



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 9B7J / pdb_00009b7j
EMDB ID : EMD-44306
Title : Cryo-EM structure of human dynactin complex bound to Chlamydia effector Dre1
Authors : Pawar, K.I.; Verba, K.A.
Deposited on : 2024-03-27
Resolution : 3.49 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

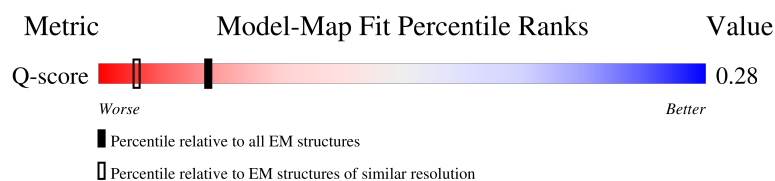
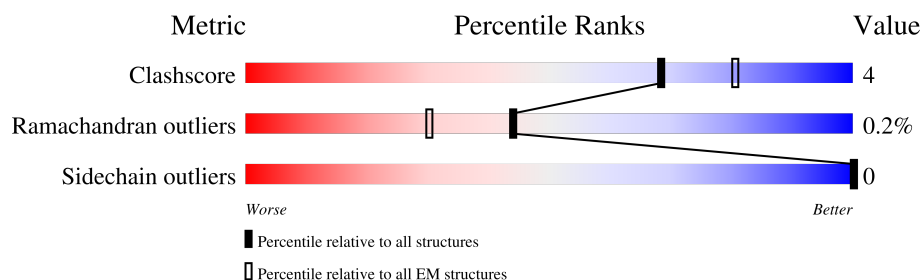
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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.



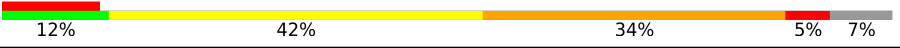
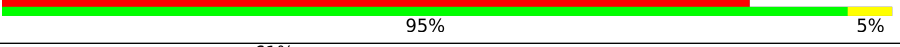
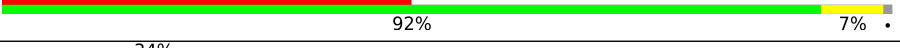
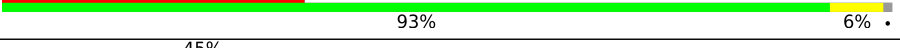
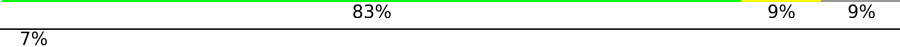
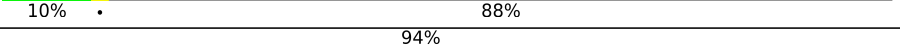
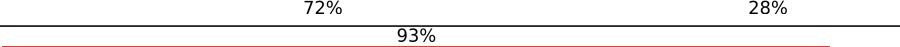
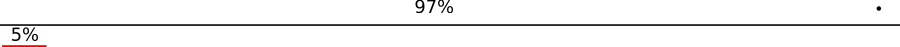
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

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	10% 92% 7% .
1	B	376	90% 8% .
1	C	376	92% 8% .
1	D	376	88% 11% .

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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	
10	R	186	
10	r	186	
11	S	1278	
12	T	83	
13	U	87	
14	s	1278	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 113042 atoms, of which 56723 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	284	Total	C	H	N	O	S	0	0
			4532	1454	2221	402	449	6		

- 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	339	Total	C	H	N	O	S	0	0
			5411	1672	2739	462	533	5		
9	Q	278	Total	C	H	N	O	S	0	0
			4436	1373	2248	375	434	6		
9	p	326	Total	C	H	N	O	S	0	0
			5107	1581	2573	432	513	8		
9	q	337	Total	C	H	N	O	S	0	0
			5312	1651	2669	448	538	6		

- Molecule 10 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	179	Total	C	H	N	O	S	0	0
			2905	908	1475	249	269	4		
10	r	170	Total	C	H	N	O	S	0	0
			2786	872	1417	238	255	4		

- Molecule 11 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	154	Total	C	H	N	O	S	0	0
			2444	760	1234	218	229	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1282	ASP	SER	conflict	UNP Q14203

- Molecule 12 is a protein called Dynactin subunit 1, p150-glued.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	83	Total	C	H	N	O	0	0
			1079	332	581	83	83		

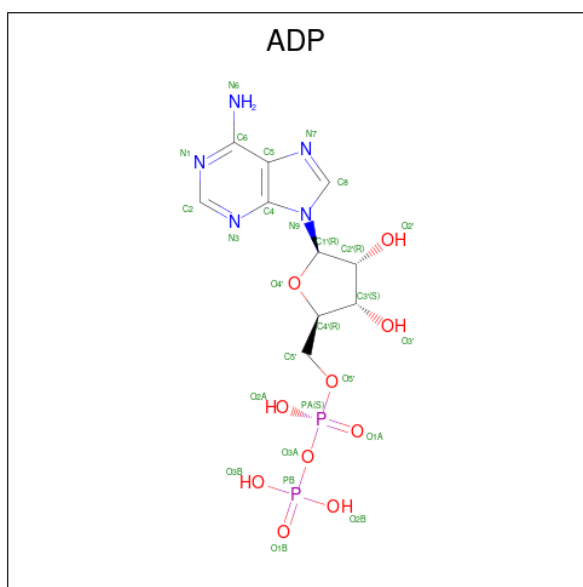
- Molecule 13 is a protein called Dynactin subunit 2, p50 dynamitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	87	Total	C	H	N	O	0	0
			1131	348	609	87	87		

- Molecule 14 is a protein called Dynactin subunit 1.

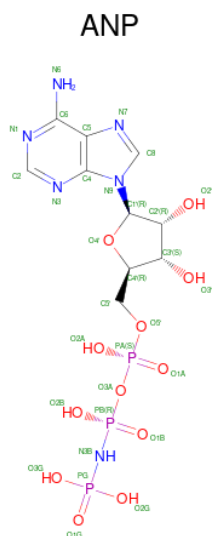
Mol	Chain	Residues	Atoms						AltConf	Trace
14	s	189	Total	C	H	N	O	S	0	0
			2940	910	1484	261	280	5		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 16 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

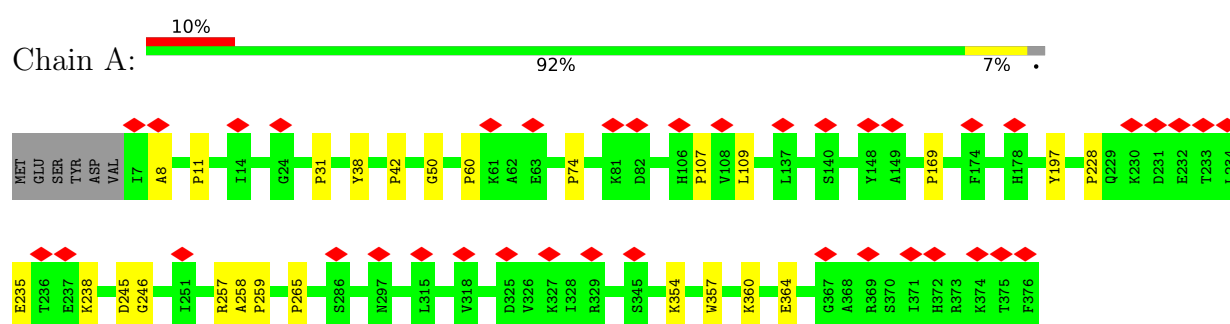
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

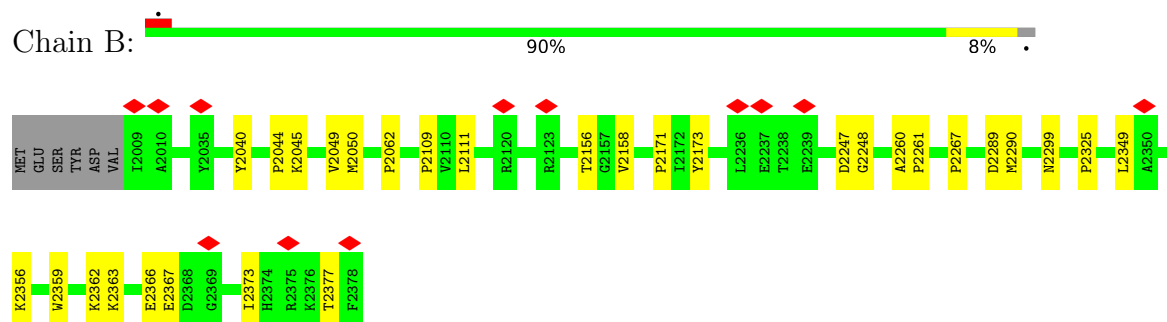
3 Residue-property plots [i](#)

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.

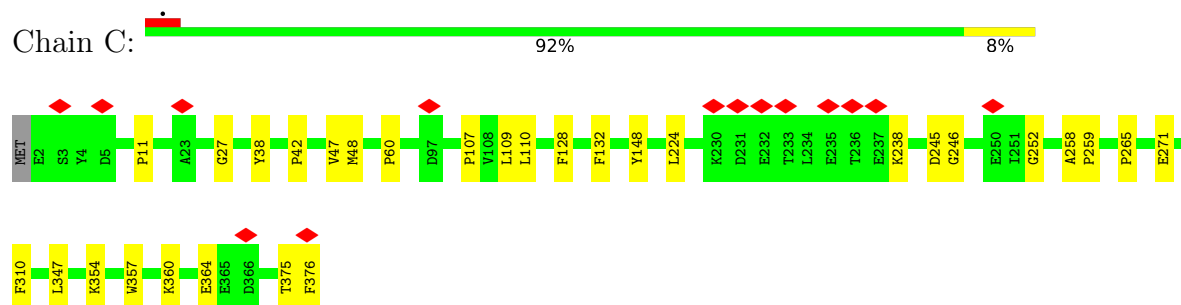
- Molecule 1: Alpha-centractin



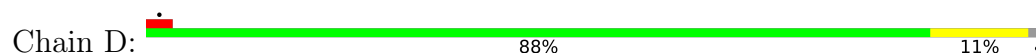
- Molecule 1: Alpha-centractin

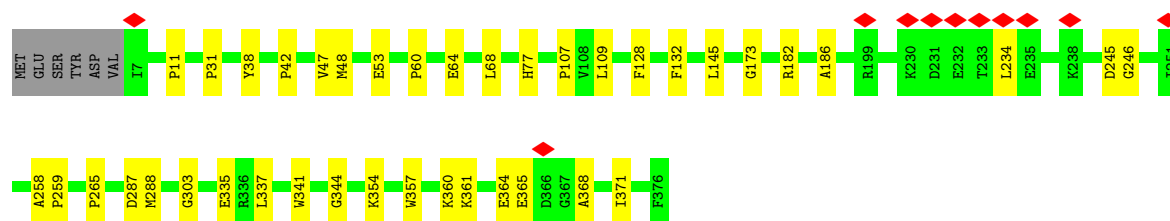


- Molecule 1: Alpha-centractin

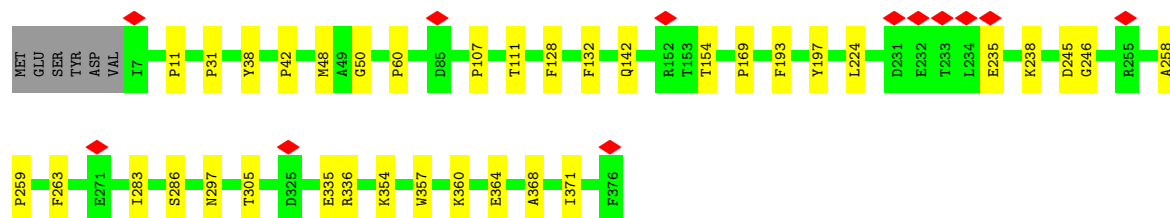
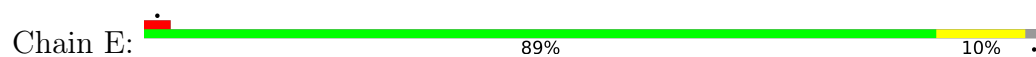


- Molecule 1: Alpha-centractin

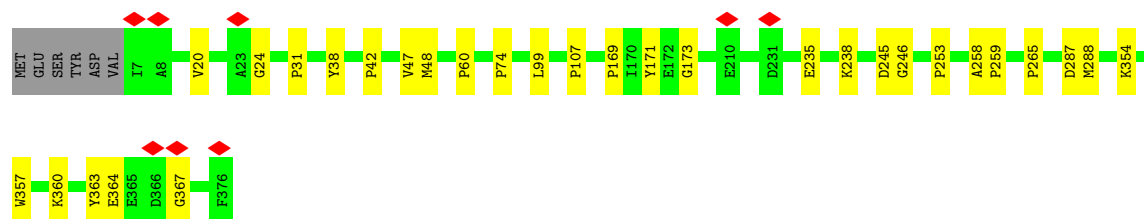
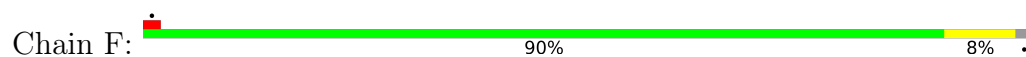




- Molecule 1: Alpha-centractin



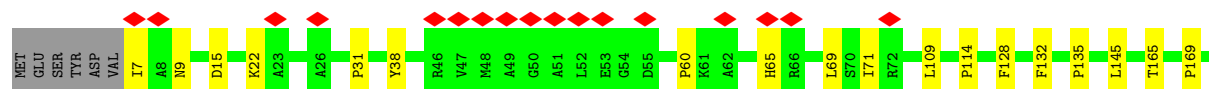
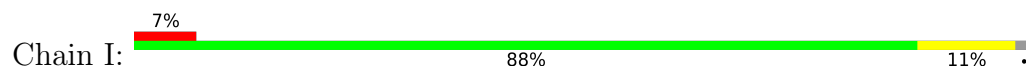
- Molecule 1: Alpha-centractin



- Molecule 1: Alpha-centractin

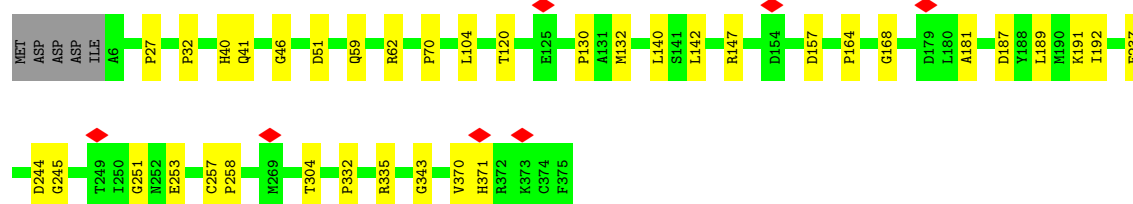
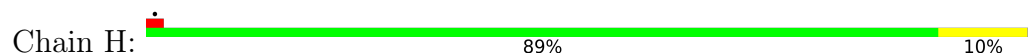


- Molecule 1: Alpha-centractin

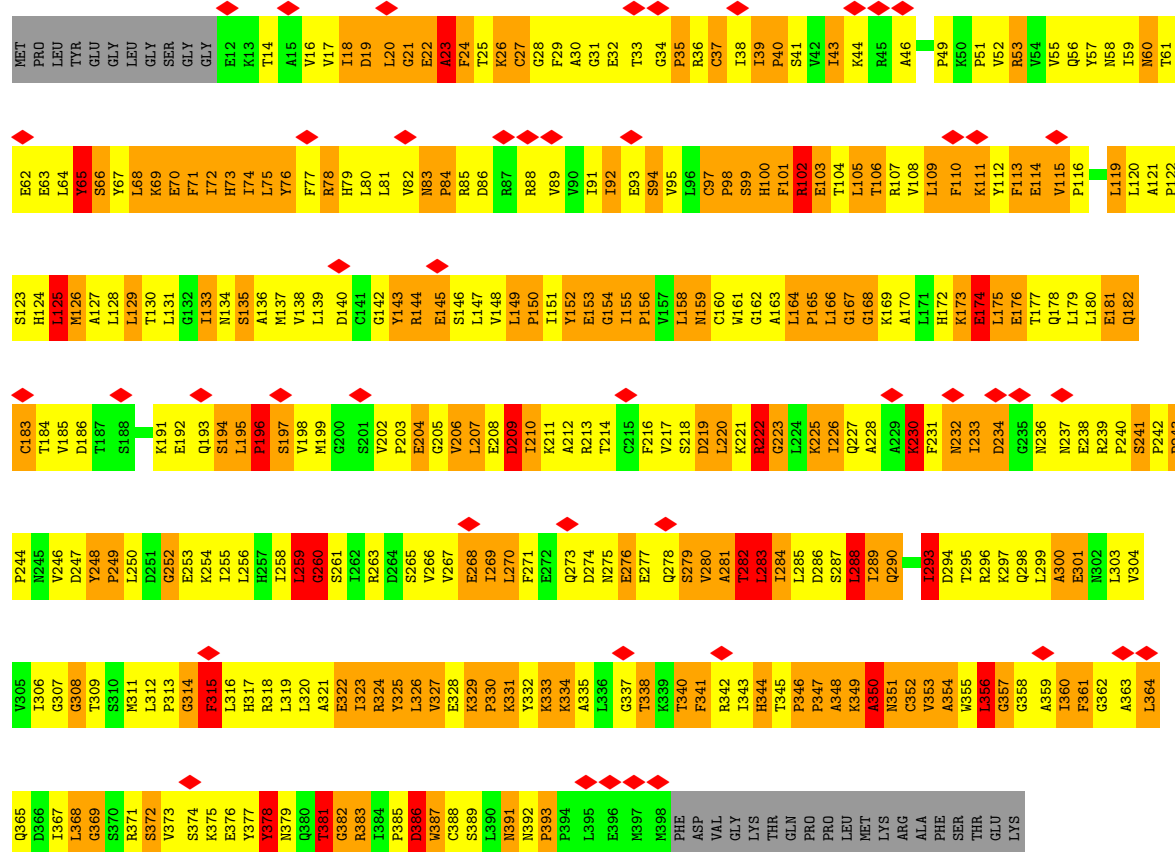




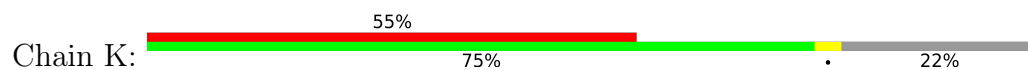
• Molecule 2: Actin, cytoplasmic 1

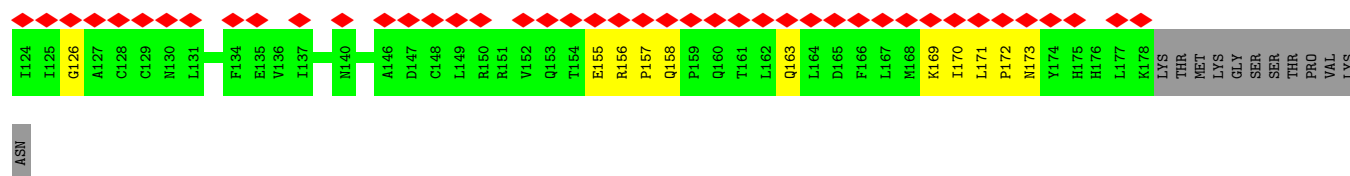


• Molecule 3: Actin-related protein 10



• Molecule 4: Dynactin subunit 4

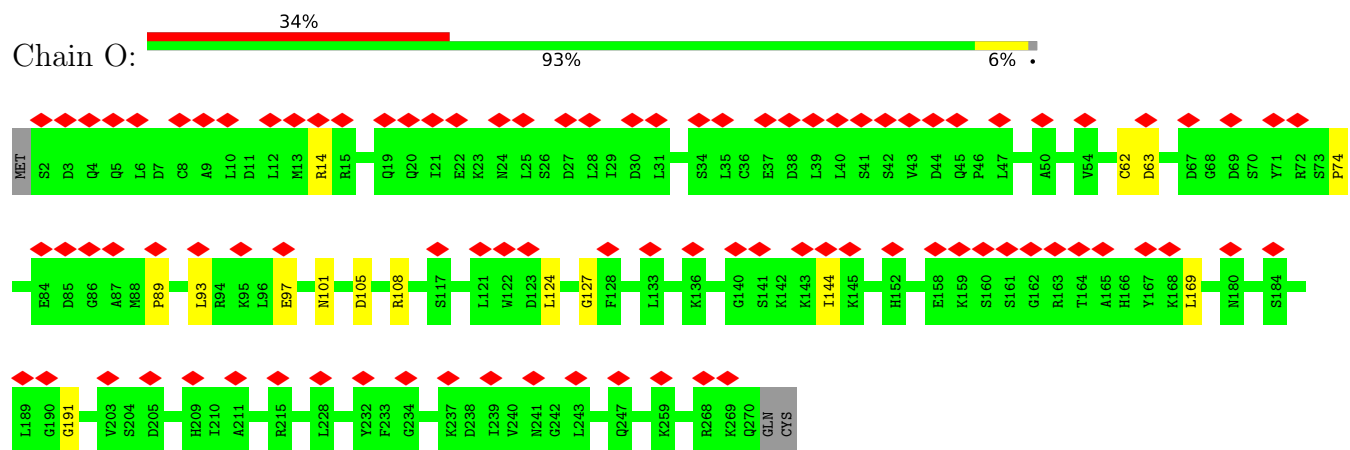




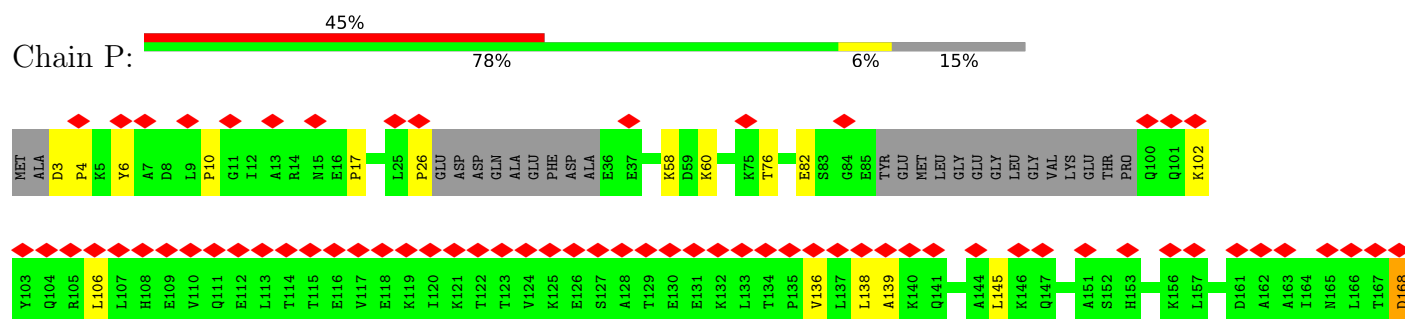
• Molecule 7: F-actin-capping protein subunit alpha-1

