54	122.49
3	J	218	SER	N-CA-C	6.00	118.97	110.50
3	J	259	LEU	CA-C-N	-6.00	110.11	120.79
3	J	259	LEU	C-N-CA	-6.00	110.11	120.79
3	J	354	ALA	O-C-N	-5.99	114.40	122.43
3	J	279	SER	CA-C-N	-5.99	110.48	120.30
3	J	279	SER	C-N-CA	-5.99	110.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	80	LEU	CA-C-N	-5.99	112.57	120.95
3	J	80	LEU	C-N-CA	-5.99	112.57	120.95
3	J	320	LEU	O-C-N	5.97	130.70	122.46
3	J	68	LEU	N-CA-C	-5.96	104.72	112.23
3	J	255	ILE	N-CA-C	5.96	116.45	107.75
3	J	138	VAL	CA-C-O	5.95	126.58	120.39
3	J	64	LEU	O-C-N	5.93	129.57	122.27
3	J	332	TYR	CA-C-O	-5.91	112.64	119.14
3	J	40	PRO	CA-C-O	-5.87	114.69	121.86
3	J	254	LYS	N-CA-C	-5.86	100.59	109.85
3	J	281	ALA	N-CA-C	5.86	119.69	112.54
3	J	322	GLU	N-CA-C	-5.85	105.03	111.82
3	J	167	GLY	CA-C-N	5.85	133.99	121.18
3	J	167	GLY	C-N-CA	5.85	133.99	121.18
3	J	26	LYS	N-CA-C	5.84	119.75	110.70
3	J	175	LEU	CA-C-O	5.83	125.82	119.24
1	D	234	LEU	CA-C-O	-5.81	114.26	120.42
3	J	33	THR	N-CA-C	5.80	120.19	113.18
3	J	378	TYR	O-C-N	-5.79	114.47	122.46
3	J	130	THR	CA-C-N	-5.79	112.25	122.26
3	J	130	THR	C-N-CA	-5.79	112.25	122.26
3	J	194	SER	CA-C-N	-5.78	107.69	121.80
3	J	194	SER	C-N-CA	-5.78	107.69	121.80
3	J	179	LEU	N-CA-C	-5.78	104.95	112.23
3	J	60	ASN	O-C-N	5.76	130.09	122.95
3	J	66	SER	N-CA-C	-5.75	105.76	112.89
3	J	34	GLY	N-CA-C	5.75	124.08	112.34
3	J	199	MET	CA-C-N	-5.75	110.14	121.41
3	J	199	MET	C-N-CA	-5.75	110.14	121.41
3	J	342	ARG	CA-C-O	-5.73	114.07	120.66
3	J	287	SER	N-CA-C	5.73	119.99	112.89
3	J	175	LEU	O-C-N	-5.72	114.69	122.36
3	J	88	ARG	O-C-N	-5.72	115.96	123.28
3	J	354	ALA	CA-C-O	-5.71	112.35	119.38
1	A	186	ALA	CA-C-N	5.71	126.43	120.03
1	A	186	ALA	C-N-CA	5.71	126.43	120.03
3	J	73	HIS	CA-C-O	-5.71	114.37	120.42
3	J	241	SER	CA-C-N	5.70	126.25	120.38
3	J	241	SER	C-N-CA	5.70	126.25	120.38
3	J	283	LEU	CA-C-O	5.70	128.66	120.51
3	J	126	MET	CA-C-N	5.70	128.48	120.28
3	J	126	MET	C-N-CA	5.70	128.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	65	TYR	CA-C-O	5.68	126.58	120.55
3	J	330	PRO	CA-N-CD	5.68	119.96	112.00
3	J	286	ASP	CA-C-N	-5.68	111.20	121.14
3	J	286	ASP	C-N-CA	-5.68	111.20	121.14
3	J	28	GLY	N-CA-C	-5.68	101.96	110.42
3	J	347	PRO	CA-C-N	-5.68	109.40	121.32
3	J	347	PRO	C-N-CA	-5.68	109.40	121.32
3	J	304	VAL	CA-C-N	5.67	130.64	123.10
3	J	304	VAL	C-N-CA	5.67	130.64	123.10
3	J	193	GLN	CA-C-N	-5.67	112.20	120.75
3	J	193	GLN	C-N-CA	-5.67	112.20	120.75
3	J	265	SER	N-CA-C	5.66	119.91	112.89
3	J	166	LEU	N-CA-C	-5.66	95.16	111.00
3	J	30	ALA	N-CA-C	5.65	117.98	110.53
3	J	381	THR	CA-C-O	-5.64	112.93	119.64
3	J	81	LEU	CA-C-N	-5.64	117.18	123.16
3	J	81	LEU	C-N-CA	-5.64	117.18	123.16
3	J	176	GLU	O-C-N	5.63	129.55	122.23
3	J	139	LEU	CA-C-O	-5.62	114.26	120.38
3	J	150	PRO	N-CA-C	-5.61	102.39	111.19
3	J	323	ILE	O-C-N	5.59	129.48	121.82
3	J	93	GLU	N-CA-C	-5.58	94.69	107.48
3	J	278	GLN	CA-C-O	-5.57	115.15	121.66
3	J	138	VAL	CA-C-N	-5.56	115.33	123.00
3	J	138	VAL	C-N-CA	-5.56	115.33	123.00
3	J	95	VAL	N-CA-C	-5.54	95.50	111.00
3	J	278	GLN	O-C-N	5.53	130.04	122.41
3	J	168	GLY	CA-C-N	-5.53	111.35	121.52
3	J	168	GLY	C-N-CA	-5.53	111.35	121.52
3	J	233	ILE	N-CA-C	5.52	115.27	106.88
9	P	58	LYS	N-CA-C	5.50	117.28	111.28
3	J	227	GLN	O-C-N	5.50	129.54	122.39
3	J	161	TRP	CA-C-N	-5.47	117.93	121.65
3	J	161	TRP	C-N-CA	-5.47	117.93	121.65
3	J	275	ASN	O-C-N	5.47	129.21	122.20
3	J	315	PHE	O-C-N	-5.46	116.33	122.12
3	J	226	ILE	CA-C-O	-5.45	115.07	120.85
2	H	181	ALA	CA-C-N	5.39	126.06	120.03
2	H	181	ALA	C-N-CA	5.39	126.06	120.03
3	J	338	THR	CA-C-O	-5.38	115.17	121.46
3	J	135	SER	N-CA-C	5.37	118.38	110.59
3	J	377	TYR	N-CA-C	-5.36	105.61	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	250	LEU	N-CA-C	-5.35	101.39	109.85
3	J	386	ASP	CA-C-N	-5.35	111.77	121.14
3	J	386	ASP	C-N-CA	-5.35	111.77	121.14
3	J	140	ASP	CA-C-O	5.35	126.02	120.40
3	J	61	THR	N-CA-C	5.31	118.86	112.38
3	J	293	ILE	CA-C-N	-5.31	110.67	121.18
3	J	293	ILE	C-N-CA	-5.31	110.67	121.18
9	P	76	THR	CB-CA-C	-5.31	108.89	115.89
3	J	170	ALA	CA-C-O	-5.30	112.32	119.11
3	J	135	SER	CA-C-N	5.30	131.03	121.06
3	J	135	SER	C-N-CA	5.30	131.03	121.06
3	J	138	VAL	O-C-N	-5.30	117.59	123.20
3	J	35	PRO	N-CA-C	-5.29	103.82	111.22
3	J	357	GLY	CA-C-N	5.29	133.61	121.34
3	J	357	GLY	C-N-CA	5.29	133.61	121.34
3	J	20	LEU	N-CA-C	5.28	119.48	112.30
3	J	111	LYS	CA-C-O	-5.27	112.89	119.38
3	J	316	LEU	O-C-N	5.26	129.87	122.41
9	p	81	TYR	N-CA-C	5.26	117.07	110.24
3	J	263	ARG	N-CA-C	-5.25	105.73	111.82
3	J	353	VAL	O-C-N	-5.25	114.88	122.12
3	J	133	ILE	N-CA-C	5.24	116.13	108.58
3	J	288	LEU	N-CA-C	-5.23	105.75	111.82
3	J	312	LEU	O-C-N	5.23	126.04	121.18
3	J	183	CYS	N-CA-CB	-5.23	102.81	110.86
3	J	226	ILE	O-C-N	5.22	127.21	121.83
3	J	63	GLU	O-C-N	5.22	127.73	122.09
3	J	89	VAL	N-CA-C	5.21	115.54	107.78
3	J	21	GLY	CA-C-N	-5.20	112.04	121.14
3	J	21	GLY	C-N-CA	-5.20	112.04	121.14
3	J	307	GLY	CA-C-N	5.20	130.04	120.79
3	J	307	GLY	C-N-CA	5.20	130.04	120.79
3	J	49	PRO	CA-C-N	-5.19	114.45	124.01
3	J	49	PRO	C-N-CA	-5.19	114.45	124.01
3	J	133	ILE	O-C-N	-5.19	117.04	122.95
3	J	103	GLU	CA-C-O	-5.18	114.92	120.42
3	J	162	GLY	N-CA-C	5.17	120.52	111.46
3	J	266	VAL	CA-C-O	-5.16	114.90	120.47
3	J	238	GLU	N-CA-C	-5.15	105.71	112.41
3	J	345	THR	CA-C-N	-5.15	115.07	120.38
3	J	345	THR	C-N-CA	-5.15	115.07	120.38
3	J	258	ILE	CA-C-N	-5.15	112.85	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	258	ILE	C-N-CA	-5.15	112.85	120.94
3	J	112	TYR	CA-C-N	-5.15	114.85	122.41
3	J	112	TYR	C-N-CA	-5.15	114.85	122.41
3	J	369	GLY	O-C-N	-5.14	114.41	122.18
3	J	68	LEU	O-C-N	-5.14	115.45	122.33
3	J	209	ASP	CA-C-O	5.12	125.67	119.31
3	J	30	ALA	CA-C-N	5.12	130.91	121.70
3	J	30	ALA	C-N-CA	5.12	130.91	121.70
3	J	217	VAL	N-CA-C	5.10	115.44	107.99
1	A	8	ALA	CA-C-N	5.10	128.34	121.05
1	A	8	ALA	C-N-CA	5.10	128.34	121.05
3	J	327	VAL	CA-C-N	5.10	131.52	121.58
3	J	327	VAL	C-N-CA	5.10	131.52	121.58
3	J	230	LYS	N-CA-CB	5.08	118.07	110.19
3	J	320	LEU	CA-C-N	-5.08	113.08	120.29
3	J	320	LEU	C-N-CA	-5.08	113.08	120.29
3	J	247	ASP	CA-C-N	-5.08	115.04	121.74
3	J	247	ASP	C-N-CA	-5.08	115.04	121.74
3	J	170	ALA	N-CA-C	5.05	119.30	113.18
3	J	261	SER	N-CA-C	5.05	118.55	112.38
3	J	248	TYR	O-C-N	-5.04	117.15	121.23
3	J	248	TYR	C-N-CD	5.04	145.64	125.00
1	D	64	GLU	N-CA-C	5.03	116.85	111.36
3	J	148	VAL	CA-C-N	-5.02	109.56	121.80
3	J	148	VAL	C-N-CA	-5.02	109.56	121.80
3	J	226	ILE	N-CA-C	-5.02	105.65	110.72
3	J	347	PRO	N-CA-C	-5.02	107.21	114.18
3	J	375	LYS	N-CA-C	-5.02	105.94	111.71
3	J	192	GLU	CA-C-N	-5.01	114.73	122.59
3	J	192	GLU	C-N-CA	-5.01	114.73	122.59
3	J	151	ILE	CA-C-N	-5.01	112.56	122.02
3	J	151	ILE	C-N-CA	-5.01	112.56	122.02

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	102	ARG	Mainchain
3	J	125	LEU	Mainchain
3	J	129	LEU	Mainchain
3	J	174	GLU	Mainchain
3	J	181	GLU	Mainchain