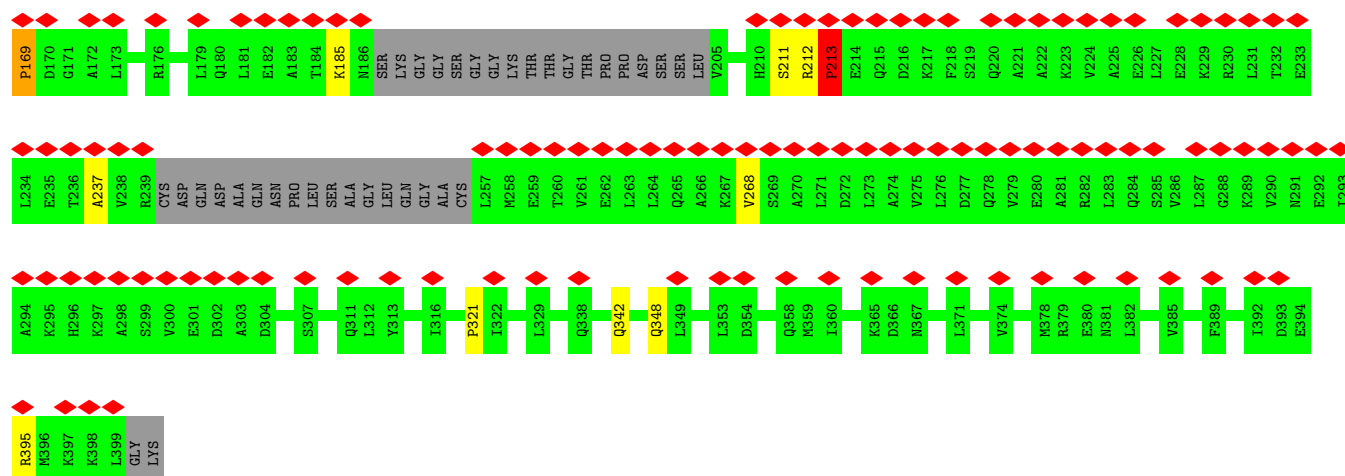


• Molecule 8: F-actin-capping protein subunit beta

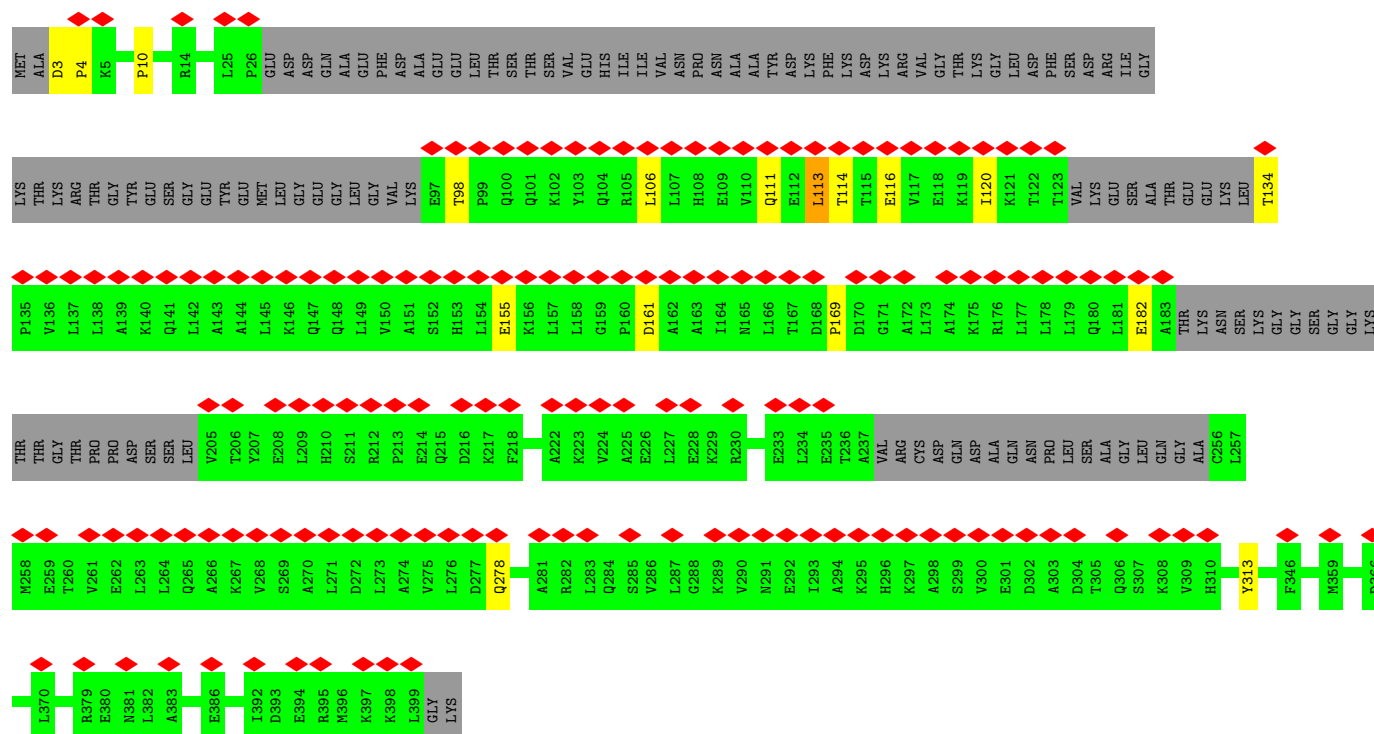
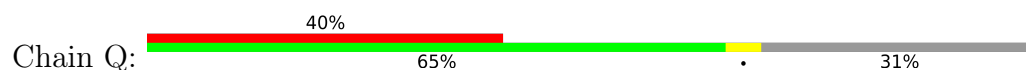


• Molecule 9: Dynactin subunit 2

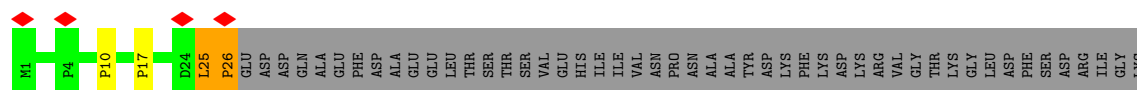
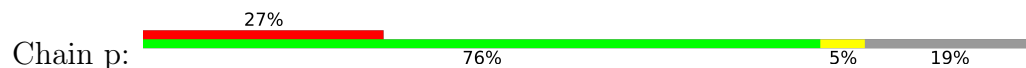


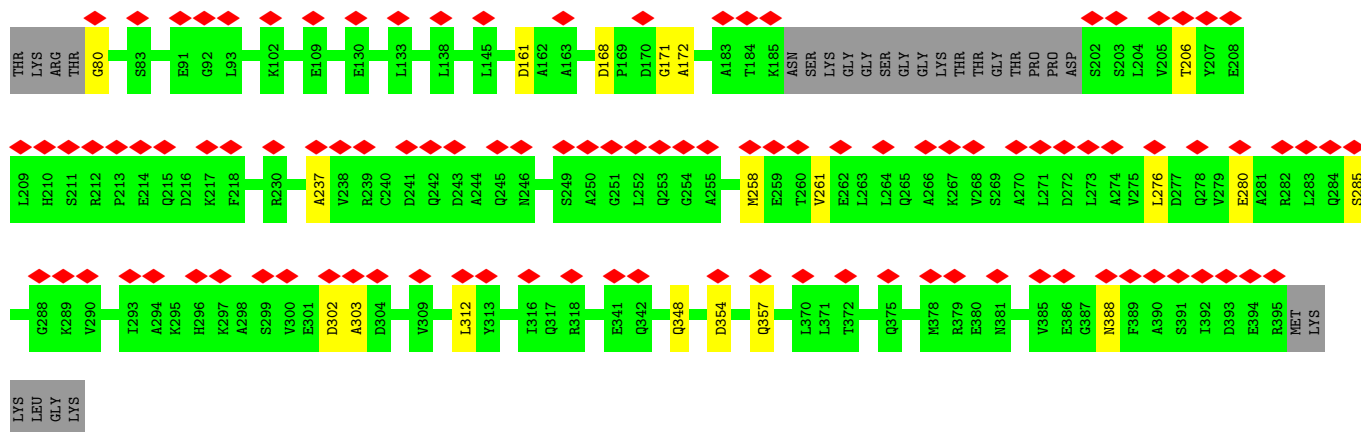


• Molecule 9: Dynactin subunit 2

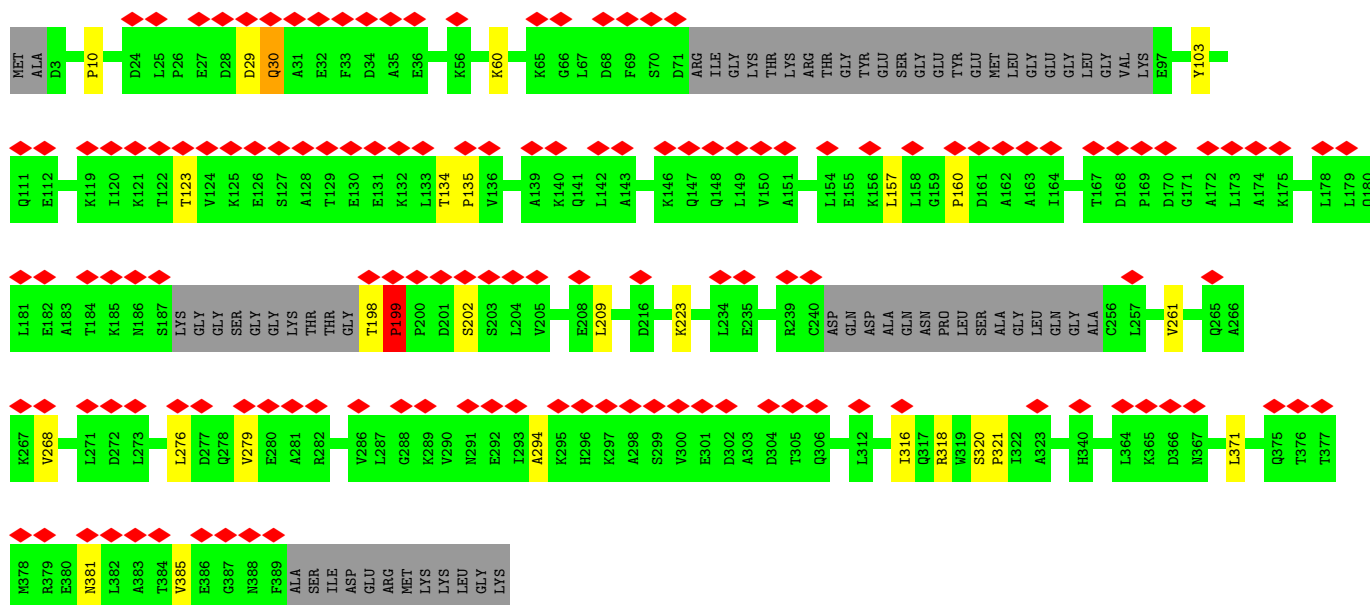
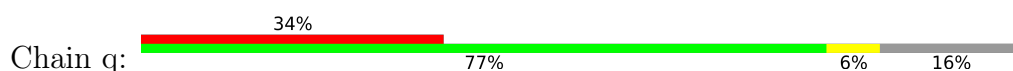


• Molecule 9: Dynactin subunit 2

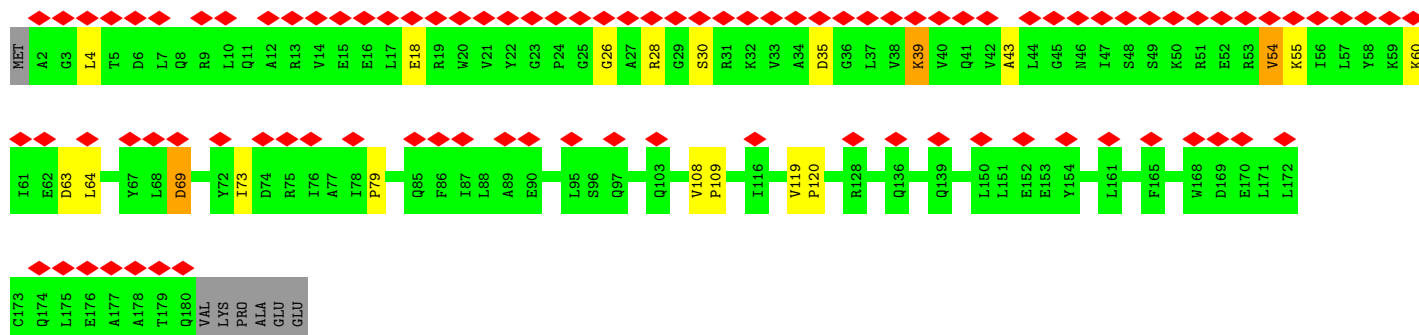
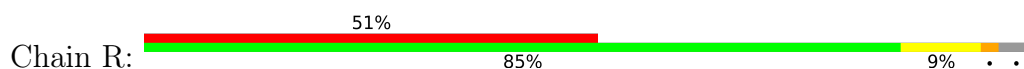