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Mol	Chain	Res	Type	Group
3	J	196	PRO	Mainchain
3	J	209	ASP	Mainchain
3	J	222	ARG	Mainchain
3	J	230	LYS	Mainchain
3	J	259	LEU	Mainchain
3	J	260	GLY	Mainchain
3	J	268	GLU	Mainchain
3	J	282	THR	Mainchain
3	J	288	LEU	Mainchain
3	J	293	ILE	Mainchain
3	J	315	PHE	Mainchain
3	J	338	THR	Mainchain
3	J	350	ALA	Mainchain
3	J	354	ALA	Mainchain
3	J	356	LEU	Mainchain
3	J	378	TYR	Mainchain
3	J	381	THR	Mainchain
3	J	386	ASP	Mainchain
3	J	50	LYS	Peptide
3	J	53	ARG	Mainchain
3	J	65	TYR	Mainchain
3	J	78	ARG	Mainchain
3	J	92	ILE	Mainchain
3	J	99	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2956	2951	2950	11	0
1	B	2956	2951	2950	16	0
1	C	2998	2984	2983	20	0
1	D	2956	2951	2950	19	0
1	E	2956	2951	2950	19	0
1	F	2956	2951	2950	23	0
1	G	2956	2951	2950	10	0
1	I	2956	2951	2950	18	0
2	H	2885	2857	2856	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	3027	3113	3108	124	0
4	K	2913	2982	2975	4	0
5	L	1408	1438	1440	3	0
6	M	1191	1217	1215	8	0
7	N	2324	2235	2237	12	0
8	O	2122	2114	2113	5	0
9	P	581	560	558	6	0
9	Q	188	173	172	0	0
9	p	286	257	258	6	0
9	q	379	354	352	2	0
10	A	27	12	12	0	0
10	B	27	12	12	1	0
10	C	27	12	12	0	0
10	D	27	12	12	0	0
10	E	27	12	12	0	0
10	F	27	12	12	0	0
10	G	27	12	12	0	0
10	I	27	12	12	0	0
11	H	31	15	13	0	0
12	K	3	0	0	0	0
All	All	41244	41052	41026	298	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 (298) 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)
3:J:109:LEU:O	3:J:110:PHE:C	1.82	1.08
3:J:109:LEU:O	3:J:111:LYS:N	2.06	0.89
3:J:109:LEU:O	3:J:110:PHE:HB3	1.77	0.83
3:J:166:LEU:HB2	3:J:167:GLY:HA2	1.61	0.82
3:J:233:ILE:O	3:J:234:ASP:C	2.16	0.79
3:J:352:CYS:O	3:J:353:VAL:C	2.05	0.79
3:J:356:LEU:O	3:J:357:GLY:C	2.12	0.76
3:J:105:LEU:O	3:J:106:THR:C	2.20	0.75
3:J:65:TYR:O	3:J:66:SER:C	2.23	0.74
3:J:23:ALA:O	3:J:24:PHE:C	2.13	0.73
3:J:125:LEU:O	3:J:126:MET:C	2.21	0.73
3:J:322:GLU:O	3:J:323:ILE:C	2.13	0.73
3:J:283:LEU:O	3:J:284:ILE:C	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:209:ASP:O	3:J:210:ILE:C	2.30	0.71
3:J:391:ASN:O	3:J:392:ASN:C	2.30	0.69
3:J:152:TYR:CG	3:J:153:GLU:N	2.57	0.69
1:E:238:LYS:HA	1:E:252:GLY:HA2	1.75	0.68
3:J:72:ILE:O	3:J:73:HIS:C	2.26	0.68
1:E:50:GLY:HA2	9:P:60:LYS:HD2	1.76	0.67
3:J:259:LEU:O	3:J:260:GLY:C	2.32	0.67
3:J:326:LEU:O	3:J:327:VAL:C	2.26	0.67
3:J:69:LYS:O	3:J:70:GLU:C	2.20	0.67
3:J:152:TYR:O	3:J:153:GLU:C	2.29	0.66
1:C:360:LYS:NZ	1:C:364:GLU:OE2	2.27	0.66
3:J:113:PHE:O	3:J:114:GLU:C	2.32	0.66
3:J:282:THR:OG1	3:J:283:LEU:N	2.27	0.65
3:J:299:LEU:C	3:J:300:ALA:O	2.22	0.65
3:J:378:TYR:O	3:J:379:ASN:C	2.30	0.65
3:J:220:LEU:O	3:J:221:LYS:C	2.33	0.65
3:J:282:THR:C	3:J:284:ILE:N	2.56	0.63
4:K:424:ASP:OD2	4:K:426:LYS:NZ	2.30	0.63
3:J:175:LEU:O	3:J:176:GLU:C	2.31	0.63
1:C:238:LYS:HA	1:C:252:GLY:HA2	1.79	0.62
3:J:195:LEU:O	3:J:196:PRO:C	2.16	0.62
1:A:197:TYR:OH	1:A:257:ARG:NH1	2.32	0.62
3:J:378:TYR:CD1	3:J:382:GLY:HA2	2.34	0.62
3:J:330:PRO:O	3:J:331:LYS:C	2.35	0.61
3:J:164:LEU:CB	3:J:165:PRO:O	2.49	0.61
3:J:39:ILE:O	3:J:40:PRO:C	2.33	0.60
2:H:51:ASP:OD2	4:K:165:LYS:NZ	2.34	0.60
3:J:68:LEU:O	3:J:69:LYS:C	2.34	0.60
3:J:158:LEU:O	3:J:159:ASN:C	2.35	0.60
2:H:237:GLU:HG2	2:H:251:GLY:HA2	1.83	0.60
3:J:252:GLY:O	3:J:253:GLU:C	2.38	0.60
3:J:142:GLY:HA2	3:J:309:THR:HG23	1.84	0.59
1:G:235:GLU:OE2	1:G:238:LYS:NZ	2.35	0.59
3:J:233:ILE:O	3:J:234:ASP:HB2	2.03	0.59
3:J:102:ARG:O	3:J:103:GLU:C	2.43	0.58
3:J:173:LYS:O	3:J:174:GLU:C	2.33	0.58
1:F:235:GLU:OE2	1:F:238:LYS:NZ	2.36	0.58
1:I:41:ARG:O	1:I:70:SER:N	2.32	0.58
1:E:48:MET:HB3	1:G:173:GLY:HA2	1.85	0.58
3:J:152:TYR:O	3:J:154:GLY:N	2.36	0.57
3:J:164:LEU:C	3:J:165:PRO:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ALA:O	1:F:116:ASN:ND2	2.37	0.57
1:E:235:GLU:OE2	1:E:238:LYS:NZ	2.37	0.57
3:J:248:TYR:O	3:J:249:PRO:C	2.34	0.57
9:p:25:LEU:CB	9:p:26:PRO:CD	2.83	0.57
3:J:84:PRO:O	3:J:85:ARG:C	2.38	0.57
1:E:354:LYS:O	1:E:357:TRP:NE1	2.38	0.56
1:D:238:LYS:HA	1:D:252:GLY:HA2	1.87	0.56
1:D:354:LYS:O	1:D:357:TRP:NE1	2.39	0.56
3:J:308:GLY:O	3:J:309:THR:C	2.33	0.55
3:J:115:VAL:O	3:J:115:VAL:HG13	2.07	0.55
3:J:333:LYS:O	3:J:334:LYS:C	2.39	0.55
1:I:114:PRO:O	1:I:182:ARG:NH1	2.40	0.54
3:J:182:GLN:O	3:J:183:CYS:HB2	2.07	0.54
3:J:204:GLU:O	3:J:205:GLY:C	2.46	0.54
1:C:151:GLY:HA2	9:q:57:PHE:HE1	1.72	0.54
3:J:346:PRO:CB	3:J:347:PRO:HD2	2.35	0.54
3:J:349:LYS:O	3:J:350:ALA:C	2.47	0.54
3:J:346:PRO:HB2	3:J:348:ALA:H	1.72	0.54
3:J:94:SER:OG	3:J:97:CYS:N	2.40	0.54
1:I:360:LYS:NZ	1:I:364:GLU:OE2	2.41	0.54
3:J:357:GLY:HA2	3:J:360:ILE:HD12	1.90	0.53
3:J:182:GLN:O	3:J:183:CYS:CB	2.44	0.53
6:M:163:GLN:OE1	6:M:163:GLN:N	2.42	0.53
1:F:268:ILE:O	1:G:178:HIS:CD2	2.62	0.53
1:A:235:GLU:OE2	1:A:238:LYS:NZ	2.41	0.53
1:I:366:ASP:O	1:I:369:ARG:NH1	2.41	0.53
7:N:261:GLN:OE1	8:O:225:ARG:NH1	2.42	0.53
9:p:25:LEU:HB2	9:p:26:PRO:HD2	1.91	0.52
3:J:155:ILE:HG22	3:J:156:PRO:O	2.10	0.52
3:J:142:GLY:O	3:J:143:TYR:C	2.51	0.52
3:J:22:GLU:C	3:J:24:PHE:N	2.65	0.52
1:B:2356:LYS:O	1:B:2359:TRP:NE1	2.43	0.52
3:J:165:PRO:CB	3:J:166:LEU:HA	2.39	0.52
1:B:2237:GLU:OE2	1:B:2240:LYS:NZ	2.43	0.52
3:J:109:LEU:C	3:J:110:PHE:O	2.27	0.52
2:H:303:THR:O	2:H:303:THR:HG22	2.09	0.52
3:J:149:LEU:O	3:J:150:PRO:C	2.52	0.51
3:J:386:ASP:O	3:J:387:TRP:C	2.48	0.51
3:J:166:LEU:CB	3:J:167:GLY:HA2	2.32	0.51
3:J:225:LYS:O	3:J:226:ILE:C	2.44	0.51
1:F:245:ASP:OD1	1:F:246:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:LYS:O	1:F:357:TRP:NE1	2.43	0.51
3:J:239:ARG:NH1	3:J:240:PRO:O	2.43	0.51
1:E:201:GLU:OE2	1:F:118:ARG:NH2	2.44	0.51
1:D:48:MET:HB3	1:F:173:GLY:HA2	1.93	0.51
7:N:175:SER:OG	7:N:177:TRP:NE1	2.44	0.51
1:A:354:LYS:O	1:A:357:TRP:NE1	2.44	0.50
3:J:59:ILE:O	3:J:60:ASN:C	2.51	0.50
3:J:222:ARG:O	3:J:223:GLY:C	2.50	0.50
3:J:27:CYS:O	3:J:37:CYS:N	2.40	0.50
3:J:340:THR:OG1	3:J:341:PHE:N	2.44	0.50
9:p:25:LEU:HB3	9:p:26:PRO:HD3	1.93	0.50
3:J:43:ILE:HA	3:J:44:LYS:HB2	1.94	0.50
3:J:155:ILE:O	3:J:156:PRO:C	2.46	0.50
6:M:169:LYS:O	6:M:173:ASN:ND2	2.44	0.50
3:J:22:GLU:C	3:J:24:PHE:H	2.19	0.50
3:J:280:VAL:CG1	3:J:281:ALA:N	2.75	0.50
1:A:245:ASP:OD1	1:A:246:GLY:N	2.44	0.50
3:J:21:GLY:O	3:J:24:PHE:CD1	2.65	0.50
3:J:282:THR:O	3:J:283:LEU:HB2	2.12	0.50
3:J:344:HIS:CE1	4:K:221:ALA:HB2	2.47	0.49
1:I:7:ILE:HG22	1:I:9:ASN:H	1.76	0.49
1:G:245:ASP:OD1	1:G:246:GLY:N	2.45	0.49
3:J:57:TYR:O	3:J:58:ASN:HB2	2.13	0.49
3:J:75:LEU:O	3:J:76:TYR:C	2.50	0.49
3:J:166:LEU:CB	3:J:167:GLY:CA	2.90	0.49
6:M:157:PRO:O	6:M:158:GLN:C	2.55	0.49
3:J:18:ILE:HG21	3:J:91:ILE:H	1.77	0.49
5:L:37:ASN:OD1	5:L:38:GLY:N	2.46	0.49
1:F:360:LYS:NZ	1:F:364:GLU:OE2	2.44	0.48
3:J:288:LEU:O	3:J:289:ILE:C	2.51	0.48
3:J:144:ARG:CG	3:J:144:ARG:O	2.59	0.48
1:G:360:LYS:NZ	1:G:364:GLU:OE2	2.44	0.48
1:C:151:GLY:HA2	9:q:57:PHE:CE1	2.48	0.48
3:J:281:ALA:C	3:J:282:THR:O	2.51	0.48
1:A:7:ILE:HG22	1:A:9:ASN:H	1.78	0.47
1:F:114:PRO:O	1:F:182:ARG:NH1	2.47	0.47
1:I:305:THR:OG1	1:I:336:ARG:NE	2.46	0.47
3:J:252:GLY:O	3:J:253:GLU:HB2	2.14	0.47
9:p:25:LEU:HB3	9:p:26:PRO:CD	2.44	0.47
1:B:2111:LEU:C	1:B:2111:LEU:HD23	2.39	0.47
1:F:109:LEU:HD23	1:F:109:LEU:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ARG:NH1	9:P:73:ILE:O	2.47	0.47
1:D:109:LEU:C	1:D:109:LEU:HD23	2.40	0.47
1:E:109:LEU:C	1:E:109:LEU:HD23	2.40	0.47
2:H:253:GLU:OE1	2:H:253:GLU:N	2.44	0.47
2:H:257:CYS:N	2:H:258:PRO:HD2	2.29	0.47
3:J:74:ILE:O	3:J:75:LEU:C	2.47	0.47
3:J:144:ARG:O	3:J:144:ARG:HG3	2.14	0.47
3:J:329:LYS:CB	3:J:330:PRO:HD2	2.43	0.47
1:A:360:LYS:NZ	1:A:364:GLU:OE2	2.46	0.47
3:J:194:SER:HB2	3:J:197:SER:H	1.80	0.47
1:B:2362:LYS:NZ	1:B:2366:GLU:OE2	2.48	0.47
1:C:109:LEU:C	1:C:109:LEU:HD23	2.40	0.47
1:E:258:ALA:N	1:E:259:PRO:HD2	2.30	0.47
3:J:164:LEU:HB3	3:J:165:PRO:O	2.13	0.47
6:M:171:LEU:N	6:M:172:PRO:HD2	2.29	0.47
1:C:245:ASP:OD1	1:C:246:GLY:N	2.48	0.46
3:J:329:LYS:HB3	3:J:330:PRO:HD2	1.96	0.46
1:D:258:ALA:N	1:D:259:PRO:HD2	2.31	0.46
7:N:203:ASN:O	8:O:191:GLY:HA2	2.16	0.46
1:B:2220:LYS:NZ	10:B:2401:ADP:O2'	2.49	0.46
1:E:245:ASP:OD1	1:E:246:GLY:N	2.48	0.46
3:J:206:VAL:O	3:J:207:LEU:C	2.42	0.46
1:E:371:ILE:O	1:E:375:THR:OG1	2.28	0.46
1:I:109:LEU:C	1:I:109:LEU:HD23	2.41	0.46
3:J:230:LYS:O	3:J:232:ASN:N	2.48	0.46
1:C:38:TYR:CD1	1:C:38:TYR:C	2.93	0.46
1:D:334:GLN:OE1	9:p:14:ARG:NH1	2.49	0.46
1:G:183:ILE:HG22	1:G:185:ILE:H	1.80	0.46
3:J:83:ASN:N	3:J:84:PRO:CD	2.77	0.46
3:J:282:THR:C	3:J:284:ILE:H	2.22	0.46
1:D:335:GLU:O	1:D:335:GLU:HG2	2.15	0.46
3:J:293:ILE:O	3:J:294:ASP:C	2.52	0.46
3:J:361:PHE:O	3:J:364:LEU:HB3	2.15	0.46
1:E:236:THR:OG1	1:E:255:ARG:NH2	2.46	0.45
3:J:19:ASP:O	3:J:20:LEU:HD23	2.16	0.45
3:J:214:THR:O	3:J:263:ARG:HD2	2.17	0.45
1:B:2040:TYR:CD1	1:B:2040:TYR:C	2.94	0.45
1:I:136:ALA:HB1	1:I:357:TRP:CE3	2.51	0.45
1:F:258:ALA:N	1:F:259:PRO:HD2	2.31	0.45
2:H:104:LEU:C	2:H:104:LEU:HD23	2.41	0.45
1:I:354:LYS:HA	1:I:357:TRP:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:279:SER:O	3:J:280:VAL:C	2.50	0.45
7:N:61:GLN:HE22	7:N:172:ARG:HH21	1.63	0.45
3:J:273:GLN:NE2	3:J:276:GLU:O	2.49	0.45
3:J:353:VAL:HG12	3:J:353:VAL:O	2.14	0.45
3:J:368:LEU:O	3:J:372:SER:OG	2.24	0.45
1:D:287:ASP:OD1	1:D:288:MET:N	2.49	0.45
1:E:38:TYR:CD1	1:E:38:TYR:C	2.95	0.45
7:N:62:PHE:N	7:N:62:PHE:CD1	2.85	0.45
5:L:85:LEU:HD23	5:L:85:LEU:C	2.41	0.45
1:A:305:THR:O	1:A:336:ARG:NH1	2.49	0.45
1:B:2289:ASP:OD1	1:B:2290:MET:N	2.48	0.45
1:I:38:TYR:CD1	1:I:38:TYR:C	2.95	0.45
3:J:100:HIS:HB2	3:J:101:PHE:HA	1.99	0.45
6:M:95:TYR:OH	6:M:97:GLN:NE2	2.49	0.45
1:A:258:ALA:N	1:A:259:PRO:HD2	2.32	0.45
1:D:38:TYR:CD1	1:D:38:TYR:C	2.94	0.45
1:D:371:ILE:O	1:D:375:THR:OG1	2.32	0.45
8:O:219:ASP:OD2	8:O:223:LYS:NZ	2.50	0.45
1:C:296:SER:O	1:C:329:ARG:HB2	2.16	0.45
1:E:305:THR:OG1	1:E:336:ARG:HD3	2.17	0.45
3:J:146:SER:N	3:J:164:LEU:O	2.48	0.45
1:E:368:ALA:O	1:E:371:ILE:HG12	2.18	0.44
1:F:232:GLU:OE1	9:P:73:ILE:N	2.49	0.44
9:P:6:TYR:CD1	9:P:6:TYR:C	2.95	0.44
1:D:245:ASP:OD1	1:D:246:GLY:N	2.51	0.44
1:B:2247:ASP:OD1	1:B:2248:GLY:N	2.50	0.44
1:C:136:ALA:HB1	1:C:357:TRP:CE3	2.52	0.44
1:E:363:TYR:O	1:E:367:GLY:HA2	2.17	0.44
2:H:257:CYS:HB3	2:H:258:PRO:HD3	1.98	0.44
7:N:224:THR:HG22	7:N:228:PHE:CE2	2.52	0.44
1:I:145:LEU:HD22	1:I:344:GLY:HA2	2.00	0.44
3:J:248:TYR:CD2	3:J:249:PRO:O	2.70	0.44
3:J:329:LYS:C	3:J:331:LYS:N	2.73	0.44
1:I:334:GLN:OE1	1:I:334:GLN:N	2.48	0.44
1:B:2050:MET:HB3	1:D:173:GLY:HA2	1.99	0.44
1:D:360:LYS:NZ	1:D:364:GLU:OE2	2.49	0.44
1:D:368:ALA:O	1:D:371:ILE:HG12	2.18	0.44
7:N:179:PHE:CD2	7:N:228:PHE:CD1	3.05	0.44
1:D:154:THR:O	1:D:297:ASN:ND2	2.51	0.44
1:A:154:THR:O	1:A:297:ASN:ND2	2.52	0.43
1:C:101:THR:OG1	1:C:106:HIS:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:PRO:O	1:D:336:ARG:HG3	2.18	0.43
3:J:243:PRO:HA	3:J:244:PRO:HD3	1.76	0.43
1:B:2035:TYR:CD2	1:B:2100:GLN:HA	2.53	0.43
1:B:2260:ALA:N	1:B:2261:PRO:HD2	2.33	0.43
1:F:44:HIS:CE1	2:H:171:LEU:HG	2.53	0.43
1:B:2349:LEU:C	1:B:2349:LEU:HD23	2.44	0.43
1:I:258:ALA:N	1:I:259:PRO:HD2	2.34	0.43
1:D:113:ALA:O	1:D:116:ASN:ND2	2.51	0.43
1:A:324:LYS:NZ	1:A:325:ASP:OD1	2.48	0.43
1:C:9:ASN:ND2	1:C:105:GLU:O	2.52	0.43
6:M:170:ILE:HG23	6:M:174:TYR:CE2	2.54	0.43
7:N:99:ASP:O	7:N:103:LYS:N	2.52	0.42
1:A:357:TRP:C	1:A:357:TRP:CD1	2.98	0.42
1:B:2363:LYS:NZ	1:B:2367:GLU:OE2	2.50	0.42
2:H:361:GLU:OE1	2:H:373:LYS:NZ	2.52	0.42
6:M:165:ASP:OD1	6:M:169:LYS:NZ	2.52	0.42
7:N:94:ILE:C	7:N:94:ILE:HD12	2.44	0.42
1:C:361:LYS:NZ	1:C:365:GLU:OE2	2.47	0.42
1:E:360:LYS:NZ	1:E:364:GLU:OE2	2.50	0.42
1:F:229:GLN:OE1	1:F:229:GLN:N	2.49	0.42
1:F:137:LEU:C	1:F:137:LEU:HD23	2.45	0.42
3:J:179:LEU:O	3:J:182:GLN:HG2	2.19	0.42
1:C:47:VAL:HG23	1:C:48:MET:N	2.34	0.42
1:C:136:ALA:CB	1:C:357:TRP:CE3	3.02	0.42
1:D:145:LEU:HD22	1:D:344:GLY:HA2	2.02	0.42
1:G:258:ALA:N	1:G:259:PRO:HD2	2.34	0.42
7:N:269:ILE:O	7:N:269:ILE:HG23	2.19	0.42
3:J:71:PHE:O	3:J:74:ILE:HB	2.20	0.42
3:J:368:LEU:O	3:J:369:GLY:C	2.39	0.42
1:G:363:TYR:O	1:G:367:GLY:N	2.50	0.42
6:M:108:GLU:OE1	6:M:126:GLY:HA2	2.19	0.42
1:C:354:LYS:HA	1:C:357:TRP:HE1	1.85	0.42
1:D:47:VAL:HG23	1:D:48:MET:N	2.34	0.42
1:F:361:LYS:NZ	1:F:365:GLU:OE2	2.50	0.42
3:J:72:ILE:O	3:J:73:HIS:O	2.38	0.42
3:J:300:ALA:O	3:J:301:GLU:HB2	2.18	0.42
1:F:38:TYR:CD1	1:F:38:TYR:C	2.98	0.41
1:C:144:VAL:HG23	1:C:145:LEU:N	2.35	0.41
1:C:368:ALA:O	1:C:371:ILE:HG12	2.21	0.41
1:G:38:TYR:CD1	1:G:38:TYR:C	2.98	0.41
3:J:92:ILE:O	3:J:122:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:LEU:HB3	3:J:133:ILE:O	2.20	0.41
5:L:6:LEU:N	5:L:175:LYS:O	2.52	0.41
1:E:225:SER:OG	1:E:231:ASP:OD2	2.30	0.41
1:B:2359:TRP:HD1	1:B:2359:TRP:O	2.04	0.41
1:C:113:ALA:O	1:C:116:ASN:ND2	2.53	0.41
1:F:357:TRP:C	1:F:357:TRP:CD1	2.98	0.41
1:I:276:HIS:CE1	1:I:277:GLU:HG2	2.56	0.41
3:J:21:GLY:C	3:J:23:ALA:N	2.63	0.41
1:B:2049:VAL:HG23	1:B:2050:MET:N	2.35	0.41
1:E:357:TRP:CD1	1:E:357:TRP:C	2.97	0.41
3:J:314:GLY:O	3:J:315:PHE:O	2.38	0.41
9:P:3:ASP:HB2	9:P:4:PRO:CD	2.50	0.41
3:J:391:ASN:O	3:J:393:PRO:N	2.52	0.41
1:I:38:TYR:CG	1:I:71:ILE:HG23	2.56	0.41
3:J:386:ASP:OD1	3:J:387:TRP:N	2.53	0.41
9:p:25:LEU:CB	9:p:26:PRO:HD2	2.50	0.41
1:F:48:MET:CG	2:H:168:GLY:HA2	2.51	0.41
1:F:363:TYR:O	1:F:367:GLY:N	2.52	0.41
1:I:20:VAL:O	1:I:20:VAL:HG23	2.21	0.41
3:J:78:ARG:O	3:J:79:HIS:C	2.60	0.41
1:C:375:THR:O	1:C:376:PHE:HB3	2.21	0.41
7:N:197:HIS:NE2	7:N:203:ASN:OD1	2.52	0.41
1:C:258:ALA:N	1:C:259:PRO:HD2	2.36	0.40
1:E:50:GLY:HA2	9:P:60:LYS:CD	2.48	0.40
1:F:226:ILE:HG23	1:F:227:ASN:N	2.36	0.40
2:H:64:ILE:HG13	2:H:65:LEU:N	2.36	0.40
3:J:57:TYR:O	3:J:58:ASN:C	2.63	0.40
2:H:244:ASP:OD1	2:H:245:GLY:N	2.53	0.40
1:I:229:GLN:OE1	1:I:229:GLN:N	2.50	0.40
3:J:55:VAL:C	3:J:56:GLN:N	2.80	0.40
4:K:393:ALA:N	4:K:401:GLY:O	2.54	0.40
7:N:246:ASN:HD21	8:O:184:SER:CB	2.35	0.40
1:F:128:PHE:O	1:F:132:PHE:O	2.39	0.40
3:J:240:PRO:O	3:J:241:SER:C	2.61	0.40
3:J:288:LEU:O	3:J:290:GLN:N	2.55	0.40
1:G:48:MET:SD	1:I:173:GLY:HA2	2.62	0.40
3:J:39:ILE:C	3:J:40:PRO:O	2.47	0.40
1:B:2020:SER:O	1:B:2190:ARG:NH2	2.55	0.40
8:O:97:GLU:O	8:O:101:ASN:ND2	2.49	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	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	373/376 (99%)	365 (98%)	8 (2%)	0	100	100
1	D	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	E	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	F	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	379/417 (91%)	357 (94%)	19 (5%)	3 (1%)	16	49
4	K	349/460 (76%)	342 (98%)	7 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	3 (2%)	1 (1%)	21	53
6	M	152/190 (80%)	145 (95%)	7 (5%)	0	100	100
7	N	284/286 (99%)	279 (98%)	5 (2%)	0	100	100
8	O	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
9	P	70/401 (18%)	65 (93%)	4 (6%)	1 (1%)	9	38
9	Q	22/401 (6%)	21 (96%)	1 (4%)	0	100	100
9	p	33/401 (8%)	28 (85%)	4 (12%)	1 (3%)	3	25
9	q	44/401 (11%)	42 (96%)	2 (4%)	0	100	100
All	All	5097/6794 (75%)	4935 (97%)	156 (3%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	p	25	LEU