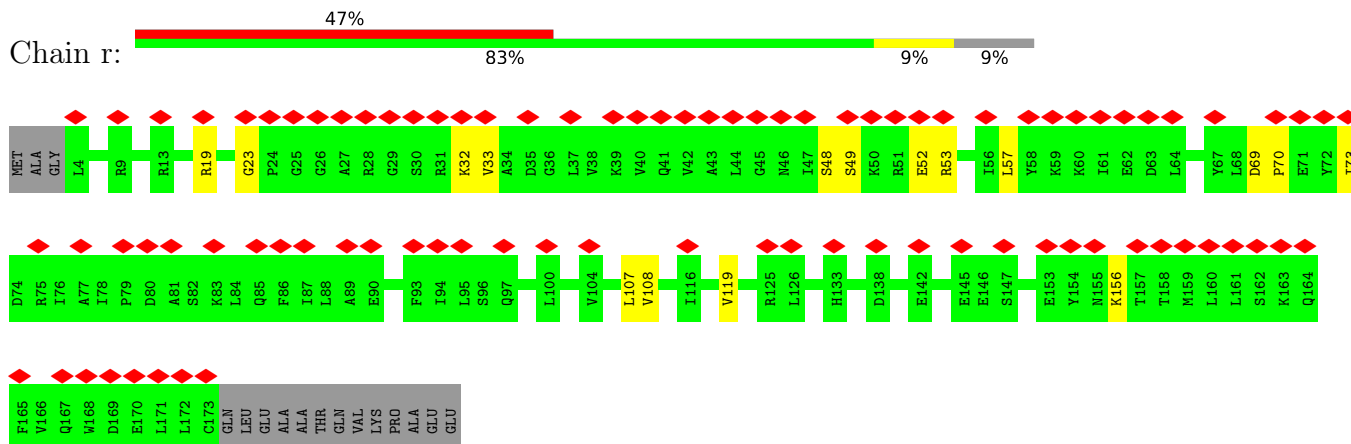
• Molecule 9: Dynactin subunit 2



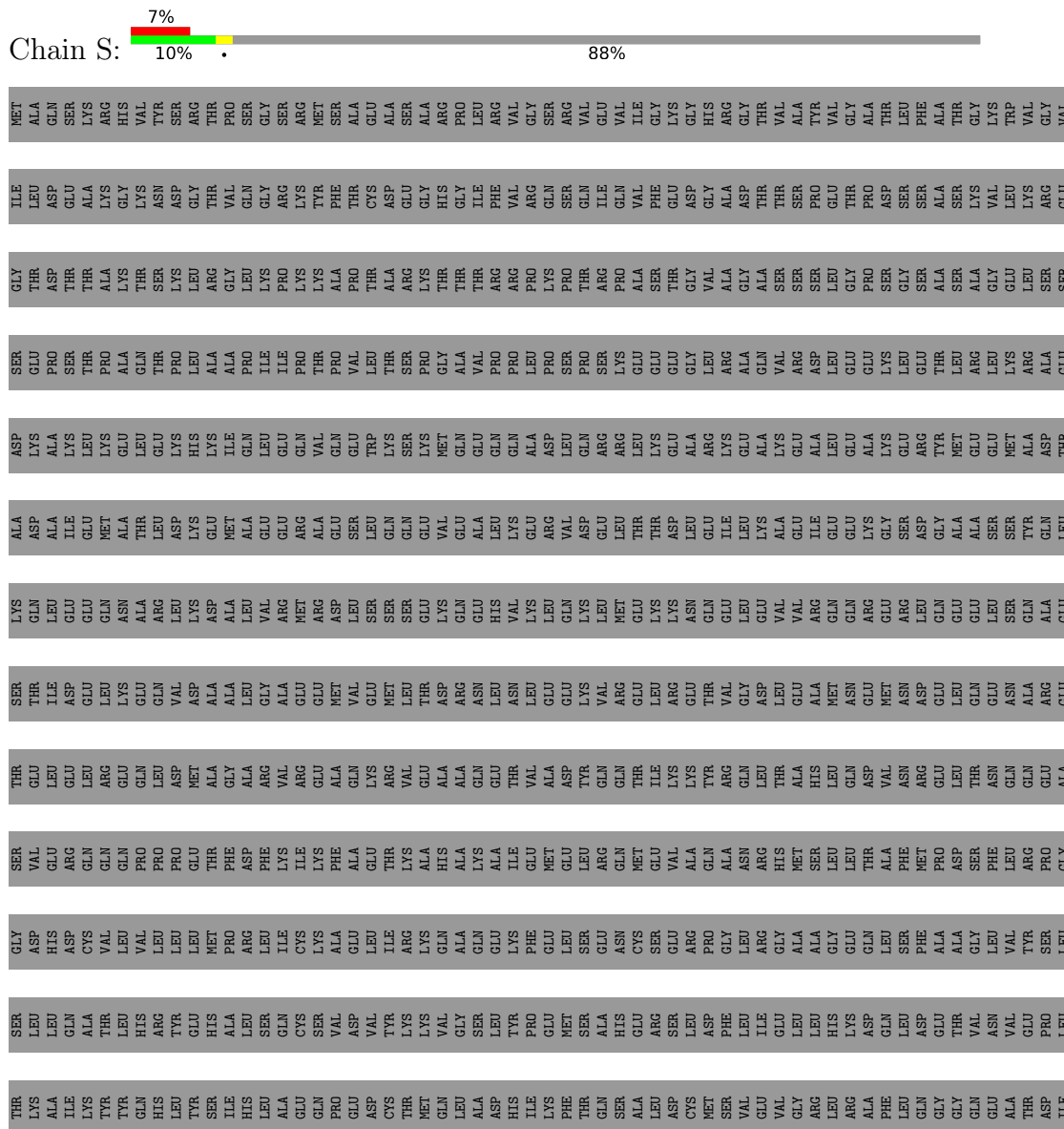
• Molecule 10: Dynactin subunit 3

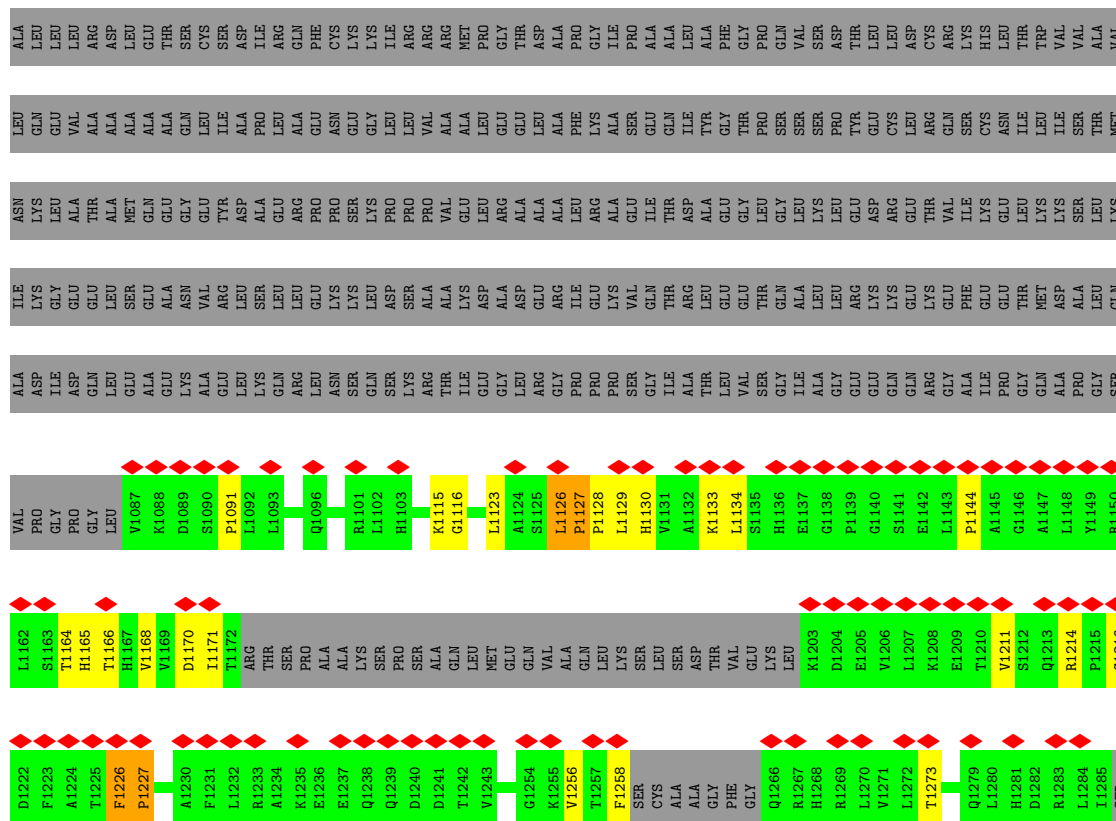


Chain r:

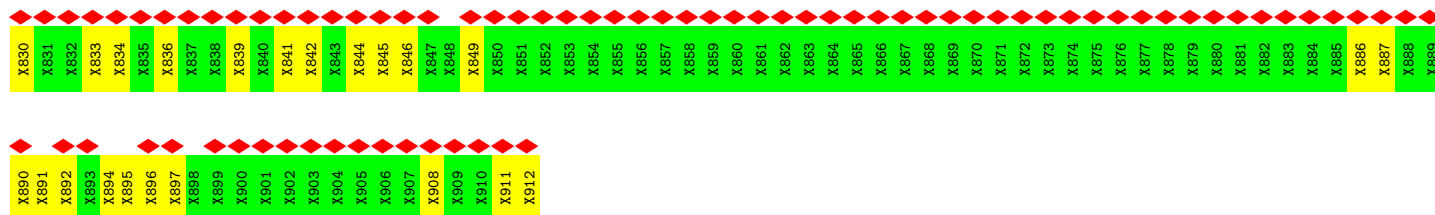
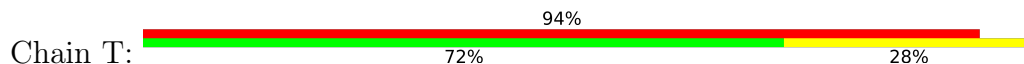


Chain S:

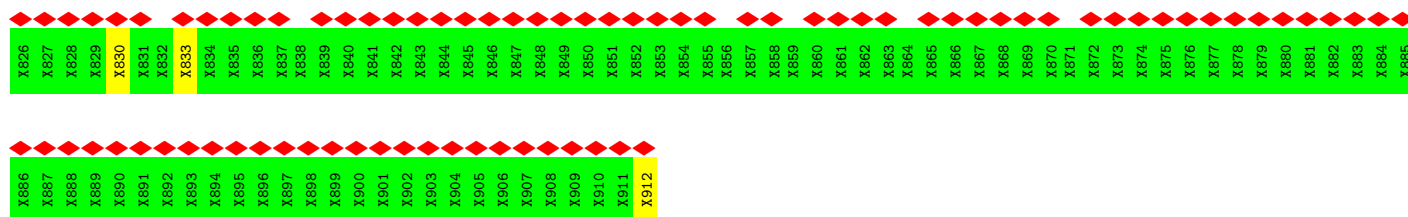




• Molecule 12: Dynactin subunit 1, p150-glued



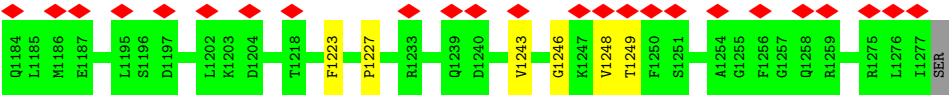
• Molecule 13: Dynactin subunit 2, p50 dynamitin



• Molecule 14: Dynactin subunit 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45091	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	30.993	Depositor
Minimum map value	-14.456	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.573	Depositor
Recommended contour level	6	Depositor
Map size (Å)	721.44, 721.44, 721.44	wwPDB
Map dimensions	864, 864, 864	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ADP, ZN, ANP

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	1.19	9/3025 (0.3%)	1.48	2/4085 (0.0%)
1	B	1.16	6/3025 (0.2%)	1.47	0/4085
1	C	1.17	5/3068 (0.2%)	1.46	0/4144
1	D	1.15	5/3025 (0.2%)	1.47	4/4085 (0.1%)
1	E	1.15	6/3025 (0.2%)	1.46	0/4085
1	F	1.18	8/3025 (0.3%)	1.49	0/4085
1	G	1.18	8/3025 (0.3%)	1.50	0/4085
1	I	1.17	5/3025 (0.2%)	1.48	0/4085
2	H	1.17	5/2948 (0.2%)	1.53	2/3991 (0.1%)
3	J	3.17	354/3088 (11.5%)	3.95	611/4188 (14.6%)
4	K	0.71	3/2970 (0.1%)	0.85	0/4005
5	L	0.69	1/1435 (0.1%)	0.87	0/1941
6	M	0.68	0/1209	0.89	0/1641
7	N	0.72	2/2363 (0.1%)	0.89	0/3197
8	O	1.18	2/2156 (0.1%)	1.54	0/2906
9	P	0.86	6/2700 (0.2%)	1.37	9/3646 (0.2%)
9	Q	0.91	6/2211 (0.3%)	1.51	12/2993 (0.4%)
9	p	0.83	3/2562 (0.1%)	1.36	5/3469 (0.1%)
9	q	0.87	3/2675 (0.1%)	1.38	14/3626 (0.4%)
10	R	0.83	1/1449 (0.1%)	1.51	15/1957 (0.8%)
10	r	0.85	0/1388	1.44	9/1874 (0.5%)
11	S	0.99	3/1229 (0.2%)	1.66	27/1660 (1.6%)
14	s	0.83	1/1481 (0.1%)	1.34	3/2005 (0.1%)
All	All	1.25	442/56107 (0.8%)	1.64	713/75838 (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
3	J	0	29

All (442) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	83	ASN	CA-C	-20.15	1.38	1.53
3	J	206	VAL	CA-C	-18.28	1.27	1.52
3	J	102	ARG	N-CA	-17.75	1.23	1.46
3	J	318	ARG	CA-C	-17.30	1.29	1.52
3	J	346	PRO	CA-C	-14.82	1.38	1.52
3	J	144	ARG	CA-C	-14.69	1.34	1.52
3	J	184	THR	C-O	14.44	1.40	1.23
3	J	230	LYS	CA-C	-14.22	1.34	1.53
3	J	319	LEU	CA-C	-14.09	1.34	1.52
3	J	330	PRO	N-CA	-13.98	1.29	1.47
3	J	377	TYR	CA-C	-13.61	1.35	1.52
3	J	316	LEU	CA-C	-13.45	1.34	1.52
3	J	331	LYS	N-CA	-13.17	1.28	1.46
3	J	322	GLU	CA-C	-12.77	1.35	1.52
3	J	82	VAL	CA-C	12.59	1.66	1.52
3	J	155	ILE	CA-C	-12.51	1.39	1.52
3	J	164	LEU	CA-C	-12.51	1.39	1.52
3	J	109	LEU	CA-C	-12.29	1.36	1.52
3	J	186	ASP	N-CA	-12.23	1.30	1.46
3	J	329	LYS	CA-C	-12.21	1.39	1.52
3	J	319	LEU	N-CA	-12.09	1.31	1.46
3	J	162	GLY	CA-C	12.08	1.61	1.52
3	J	183	CYS	N-CA	-12.07	1.30	1.46
3	J	65	TYR	CA-C	-11.96	1.37	1.52
3	J	352	CYS	C-N	-11.72	1.21	1.34
3	J	82	VAL	C-N	11.65	1.46	1.33
3	J	112	TYR	CA-C	-11.63	1.38	1.53
3	J	322	GLU	C-N	-11.51	1.19	1.33
3	J	71	PHE	CA-C	-11.24	1.38	1.52
3	J	276	GLU	N-CA	-11.22	1.32	1.45
3	J	77	PHE	N-CA	-11.15	1.32	1.46
3	J	109	LEU	C-N	-11.02	1.21	1.33
3	J	381	THR	CA-C	-10.99	1.39	1.52
3	J	209	ASP	CA-C	-10.92	1.37	1.52
3	J	83	ASN	C-O	-10.86	1.18	1.23
3	J	360	ILE	CA-C	-10.72	1.39	1.52
3	J	329	LYS	C-N	-10.71	1.20	1.33
3	J	89	VAL	C-N	-10.71	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	152	TYR	CA-C	-10.59	1.39	1.53
3	J	91	ILE	CA-C	-10.51	1.39	1.52
3	J	182	GLN	C-O	10.51	1.35	1.23
3	J	25	THR	CA-C	10.50	1.67	1.52
3	J	38	ILE	C-N	-10.42	1.23	1.33
3	J	368	LEU	CA-C	-10.38	1.38	1.52
9	Q	116	GLU	CA-C	10.34	1.66	1.52
3	J	172	HIS	N-CA	-10.28	1.33	1.46
3	J	317	HIS	CA-C	-10.17	1.40	1.52
3	J	198	VAL	N-CA	-10.16	1.36	1.46
3	J	209	ASP	C-N	-10.14	1.21	1.33
3	J	364	LEU	N-CA	-10.12	1.32	1.46
3	J	82	VAL	N-CA	10.08	1.55	1.46
3	J	313	PRO	CA-C	-10.08	1.39	1.52
3	J	39	ILE	CA-C	-10.00	1.42	1.52
3	J	164	LEU	N-CA	9.98	1.54	1.45
3	J	321	ALA	N-CA	-9.95	1.34	1.46
3	J	101	PHE	C-N	-9.91	1.19	1.33
3	J	156	PRO	CA-C	-9.88	1.40	1.52
3	J	288	LEU	C-N	-9.88	1.23	1.34
3	J	343	ILE	CA-C	-9.88	1.40	1.52
3	J	185	VAL	CA-C	-9.83	1.40	1.52
3	J	313	PRO	N-CA	-9.81	1.35	1.47
3	J	102	ARG	CA-C	-9.80	1.39	1.52
3	J	324	ARG	C-N	-9.71	1.21	1.33
3	J	37	CYS	N-CA	-9.70	1.34	1.46
3	J	356	LEU	C-N	-9.69	1.17	1.33
3	J	276	GLU	CA-C	9.68	1.64	1.52
3	J	300	ALA	CA-C	-9.62	1.39	1.53
3	J	153	GLU	CA-C	-9.55	1.40	1.52
3	J	248	TYR	CA-C	-9.48	1.41	1.52
3	J	237	ASN	CA-C	-9.35	1.42	1.52
3	J	393	PRO	CA-C	-9.33	1.45	1.52
3	J	212	ALA	CA-C	-9.31	1.40	1.52
3	J	158	LEU	CA-C	-9.29	1.40	1.52
3	J	236	ASN	N-CA	-9.23	1.35	1.46
3	J	242	PRO	CA-C	-9.22	1.43	1.52
3	J	93	GLU	CA-C	-9.21	1.40	1.53
3	J	340	THR	CA-C	-9.19	1.41	1.53
3	J	388	CYS	N-CA	-9.17	1.33	1.46
3	J	74	ILE	C-N	-9.14	1.20	1.33
3	J	24	PHE	C-N	-9.10	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	93	GLU	N-CA	-9.10	1.34	1.46
3	J	266	VAL	CA-C	-9.09	1.39	1.52
3	J	320	LEU	N-CA	-9.08	1.34	1.46
3	J	318	ARG	N-CA	-9.02	1.34	1.46
3	J	83	ASN	N-CA	-9.02	1.39	1.46
9	P	213	PRO	N-CD	-9.02	1.35	1.47
3	J	154	GLY	N-CA	-8.97	1.36	1.46
3	J	177	THR	CA-C	-8.90	1.41	1.52
3	J	269	ILE	CA-C	-8.85	1.41	1.53
3	J	198	VAL	CA-C	-8.84	1.41	1.52
3	J	268	GLU	CA-C	-8.82	1.41	1.53
3	J	36	ARG	C-N	-8.82	1.21	1.33
3	J	100	HIS	CA-C	-8.81	1.41	1.52
11	S	1144	PRO	N-CD	-8.79	1.35	1.47
3	J	208	GLU	N-CA	-8.75	1.35	1.46
3	J	66	SER	N-CA	-8.74	1.34	1.46
3	J	290	GLN	N-CA	-8.74	1.34	1.46
3	J	92	ILE	CA-C	-8.74	1.41	1.52
3	J	120	LEU	N-CA	-8.74	1.35	1.46
3	J	231	PHE	N-CA	-8.73	1.34	1.46
3	J	61	THR	CA-C	-8.69	1.40	1.52
3	J	78	ARG	CA-C	-8.69	1.43	1.52
3	J	29	PHE	CA-C	-8.66	1.41	1.52
3	J	367	ILE	CA-C	-8.65	1.43	1.52
3	J	102	ARG	C-N	-8.63	1.22	1.33
3	J	376	GLU	CA-C	-8.54	1.41	1.52
3	J	173	LYS	CA-C	-8.53	1.41	1.52
3	J	311	MET	N-CA	-8.53	1.33	1.45
3	J	266	VAL	N-CA	-8.52	1.35	1.46
3	J	185	VAL	C-N	-8.43	1.19	1.33
3	J	382	GLY	CA-C	-8.42	1.41	1.51
3	J	387	TRP	CA-C	-8.41	1.41	1.52
3	J	230	LYS	C-O	-8.40	1.13	1.23
3	J	346	PRO	C-N	-8.40	1.23	1.34
3	J	363	ALA	C-N	-8.37	1.22	1.33
3	J	372	SER	N-CA	-8.36	1.34	1.45
3	J	357	GLY	CA-C	8.33	1.65	1.51
3	J	78	ARG	N-CA	-8.28	1.36	1.46
3	J	296	ARG	C-N	-8.23	1.22	1.33
3	J	256	LEU	N-CA	-8.18	1.35	1.46
3	J	326	LEU	C-N	-8.18	1.25	1.34
3	J	248	TYR	C-N	-8.17	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	210	ILE	N-CA	-8.15	1.36	1.46
3	J	60	ASN	CA-C	-8.10	1.42	1.52
3	J	19	ASP	CA-C	-8.09	1.42	1.52
3	J	371	ARG	C-N	-8.06	1.22	1.33
3	J	151	ILE	CA-C	8.04	1.63	1.52
3	J	93	GLU	C-N	-7.94	1.22	1.33
3	J	123	SER	CA-C	-7.88	1.41	1.52
3	J	282	THR	CA-C	-7.87	1.42	1.52
3	J	365	GLN	CA-C	7.85	1.63	1.52
3	J	110	PHE	N-CA	-7.85	1.33	1.47
3	J	323	ILE	CA-C	-7.83	1.40	1.52
3	J	277	GLU	N-CA	7.82	1.56	1.45
3	J	122	PRO	C-O	-7.80	1.14	1.23
3	J	130	THR	CA-C	-7.78	1.42	1.52
3	J	152	TYR	N-CA	7.78	1.55	1.45
3	J	153	GLU	N-CA	-7.77	1.36	1.46
3	J	88	ARG	C-N	7.77	1.43	1.33
3	J	177	THR	N-CA	-7.75	1.37	1.46
3	J	92	ILE	C-N	-7.73	1.23	1.33
3	J	316	LEU	N-CA	-7.71	1.35	1.46
3	J	110	PHE	CA-C	-7.70	1.45	1.53
3	J	365	GLN	N-CA	7.69	1.56	1.46
3	J	359	ALA	N-CA	-7.67	1.36	1.46
3	J	25	THR	N-CA	-7.63	1.35	1.46
3	J	155	ILE	N-CA	7.62	1.55	1.46
3	J	76	TYR	C-N	-7.59	1.24	1.33
3	J	91	ILE	N-CA	-7.58	1.37	1.46
3	J	70	GLU	N-CA	-7.57	1.36	1.46
3	J	101	PHE	CA-C	-7.56	1.37	1.52
3	J	178	GLN	CA-C	-7.55	1.42	1.52
3	J	307	GLY	C-O	-7.55	1.16	1.24
3	J	212	ALA	N-CA	-7.51	1.37	1.46
3	J	356	LEU	CA-C	-7.50	1.42	1.52
3	J	306	ILE	N-CA	7.49	1.54	1.46
3	J	307	GLY	CA-C	-7.48	1.43	1.52
3	J	32	GLU	CA-C	-7.48	1.42	1.52
3	J	375	LYS	N-CA	-7.48	1.36	1.46
1	I	135	PRO	N-CD	-7.47	1.37	1.47
3	J	39	ILE	C-N	-7.47	1.24	1.33
3	J	19	ASP	C-N	-7.42	1.22	1.33
3	J	280	VAL	CA-C	-7.42	1.42	1.52
3	J	46	ALA	CA-C	-7.40	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	94	SER	CA-C	-7.36	1.37	1.52
3	J	62	GLU	CA-C	-7.35	1.42	1.52
3	J	347	PRO	N-CA	-7.33	1.37	1.47
3	J	166	LEU	N-CA	-7.32	1.32	1.46
3	J	378	TYR	C-N	-7.30	1.23	1.34
3	J	331	LYS	C-O	-7.30	1.14	1.24
3	J	222	ARG	N-CA	-7.29	1.36	1.46
3	J	130	THR	C-N	-7.29	1.23	1.33
1	G	135	PRO	N-CD	-7.25	1.37	1.47
3	J	308	GLY	C-N	-7.25	1.23	1.33
3	J	350	ALA	C-N	-7.25	1.24	1.33
3	J	159	ASN	N-CA	-7.24	1.36	1.46
3	J	23	ALA	N-CA	-7.23	1.36	1.46
3	J	237	ASN	N-CA	-7.22	1.38	1.46
9	Q	116	GLU	C-N	-7.22	1.25	1.33
3	J	301	GLU	C-O	-7.22	1.14	1.24
9	P	169	PRO	N-CD	-7.20	1.37	1.47
3	J	122	PRO	N-CD	-7.18	1.37	1.47
3	J	301	GLU	N-CA	-7.15	1.36	1.46
3	J	283	LEU	C-N	-7.15	1.24	1.33
3	J	267	VAL	N-CA	-7.13	1.37	1.46
3	J	75	LEU	N-CA	-7.12	1.36	1.46
3	J	361	PHE	N-CA	-7.09	1.36	1.46
3	J	381	THR	C-N	-7.06	1.25	1.33
3	J	248	TYR	N-CA	-7.03	1.37	1.46
3	J	167	GLY	N-CA	-7.02	1.34	1.45
3	J	65	TYR	N-CA	-7.01	1.37	1.46
3	J	71	PHE	C-N	-7.01	1.25	1.33
3	J	233	ILE	C-N	-7.01	1.24	1.33
3	J	330	PRO	C-N	-7.01	1.23	1.33
3	J	197	SER	CA-C	-7.00	1.43	1.53
3	J	77	PHE	CA-C	-6.95	1.43	1.52
3	J	92	ILE	N-CA	-6.95	1.37	1.46
3	J	156	PRO	N-CA	-6.93	1.39	1.46
3	J	323	ILE	C-N	-6.92	1.24	1.33
3	J	203	PRO	N-CA	-6.91	1.38	1.47
3	J	43	ILE	C-O	-6.90	1.17	1.24
14	s	1227	PRO	N-CD	-6.90	1.38	1.47
3	J	21	GLY	C-N	6.89	1.44	1.33
9	p	26	PRO	N-CD	-6.86	1.38	1.47
3	J	72	ILE	CA-C	-6.79	1.42	1.52
3	J	368	LEU	C-N	-6.78	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	166	LEU	C-N	-6.77	1.23	1.33
3	J	209	ASP	C-O	-6.73	1.15	1.24
3	J	315	PHE	CA-C	-6.73	1.43	1.52
3	J	69	LYS	C-N	-6.73	1.24	1.33
3	J	165	PRO	N-CA	-6.73	1.39	1.47
3	J	131	LEU	N-CA	-6.71	1.36	1.45
3	J	158	LEU	C-N	-6.68	1.23	1.33
3	J	143	TYR	CA-C	-6.65	1.44	1.52
3	J	166	LEU	CA-C	-6.65	1.39	1.52
3	J	231	PHE	CA-C	-6.64	1.44	1.53
3	J	182	GLN	CA-C	-6.64	1.44	1.52
3	J	326	LEU	CA-C	-6.63	1.43	1.52
3	J	355	TRP	CA-C	-6.63	1.43	1.52
3	J	199	MET	CA-C	-6.63	1.44	1.52
3	J	230	LYS	N-CA	-6.62	1.37	1.46
3	J	228	ALA	N-CA	6.61	1.55	1.46
3	J	249	PRO	N-CA	-6.59	1.39	1.47
3	J	183	CYS	CA-C	-6.58	1.46	1.53
1	D	107	PRO	N-CD	-6.57	1.38	1.47
1	A	265	PRO	N-CD	-6.57	1.38	1.47
3	J	103	GLU	CA-C	-6.57	1.44	1.52
3	J	75	LEU	C-N	-6.56	1.24	1.33
3	J	317	HIS	N-CA	-6.56	1.38	1.46
4	K	256	PRO	N-CD	-6.55	1.38	1.47
3	J	204	GLU	C-N	-6.54	1.26	1.33
3	J	364	LEU	C-O	-6.52	1.15	1.24
3	J	40	PRO	N-CA	-6.51	1.39	1.46
3	J	361	PHE	C-N	-6.51	1.25	1.34
1	B	2109	PRO	N-CD	-6.51	1.38	1.47
3	J	121	ALA	C-O	-6.51	1.16	1.24
4	K	460	PRO	N-CD	-6.50	1.38	1.47
3	J	219	ASP	CA-C	-6.49	1.44	1.52
3	J	213	ARG	N-CA	-6.48	1.36	1.45
3	J	176	GLU	CA-C	-6.48	1.44	1.52
3	J	83	ASN	C-N	6.45	1.41	1.33
3	J	160	CYS	N-CA	-6.44	1.37	1.46
1	I	60	PRO	N-CD	-6.42	1.38	1.47
3	J	333	LYS	C-N	-6.39	1.24	1.33
1	A	228	PRO	N-CD	-6.39	1.38	1.47
3	J	73	HIS	N-CA	-6.38	1.38	1.46
3	J	61	THR	N-CA	-6.38	1.38	1.46
1	C	107	PRO	N-CD	-6.37	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	269	ILE	C-N	-6.37	1.25	1.33
3	J	334	LYS	CA-C	-6.37	1.44	1.52
3	J	76	TYR	N-CA	-6.37	1.38	1.46
3	J	275	ASN	C-N	-6.36	1.24	1.33
8	O	74	PRO	N-CD	-6.35	1.38	1.47
3	J	149	LEU	C-N	-6.35	1.26	1.33
3	J	100	HIS	C-N	-6.32	1.24	1.33
11	S	1091	PRO	N-CD	-6.31	1.39	1.47
3	J	53	ARG	CA-C	-6.30	1.45	1.52
3	J	137	MET	N-CA	6.28	1.58	1.46
3	J	103	GLU	N-CA	-6.28	1.38	1.46
1	A	107	PRO	N-CD	-6.25	1.39	1.47
3	J	375	LYS	CA-C	-6.24	1.44	1.52
3	J	367	ILE	C-O	-6.24	1.17	1.23
3	J	298	GLN	N-CA	-6.21	1.38	1.46
3	J	275	ASN	CA-C	-6.19	1.45	1.53
1	E	11	PRO	N-CD	-6.19	1.39	1.47
2	H	164	PRO	N-CD	-6.18	1.39	1.47
3	J	278	GLN	CA-C	-6.16	1.44	1.52
3	J	20	LEU	N-CA	-6.15	1.38	1.46
3	J	40	PRO	CA-C	-6.13	1.44	1.52
2	H	130	PRO	N-CD	-6.11	1.39	1.47
3	J	227	GLN	CA-C	-6.11	1.44	1.52
1	A	60	PRO	N-CD	-6.10	1.39	1.47
11	S	1227	PRO	N-CD	-6.10	1.39	1.47
8	O	89	PRO	N-CD	-6.09	1.39	1.47
3	J	297	LYS	N-CA	-6.09	1.38	1.46
1	G	11	PRO	N-CD	-6.04	1.39	1.47
1	E	107	PRO	N-CD	-6.04	1.39	1.47
3	J	124	HIS	N-CA	-6.03	1.38	1.46
3	J	343	ILE	C-N	-6.01	1.25	1.33
3	J	120	LEU	CA-C	-6.00	1.45	1.52
1	F	60	PRO	N-CD	-5.99	1.39	1.47
1	G	60	PRO	N-CD	-5.99	1.39	1.47
3	J	17	VAL	CA-C	5.99	1.60	1.52
1	F	169	PRO	N-CD	-5.98	1.39	1.47
3	J	242	PRO	C-N	-5.97	1.26	1.33
3	J	207	LEU	C-N	-5.95	1.25	1.33
3	J	330	PRO	C-O	-5.95	1.16	1.24
3	J	144	ARG	C-N	5.94	1.42	1.33
9	P	321	PRO	N-CD	-5.94	1.39	1.47
3	J	192	GLU	CA-C	-5.93	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	199	MET	N-CA	-5.93	1.39	1.46
3	J	270	LEU	N-CA	-5.92	1.39	1.46
3	J	179	LEU	CA-C	-5.92	1.44	1.52
3	J	241	SER	C-N	-5.90	1.26	1.33
3	J	315	PHE	C-N	-5.90	1.24	1.33
1	C	11	PRO	N-CD	-5.89	1.39	1.47
1	A	11	PRO	N-CD	-5.88	1.39	1.47
3	J	98	PRO	N-CD	-5.87	1.39	1.47
1	B	2044	PRO	N-CD	-5.86	1.39	1.47
1	D	42	PRO	N-CD	-5.85	1.39	1.47
1	D	60	PRO	N-CD	-5.85	1.39	1.47
3	J	193	GLN	N-CA	-5.83	1.38	1.45
3	J	216	PHE	CA-C	-5.81	1.45	1.52
3	J	263	ARG	C-O	5.81	1.31	1.24
1	I	169	PRO	N-CD	-5.81	1.39	1.47
1	C	60	PRO	N-CD	-5.80	1.39	1.47
3	J	184	THR	CA-C	5.80	1.59	1.52
3	J	104	THR	CA-C	-5.80	1.45	1.52
3	J	333	LYS	CA-C	-5.80	1.45	1.52
3	J	63	GLU	N-CA	-5.78	1.39	1.46
1	F	107	PRO	N-CD	-5.78	1.39	1.47
1	E	42	PRO	N-CD	-5.77	1.39	1.47
3	J	68	LEU	C-N	-5.77	1.26	1.33
3	J	222	ARG	CA-C	-5.76	1.45	1.52
3	J	332	TYR	C-N	-5.76	1.26	1.33
1	C	42	PRO	N-CD	-5.72	1.39	1.47
3	J	383	ARG	N-CA	-5.71	1.39	1.46
3	J	282	THR	C-N	-5.71	1.25	1.33
1	B	2062	PRO	N-CD	-5.71	1.39	1.47
3	J	123	SER	C-N	-5.70	1.25	1.33
3	J	173	LYS	C-N	-5.70	1.25	1.33
1	E	60	PRO	N-CD	-5.69	1.39	1.47
3	J	84	PRO	C-N	-5.69	1.26	1.33
3	J	282	THR	C-O	-5.69	1.16	1.24
3	J	43	ILE	CA-C	-5.68	1.45	1.52
3	J	107	ARG	N-CA	-5.66	1.39	1.46
3	J	127	ALA	CA-C	-5.65	1.45	1.52
3	J	27	CYS	C-N	-5.63	1.26	1.33
3	J	28	GLY	N-CA	-5.63	1.39	1.45
3	J	327	VAL	N-CA	-5.62	1.38	1.46
3	J	98	PRO	CA-C	5.62	1.59	1.52
3	J	206	VAL	C-O	-5.62	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	289	ILE	CA-C	-5.60	1.45	1.52
1	F	42	PRO	N-CD	-5.60	1.40	1.47
1	E	169	PRO	N-CD	-5.60	1.40	1.47
9	q	10	PRO	N-CD	-5.60	1.40	1.47
9	Q	10	PRO	N-CD	-5.59	1.40	1.47
3	J	143	TYR	C-N	-5.58	1.26	1.33
3	J	378	TYR	N-CA	-5.58	1.38	1.46
3	J	145	GLU	N-CA	5.57	1.53	1.46
1	A	42	PRO	N-CD	-5.57	1.40	1.47
9	p	17	PRO	N-CD	-5.57	1.40	1.47
3	J	105	LEU	C-N	-5.56	1.25	1.33
3	J	226	ILE	N-CA	-5.55	1.40	1.46
3	J	318	ARG	C-N	-5.55	1.26	1.33
3	J	202	VAL	C-N	-5.54	1.26	1.33
1	G	42	PRO	N-CD	-5.53	1.40	1.47
3	J	197	SER	C-N	-5.53	1.27	1.33
2	H	32	PRO	N-CD	-5.51	1.40	1.47
1	G	107	PRO	N-CD	-5.51	1.40	1.47
10	R	79	PRO	N-CD	-5.50	1.40	1.47
2	H	70	PRO	N-CD	-5.50	1.40	1.47
3	J	388	CYS	C-N	5.50	1.41	1.33
1	C	265	PRO	N-CD	-5.50	1.40	1.47
1	A	169	PRO	N-CD	-5.49	1.40	1.47
3	J	293	ILE	C-N	-5.48	1.26	1.33
1	B	2267	PRO	N-CD	-5.46	1.40	1.47
1	B	2325	PRO	N-CD	-5.45	1.40	1.47
3	J	158	LEU	N-CA	-5.44	1.39	1.46
1	D	11	PRO	N-CD	-5.43	1.40	1.47
3	J	163	ALA	N-CA	5.43	1.52	1.46
9	q	160	PRO	N-CD	-5.40	1.40	1.47
3	J	139	LEU	CA-C	-5.39	1.46	1.52
3	J	320	LEU	CA-C	-5.38	1.45	1.52
3	J	114	GLU	CA-C	-5.37	1.46	1.52
3	J	363	ALA	CA-C	-5.36	1.45	1.52
3	J	328	GLU	N-CA	-5.35	1.39	1.46
9	q	199	PRO	CA-C	5.35	1.57	1.52
1	F	253	PRO	N-CD	-5.34	1.40	1.47
3	J	62	GLU	N-CA	-5.34	1.39	1.46
3	J	289	ILE	C-N	-5.32	1.25	1.33
3	J	356	LEU	C-O	-5.32	1.17	1.24
2	H	27	PRO	N-CD	-5.32	1.40	1.47
1	I	31	PRO	N-CD	-5.31	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	31	PRO	N-CD	-5.31	1.40	1.47
3	J	166	LEU	C-O	-5.30	1.12	1.23
3	J	67	TYR	CA-C	-5.29	1.45	1.52
3	J	321	ALA	CA-C	-5.29	1.46	1.52
3	J	391	ASN	CA-C	-5.28	1.46	1.53
3	J	69	LYS	CA-C	-5.28	1.46	1.52
1	A	74	PRO	N-CD	-5.28	1.40	1.47
3	J	377	TYR	N-CA	-5.28	1.39	1.46
3	J	358	GLY	C-N	-5.27	1.25	1.33
1	F	74	PRO	N-CD	-5.27	1.40	1.47
3	J	341	PHE	N-CA	-5.27	1.39	1.45
3	J	136	ALA	N-CA	5.26	1.52	1.45
1	A	31	PRO	N-CD	-5.26	1.40	1.47
1	G	74	PRO	N-CD	-5.26	1.40	1.47
3	J	64	LEU	CA-C	-5.26	1.45	1.52
3	J	208	GLU	CA-C	-5.25	1.46	1.52
7	N	165	PRO	N-CD	-5.24	1.40	1.47
3	J	280	VAL	C-N	-5.23	1.26	1.33
1	I	228	PRO	N-CD	-5.23	1.40	1.47
3	J	23	ALA	C-O	-5.22	1.17	1.24
3	J	128	LEU	N-CA	-5.21	1.39	1.46
3	J	337	GLY	N-CA	5.21	1.52	1.45
1	B	2171	PRO	N-CD	-5.21	1.40	1.47
9	P	185	LYS	C-O	-5.20	1.17	1.23
3	J	140	ASP	CA-C	5.20	1.59	1.52
3	J	219	ASP	C-N	-5.19	1.26	1.33
9	Q	114	THR	CA-C	-5.18	1.46	1.52
3	J	344	HIS	N-CA	-5.18	1.39	1.46
3	J	325	TYR	N-CA	-5.18	1.40	1.46
3	J	284	ILE	N-CA	-5.18	1.40	1.46
3	J	236	ASN	C-N	-5.17	1.26	1.33
1	D	265	PRO	N-CD	-5.16	1.40	1.47
1	F	31	PRO	N-CD	-5.15	1.40	1.47
3	J	147	LEU	CA-C	5.15	1.58	1.52
3	J	173	LYS	N-CA	5.14	1.52	1.46
3	J	378	TYR	CA-C	-5.14	1.45	1.52
3	J	133	ILE	CA-C	-5.13	1.46	1.52
3	J	385	PRO	N-CD	-5.13	1.40	1.47
3	J	360	ILE	C-N	-5.12	1.27	1.33
3	J	195	LEU	C-O	-5.12	1.17	1.24
1	G	323	PRO	N-CD	-5.12	1.40	1.47
9	P	26	PRO	N-CD	-5.11	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	10	PRO	N-CD	-5.10	1.40	1.47
3	J	389	SER	N-CA	5.09	1.52	1.46
3	J	271	PHE	N-CA	-5.09	1.40	1.46
9	Q	120	ILE	CA-C	-5.09	1.46	1.52
3	J	271	PHE	CA-C	5.09	1.60	1.52
3	J	79	HIS	N-CA	-5.08	1.40	1.46
3	J	124	HIS	C-N	-5.07	1.26	1.33
3	J	241	SER	CA-C	-5.07	1.48	1.53
3	J	73	HIS	C-O	-5.07	1.18	1.24
9	Q	169	PRO	N-CD	-5.07	1.40	1.47
5	L	141	PRO	N-CD	-5.05	1.40	1.47
7	N	25	PRO	CA-C	5.05	1.54	1.51
3	J	68	LEU	CA-C	-5.05	1.45	1.52
3	J	111	LYS	N-CA	-5.05	1.39	1.46
3	J	326	LEU	N-CA	-5.04	1.39	1.46
1	E	31	PRO	N-CD	-5.03	1.40	1.47
3	J	387	TRP	C-N	-5.03	1.26	1.33
3	J	180	LEU	N-CA	-5.02	1.39	1.46
1	F	265	PRO	N-CD	-5.02	1.40	1.47
9	P	17	PRO	N-CD	-5.02	1.40	1.47
3	J	355	TRP	C-N	-5.02	1.26	1.33
3	J	371	ARG	CA-C	-5.02	1.46	1.52
4	K	457	PRO	N-CD	-5.00	1.40	1.47
3	J	296	ARG	CA-C	-5.00	1.45	1.52
3	J	316	LEU	C-N	-5.00	1.27	1.33
3	J	317	HIS	C-N	-5.00	1.26	1.33