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Mol	Chain	Res	Type
3	J	23	ALA
3	J	145	GLU
5	L	179	LEU
9	P	10	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/324 (98%)	318 (100%)	0	100	100
1	B	318/324 (98%)	318 (100%)	0	100	100
1	C	323/324 (100%)	323 (100%)	0	100	100
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	318 (100%)	0	100	100
1	F	318/324 (98%)	318 (100%)	0	100	100
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	318/324 (98%)	318 (100%)	0	100	100
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	339/363 (93%)	339 (100%)	0	100	100
4	K	330/412 (80%)	330 (100%)	0	100	100
5	L	163/163 (100%)	163 (100%)	0	100	100
6	M	132/164 (80%)	132 (100%)	0	100	100
7	N	252/252 (100%)	252 (100%)	0	100	100
8	O	238/241 (99%)	238 (100%)	0	100	100
9	P	64/343 (19%)	64 (100%)	0	100	100
9	Q	21/343 (6%)	21 (100%)	0	100	100
9	p	30/343 (9%)	30 (100%)	0	100	100
9	q	43/343 (12%)	43 (100%)	0	100	100
All	All	4474/5877 (76%)	4474 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	C	29	GLN
1	C	44	HIS
1	C	133	ASN
1	E	284	GLN
1	F	91	GLN
1	F	133	ASN
1	F	284	GLN
1	G	120	ASN
2	H	40	HIS
2	H	128	ASN
1	I	133	ASN
1	I	166	HIS
3	J	73	HIS
4	K	81	HIS
4	K	266	HIS
5	L	60	HIS
5	L	103	GLN
7	N	246	ASN
8	O	20	GLN
8	O	178	GLN
8	O	180	ASN
8	O	188	ASN
8	O	196	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ADP	A	800	-	28,29,29	0.44	0	43,45,45	0.43	0
10	ADP	I	800	-	28,29,29	0.47	0	43,45,45	0.44	0
10	ADP	G	800	-	28,29,29	0.43	0	43,45,45	0.43	0
11	ANP	H	401	-	33,33,33	1.94	9 (27%)	45,52,52	1.99	15 (33%)
10	ADP	C	800	-	28,29,29	0.47	0	43,45,45	0.44	0
10	ADP	B	2401	-	28,29,29	0.45	0	43,45,45	0.43	0
10	ADP	F	800	-	28,29,29	0.46	0	43,45,45	0.44	0
10	ADP	D	800	-	28,29,29	0.44	0	43,45,45	0.45	0
10	ADP	E	800	-	28,29,29	0.43	0	43,45,45	0.44	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
10	ADP	A	800	-	-	7/16/32/32	0/3/3/3
10	ADP	I	800	-	-	4/16/32/32	0/3/3/3
10	ADP	G	800	-	-	4/16/32/32	0/3/3/3
11	ANP	H	401	-	-	7/18/38/38	0/3/3/3
10	ADP	C	800	-	-	4/16/32/32	0/3/3/3
10	ADP	B	2401	-	-	3/16/32/32	0/3/3/3
10	ADP	F	800	-	-	4/16/32/32	0/3/3/3
10	ADP	D	800	-	-	4/16/32/32	0/3/3/3
10	ADP	E	800	-	-	4/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	401	ANP	C5-C4	5.01	1.48	1.39
11	H	401	ANP	PG-N3B	4.34	1.74	1.63
11	H	401	ANP	PG-O1G	3.93	1.52	1.46
11	H	401	ANP	PB-N3B	3.58	1.72	1.63
11	H	401	ANP	PB-O1B	3.43	1.51	1.46
11	H	401	ANP	C8-N7	2.74	1.37	1.31
11	H	401	ANP	C5-C6	2.64	1.48	1.41
11	H	401	ANP	PB-O2B	-2.38	1.50	1.56
11	H	401	ANP	C4-N9	-2.37	1.32	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	401	ANP	C5-C4-N3	-5.14	119.64	126.72
11	H	401	ANP	N3-C4-N9	4.53	134.88	127.17
11	H	401	ANP	C4-N9-C8	3.94	109.88	105.74
11	H	401	ANP	C2-N3-C4	3.74	120.95	111.83
11	H	401	ANP	N3-C2-N1	-3.60	123.13	128.58
11	H	401	ANP	O1B-PB-N3B	-3.48	106.65	111.77
11	H	401	ANP	O1G-PG-N3B	-2.76	107.70	111.77
11	H	401	ANP	C4-C5-N7	-2.72	107.47	110.58
11	H	401	ANP	O2A-PA-O1A	2.65	124.77	112.44
11	H	401	ANP	O2B-PB-O1B	2.64	115.52	109.87
11	H	401	ANP	N9-C8-N7	-2.40	110.54	113.94
11	H	401	ANP	O3A-PB-N3B	2.23	112.77	106.59
11	H	401	ANP	C6-C5-N7	2.21	136.35	132.09
11	H	401	ANP	O2G-PG-O3G	2.03	113.06	107.59
11	H	401	ANP	C5-N7-C8	2.02	106.62	103.45