All (713) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	196	PRO	CA-C-N	-45.23	62.42	123.03
3	J	196	PRO	C-N-CA	-45.23	62.42	123.03
3	J	144	ARG	O-C-N	35.68	165.94	123.12
3	J	195	LEU	CA-C-N	-26.54	86.66	119.84
3	J	195	LEU	C-N-CA	-26.54	86.66	119.84
3	J	144	ARG	CA-C-O	-24.75	94.34	121.07
3	J	230	LYS	CA-C-N	-20.27	93.14	123.14
3	J	230	LYS	C-N-CA	-20.27	93.14	123.14
3	J	182	GLN	CA-C-N	-19.53	93.99	121.33
3	J	182	GLN	C-N-CA	-19.53	93.99	121.33
3	J	248	TYR	CA-C-N	-18.94	100.72	119.85
3	J	248	TYR	C-N-CA	-18.94	100.72	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	237	ASN	CA-C-N	-18.68	93.16	122.49
3	J	237	ASN	C-N-CA	-18.68	93.16	122.49
3	J	230	LYS	N-CA-C	-18.35	85.61	112.04
3	J	198	VAL	N-CA-C	-18.23	95.66	113.53
3	J	22	GLU	N-CA-C	-17.48	91.21	112.89
3	J	308	GLY	CA-C-N	-16.79	88.85	121.58
3	J	308	GLY	C-N-CA	-16.79	88.85	121.58
3	J	34	GLY	CA-C-N	-16.49	104.38	120.21
3	J	34	GLY	C-N-CA	-16.49	104.38	120.21
3	J	115	VAL	CA-C-N	-16.37	104.27	120.31
3	J	115	VAL	C-N-CA	-16.37	104.27	120.31
3	J	39	ILE	CA-C-N	-16.36	102.80	120.14
3	J	39	ILE	C-N-CA	-16.36	102.80	120.14
3	J	300	ALA	N-CA-C	-15.84	87.62	110.59
3	J	17	VAL	CA-C-N	15.84	147.84	122.50
3	J	17	VAL	C-N-CA	15.84	147.84	122.50
3	J	40	PRO	CA-C-N	-15.53	101.11	123.00
3	J	40	PRO	C-N-CA	-15.53	101.11	123.00
3	J	352	CYS	CA-C-N	-15.51	94.89	120.64
3	J	352	CYS	C-N-CA	-15.51	94.89	120.64
3	J	165	PRO	N-CA-C	-15.12	90.05	111.22
3	J	155	ILE	CA-C-N	-15.12	104.12	120.14
3	J	155	ILE	C-N-CA	-15.12	104.12	120.14
3	J	144	ARG	N-CA-C	14.79	131.06	110.35
3	J	18	ILE	CA-C-N	14.63	142.30	121.24
3	J	18	ILE	C-N-CA	14.63	142.30	121.24
3	J	197	SER	N-CA-C	14.53	132.46	108.49
3	J	125	LEU	CA-C-O	13.82	134.34	119.14
3	J	19	ASP	CA-C-N	-13.72	100.26	122.08
3	J	19	ASP	C-N-CA	-13.72	100.26	122.08
3	J	329	LYS	CA-C-N	13.61	134.25	119.28
3	J	329	LYS	C-N-CA	13.61	134.25	119.28
3	J	173	LYS	N-CA-C	-13.53	95.18	112.23
3	J	151	ILE	O-C-N	-13.46	108.93	123.20
3	J	169	LYS	N-CA-C	-13.39	95.36	112.90
9	Q	116	GLU	N-CA-C	-13.38	96.75	111.07
3	J	152	TYR	CA-C-N	-13.25	102.14	120.82
3	J	152	TYR	C-N-CA	-13.25	102.14	120.82
3	J	16	VAL	N-CA-C	13.24	127.54	108.48
3	J	248	TYR	CA-C-O	13.16	127.84	119.29
3	J	225	LYS	N-CA-C	-13.13	96.95	113.23
3	J	183	CYS	N-CA-C	13.08	129.43	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	69	LYS	CA-C-N	-13.05	98.49	120.68
3	J	69	LYS	C-N-CA	-13.05	98.49	120.68
3	J	23	ALA	CA-C-N	-13.04	95.36	121.18
3	J	23	ALA	C-N-CA	-13.04	95.36	121.18
3	J	315	PHE	CA-C-O	-13.02	106.56	120.63
3	J	322	GLU	CA-C-N	-13.01	97.91	120.29
3	J	322	GLU	C-N-CA	-13.01	97.91	120.29
3	J	43	ILE	N-CA-C	-12.94	89.18	108.46
3	J	306	ILE	O-C-N	12.86	137.32	123.04
3	J	268	GLU	CA-C-N	-12.57	101.33	120.82
3	J	268	GLU	C-N-CA	-12.57	101.33	120.82
3	J	100	HIS	N-CA-C	-12.55	90.38	110.20
3	J	105	LEU	CA-C-N	-12.52	99.40	120.68
3	J	105	LEU	C-N-CA	-12.52	99.40	120.68
3	J	332	TYR	N-CA-C	-12.23	98.45	113.50
3	J	173	LYS	CA-C-N	-12.19	97.81	121.58
3	J	173	LYS	C-N-CA	-12.19	97.81	121.58
3	J	78	ARG	CA-C-N	-12.16	103.91	120.44
3	J	78	ARG	C-N-CA	-12.16	103.91	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	391	ASN	CA-C-N	-12.06	104.25	120.65
3	J	391	ASN	C-N-CA	-12.06	104.25	120.65
3	J	76	TYR	CA-C-N	12.04	136.80	120.54
3	J	76	TYR	C-N-CA	12.04	136.80	120.54
3	J	164	LEU	CA-C-N	12.04	131.77	120.21
3	J	164	LEU	C-N-CA	12.04	131.77	120.21
3	J	296	ARG	CA-C-O	12.01	134.67	119.05
3	J	158	LEU	CA-C-N	-11.95	98.28	121.58
3	J	158	LEU	C-N-CA	-11.95	98.28	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	40	PRO	N-CA-C	-11.91	91.80	111.68
3	J	112	TYR	N-CA-C	-11.91	94.89	112.04
3	J	212	ALA	CA-C-N	-11.79	103.72	122.23
3	J	212	ALA	C-N-CA	-11.79	103.72	122.23
3	J	325	TYR	N-CA-C	-11.73	98.47	111.14
3	J	110	PHE	N-CA-C	-11.70	90.68	108.00
3	J	65	TYR	CA-C-N	-11.55	100.93	121.14
3	J	65	TYR	C-N-CA	-11.55	100.93	121.14
3	J	352	CYS	O-C-N	-11.54	107.08	122.43
3	J	74	ILE	CA-C-O	11.49	132.90	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	352	CYS	CA-C-O	11.49	133.58	119.10
9	Q	116	GLU	CA-C-N	11.41	135.32	120.60
9	Q	116	GLU	C-N-CA	11.41	135.32	120.60
3	J	127	ALA	N-CA-C	11.29	124.69	111.71
3	J	313	PRO	O-C-N	11.19	136.82	123.06
3	J	225	LYS	CA-C-N	-11.14	105.20	120.46
3	J	225	LYS	C-N-CA	-11.14	105.20	120.46
3	J	210	ILE	N-CA-C	-11.02	100.17	110.53
3	J	37	CYS	CA-C-O	11.00	133.46	120.81
3	J	219	ASP	CA-C-N	10.97	142.50	121.54
3	J	219	ASP	C-N-CA	10.97	142.50	121.54
3	J	313	PRO	CA-C-N	10.95	141.86	122.05
3	J	313	PRO	C-N-CA	10.95	141.86	122.05
3	J	175	LEU	CA-C-N	-10.89	104.83	120.29
3	J	175	LEU	C-N-CA	-10.89	104.83	120.29
3	J	350	ALA	O-C-N	-10.88	109.49	122.22
3	J	63	GLU	N-CA-C	-10.87	99.40	111.14
3	J	99	SER	CA-C-O	-10.78	107.92	120.10
3	J	256	LEU	CA-C-N	-10.78	106.00	121.42
3	J	256	LEU	C-N-CA	-10.78	106.00	121.42
3	J	223	GLY	N-CA-C	-10.77	98.99	112.77
3	J	41	SER	N-CA-C	10.66	125.79	108.41
3	J	23	ALA	O-C-N	-10.65	108.42	122.59
3	J	125	LEU	O-C-N	-10.57	108.33	122.49
3	J	330	PRO	CA-C-N	-10.52	102.73	121.14
3	J	330	PRO	C-N-CA	-10.52	102.73	121.14
3	J	68	LEU	CA-C-O	10.49	132.17	119.79
9	Q	116	GLU	O-C-N	-10.40	111.36	122.07
3	J	270	LEU	N-CA-C	-10.39	99.96	111.28
3	J	121	ALA	CA-C-N	10.38	130.31	120.03
3	J	121	ALA	C-N-CA	10.38	130.31	120.03
3	J	67	TYR	N-CA-C	10.38	123.86	111.82
3	J	184	THR	CA-C-N	-10.36	108.59	122.99
3	J	184	THR	C-N-CA	-10.36	108.59	122.99
3	J	195	LEU	O-C-N	-10.31	109.46	121.32
3	J	71	PHE	O-C-N	10.30	133.03	122.12
3	J	306	ILE	CA-C-O	-10.28	110.87	121.67
3	J	109	LEU	CA-C-N	-10.27	100.37	122.04
3	J	109	LEU	C-N-CA	-10.27	100.37	122.04
3	J	122	PRO	N-CA-C	10.23	126.76	111.41
3	J	81	LEU	N-CA-C	-10.23	94.62	109.96
3	J	311	MET	N-CA-C	-10.20	99.94	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	355	TRP	N-CA-C	-10.18	99.56	112.90
3	J	105	LEU	CA-C-O	10.13	131.62	119.97
3	J	357	GLY	N-CA-C	-10.04	98.44	115.62
3	J	43	ILE	CA-C-O	-10.04	109.43	120.67
3	J	206	VAL	CA-C-N	-9.91	105.24	120.31
3	J	206	VAL	C-N-CA	-9.91	105.24	120.31
3	J	129	LEU	CA-C-O	-9.90	108.91	120.10
3	J	86	ASP	N-CA-C	9.85	125.37	113.16
3	J	233	ILE	CA-C-N	-9.84	108.13	122.40
3	J	233	ILE	C-N-CA	-9.84	108.13	122.40
3	J	195	LEU	CA-C-O	9.81	133.60	120.16
3	J	356	LEU	CA-C-N	-9.80	96.00	122.46
3	J	356	LEU	C-N-CA	-9.80	96.00	122.46
3	J	111	LYS	N-CA-C	9.78	124.48	112.54
3	J	275	ASN	CA-C-N	9.75	138.56	122.87
3	J	275	ASN	C-N-CA	9.75	138.56	122.87
3	J	164	LEU	O-C-N	9.71	129.13	121.55
11	S	1214	ARG	CA-C-N	9.55	129.65	119.05
11	S	1214	ARG	C-N-CA	9.55	129.65	119.05
3	J	204	GLU	CA-C-O	9.53	131.02	119.49
3	J	116	PRO	N-CA-C	-9.51	97.11	111.57
3	J	382	GLY	CA-C-N	-9.51	109.88	123.00
3	J	382	GLY	C-N-CA	-9.51	109.88	123.00
3	J	243	PRO	CA-C-N	9.50	129.59	119.90
3	J	243	PRO	C-N-CA	9.50	129.59	119.90
3	J	377	TYR	O-C-N	9.50	132.98	122.15
3	J	368	LEU	CA-C-N	-9.44	96.97	122.46
3	J	368	LEU	C-N-CA	-9.44	96.97	122.46
3	J	256	LEU	O-C-N	-9.40	111.87	123.05
3	J	349	LYS	CA-C-O	9.38	132.19	121.87
3	J	359	ALA	N-CA-C	-9.37	100.62	112.90
3	J	283	LEU	CA-C-N	-9.37	107.12	120.42
3	J	283	LEU	C-N-CA	-9.37	107.12	120.42
3	J	276	GLU	N-CA-C	-9.36	95.06	109.95
3	J	374	SER	N-CA-C	9.35	123.68	110.50
3	J	72	ILE	CA-C-N	-9.33	107.05	120.29
3	J	72	ILE	C-N-CA	-9.33	107.05	120.29
3	J	75	LEU	CA-C-O	9.26	130.71	119.79
3	J	259	LEU	O-C-N	-9.26	111.94	122.86
3	J	105	LEU	O-C-N	-9.23	110.91	122.27
3	J	177	THR	O-C-N	9.23	131.58	122.07
3	J	368	LEU	O-C-N	-9.22	111.43	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	346	PRO	CA-C-N	9.22	128.95	119.64
3	J	346	PRO	C-N-CA	9.22	128.95	119.64
3	J	178	GLN	CA-C-N	-9.21	105.02	120.68
3	J	178	GLN	C-N-CA	-9.21	105.02	120.68
3	J	69	LYS	CA-C-O	9.20	130.17	120.42
3	J	378	TYR	CA-C-N	-9.18	106.35	120.31
3	J	378	TYR	C-N-CA	-9.18	106.35	120.31
3	J	71	PHE	CA-C-O	-9.17	110.83	120.55
3	J	308	GLY	N-CA-C	-9.17	103.06	114.16
3	J	73	HIS	CA-C-N	9.15	133.00	120.46
3	J	73	HIS	C-N-CA	9.15	133.00	120.46
3	J	69	LYS	O-C-N	-9.12	111.75	122.15
11	S	1126	LEU	CA-C-N	9.11	129.76	120.38
11	S	1126	LEU	C-N-CA	9.11	129.76	120.38
3	J	191	LYS	CA-C-N	-9.09	110.03	122.30
3	J	191	LYS	C-N-CA	-9.09	110.03	122.30
3	J	360	ILE	O-C-N	9.07	130.67	121.87
3	J	318	ARG	O-C-N	9.03	134.43	122.33
3	J	89	VAL	O-C-N	-9.03	113.73	123.03
3	J	318	ARG	CA-C-N	-8.99	108.23	120.28
3	J	318	ARG	C-N-CA	-8.99	108.23	120.28
3	J	128	LEU	N-CA-C	-8.99	102.33	113.38
3	J	37	CYS	CA-C-N	-8.96	111.19	122.93
3	J	37	CYS	C-N-CA	-8.96	111.19	122.93
3	J	137	MET	CA-C-N	-8.92	111.45	123.14
3	J	137	MET	C-N-CA	-8.92	111.45	123.14
3	J	333	LYS	CA-C-N	-8.92	105.52	120.68
3	J	333	LYS	C-N-CA	-8.92	105.52	120.68
3	J	285	LEU	CA-C-N	-8.91	105.53	120.68
3	J	285	LEU	C-N-CA	-8.91	105.53	120.68
3	J	315	PHE	CA-C-N	-8.89	105.52	122.06
3	J	315	PHE	C-N-CA	-8.89	105.52	122.06
3	J	125	LEU	CA-C-N	-8.89	105.59	121.14
3	J	125	LEU	C-N-CA	-8.89	105.59	121.14
3	J	288	LEU	O-C-N	-8.88	111.34	122.27
3	J	337	GLY	CA-C-N	-8.87	107.90	122.81
3	J	337	GLY	C-N-CA	-8.87	107.90	122.81
3	J	371	ARG	CA-C-N	8.86	136.09	121.39
3	J	371	ARG	C-N-CA	8.86	136.09	121.39
3	J	348	ALA	N-CA-C	-8.84	98.62	110.55
3	J	333	LYS	CA-C-O	8.84	129.79	120.42
3	J	335	ALA	N-CA-C	8.80	120.96	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	103	GLU	O-C-N	8.80	132.18	122.15
3	J	232	ASN	N-CA-C	-8.78	91.41	107.75
3	J	156	PRO	CA-C-N	-8.77	111.18	123.11
3	J	156	PRO	C-N-CA	-8.77	111.18	123.11
3	J	306	ILE	N-CA-C	-8.76	94.49	108.95
3	J	334	LYS	N-CA-C	-8.75	101.21	112.23
3	J	69	LYS	N-CA-C	-8.73	101.84	111.36
3	J	136	ALA	CA-C-N	8.73	137.41	121.70
3	J	136	ALA	C-N-CA	8.73	137.41	121.70
3	J	162	GLY	O-C-N	-8.72	115.29	123.48
3	J	300	ALA	CA-C-O	-8.70	111.72	121.89
3	J	356	LEU	O-C-N	-8.65	109.79	122.43
3	J	170	ALA	O-C-N	8.65	134.39	122.46
3	J	51	PRO	CA-C-N	8.59	133.84	123.19
3	J	51	PRO	C-N-CA	8.59	133.84	123.19
3	J	83	ASN	CA-C-N	8.57	128.30	119.56
3	J	83	ASN	C-N-CA	8.57	128.30	119.56
3	J	387	TRP	CA-C-N	-8.55	107.85	122.56
3	J	387	TRP	C-N-CA	-8.55	107.85	122.56
3	J	266	VAL	CA-C-N	-8.54	106.59	121.97
3	J	266	VAL	C-N-CA	-8.54	106.59	121.97
3	J	193	GLN	N-CA-C	8.54	122.76	109.52
3	J	246	VAL	O-C-N	-8.53	114.05	123.26
3	J	393	PRO	CA-C-O	-8.53	113.99	120.73
3	J	378	TYR	N-CA-C	-8.51	102.34	112.89
3	J	220	LEU	CA-C-N	-8.48	106.55	120.72
3	J	220	LEU	C-N-CA	-8.48	106.55	120.72
14	s	1143	LEU	CA-C-N	8.38	128.59	119.87
14	s	1143	LEU	C-N-CA	8.38	128.59	119.87
3	J	255	ILE	CA-C-N	-8.37	111.96	122.84
3	J	255	ILE	C-N-CA	-8.37	111.96	122.84
3	J	246	VAL	N-CA-C	8.36	119.82	108.11
3	J	82	VAL	CA-C-N	8.35	131.85	122.83
3	J	82	VAL	C-N-CA	8.35	131.85	122.83
3	J	145	GLU	CA-C-N	8.34	132.71	120.87
3	J	145	GLU	C-N-CA	8.34	132.71	120.87
3	J	268	GLU	N-CA-C	-8.33	101.27	112.26
3	J	14	THR	CA-C-N	8.29	136.63	121.70
3	J	14	THR	C-N-CA	8.29	136.63	121.70
3	J	350	ALA	CA-C-N	-8.28	108.54	120.29
3	J	350	ALA	C-N-CA	-8.28	108.54	120.29
3	J	191	LYS	O-C-N	-8.26	113.81	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	60	ASN	N-CA-C	-8.20	97.88	110.10
3	J	298	GLN	O-C-N	8.19	133.99	122.36
3	J	303	LEU	O-C-N	-8.18	113.64	123.29
3	J	319	LEU	CA-C-N	-8.16	106.86	121.14
3	J	319	LEU	C-N-CA	-8.16	106.86	121.14
3	J	72	ILE	N-CA-C	-8.16	100.89	111.09
3	J	386	ASP	O-C-N	-8.15	112.59	123.19
3	J	181	GLU	CA-C-O	-8.15	109.56	119.59
3	J	234	ASP	N-CA-C	-8.14	101.83	112.24
3	J	319	LEU	O-C-N	8.08	130.69	122.12
10	r	70	PRO	N-CA-C	-8.08	105.31	114.92
3	J	134	ASN	N-CA-C	-8.06	103.02	113.17
3	J	381	THR	N-CA-C	-8.02	103.33	113.43
3	J	147	LEU	CA-C-N	-8.01	113.26	123.19
3	J	147	LEU	C-N-CA	-8.01	113.26	123.19
3	J	126	MET	N-CA-C	-7.98	103.00	112.89
3	J	74	ILE	O-C-N	-7.96	114.14	121.87
3	J	280	VAL	N-CA-C	-7.92	101.20	111.09
3	J	176	GLU	N-CA-C	-7.91	102.73	111.36
3	J	322	GLU	CA-C-O	7.91	129.07	119.97
3	J	17	VAL	O-C-N	-7.90	114.67	123.20
3	J	231	PHE	N-CA-C	7.90	123.19	107.62
3	J	97	CYS	CA-C-N	-7.88	112.65	120.21
3	J	97	CYS	C-N-CA	-7.88	112.65	120.21
3	J	256	LEU	CA-C-O	7.86	128.72	120.54
3	J	374	SER	O-C-N	7.85	132.13	122.86
3	J	337	GLY	N-CA-C	-7.85	98.45	112.58
3	J	260	GLY	N-CA-C	-7.84	104.68	114.16
3	J	65	TYR	O-C-N	-7.82	113.83	122.12
3	J	246	VAL	CA-C-N	-7.81	112.03	122.42
3	J	246	VAL	C-N-CA	-7.81	112.03	122.42
3	J	73	HIS	O-C-N	7.81	131.05	122.15
3	J	14	THR	N-CA-C	-7.77	97.58	109.85
3	J	388	CYS	N-CA-C	7.75	122.32	113.02
3	J	331	LYS	CA-C-N	-7.71	108.58	121.92
3	J	331	LYS	C-N-CA	-7.71	108.58	121.92
3	J	68	LEU	CA-C-N	-7.71	109.35	120.29
3	J	68	LEU	C-N-CA	-7.71	109.35	120.29
3	J	252	GLY	CA-C-N	-7.71	111.42	122.36
3	J	252	GLY	C-N-CA	-7.71	111.42	122.36
3	J	368	LEU	CA-C-O	7.69	128.79	120.10
3	J	181	GLU	CA-C-N	-7.68	109.42	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	181	GLU	C-N-CA	-7.68	109.42	122.33
3	J	119	LEU	CA-C-O	7.68	129.33	120.80
3	J	163	ALA	N-CA-C	7.68	121.88	108.75
3	J	373	VAL	O-C-N	-7.68	113.25	122.77
3	J	191	LYS	CA-C-O	7.67	130.57	121.36
3	J	267	VAL	N-CA-C	7.65	125.25	109.34
3	J	122	PRO	O-C-N	-7.62	113.70	123.00
3	J	122	PRO	CA-C-N	-7.62	107.81	121.14
3	J	122	PRO	C-N-CA	-7.62	107.81	121.14
3	J	212	ALA	N-CA-C	-7.60	103.00	111.28
3	J	49	PRO	N-CA-C	-7.59	99.14	111.21
3	J	293	ILE	CA-C-O	7.58	128.66	120.47
3	J	105	LEU	N-CA-C	-7.58	103.03	111.82
3	J	287	SER	CA-C-N	-7.56	108.83	120.31
3	J	287	SER	C-N-CA	-7.56	108.83	120.31
3	J	124	HIS	N-CA-C	-7.55	104.04	113.18
3	J	131	LEU	N-CA-C	-7.55	103.91	113.72
3	J	204	GLU	CA-C-N	-7.54	107.37	120.79
3	J	204	GLU	C-N-CA	-7.54	107.37	120.79
3	J	108	VAL	O-C-N	7.53	132.28	122.26
3	J	147	LEU	O-C-N	-7.53	114.34	123.30
3	J	338	THR	O-C-N	-7.51	113.05	123.11
3	J	52	VAL	CA-C-N	-7.49	112.46	122.42
3	J	52	VAL	C-N-CA	-7.49	112.46	122.42
3	J	82	VAL	O-C-N	-7.47	116.23	121.98
3	J	109	LEU	N-CA-C	-7.44	94.95	110.80
3	J	203	PRO	CA-C-N	7.42	132.47	120.60
3	J	203	PRO	C-N-CA	7.42	132.47	120.60
3	J	369	GLY	N-CA-C	-7.39	102.98	115.62
3	J	169	LYS	CA-C-N	-7.35	106.62	121.18
3	J	169	LYS	C-N-CA	-7.35	106.62	121.18
3	J	314	GLY	N-CA-C	-7.35	105.18	115.32
3	J	147	LEU	N-CA-C	7.34	120.87	108.90
3	J	319	LEU	CA-C-O	-7.34	112.77	120.55
11	S	1218	THR	CA-C-N	7.34	126.20	120.33
11	S	1218	THR	C-N-CA	7.34	126.20	120.33
3	J	326	LEU	CA-C-N	-7.33	108.63	120.86
3	J	326	LEU	C-N-CA	-7.33	108.63	120.86
3	J	23	ALA	CA-C-O	7.31	130.97	120.51
3	J	326	LEU	CA-C-O	7.31	128.37	119.38
3	J	268	GLU	CA-C-O	-7.30	111.71	120.55
3	J	133	ILE	CA-C-N	-7.29	110.51	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	133	ILE	C-N-CA	-7.29	110.51	122.54
3	J	329	LYS	N-CA-C	-7.28	100.47	109.65
3	J	175	LEU	N-CA-C	-7.27	104.94	113.88
11	S	1211	VAL	CA-C-O	-7.27	113.15	120.85
3	J	252	GLY	N-CA-C	-7.26	105.20	115.30
3	J	326	LEU	O-C-N	-7.26	112.70	122.43
3	J	43	ILE	CA-C-N	7.23	134.71	121.70
3	J	43	ILE	C-N-CA	7.23	134.71	121.70
3	J	160	CYS	N-CA-C	-7.22	92.83	107.41
3	J	185	VAL	N-CA-C	-7.20	97.76	108.12
3	J	288	LEU	CA-C-O	7.18	128.22	119.97
3	J	281	ALA	CA-C-N	-7.17	107.85	121.54
3	J	281	ALA	C-N-CA	-7.17	107.85	121.54
3	J	343	ILE	CA-C-N	-7.15	112.86	122.72
3	J	343	ILE	C-N-CA	-7.15	112.86	122.72
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	317	HIS	O-C-N	7.14	129.80	122.09
3	J	147	LEU	CA-C-O	7.12	128.04	120.36
3	J	114	GLU	N-CA-C	-7.11	99.92	110.23
3	J	184	THR	O-C-N	7.11	132.03	123.36
3	J	129	LEU	O-C-N	-7.09	113.92	122.22
3	J	111	LYS	CA-C-N	-7.09	106.50	121.80
3	J	111	LYS	C-N-CA	-7.09	106.50	121.80
3	J	220	LEU	O-C-N	-7.08	113.17	122.59
3	J	36	ARG	N-CA-C	-7.05	92.93	107.67
3	J	14	THR	CA-C-O	-7.05	113.21	121.46
3	J	393	PRO	CA-C-N	-7.04	111.04	119.84
3	J	393	PRO	C-N-CA	-7.04	111.04	119.84
3	J	183	CYS	CA-C-O	7.04	127.20	120.09
3	J	303	LEU	CA-C-O	7.02	128.03	120.38
3	J	186	ASP	CA-C-O	7.01	128.42	120.84
3	J	258	ILE	O-C-N	-7.00	115.69	123.26
3	J	349	LYS	N-CA-C	7.00	119.59	110.43
3	J	37	CYS	O-C-N	-6.98	114.34	122.93
3	J	84	PRO	CA-C-N	-6.97	109.08	120.72
3	J	84	PRO	C-N-CA	-6.97	109.08	120.72
3	J	312	LEU	CA-C-O	-6.97	112.59	119.49
3	J	376	GLU	CA-C-O	-6.96	113.04	120.42
11	S	1219	VAL	O-C-N	-6.96	115.97	120.42
3	J	75	LEU	O-C-N	-6.95	113.02	122.33
10	R	63	ASP	CA-C-N	6.95	130.16	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	63	ASP	C-N-CA	6.95	130.16	120.29
3	J	138	VAL	N-CA-C	6.91	117.78	108.11
3	J	376	GLU	O-C-N	6.86	129.97	122.15
3	J	83	ASN	O-C-N	6.83	129.18	121.32
3	J	356	LEU	CA-C-O	6.83	127.85	119.11
3	J	172	HIS	CA-C-O	-6.81	112.14	119.97
3	J	322	GLU	O-C-N	-6.81	113.90	122.27
3	J	324	ARG	CA-C-O	6.80	127.74	119.38
3	J	74	ILE	N-CA-C	6.78	117.54	110.62
3	J	341	PHE	N-CA-C	-6.78	98.78	109.50
3	J	214	THR	N-CA-C	6.78	121.83	113.50
3	J	349	LYS	O-C-N	-6.77	114.83	122.75
10	R	54	VAL	N-CA-C	6.77	117.55	110.72
3	J	333	LYS	N-CA-C	6.75	118.72	111.36
11	S	1226	PHE	CA-C-N	6.74	126.53	119.05
11	S	1226	PHE	C-N-CA	6.74	126.53	119.05
3	J	386	ASP	CA-C-O	6.71	128.69	121.11
3	J	110	PHE	CA-C-N	-6.71	109.52	120.72
3	J	110	PHE	C-N-CA	-6.71	109.52	120.72
3	J	393	PRO	O-C-N	6.70	124.30	121.15
3	J	365	GLN	O-C-N	-6.70	113.68	122.59
3	J	75	LEU	N-CA-C	-6.69	103.81	112.23
3	J	389	SER	N-CA-C	6.68	120.12	109.24
3	J	362	GLY	N-CA-C	-6.67	106.39	114.66
10	R	73	ILE	CA-C-N	6.64	129.18	120.28
10	R	73	ILE	C-N-CA	6.64	129.18	120.28
3	J	106	THR	CA-C-N	6.61	129.79	120.28
3	J	106	THR	C-N-CA	6.61	129.79	120.28
9	Q	134	THR	CA-C-N	6.61	126.85	119.32
9	Q	134	THR	C-N-CA	6.61	126.85	119.32
3	J	321	ALA	N-CA-C	-6.61	104.16	111.36
3	J	72	ILE	CA-C-O	6.60	127.60	120.47
3	J	266	VAL	O-C-N	6.57	129.23	121.80
3	J	364	LEU	CA-C-O	-6.57	110.51	119.05
3	J	134	ASN	CA-C-O	6.57	127.03	119.35
3	J	282	THR	CA-C-O	-6.56	111.13	120.51
3	J	174	GLU	N-CA-C	6.55	121.11	113.18
3	J	196	PRO	O-C-N	-6.54	113.82	122.64
3	J	208	GLU	CA-C-N	-6.49	109.79	121.14
3	J	208	GLU	C-N-CA	-6.49	109.79	121.14
3	J	176	GLU	O-C-N	6.48	129.53	122.15
3	J	166	LEU	CA-C-O	-6.47	109.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	84	PRO	O-C-N	-6.46	113.58	122.24
3	J	207	LEU	O-C-N	6.46	130.21	122.27
3	J	61	THR	O-C-N	6.45	130.77	122.39
3	J	263	ARG	CA-C-O	6.44	127.25	120.42
3	J	313	PRO	CA-C-O	-6.44	113.81	121.67
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	148	VAL	O-C-N	-6.41	116.45	123.18
3	J	144	ARG	CB-CA-C	-6.39	99.51	109.61
3	J	130	THR	CA-C-N	-6.38	112.11	122.26
3	J	130	THR	C-N-CA	-6.38	112.11	122.26
3	J	177	THR	CA-C-O	-6.35	114.15	120.82
3	J	304	VAL	CA-C-O	-6.32	113.75	120.39
3	J	113	PHE	N-CA-C	6.31	119.10	107.99
3	J	298	GLN	N-CA-C	-6.31	105.71	113.41
3	J	351	ASN	CA-C-N	6.30	132.70	120.99
3	J	351	ASN	C-N-CA	6.30	132.70	120.99
3	J	46	ALA	N-CA-C	6.28	118.93	111.71
3	J	103	GLU	N-CA-C	-6.28	104.52	111.36
3	J	283	LEU	O-C-N	-6.28	114.24	122.59
10	r	52	GLU	CB-CA-C	-6.25	109.35	116.54
3	J	156	PRO	CA-C-O	-6.25	114.23	121.86
9	p	80	GLY	CA-C-N	6.23	130.59	121.31
9	p	80	GLY	C-N-CA	6.23	130.59	121.31
3	J	64	LEU	CA-C-O	-6.23	112.81	119.97
3	J	334	LYS	CA-C-N	-6.22	111.45	120.29
3	J	334	LYS	C-N-CA	-6.22	111.45	120.29
3	J	148	VAL	CA-C-O	6.22	127.07	120.48
10	R	30	SER	CB-CA-C	-6.22	109.42	116.63
3	J	330	PRO	CA-C-O	6.21	128.99	119.55
10	r	73	ILE	CA-C-N	6.20	128.59	120.28
10	r	73	ILE	C-N-CA	6.20	128.59	120.28
3	J	277	GLU	CA-C-N	-6.20	111.41	122.32
3	J	277	GLU	C-N-CA	-6.20	111.41	122.32
3	J	258	ILE	CA-C-O	6.19	126.89	120.39
11	S	1216	GLY	CA-C-N	6.18	133.80	122.79
11	S	1216	GLY	C-N-CA	6.18	133.80	122.79
3	J	31	GLY	N-CA-C	-6.18	95.37	113.30
11	S	1127	PRO	CA-C-O	-6.18	111.59	120.56
10	r	107	LEU	CA-C-N	6.17	124.13	120.24
10	r	107	LEU	C-N-CA	6.17	124.13	120.24
3	J	98	PRO	CA-C-N	-6.14	111.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	98	PRO	C-N-CA	-6.14	111.44	120.28
3	J	204	GLU	O-C-N	-6.14	114.41	122.39
3	J	210	ILE	CA-C-N	6.13	128.50	120.28
3	J	210	ILE	C-N-CA	6.13	128.50	120.28
11	S	1130	HIS	CA-C-N	6.13	129.51	120.74
11	S	1130	HIS	C-N-CA	6.13	129.51	120.74
3	J	293	ILE	O-C-N	-6.12	114.89	121.80
3	J	164	LEU	N-CA-C	-6.11	98.45	109.09
3	J	242	PRO	CA-C-N	-6.10	114.10	120.38
3	J	242	PRO	C-N-CA	-6.10	114.10	120.38
3	J	350	ALA	CA-C-O	6.07	126.96	120.10
3	J	346	PRO	O-C-N	6.05	128.60	121.46
3	J	63	GLU	CA-C-N	-6.05	111.11	120.31
3	J	63	GLU	C-N-CA	-6.05	111.11	120.31
3	J	61	THR	CA-C-O	-6.05	112.17	119.49
3	J	60	ASN	CA-C-O	-6.04	114.03	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	209	ASP	O-C-N	-6.04	114.12	122.46
3	J	354	ALA	O-C-N	-6.03	114.36	122.43
3	J	279	SER	CA-C-N	-6.01	110.45	120.30
3	J	279	SER	C-N-CA	-6.01	110.45	120.30
3	J	161	TRP	CA-C-N	-6.00	117.95	122.33
3	J	161	TRP	C-N-CA	-6.00	117.95	122.33
3	J	320	LEU	O-C-N	6.00	130.74	122.46
3	J	218	SER	N-CA-C	6.00	118.96	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	361	PHE	CA-C-N	-6.00	110.29	120.79
3	J	361	PHE	C-N-CA	-6.00	110.29	120.79
3	J	332	TYR	O-C-N	5.99	130.51	122.49
3	J	255	ILE	N-CA-C	5.98	116.48	107.75
3	J	80	LEU	CA-C-N	-5.97	112.59	120.95
3	J	80	LEU	C-N-CA	-5.97	112.59	120.95
3	J	64	LEU	O-C-N	5.97	129.61	122.27
11	S	1219	VAL	CA-C-N	5.97	125.85	119.28
11	S	1219	VAL	C-N-CA	5.97	125.85	119.28
9	P	213	PRO	N-CA-C	5.94	124.71	112.47
3	J	68	LEU	N-CA-C	-5.93	104.76	112.23
3	J	175	LEU	CA-C-O	5.92	125.92	119.24
3	J	322	GLU	N-CA-C	-5.91	104.97	111.82
10	R	43	ALA	CA-C-N	5.89	128.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	43	ALA	C-N-CA	5.89	128.17	120.28
3	J	254	LYS	N-CA-C	-5.89	100.55	109.85
3	J	332	TYR	CA-C-O	-5.88	112.67	119.14
3	J	167	GLY	CA-C-N	5.88	134.06	121.18
3	J	167	GLY	C-N-CA	5.88	134.06	121.18
1	D	234	LEU	CA-C-O	-5.88	114.19	120.42
3	J	40	PRO	CA-C-O	-5.86	114.71	121.86
3	J	330	PRO	CA-N-CD	5.86	120.21	112.00
9	Q	113	LEU	CA-C-N	5.85	128.12	120.28
9	Q	113	LEU	C-N-CA	5.85	128.12	120.28
3	J	26	LYS	N-CA-C	5.84	119.76	110.70
3	J	281	ALA	N-CA-C	5.83	119.65	112.54
9	Q	134	THR	O-C-N	-5.83	113.67	123.00
3	J	65	TYR	CA-C-O	5.81	126.71	120.55
3	J	138	VAL	CA-C-O	5.81	126.49	120.39
3	J	179	LEU	N-CA-C	-5.81	104.91	112.23
3	J	33	THR	N-CA-C	5.79	120.18	113.18
9	q	268	VAL	CA-C-N	5.78	127.96	120.44
9	q	268	VAL	C-N-CA	5.78	127.96	120.44
11	S	1115	LYS	CA-C-N	5.77	127.35	120.14
11	S	1115	LYS	C-N-CA	5.77	127.35	120.14
3	J	378	TYR	O-C-N	-5.77	114.50	122.46
3	J	66	SER	N-CA-C	-5.76	105.74	112.89
3	J	287	SER	N-CA-C	5.76	120.03	112.89
3	J	342	ARG	CA-C-O	-5.75	114.05	120.66
3	J	199	MET	CA-C-N	-5.74	110.16	121.41
3	J	199	MET	C-N-CA	-5.74	110.16	121.41
11	S	1129	LEU	CA-C-N	5.74	127.97	120.28
11	S	1129	LEU	C-N-CA	5.74	127.97	120.28
3	J	60	ASN	O-C-N	5.74	130.06	122.95
3	J	194	SER	CA-C-N	-5.74	107.81	121.80
3	J	194	SER	C-N-CA	-5.74	107.81	121.80
3	J	197	SER	CB-CA-C	-5.73	103.42	111.85
3	J	73	HIS	CA-C-O	-5.72	114.35	120.42
3	J	283	LEU	CA-C-O	5.72	128.69	120.51
3	J	354	ALA	CA-C-O	-5.72	112.35	119.38
3	J	304	VAL	CA-C-N	5.71	130.70	123.10
3	J	304	VAL	C-N-CA	5.71	130.70	123.10
3	J	34	GLY	N-CA-C	5.71	123.98	112.34
9	p	237	ALA	N-CA-C	5.71	117.58	111.36
3	J	126	MET	CA-C-N	5.69	128.47	120.28
3	J	126	MET	C-N-CA	5.69	128.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	175	LEU	O-C-N	-5.69	114.74	122.36
10	r	32	LYS	N-CA-C	5.67	117.55	110.91
3	J	347	PRO	CA-C-N	-5.67	109.41	121.32
3	J	347	PRO	C-N-CA	-5.67	109.41	121.32
3	J	166	LEU	N-CA-C	-5.67	95.14	111.00
3	J	226	ILE	CA-C-O	-5.67	115.06	120.95
3	J	88	ARG	O-C-N	-5.64	116.06	123.28
3	J	286	ASP	CA-C-N	-5.64	111.27	121.14
3	J	286	ASP	C-N-CA	-5.64	111.27	121.14
3	J	30	ALA	N-CA-C	5.63	117.97	110.53
3	J	193	GLN	CA-C-N	-5.63	112.25	120.75
3	J	193	GLN	C-N-CA	-5.63	112.25	120.75
3	J	241	SER	CA-C-N	5.62	126.17	120.38
3	J	241	SER	C-N-CA	5.62	126.17	120.38
3	J	323	ILE	O-C-N	5.61	129.51	121.82
3	J	81	LEU	CA-C-N	-5.59	117.23	123.16
3	J	81	LEU	C-N-CA	-5.59	117.23	123.16
3	J	138	VAL	CA-C-N	-5.59	115.28	123.00
3	J	138	VAL	C-N-CA	-5.59	115.28	123.00
3	J	139	LEU	CA-C-O	-5.59	114.28	120.38
3	J	278	GLN	CA-C-O	-5.59	115.12	121.66
3	J	357	GLY	CA-C-N	5.56	133.59	121.19
3	J	357	GLY	C-N-CA	5.56	133.59	121.19
3	J	381	THR	CA-C-O	-5.56	113.02	119.64
3	J	226	ILE	O-C-N	5.56	127.26	121.87
3	J	150	PRO	N-CA-C	-5.55	102.41	110.80
3	J	93	GLU	N-CA-C	-5.55	94.77	107.48
3	J	95	VAL	N-CA-C	-5.54	95.49	111.00
9	P	58	LYS	N-CA-C	5.54	117.32	111.28
3	J	233	ILE	N-CA-C	5.53	115.29	106.88
11	S	1273	THR	CB-CA-C	-5.52	110.19	116.54
3	J	168	GLY	CA-C-N	-5.52	111.36	121.52
3	J	168	GLY	C-N-CA	-5.52	111.36	121.52
9	q	276	LEU	N-CA-C	5.50	117.36	111.36
3	J	353	VAL	O-C-N	-5.50	114.85	122.05
3	J	227	GLN	O-C-N	5.48	129.52	122.39
3	J	278	GLN	O-C-N	5.47	129.96	122.41
3	J	275	ASN	O-C-N	5.45	129.18	122.20
10	R	69	ASP	O-C-N	-5.42	115.09	121.32
10	R	4	LEU	CA-C-N	5.40	127.52	120.28
10	R	4	LEU	C-N-CA	5.40	127.52	120.28
3	J	135	SER	N-CA-C	5.39	118.41	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	265	SER	N-CA-C	5.39	119.92	113.23
3	J	315	PHE	O-C-N	-5.39	116.41	122.12
3	J	386	ASP	CA-C-N	-5.39	111.71	121.14
3	J	386	ASP	C-N-CA	-5.39	111.71	121.14
9	P	395	ARG	CA-C-N	5.39	128.50	120.31
9	P	395	ARG	C-N-CA	5.39	128.50	120.31
2	H	181	ALA	CA-C-N	5.38	126.06	120.03
2	H	181	ALA	C-N-CA	5.38	126.06	120.03
3	J	61	THR	N-CA-C	5.37	118.93	112.38
3	J	250	LEU	N-CA-C	-5.37	101.36	109.85
3	J	140	ASP	CA-C-O	5.36	126.03	120.40
3	J	162	GLY	N-CA-C	5.35	120.52	111.04
11	S	1123	LEU	N-CA-C	-5.34	106.27	112.89
1	D	186	ALA	CA-C-N	5.34	126.02	119.99
1	D	186	ALA	C-N-CA	5.34	126.02	119.99
3	J	338	THR	CA-C-O	-5.33	115.22	121.46
3	J	35	PRO	N-CA-C	-5.33	103.76	111.22
9	q	279	VAL	CA-C-N	5.32	127.85	120.29
9	q	279	VAL	C-N-CA	5.32	127.85	120.29
3	J	135	SER	CA-C-N	5.32	131.06	121.06
3	J	135	SER	C-N-CA	5.32	131.06	121.06
9	P	76	THR	CB-CA-C	-5.32	108.87	115.89
9	q	30	GLN	N-CA-C	5.31	115.85	108.00
3	J	293	ILE	CA-C-N	-5.30	110.68	121.18
3	J	293	ILE	C-N-CA	-5.30	110.68	121.18
14	s	1243	VAL	N-CA-C	5.30	116.03	110.62
9	q	30	GLN	CB-CA-C	-5.30	108.92	116.34
10	r	108	VAL	CB-CA-C	-5.29	108.74	114.35
3	J	111	LYS	CA-C-O	-5.29	112.88	119.38
3	J	28	GLY	N-CA-C	-5.27	101.90	110.55
3	J	170	ALA	N-CA-C	5.27	119.33	113.01
11	S	1211	VAL	CA-C-N	5.27	128.32	120.31
11	S	1211	VAL	C-N-CA	5.27	128.32	120.31
3	J	288	LEU	N-CA-C	-5.26	105.72	111.82
3	J	312	LEU	O-C-N	5.26	126.07	121.18
3	J	316	LEU	O-C-N	5.25	129.87	122.41
3	J	63	GLU	O-C-N	5.25	127.76	122.09
3	J	183	CYS	N-CA-CB	-5.25	102.78	110.86
3	J	377	TYR	N-CA-C	-5.25	105.64	111.36
3	J	133	ILE	N-CA-C	5.24	116.12	108.58
3	J	21	GLY	CA-C-N	-5.23	111.99	121.14
3	J	21	GLY	C-N-CA	-5.23	111.99	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	112	TYR	CA-C-N	-5.23	114.73	122.41
3	J	112	TYR	C-N-CA	-5.23	114.73	122.41
3	J	133	ILE	O-C-N	-5.22	117.00	122.95
3	J	266	VAL	CA-C-O	-5.21	114.84	120.47
3	J	89	VAL	N-CA-C	5.20	115.53	107.78
11	S	1116	GLY	CA-C-N	5.20	127.68	120.29
11	S	1116	GLY	C-N-CA	5.20	127.68	120.29
3	J	263	ARG	N-CA-C	-5.20	105.69	111.36
3	J	211	LYS	CA-C-N	5.19	127.23	120.28
3	J	211	LYS	C-N-CA	5.19	127.23	120.28
3	J	258	ILE	CA-C-N	-5.19	112.80	120.94
3	J	258	ILE	C-N-CA	-5.19	112.80	120.94
3	J	49	PRO	CA-C-N	-5.18	114.47	124.01
3	J	49	PRO	C-N-CA	-5.18	114.47	124.01
3	J	307	GLY	CA-C-N	5.18	130.02	120.79
3	J	307	GLY	C-N-CA	5.18	130.02	120.79
3	J	170	ALA	CA-C-O	-5.18	112.32	119.05
3	J	345	THR	CA-C-N	-5.17	115.05	120.38
3	J	345	THR	C-N-CA	-5.17	115.05	120.38
10	R	60	LYS	CA-C-O	-5.17	114.94	120.42
3	J	138	VAL	O-C-N	-5.16	117.68	123.26
9	Q	98	THR	O-C-N	-5.16	115.38	121.32
9	p	276	LEU	CA-C-N	5.16	127.19	120.28
9	p	276	LEU	C-N-CA	5.16	127.19	120.28
3	J	369	GLY	O-C-N	-5.16	114.39	122.18
3	J	320	LEU	CA-C-N	-5.15	112.97	120.29
3	J	320	LEU	C-N-CA	-5.15	112.97	120.29
9	P	82	GLU	N-CA-C	5.15	116.58	110.97
3	J	238	GLU	N-CA-C	-5.15	105.72	112.41
3	J	30	ALA	CA-C-N	5.13	130.94	121.70
3	J	30	ALA	C-N-CA	5.13	130.94	121.70
3	J	68	LEU	O-C-N	-5.12	115.47	122.33
9	P	237	ALA	N-CA-C	5.12	116.94	111.36
3	J	327	VAL	CA-C-N	5.12	131.55	121.58
3	J	327	VAL	C-N-CA	5.12	131.55	121.58
3	J	230	LYS	N-CA-CB	5.11	118.11	110.19
9	Q	155	GLU	CB-CA-C	-5.11	109.19	116.34
3	J	357	GLY	O-C-N	5.11	129.89	122.18
10	r	119	VAL	CB-CA-C	-5.11	108.94	114.35
3	J	103	GLU	CA-C-O	-5.10	115.01	120.42
3	J	217	VAL	N-CA-C	5.10	115.44	107.99
3	J	209	ASP	CA-C-O	5.09	125.62	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	375	LYS	N-CA-C	-5.09	105.92	111.82
10	R	39	LYS	CA-C-N	5.09	127.65	120.42
10	R	39	LYS	C-N-CA	5.09	127.65	120.42
9	Q	106	LEU	N-CA-C	-5.08	104.82	111.02
9	q	294	ALA	CA-C-N	5.08	128.72	120.60
9	q	294	ALA	C-N-CA	5.08	128.72	120.60
3	J	261	SER	N-CA-C	5.08	118.57	112.38
9	q	261	VAL	CA-C-N	5.08	127.08	120.28
9	q	261	VAL	C-N-CA	5.08	127.08	120.28
9	P	168	ASP	CA-C-N	5.07	124.25	118.97
9	P	168	ASP	C-N-CA	5.07	124.25	118.97
1	A	8	ALA	CA-C-N	5.07	128.30	121.05
1	A	8	ALA	C-N-CA	5.07	128.30	121.05
9	q	318	ARG	N-CA-C	5.03	116.77	111.28
1	D	64	GLU	N-CA-C	5.03	116.84	111.36
9	q	123	THR	CA-C-N	5.03	127.56	120.42
9	q	123	THR	C-N-CA	5.03	127.56	120.42
3	J	192	GLU	CA-C-N	-5.03	114.70	122.59
3	J	192	GLU	C-N-CA	-5.03	114.70	122.59
10	R	28	ARG	N-CA-C	5.03	118.38	111.54
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	39	ILE	C-N-CD	5.02	145.56	125.00
3	J	347	PRO	N-CA-C	-5.01	107.22	114.18
3	J	349	LYS	CA-C-N	-5.00	113.07	120.28
3	J	349	LYS	C-N-CA	-5.00	113.07	120.28
3	J	40	PRO	N-CA-CB	5.00	108.00	103.15
3	J	247	ASP	CA-C-N	-5.00	115.14	121.74
3	J	247	ASP	C-N-CA	-5.00	115.14	121.74