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	800	ADP	PA-O3A-PB-O2B
10	A	800	ADP	PA-O3A-PB-O3B
10	A	800	ADP	C5'-O5'-PA-O1A
10	A	800	ADP	C5'-O5'-PA-O3A
10	C	800	ADP	C5'-O5'-PA-O1A
10	C	800	ADP	C5'-O5'-PA-O3A
10	D	800	ADP	C5'-O5'-PA-O3A
10	E	800	ADP	C5'-O5'-PA-O1A
10	E	800	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
10	F	800	ADP	C5'-O5'-PA-O1A
10	G	800	ADP	C5'-O5'-PA-O3A
10	I	800	ADP	C5'-O5'-PA-O1A
10	I	800	ADP	C5'-O5'-PA-O3A
11	H	401	ANP	PB-N3B-PG-O1G
11	H	401	ANP	PG-N3B-PB-O1B
11	H	401	ANP	PG-N3B-PB-O3A
11	H	401	ANP	C5'-O5'-PA-O2A
10	A	800	ADP	C3'-C4'-C5'-O5'
10	D	800	ADP	C3'-C4'-C5'-O5'
10	E	800	ADP	C3'-C4'-C5'-O5'
10	F	800	ADP	C3'-C4'-C5'-O5'
10	G	800	ADP	C3'-C4'-C5'-O5'
10	C	800	ADP	C3'-C4'-C5'-O5'
10	D	800	ADP	O4'-C4'-C5'-O5'
10	I	800	ADP	C3'-C4'-C5'-O5'
10	B	2401	ADP	C3'-C4'-C5'-O5'
11	H	401	ANP	PB-O3A-PA-O1A
10	E	800	ADP	O4'-C4'-C5'-O5'
10	F	800	ADP	O4'-C4'-C5'-O5'
10	A	800	ADP	O4'-C4'-C5'-O5'
10	C	800	ADP	O4'-C4'-C5'-O5'
10	G	800	ADP	O4'-C4'-C5'-O5'
10	I	800	ADP	O4'-C4'-C5'-O5'
10	B	2401	ADP	O4'-C4'-C5'-O5'
10	B	2401	ADP	PA-O3A-PB-O1B
10	D	800	ADP	C5'-O5'-PA-O1A
10	F	800	ADP	C5'-O5'-PA-O3A
10	G	800	ADP	C5'-O5'-PA-O1A
11	H	401	ANP	PB-O3A-PA-O2A
11	H	401	ANP	O4'-C4'-C5'-O5'
10	A	800	ADP	PA-O3A-PB-O1B

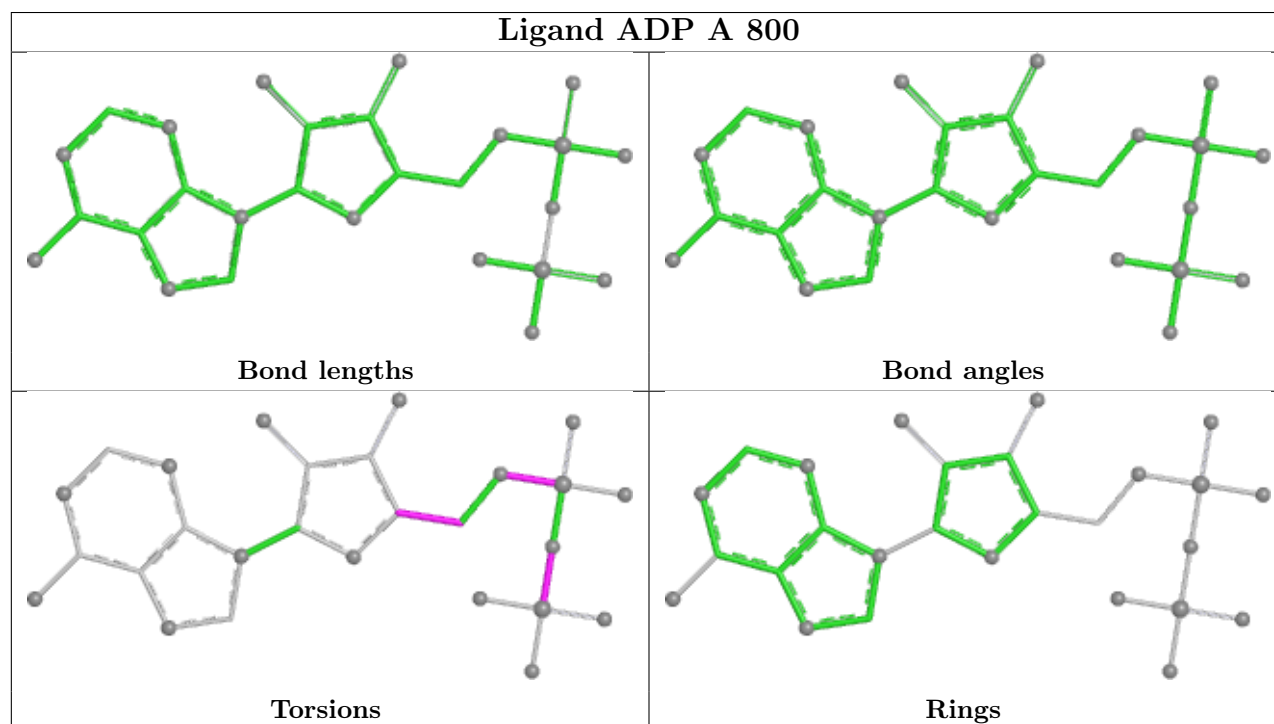
There are no ring outliers.

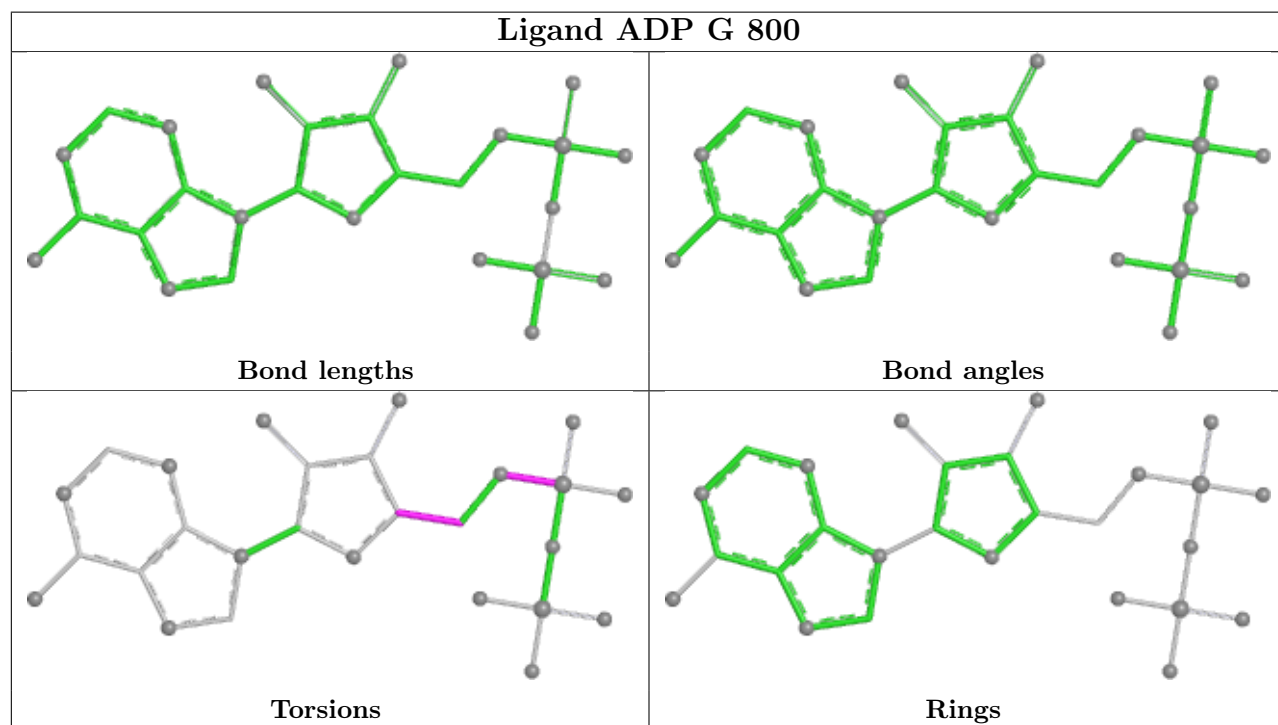
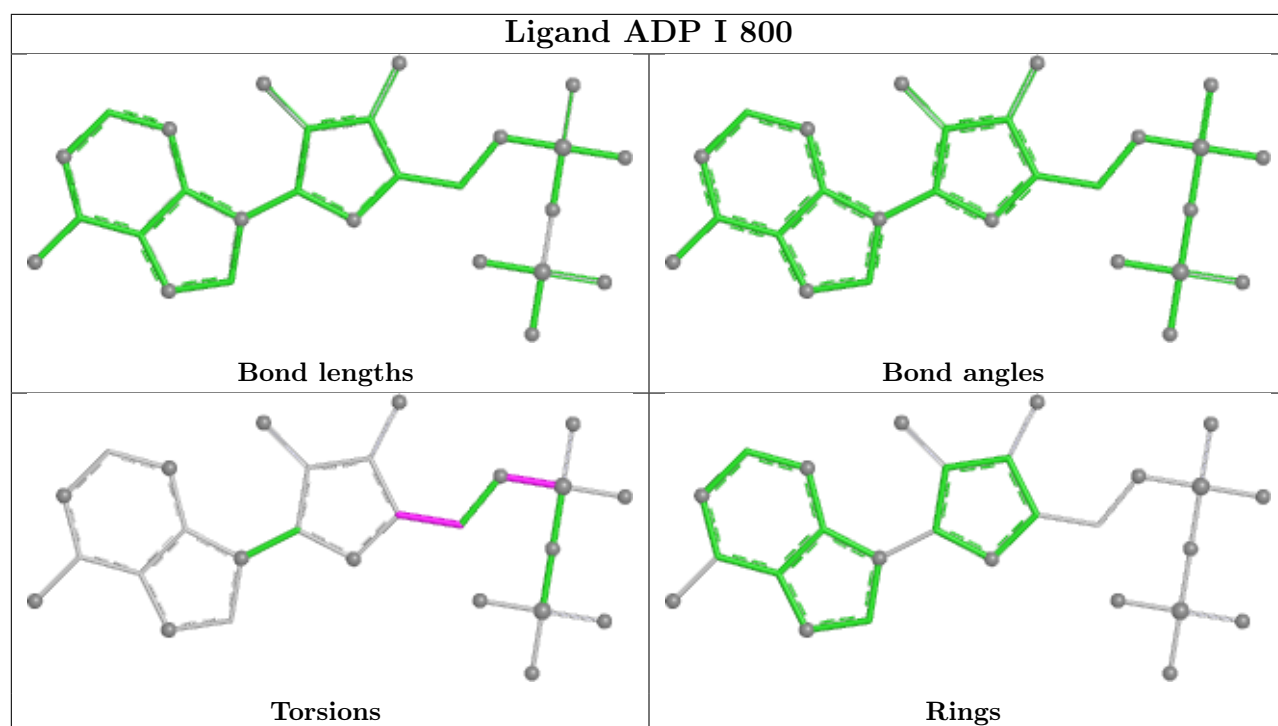
1 monomer is involved in 1 short contact:

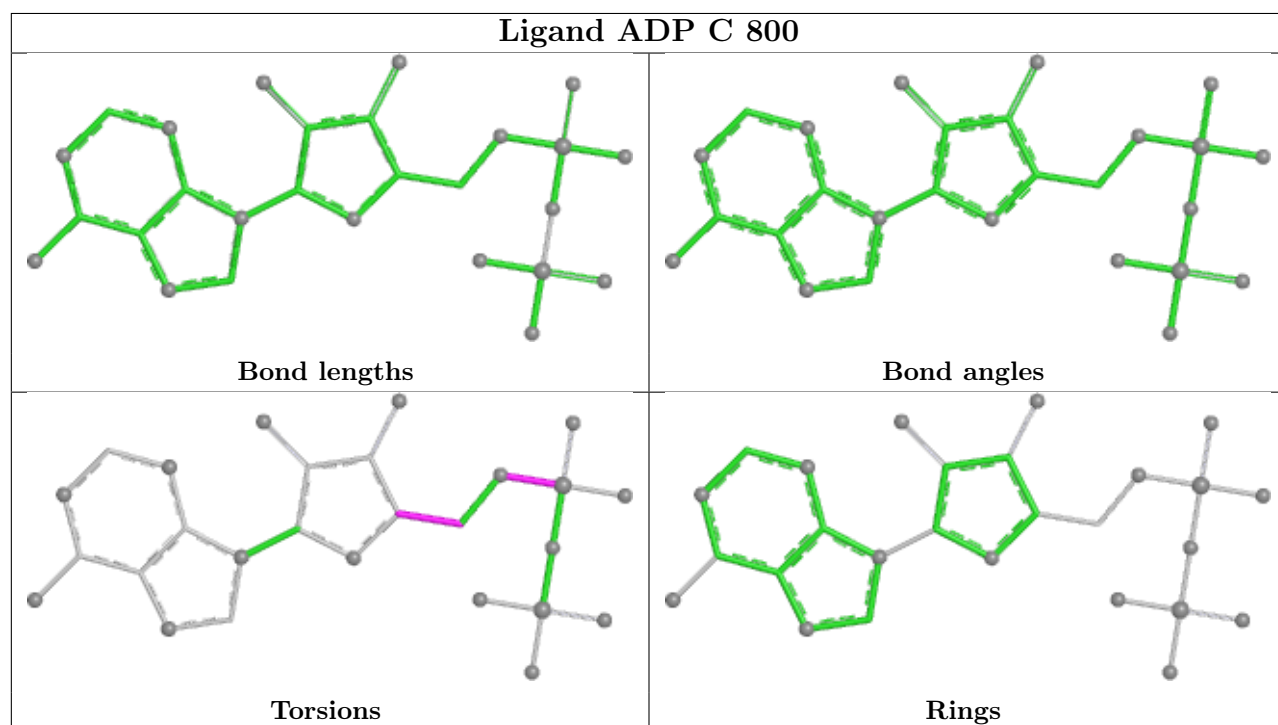
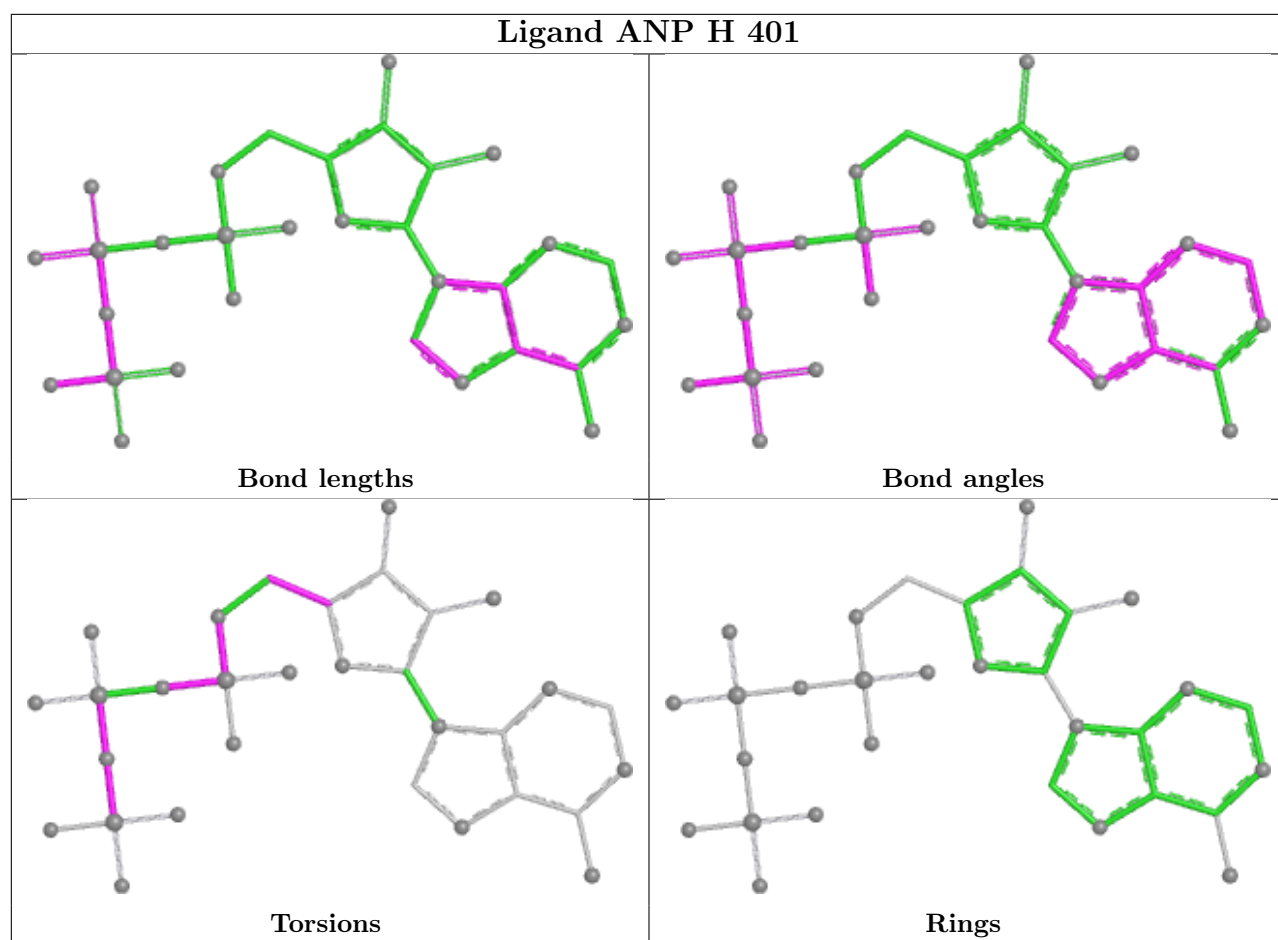
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2401	ADP	1	0

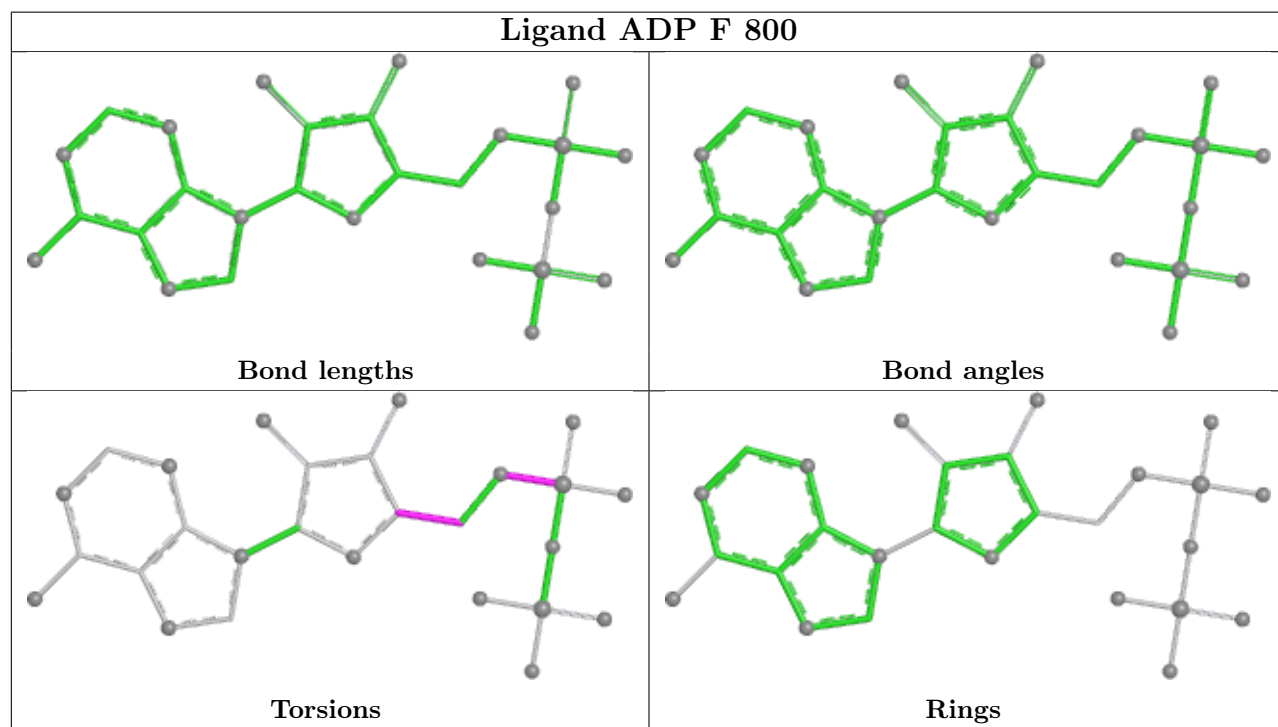
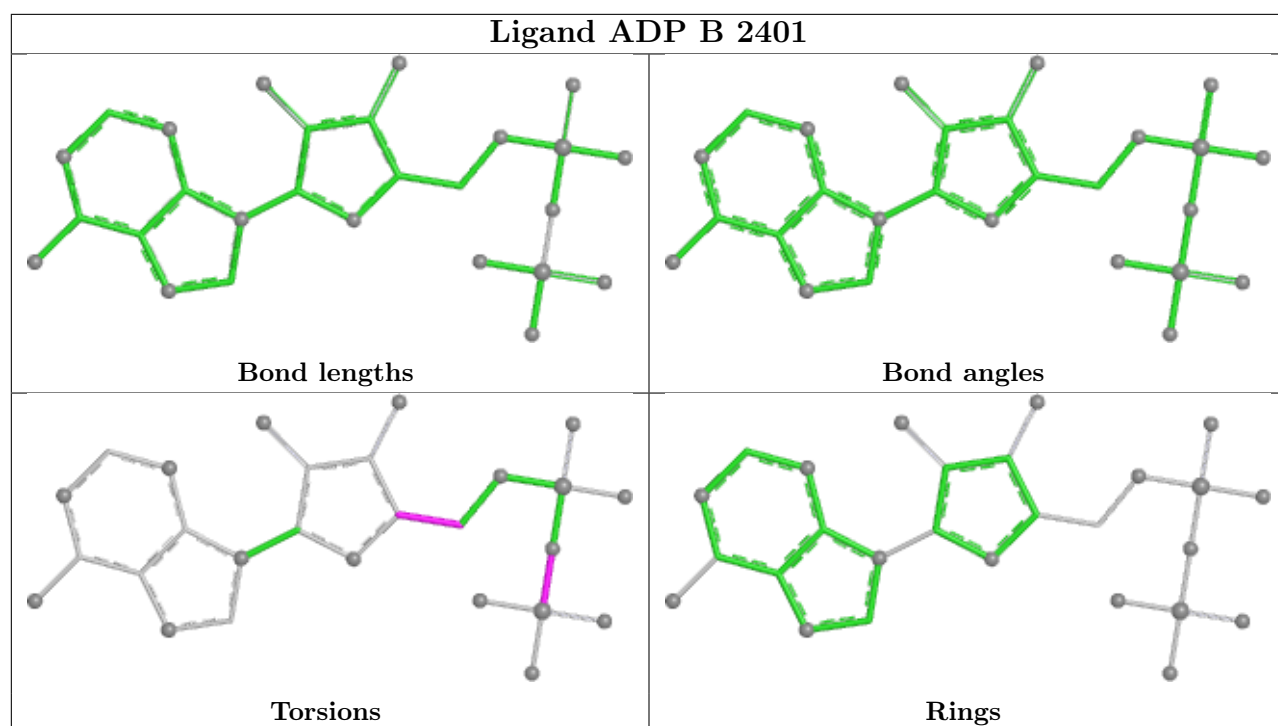
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