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
3	J	196	PRO	Mainchain
3	J	209	ASP	Mainchain
3	J	222	ARG	Mainchain

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Mol	Chain	Res	Type	Group
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	53	ARG	Mainchain
3	J	65	TYR	Mainchain
3	J	78	ARG	Peptide,Mainchain
3	J	92	ILE	Mainchain
3	J	99	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2956	2951	2950	11	0
1	B	2956	2951	2950	16	0
1	C	2998	2984	2983	15	0
1	D	2956	2951	2950	23	0
1	E	2956	2951	2950	20	0
1	F	2956	2951	2950	16	0
1	G	2956	2951	2950	10	0
1	I	2956	2951	2950	22	0
2	H	2885	2857	2856	23	0
3	J	3027	3113	3108	135	0
4	K	2913	2982	2975	8	0
5	L	1408	1438	1440	6	0
6	M	1191	1217	1215	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	2311	2221	2220	12	0
8	O	2122	2114	2113	9	0
9	P	2672	2739	2734	16	0
9	Q	2188	2248	2243	6	0
9	p	2534	2573	2573	18	0
9	q	2643	2669	2665	15	0
10	R	1430	1475	1474	7	0
10	r	1369	1417	1416	13	0
11	S	1210	1234	1230	10	0
12	T	498	581	499	25	0
13	U	522	609	524	2	0
14	s	1456	1484	1483	9	0
15	A	27	12	12	0	0
15	B	27	12	12	0	0
15	C	27	12	12	0	0
15	D	27	12	12	0	0
15	E	27	12	12	0	0
15	F	27	12	12	0	0
15	G	27	12	12	0	0
15	I	27	12	12	0	0
16	H	31	15	13	1	0
17	K	3	0	0	0	0
All	All	56319	56723	56510	416	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 (416) 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	0.88
12:T:886:UNK:HB2	10:r:53:ARG:NH1	1.90	0.87
3:J:109:LEU:O	3:J:110:PHE:HB3	1.77	0.84
3:J:352:CYS:O	3:J:353:VAL:C	2.04	0.81
3:J:233:ILE:O	3:J:234:ASP:C	2.16	0.78
3:J:166:LEU:HB2	3:J:167:GLY:HA2	1.66	0.77
2:H:237:GLU:HG2	2:H:251:GLY:HA2	1.68	0.76
3:J:356:LEU:O	3:J:357:GLY:C	2.14	0.76
1:E:50:GLY:HA2	9:P:60:LYS:HD2	1.69	0.74
3:J:152:TYR:CG	3:J:153:GLU:N	2.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:69:LYS:O	3:J:70:GLU:C	2.17	0.71
3:J:209:ASP:O	3:J:210:ILE:C	2.28	0.71
1:A:50:GLY:HA2	9:q:60:LYS:HD2	1.73	0.71
12:T:886:UNK:HB2	10:r:53:ARG:HH11	1.52	0.71
12:T:886:UNK:CB	10:r:53:ARG:NH1	2.54	0.70
3:J:72:ILE:O	3:J:73:HIS:C	2.26	0.70
3:J:113:PHE:O	3:J:114:GLU:C	2.32	0.70
3:J:125:LEU:O	3:J:126:MET:C	2.22	0.69
3:J:259:LEU:O	3:J:260:GLY:C	2.33	0.69
3:J:322:GLU:O	3:J:323:ILE:C	2.13	0.69
3:J:326:LEU:O	3:J:327:VAL:C	2.26	0.68
3:J:23:ALA:O	3:J:24:PHE:C	2.14	0.68
3:J:283:LEU:O	3:J:284:ILE:C	2.23	0.68
3:J:378:TYR:O	3:J:379:ASN:C	2.30	0.67
12:T:886:UNK:CB	10:r:53:ARG:HH11	2.06	0.67
3:J:65:TYR:O	3:J:66:SER:C	2.23	0.67
1:C:27:GLY:HA2	14:s:1223:PHE:HB2	1.77	0.66
3:J:152:TYR:O	3:J:153:GLU:C	2.25	0.66
3:J:282:THR:OG1	3:J:283:LEU:N	2.26	0.65
3:J:381:THR:OG1	3:J:383:ARG:N	2.28	0.65
7:N:203:ASN:O	8:O:191:GLY:HA2	1.96	0.65
3:J:142:GLY:HA2	3:J:309:THR:HG23	1.79	0.65
3:J:391:ASN:O	3:J:392:ASN:C	2.29	0.65
3:J:175:LEU:O	3:J:176:GLU:C	2.30	0.64
3:J:299:LEU:C	3:J:300:ALA:O	2.22	0.64
3:J:105:LEU:O	3:J:106:THR:C	2.20	0.64
3:J:282:THR:C	3:J:284:ILE:N	2.55	0.64
1:D:53:GLU:CG	12:T:834:UNK:CB	2.77	0.63
3:J:220:LEU:O	3:J:221:LYS:C	2.34	0.63
3:J:195:LEU:O	3:J:196:PRO:C	2.15	0.62
1:G:235:GLU:OE2	1:G:238:LYS:NZ	2.33	0.62
3:J:94:SER:OG	3:J:97:CYS:N	2.32	0.62
9:p:206:THR:OG1	14:s:1249:THR:OG1	2.17	0.62
3:J:39:ILE:O	3:J:40:PRO:C	2.31	0.62
1:C:354:LYS:O	1:C:357:TRP:NE1	2.33	0.62
4:K:424:ASP:OD2	4:K:426:LYS:NZ	2.31	0.62
3:J:173:LYS:O	3:J:174:GLU:C	2.37	0.61
12:T:886:UNK:HA	10:r:53:ARG:HH12	1.66	0.61
1:A:354:LYS:O	1:A:357:TRP:NE1	2.34	0.61
3:J:152:TYR:O	3:J:154:GLY:N	2.33	0.61
1:F:235:GLU:OE2	1:F:238:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:OH	1:A:257:ARG:NH1	2.34	0.60
1:D:53:GLU:CG	12:T:834:UNK:HB2	2.15	0.60
3:J:84:PRO:O	3:J:85:ARG:C	2.40	0.60
3:J:252:GLY:O	3:J:253:GLU:C	2.38	0.60
3:J:378:TYR:CD1	3:J:382:GLY:HA2	2.37	0.59
3:J:68:LEU:O	3:J:69:LYS:C	2.37	0.59
3:J:164:LEU:CB	3:J:165:PRO:O	2.50	0.59
1:E:235:GLU:OE2	1:E:238:LYS:NZ	2.36	0.59
3:J:27:CYS:O	3:J:37:CYS:N	2.35	0.59
3:J:248:TYR:O	3:J:249:PRO:C	2.29	0.58
3:J:115:VAL:O	3:J:115:VAL:HG13	2.04	0.58
3:J:346:PRO:CB	3:J:347:PRO:HD2	2.34	0.58
12:T:886:UNK:HA	10:r:53:ARG:NH1	2.19	0.58
9:p:25:LEU:CB	9:p:26:PRO:CD	2.82	0.58
3:J:233:ILE:O	3:J:234:ASP:HB2	2.02	0.58
1:E:335:GLU:HG2	1:E:335:GLU:O	2.04	0.58
3:J:239:ARG:NH1	3:J:240:PRO:O	2.36	0.58
9:q:198:THR:HB	9:q:199:PRO:CD	2.34	0.57
3:J:164:LEU:C	3:J:165:PRO:O	2.33	0.57
3:J:206:VAL:O	3:J:207:LEU:C	2.42	0.57
3:J:330:PRO:O	3:J:331:LYS:C	2.36	0.57
1:C:238:LYS:HA	1:C:252:GLY:HA2	1.86	0.56
1:A:235:GLU:OE2	1:A:238:LYS:NZ	2.38	0.56
5:L:83:PHE:CD2	5:L:84:PRO:O	2.59	0.56
1:B:2356:LYS:O	1:B:2359:TRP:NE1	2.38	0.56
1:C:360:LYS:NZ	1:C:364:GLU:OE2	2.38	0.56
3:J:225:LYS:O	3:J:226:ILE:C	2.42	0.56
2:H:51:ASP:OD2	4:K:165:LYS:NZ	2.34	0.55
1:B:2156:THR:O	1:B:2299:ASN:ND2	2.39	0.55
3:J:346:PRO:HB2	3:J:348:ALA:H	1.70	0.55
3:J:368:LEU:O	3:J:369:GLY:C	2.37	0.55
1:E:360:LYS:NZ	1:E:364:GLU:OE2	2.39	0.55
12:T:886:UNK:CA	10:r:53:ARG:NH1	2.70	0.55
1:I:183:ILE:HG22	1:I:185:ILE:H	1.71	0.55
3:J:83:ASN:N	3:J:84:PRO:CD	2.69	0.55
1:I:235:GLU:OE2	1:I:238:LYS:NZ	2.40	0.55
3:J:349:LYS:O	3:J:350:ALA:C	2.46	0.55
2:H:157:ASP:OD2	16:H:401:ANP:O3G	2.25	0.54
3:J:182:GLN:O	3:J:183:CYS:CB	2.43	0.54
1:G:154:THR:O	1:G:297:ASN:ND2	2.39	0.54
1:B:2362:LYS:NZ	1:B:2366:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:333:LYS:O	3:J:334:LYS:C	2.39	0.54
3:J:357:GLY:HA2	3:J:360:ILE:HD12	1.90	0.54
6:M:163:GLN:OE1	6:M:163:GLN:N	2.41	0.54
9:p:25:LEU:HB2	9:p:26:PRO:HD2	1.89	0.54
7:N:175:SER:OG	7:N:177:TRP:NE1	2.42	0.53
3:J:155:ILE:HG22	3:J:156:PRO:O	2.07	0.53
3:J:386:ASP:O	3:J:387:TRP:C	2.47	0.53
8:O:62:CYS:SG	8:O:63:ASP:N	2.81	0.53
3:J:204:GLU:O	3:J:205:GLY:C	2.45	0.53
9:Q:278:GLN:HE22	10:R:64:LEU:HD22	1.75	0.52
3:J:142:GLY:O	3:J:143:TYR:C	2.47	0.52
3:J:308:GLY:O	3:J:309:THR:C	2.34	0.52
8:O:93:LEU:O	8:O:97:GLU:N	2.36	0.52
6:M:169:LYS:O	6:M:173:ASN:ND2	2.43	0.52
3:J:19:ASP:O	3:J:20:LEU:HD23	2.10	0.52
3:J:102:ARG:O	3:J:103:GLU:C	2.46	0.52
3:J:182:GLN:O	3:J:183:CYS:HB2	2.06	0.51
9:P:136:VAL:HG12	9:P:138:LEU:H	1.75	0.51
1:D:335:GLU:O	1:D:335:GLU:HG2	2.09	0.51
9:q:371:LEU:HD23	9:q:371:LEU:C	2.35	0.51
1:D:303:GLY:HA2	1:D:337:LEU:HD21	1.92	0.51
3:J:165:PRO:CB	3:J:166:LEU:HA	2.40	0.51
8:O:144:ILE:O	8:O:144:ILE:HG13	2.10	0.51
9:p:25:LEU:HB3	9:p:26:PRO:CD	2.40	0.51
9:p:25:LEU:HB3	9:p:26:PRO:HD3	1.93	0.51
1:E:48:MET:HB3	1:G:173:GLY:HA2	1.91	0.51
6:M:108:GLU:OE1	6:M:126:GLY:HA2	2.10	0.51
3:J:22:GLU:C	3:J:24:PHE:N	2.66	0.51
9:Q:113:LEU:C	9:Q:113:LEU:HD12	2.36	0.51
1:I:7:ILE:HG22	1:I:9:ASN:H	1.75	0.51
3:J:21:GLY:C	3:J:23:ALA:N	2.62	0.51
3:J:155:ILE:O	3:J:156:PRO:C	2.45	0.51
3:J:273:GLN:NE2	3:J:276:GLU:O	2.44	0.50
3:J:282:THR:O	3:J:283:LEU:HB2	2.11	0.50
11:S:1127:PRO:HB2	11:S:1128:PRO:HD3	1.92	0.50
1:F:354:LYS:O	1:F:357:TRP:NE1	2.44	0.50
1:E:354:LYS:O	1:E:357:TRP:NE1	2.44	0.50
1:F:287:ASP:OD1	1:F:288:MET:N	2.44	0.50
3:J:21:GLY:H	3:J:24:PHE:N	2.08	0.50
3:J:281:ALA:C	3:J:282:THR:O	2.49	0.50
1:A:109:LEU:HD23	1:A:109:LEU:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2173:TYR:CE2	7:N:264:VAL:HG21	2.46	0.50
1:F:245:ASP:OD1	1:F:246:GLY:N	2.45	0.50
3:J:361:PHE:O	3:J:364:LEU:HB3	2.12	0.50
3:J:74:ILE:O	3:J:75:LEU:C	2.48	0.50
3:J:280:VAL:CG1	3:J:281:ALA:N	2.75	0.50
6:M:157:PRO:O	6:M:158:GLN:C	2.54	0.50
9:p:161:ASP:OD2	9:q:223:LYS:NZ	2.45	0.50
3:J:144:ARG:CG	3:J:144:ARG:O	2.58	0.50
12:T:886:UNK:CA	10:r:53:ARG:HH12	2.25	0.50
1:E:258:ALA:N	1:E:259:PRO:HD2	2.27	0.49
3:J:75:LEU:O	3:J:76:TYR:C	2.52	0.49
3:J:100:HIS:HB3	3:J:101:PHE:HA	1.94	0.49
9:p:168:ASP:OD2	9:p:171:GLY:HA2	2.12	0.49
1:A:245:ASP:OD1	1:A:246:GLY:N	2.44	0.49
1:G:245:ASP:OD1	1:G:246:GLY:N	2.45	0.49
9:P:342:GLN:NE2	14:s:1132:ALA:O	2.45	0.49
6:M:61:LEU:HD23	6:M:61:LEU:C	2.38	0.49
7:N:61:GLN:HE22	7:N:172:ARG:HH21	1.61	0.49
10:R:108:VAL:N	10:R:109:PRO:HD2	2.27	0.49
11:S:1219:VAL:HB	11:S:1220:PRO:HD3	1.93	0.49
1:I:165:THR:HG23	1:I:165:THR:O	2.13	0.49
3:J:57:TYR:O	3:J:58:ASN:HB2	2.12	0.49
9:Q:182:GLU:OE1	10:r:156:LYS:NZ	2.46	0.49
1:B:2111:LEU:C	1:B:2111:LEU:HD23	2.38	0.49
1:F:24:GLY:HA2	1:F:99:LEU:HD21	1.95	0.49
3:J:109:LEU:C	3:J:110:PHE:O	2.24	0.49
3:J:166:LEU:CB	3:J:167:GLY:HA2	2.36	0.49
3:J:282:THR:C	3:J:284:ILE:H	2.20	0.49
12:T:891:UNK:HG2	12:T:892:UNK:N	2.28	0.49
2:H:40:HIS:CD2	2:H:41:GLN:O	2.66	0.48
1:C:109:LEU:C	1:C:109:LEU:HD23	2.38	0.48
1:I:109:LEU:C	1:I:109:LEU:HD23	2.38	0.48
1:I:342:ILE:O	1:I:345:SER:OG	2.25	0.48
3:J:288:LEU:O	3:J:289:ILE:C	2.50	0.48
1:I:276:HIS:CE1	1:I:277:GLU:HG2	2.49	0.48
12:T:895:UNK:HG2	12:T:896:UNK:N	2.28	0.48