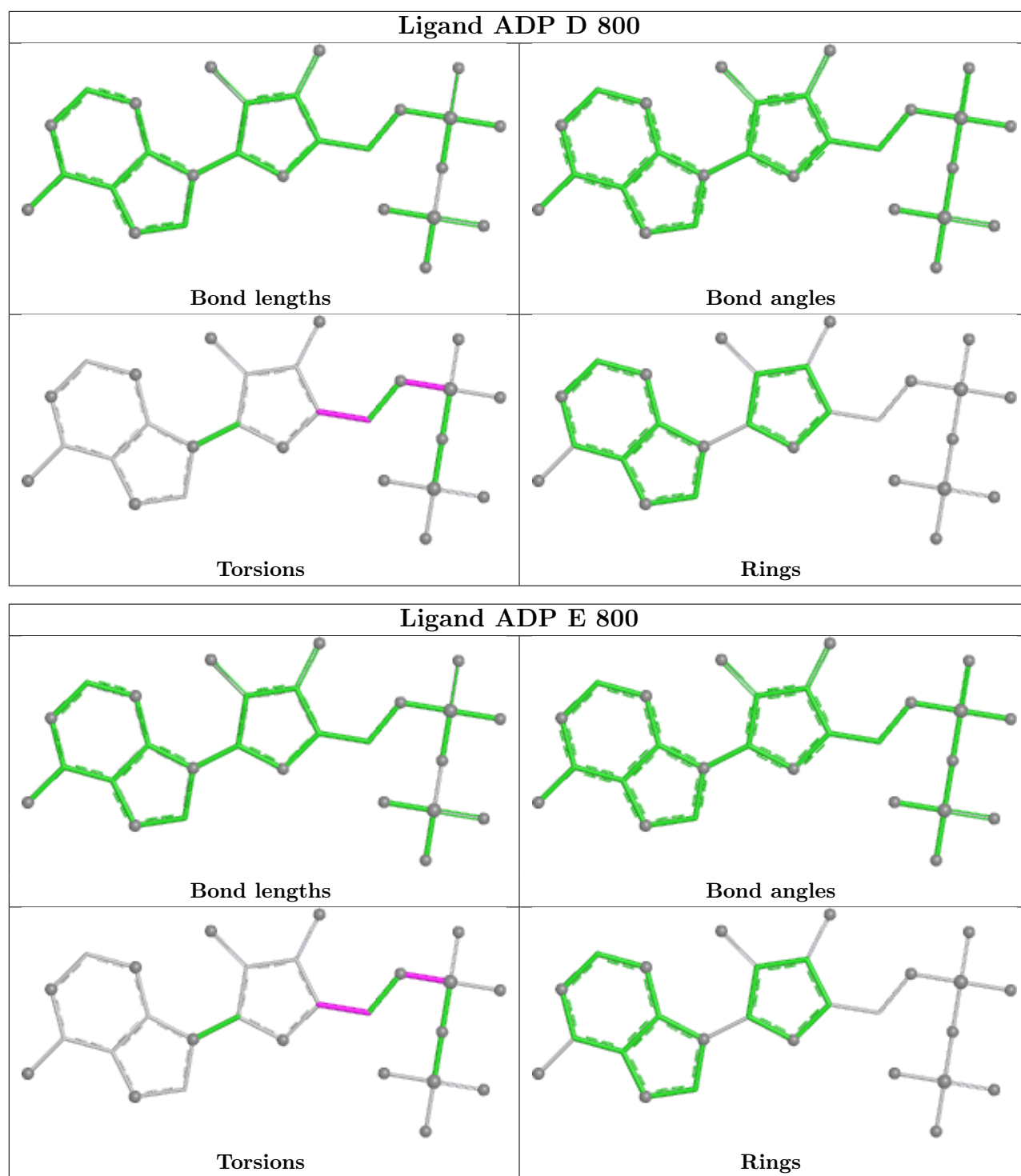
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	94:SER	C	95:VAL	N	3.80
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.80
1	J	329:LYS	C	330:PRO	N	1.20
1	J	89:VAL	C	90:VAL	N	1.19
1	J	101:PHE	C	102:ARG	N	1.19
1	J	185:VAL	C	186:ASP	N	1.19
1	J	322:GLU	C	323:ILE	N	1.19
1	J	356:LEU	C	357:GLY	N	1.18

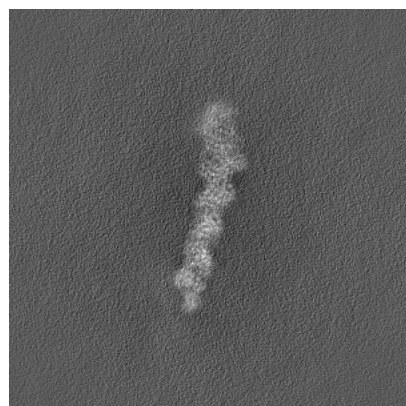
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44333. These allow visual inspection of the internal detail of the map and identification of artifacts.

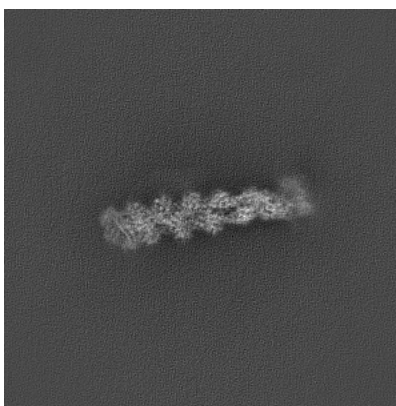
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

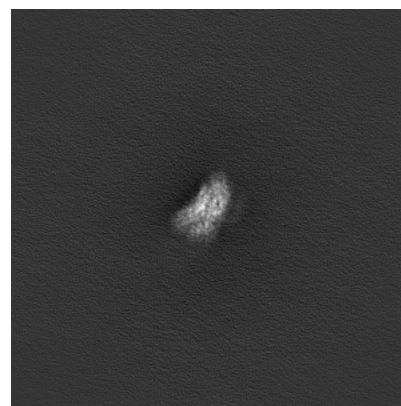
6.1.1 Primary map



X

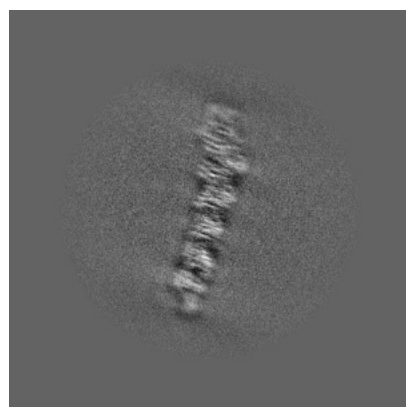


Y

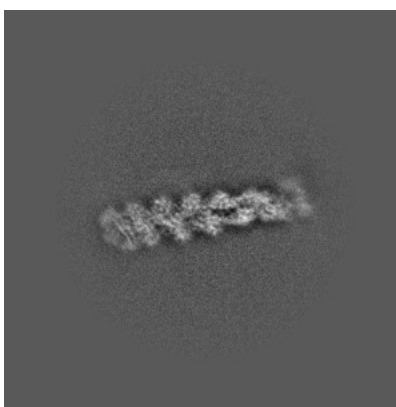


Z

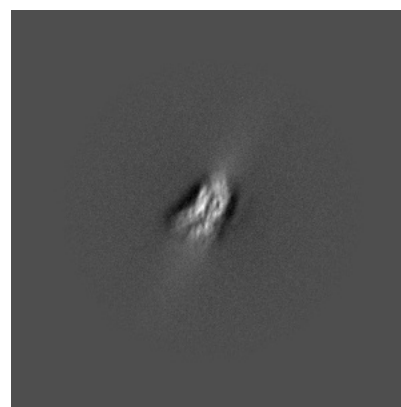
6.1.2 Raw map



X



Y



Z

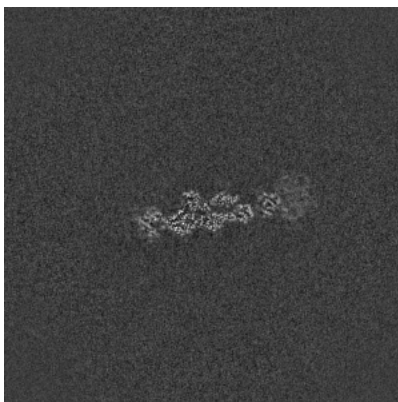
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

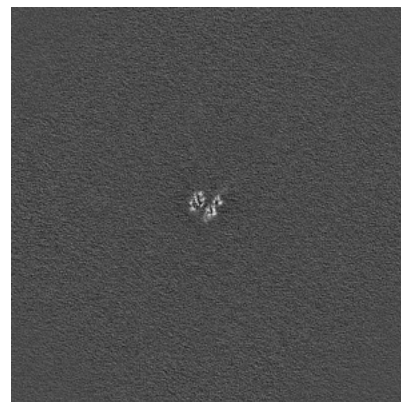
6.2.1 Primary map



X Index: 432

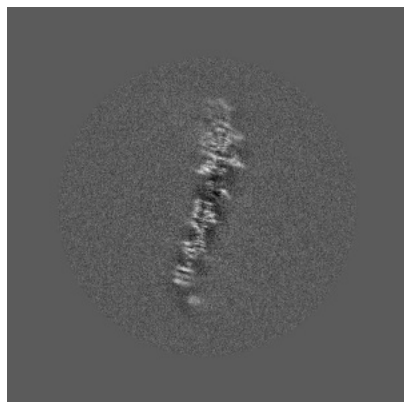


Y Index: 432

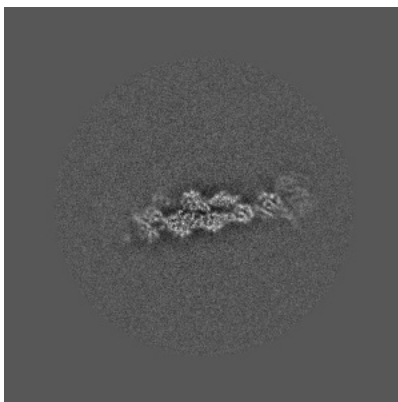


Z Index: 432

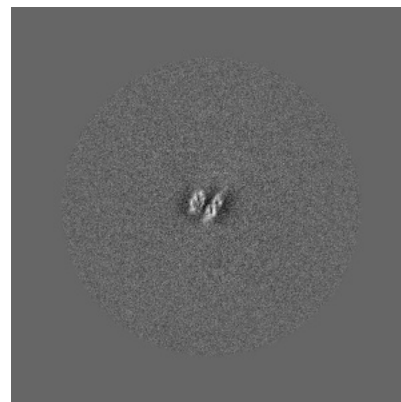
6.2.2 Raw map



X Index: 432



Y Index: 432

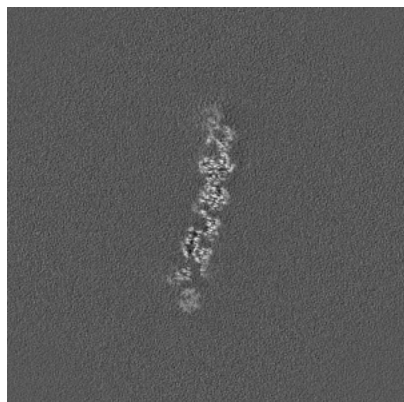


Z Index: 432

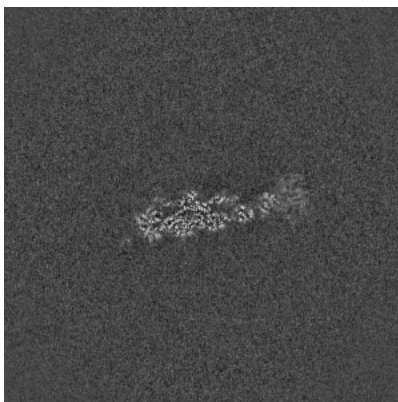
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

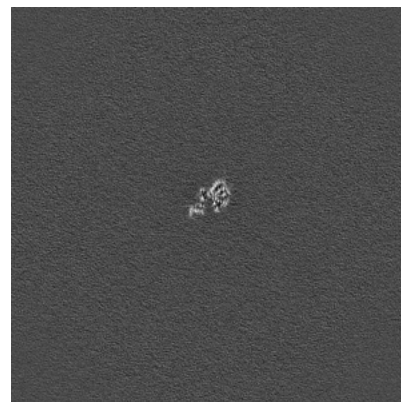
6.3.1 Primary map



X Index: 416

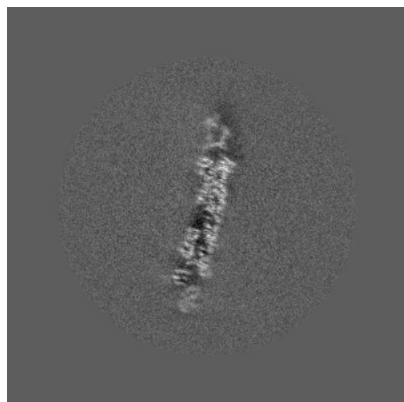


Y Index: 428

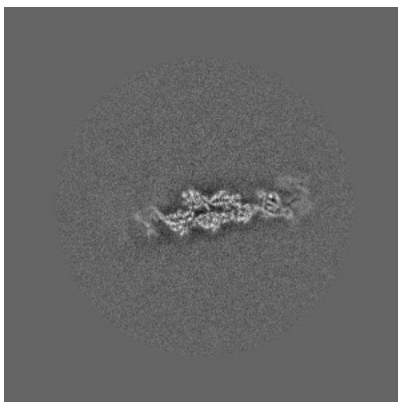


Z Index: 467

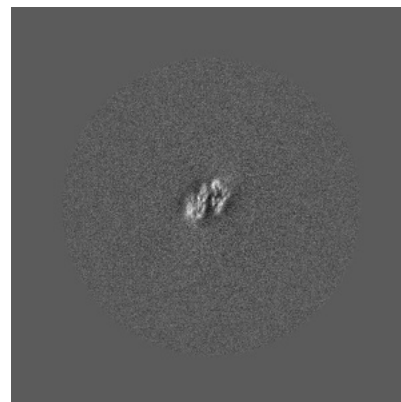
6.3.2 Raw map



X Index: 411



Y Index: 438

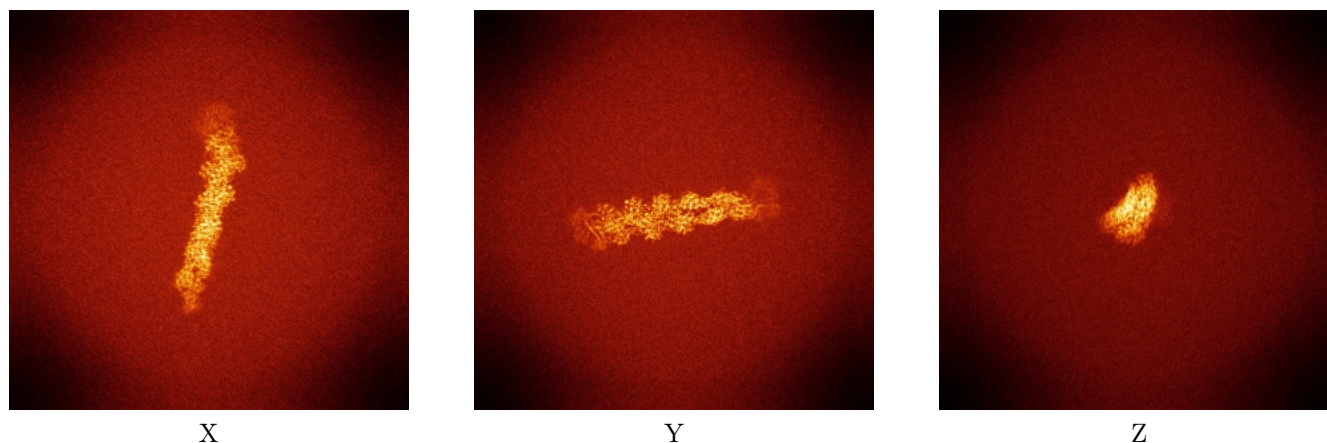


Z Index: 455

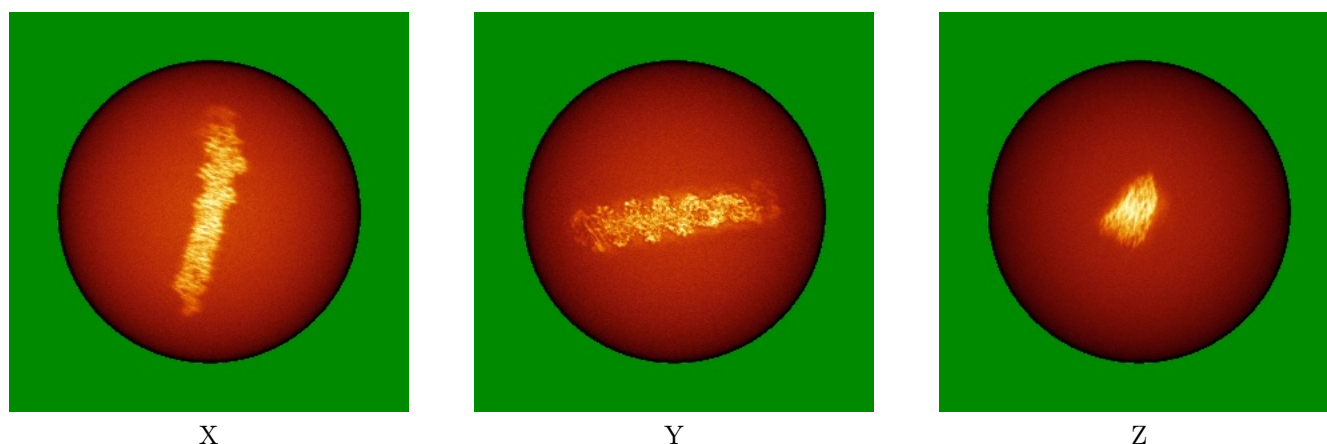
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

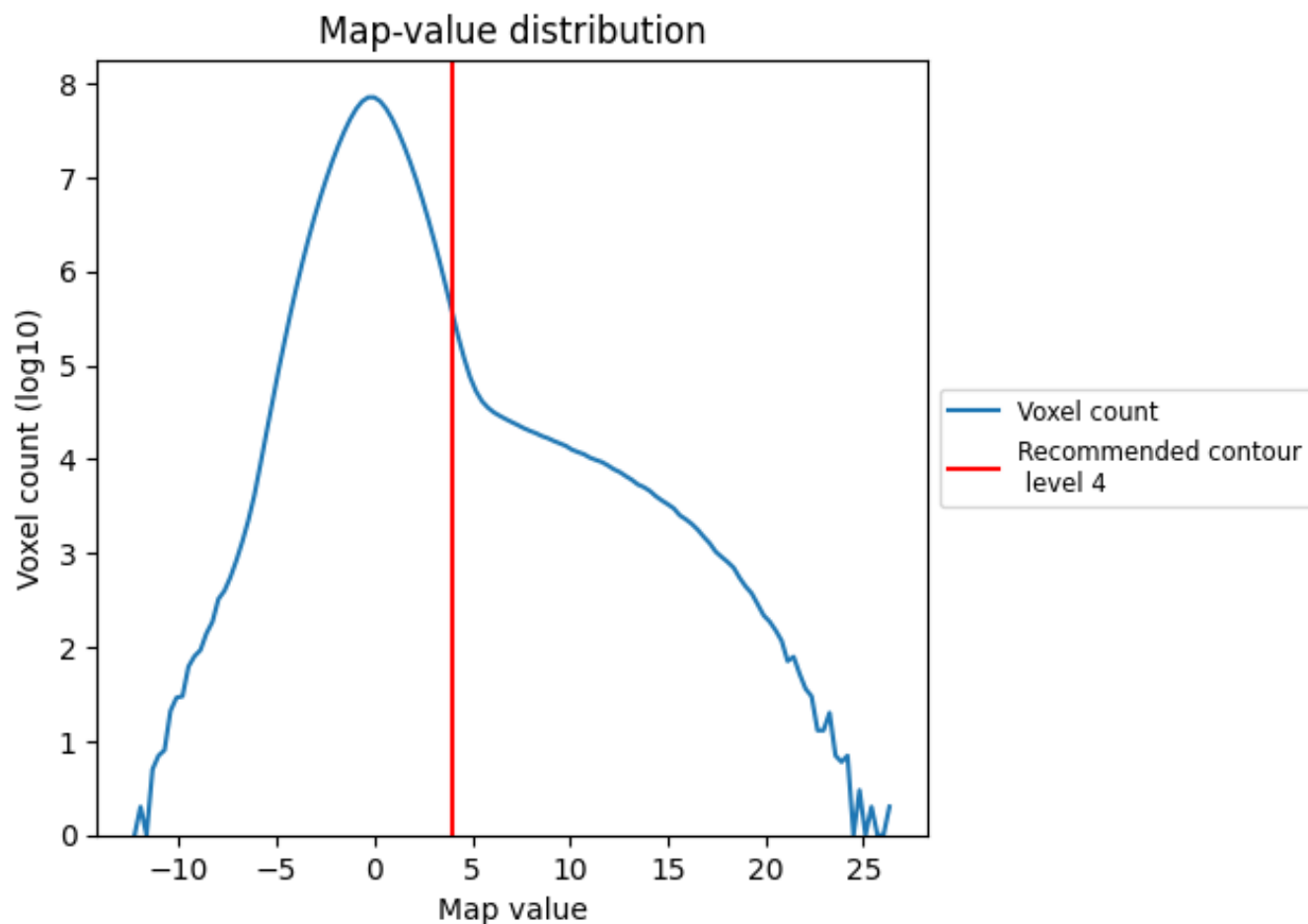
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

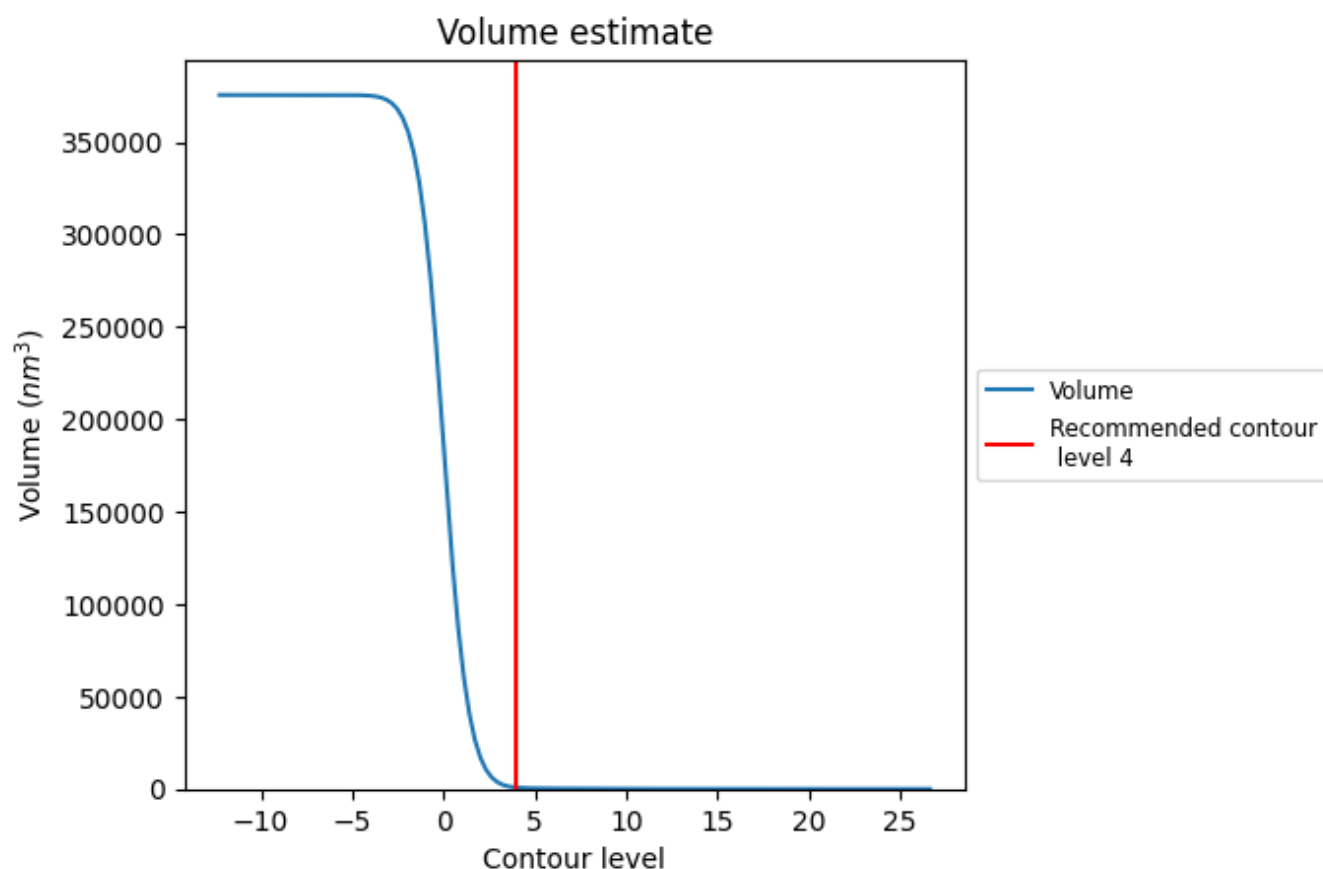
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

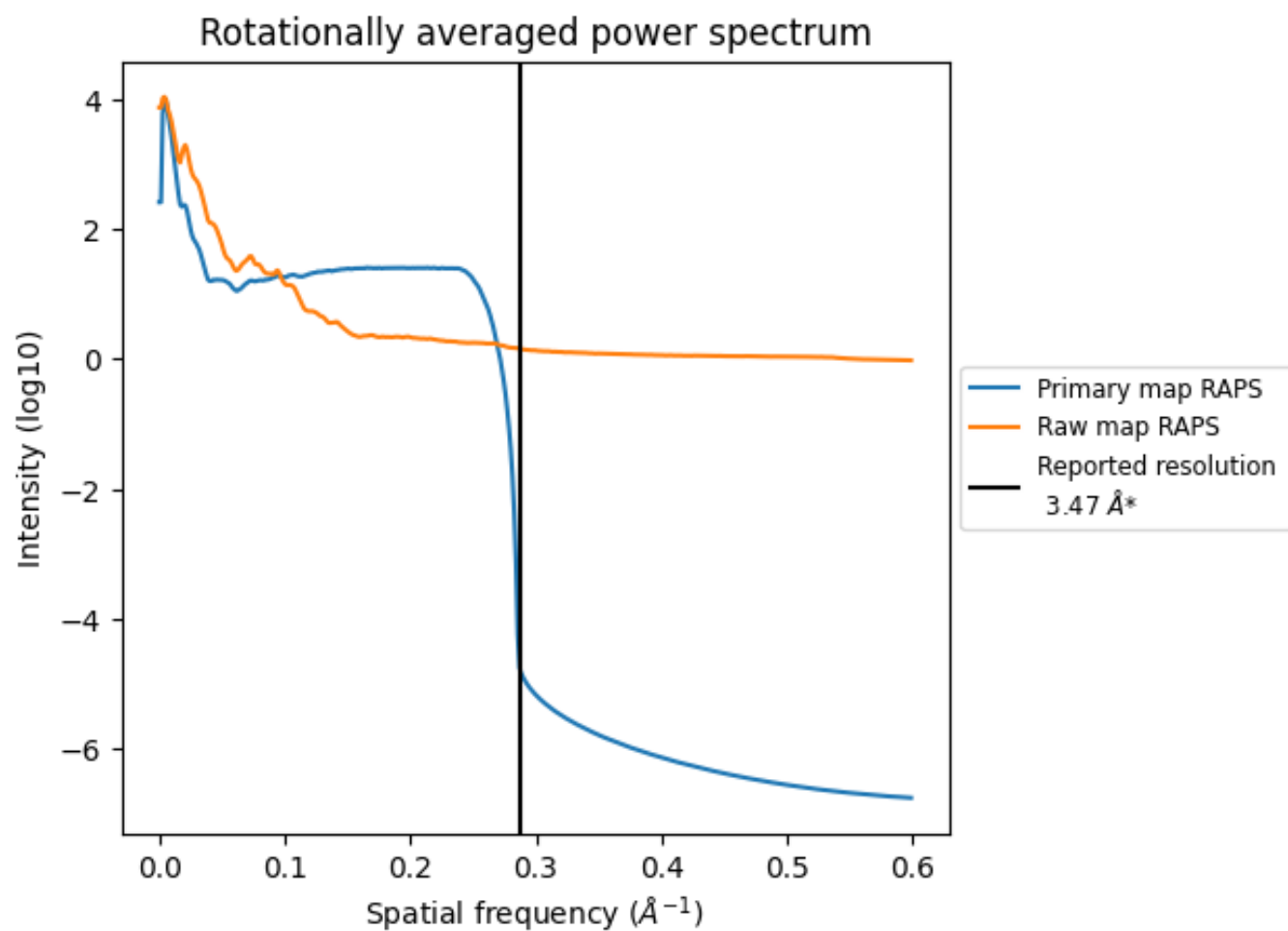
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765 nm^3 ; this corresponds to an approximate mass of 691 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 ⓘ

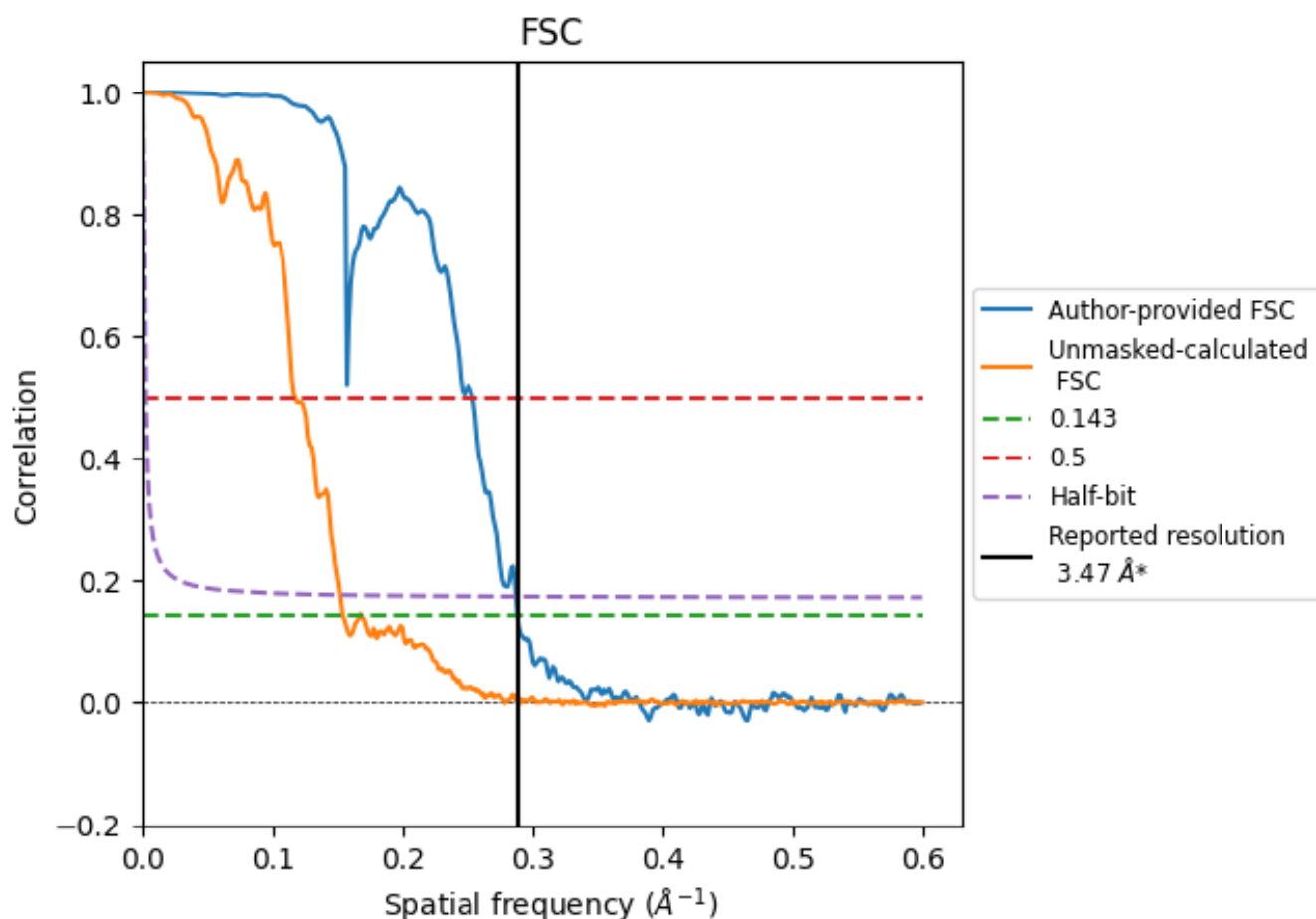


*Reported resolution corresponds to spatial frequency of 0.288 $\text{\AA}^{-1}$

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

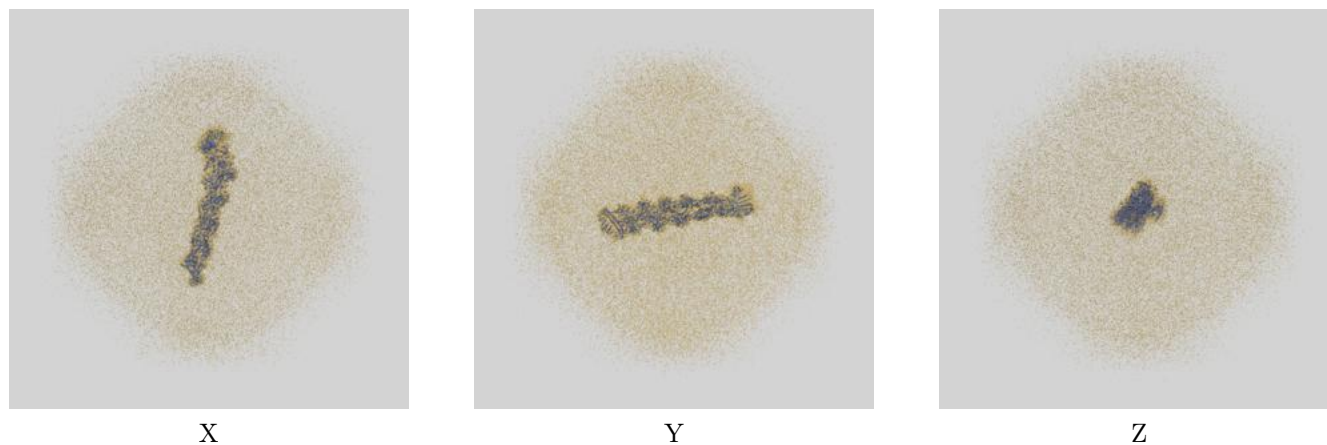
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.47	3.94	3.48
Unmasked-calculated*	6.49	8.50	6.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.49 differs from the reported value 3.47 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44333 and PDB model 9B85. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



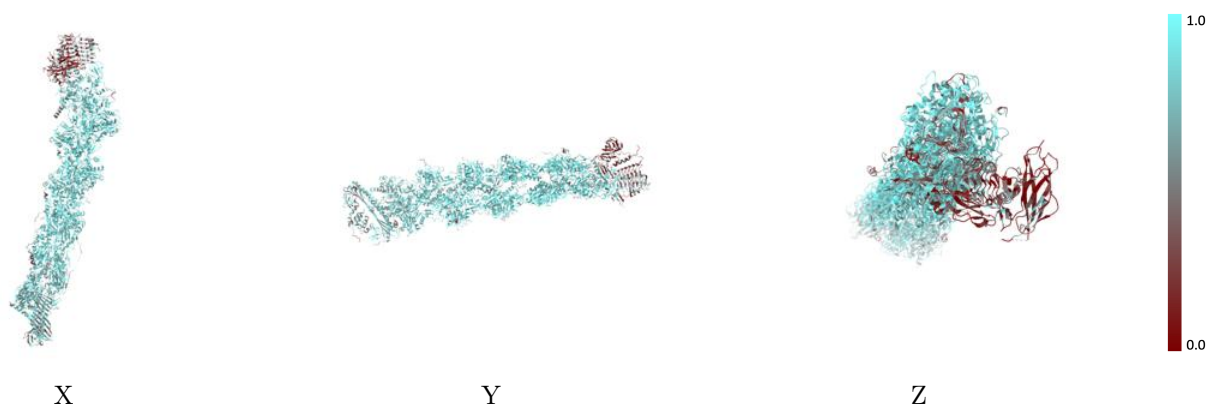
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



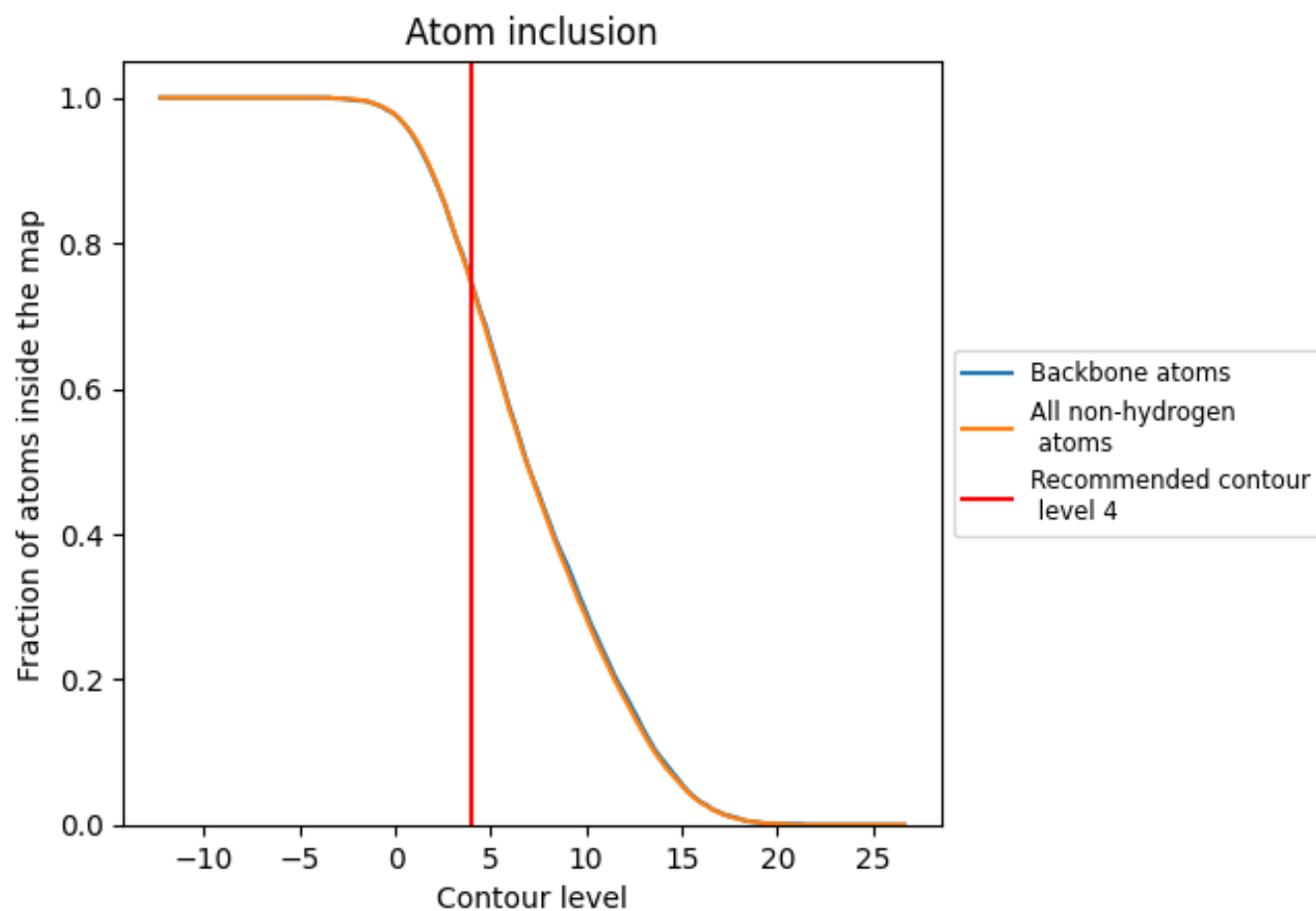
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.3060
A	 0.7800	 0.3070
B	 0.8140	 0.3470
C	 0.8420	 0.3770
D	 0.8680	 0.3910
E	 0.8560	 0.3800
F	 0.8700	 0.3870
G	 0.8630	 0.3920
H	 0.8650	 0.3760
I	 0.8220	 0.3250
J	 0.7910	 0.2870
K	 0.3990	 0.1340
L	 0.3250	 0.1000
M	 0.4630	 0.1350
N	 0.6200	 0.1810
O	 0.7150	 0.2340
P	 0.6710	 0.3050
Q	 0.4950	 0.2500
p	 0.4890	 0.2020
q	 0.4440	 0.2400