3:J:293:ILE:O	3:J:294:ASP:C	2.51	0.48
3:J:158:LEU:O	3:J:159:ASN:C	2.38	0.48
1:D:354:LYS:O	1:D:357:TRP:NE1	2.47	0.48
3:J:149:LEU:O	3:J:150:PRO:C	2.53	0.48
9:P:138:LEU:HD23	9:P:138:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:p:168:ASP:OD1	9:p:172:ALA:N	2.47	0.48
1:D:109:LEU:C	1:D:109:LEU:HD23	2.38	0.48
1:D:360:LYS:NZ	1:D:364:GLU:OE2	2.47	0.48
3:J:222:ARG:O	3:J:223:GLY:C	2.52	0.48
1:F:48:MET:CG	2:H:168:GLY:HA2	2.43	0.48
3:J:340:THR:OG1	3:J:341:PHE:N	2.44	0.48
5:L:85:LEU:HD23	5:L:85:LEU:C	2.39	0.48
3:J:21:GLY:O	3:J:24:PHE:CD1	2.67	0.47
1:B:2158:VAL:O	1:B:2158:VAL:HG13	2.14	0.47
1:E:245:ASP:OD1	1:E:246:GLY:N	2.47	0.47
2:H:257:CYS:HB3	2:H:258:PRO:HD3	1.95	0.47
4:K:237:VAL:HG13	4:K:237:VAL:O	2.14	0.47
9:p:302:ASP:OD1	9:p:303:ALA:N	2.47	0.47
3:J:144:ARG:O	3:J:144:ARG:HG3	2.13	0.47
1:D:245:ASP:OD1	1:D:246:GLY:N	2.47	0.47
1:F:258:ALA:N	1:F:259:PRO:HD2	2.30	0.47
3:J:22:GLU:C	3:J:24:PHE:H	2.22	0.47
3:J:59:ILE:O	3:J:60:ASN:C	2.50	0.47
3:J:166:LEU:CB	3:J:167:GLY:CA	2.92	0.47
2:H:104:LEU:C	2:H:104:LEU:HD23	2.39	0.47
9:P:3:ASP:HB2	9:P:4:PRO:CD	2.44	0.47
1:C:245:ASP:OD1	1:C:246:GLY:N	2.48	0.47
1:D:48:MET:HB3	1:F:173:GLY:HA2	1.97	0.47
3:J:269:ILE:HG13	3:J:270:LEU:N	2.30	0.47
8:O:169:LEU:C	8:O:169:LEU:HD23	2.40	0.47
1:D:287:ASP:OD1	1:D:288:MET:N	2.48	0.46
1:D:368:ALA:O	1:D:371:ILE:HG12	2.15	0.46
3:J:252:GLY:O	3:J:253:GLU:HB2	2.14	0.46
1:B:2289:ASP:OD1	1:B:2290:MET:N	2.48	0.46
1:I:114:PRO:O	1:I:182:ARG:NH1	2.48	0.46
10:R:119:VAL:N	10:R:120:PRO:HD2	2.31	0.46
1:E:357:TRP:CD1	1:E:357:TRP:C	2.93	0.46
1:I:145:LEU:HD22	1:I:344:GLY:HA2	1.96	0.46
3:J:230:LYS:O	3:J:232:ASN:N	2.47	0.46
1:B:2040:TYR:CD1	1:B:2040:TYR:C	2.94	0.46
1:C:38:TYR:CD1	1:C:38:TYR:C	2.93	0.46
3:J:21:GLY:H	3:J:23:ALA:C	2.23	0.46
9:Q:111:GLN:OE1	9:Q:111:GLN:N	2.47	0.46
9:q:198:THR:HB	9:q:199:PRO:HD2	1.96	0.46
1:C:128:PHE:O	1:C:132:PHE:O	2.34	0.46
3:J:43:ILE:HA	3:J:44:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:830:UNK:O	12:T:833:UNK:HG3	2.16	0.46
9:p:348:GLN:OE1	9:p:348:GLN:N	2.43	0.46
2:H:257:CYS:N	2:H:258:PRO:HD2	2.31	0.46
1:A:354:LYS:O	1:A:357:TRP:CD1	2.69	0.46
1:F:357:TRP:C	1:F:357:TRP:CD1	2.93	0.46
1:D:145:LEU:HD22	1:D:344:GLY:HA2	1.98	0.46
1:E:38:TYR:CD1	1:E:38:TYR:C	2.94	0.46
4:K:419:PHE:CD1	4:K:419:PHE:C	2.94	0.46
7:N:203:ASN:ND2	8:O:14:ARG:O	2.49	0.46
3:J:248:TYR:CD2	3:J:249:PRO:O	2.69	0.45
1:E:50:GLY:HA2	9:P:60:LYS:CD	2.43	0.45
8:O:97:GLU:O	8:O:101:ASN:ND2	2.44	0.45
9:P:211:SER:C	9:P:213:PRO:HD3	2.41	0.45
1:A:258:ALA:N	1:A:259:PRO:HD2	2.31	0.45
3:J:83:ASN:N	3:J:84:PRO:HD3	2.31	0.45
3:J:353:VAL:HG12	3:J:353:VAL:O	2.15	0.45
2:H:304:THR:O	2:H:335:ARG:NH2	2.49	0.45
3:J:274:ASP:C	3:J:276:GLU:H	2.15	0.45
10:r:19:ARG:O	10:r:23:GLY:HA2	2.16	0.45
14:s:1089:ASP:OD1	14:s:1089:ASP:C	2.59	0.45
1:D:38:TYR:CD1	1:D:38:TYR:C	2.94	0.45
1:I:128:PHE:O	1:I:132:PHE:O	2.35	0.45
10:R:54:VAL:HG13	10:R:55:LYS:N	2.32	0.45
12:T:894:UNK:HG1	9:p:285:SER:OG	2.17	0.45
11:S:1165:HIS:O	11:S:1168:VAL:HG22	2.16	0.45
1:I:38:TYR:CD1	1:I:38:TYR:C	2.94	0.45
1:I:275:ILE:O	1:I:278:VAL:HG12	2.16	0.45
9:p:280:GLU:HA	9:p:280:GLU:OE1	2.17	0.45
1:B:2373:ILE:O	1:B:2377:THR:OG1	2.30	0.45
1:E:283:ILE:O	1:E:286:SER:OG	2.33	0.45
7:N:94:ILE:C	7:N:94:ILE:HD12	2.42	0.45
9:p:25:LEU:CB	9:p:26:PRO:HD2	2.45	0.45
9:q:134:THR:HB	9:q:135:PRO:HD3	1.99	0.45
9:q:209:LEU:O	14:s:1246:GLY:N	2.45	0.45
1:D:258:ALA:N	1:D:259:PRO:HD2	2.31	0.45
1:I:360:LYS:NZ	1:I:364:GLU:OE2	2.47	0.45
1:B:2247:ASP:OD1	1:B:2248:GLY:N	2.50	0.45
9:P:138:LEU:HD23	9:P:139:ALA:N	2.32	0.45
3:J:243:PRO:HA	3:J:244:PRO:HD3	1.75	0.44
7:N:180:THR:O	7:N:186:ALA:HA	2.17	0.44
9:q:198:THR:CB	9:q:199:PRO:CD	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PHE:HB2	1:G:59:GLY:HA2	1.99	0.44
1:D:357:TRP:CD1	1:D:357:TRP:C	2.93	0.44
1:E:368:ALA:O	1:E:371:ILE:HG12	2.18	0.44
6:M:63:ILE:HG23	6:M:63:ILE:O	2.17	0.44
3:J:164:LEU:HB3	3:J:165:PRO:O	2.16	0.44
9:P:6:TYR:CD1	9:P:6:TYR:C	2.95	0.44
9:p:258:MET:O	9:p:261:VAL:HG12	2.17	0.44
11:S:1168:VAL:O	11:S:1171:ILE:HG12	2.17	0.44
2:H:46:GLY:HA2	3:J:125:LEU:HD21	2.00	0.44
9:q:320:SER:N	9:q:321:PRO:HD2	2.33	0.44
1:G:363:TYR:O	1:G:367:GLY:N	2.50	0.44
13:U:912:UNK:O	13:U:912:UNK:HG2	2.17	0.44
14:s:1166:THR:HG23	14:s:1166:THR:O	2.17	0.44
1:D:361:LYS:NZ	1:D:365:GLU:OE2	2.49	0.44
7:N:99:ASP:O	7:N:103:LYS:N	2.50	0.44
12:T:896:UNK:HG2	12:T:897:UNK:N	2.32	0.44
1:D:68:LEU:HD11	1:F:171:TYR:CD2	2.53	0.44
2:H:187:ASP:OD2	2:H:191:LYS:NZ	2.51	0.44
8:O:105:ASP:O	8:O:108:ARG:HG2	2.18	0.44
11:S:1126:LEU:HB2	11:S:1127:PRO:HD3	1.99	0.44
1:E:193:PHE:HZ	1:E:197:TYR:HH	1.63	0.43
5:L:123:LYS:C	5:L:126:CYS:HG	2.25	0.43
8:O:124:LEU:HB2	8:O:127:GLY:O	2.18	0.43
10:R:18:GLU:OE2	10:R:26:GLY:HA2	2.18	0.43
9:p:388:ASN:HD21	9:q:385:VAL:HG13	1.83	0.43
6:M:170:ILE:HG13	6:M:171:LEU:N	2.33	0.43
1:G:258:ALA:N	1:G:259:PRO:HD2	2.33	0.43
1:D:47:VAL:HG23	1:D:48:MET:N	2.33	0.43
3:J:329:LYS:HB3	3:J:330:PRO:HD2	2.00	0.43
14:s:1248:VAL:O	14:s:1248:VAL:HG13	2.19	0.43
1:C:47:VAL:HG23	1:C:48:MET:N	2.33	0.43
3:J:119:LEU:HD13	3:J:368:LEU:HD12	2.01	0.43
7:N:273:LYS:O	7:N:277:TYR:N	2.44	0.43
9:P:145:LEU:CD1	11:S:1164:THR:OG1	2.67	0.43
1:D:128:PHE:O	1:D:132:PHE:O	2.36	0.43
3:J:344:HIS:CE1	4:K:221:ALA:HB2	2.53	0.43
1:A:360:LYS:NZ	1:A:364:GLU:OE2	2.47	0.43
1:C:110:LEU:HD11	1:C:128:PHE:CE1	2.54	0.43
1:A:38:TYR:CD1	1:A:38:TYR:C	2.97	0.43
1:B:2050:MET:HB3	1:D:173:GLY:HA2	2.01	0.43
2:H:257:CYS:HB3	2:H:258:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:LYS:O	3:J:98:PRO:HA	2.19	0.43
3:J:194:SER:HB2	3:J:197:SER:H	1.84	0.43
3:J:219:ASP:O	3:J:222:ARG:HG2	2.19	0.42
7:N:269:ILE:HG23	7:N:269:ILE:O	2.18	0.42
1:E:305:THR:OG1	1:E:336:ARG:HD3	2.20	0.42
1:F:360:LYS:NZ	1:F:364:GLU:OE2	2.48	0.42
10:r:57:LEU:C	10:r:57:LEU:HD23	2.44	0.42
10:R:108:VAL:CG1	10:R:109:PRO:HD3	2.50	0.42
1:C:375:THR:O	1:C:376:PHE:HB3	2.19	0.42
1:G:183:ILE:HG22	1:G:185:ILE:H	1.83	0.42
1:I:38:TYR:CG	1:I:71:ILE:HG23	2.54	0.42
1:I:361:LYS:NZ	1:I:365:GLU:OE2	2.47	0.42
3:J:300:ALA:O	3:J:301:GLU:HB2	2.18	0.42
9:p:258:MET:SD	10:r:33:VAL:HB	2.60	0.42
1:G:83:TRP:CE2	1:G:123:ARG:HG2	2.53	0.42
2:H:120:THR:HG22	2:H:132:MET:SD	2.60	0.42
2:H:140:LEU:HD22	2:H:343:GLY:HA2	2.00	0.42
11:S:1256:VAL:HG12	11:S:1258:PHE:CE1	2.54	0.42
1:G:38:TYR:CD1	1:G:38:TYR:C	2.97	0.42
3:J:357:GLY:O	3:J:360:ILE:HB	2.19	0.42
6:M:155:GLU:O	6:M:156:ARG:C	2.62	0.42
1:I:15:ASP:OD2	1:I:22:LYS:NZ	2.51	0.42
9:P:102:LYS:O	9:P:106:LEU:HG	2.20	0.42
12:T:836:UNK:O	12:T:839:UNK:HG3	2.20	0.42
1:B:2049:VAL:HG23	1:B:2050:MET:N	2.34	0.42
1:B:2363:LYS:NZ	1:B:2367:GLU:OE2	2.51	0.42
1:E:224:LEU:HD21	1:E:263:PHE:CE1	2.54	0.42
3:J:279:SER:O	3:J:280:VAL:C	2.53	0.42
3:J:324:ARG:O	3:J:325:TYR:C	2.62	0.42
3:J:346:PRO:HA	3:J:347:PRO:HD3	1.75	0.42
1:A:50:GLY:HA2	9:q:60:LYS:CD	2.48	0.42
2:H:41:GLN:N	2:H:41:GLN:OE1	2.53	0.42
4:K:12:TYR:CE1	4:K:24:LEU:HB2	2.55	0.42
7:N:73:GLN:O	7:N:91:ARG:NH2	2.53	0.42
11:S:1133:LYS:HD3	11:S:1134:LEU:O	2.20	0.42
1:F:38:TYR:CD1	1:F:38:TYR:C	2.97	0.42
3:J:368:LEU:O	3:J:372:SER:OG	2.25	0.42
9:P:348:GLN:OE1	9:P:348:GLN:N	2.47	0.42
12:T:908:UNK:O	12:T:911:UNK:HG3	2.20	0.42
9:p:354:ASP:O	9:p:357:GLN:HG3	2.20	0.42
1:D:31:PRO:HD3	1:D:341:TRP:CE3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:HD12	1:I:310:PHE:HA	2.02	0.41
1:I:305:THR:OG1	1:I:336:ARG:NE	2.51	0.41
7:N:270:ASP:O	7:N:274:ILE:HG12	2.20	0.41
9:Q:3:ASP:CG	9:Q:4:PRO:HD2	2.44	0.41
12:T:846:UNK:O	12:T:849:UNK:HG3	2.20	0.41
1:D:357:TRP:O	1:D:357:TRP:HD1	2.03	0.41
2:H:189:LEU:O	2:H:192:ILE:HG22	2.20	0.41
1:I:229:GLN:OE1	1:I:229:GLN:N	2.47	0.41
3:J:146:SER:N	3:J:164:LEU:O	2.50	0.41
1:B:2349:LEU:C	1:B:2349:LEU:HD23	2.45	0.41
1:E:111:THR:HG22	1:E:142:GLN:HG2	2.02	0.41
1:I:65:HIS:O	1:I:69:LEU:HG	2.20	0.41
3:J:166:LEU:HB2	3:J:168:GLY:H	1.86	0.41
3:J:288:LEU:O	3:J:290:GLN:N	2.53	0.41
9:P:3:ASP:HA	9:P:6:TYR:CZ	2.55	0.41
12:T:841:UNK:O	12:T:844:UNK:HG3	2.19	0.41
9:p:312:LEU:CD2	9:q:316:ILE:HD12	2.50	0.41
1:B:2045:LYS:NZ	1:C:271:GLU:OE2	2.41	0.41
1:D:77:HIS:O	1:D:182:ARG:NH2	2.53	0.41
2:H:332:PRO:O	2:H:335:ARG:HG3	2.19	0.41
4:K:231:ASP:O	4:K:235:ARG:CB	2.69	0.41
5:L:83:PHE:CE2	5:L:84:PRO:O	2.73	0.41
5:L:146:PHE:HA	5:L:152:LEU:O	2.20	0.41
12:T:891:UNK:O	12:T:894:UNK:HG3	2.20	0.41
12:T:908:UNK:O	12:T:912:UNK:HG3	2.20	0.41
9:q:29:ASP:OD1	9:q:30:GLN:N	2.54	0.41
1:C:258:ALA:N	1:C:259:PRO:HD2	2.35	0.41
2:H:244:ASP:OD1	2:H:245:GLY:N	2.53	0.41
3:J:26:LYS:NZ	3:J:351:ASN:O	2.46	0.41
4:K:51:CYS:HB3	4:K:54:CYS:SG	2.61	0.41
1:F:47:VAL:HG23	1:F:48:MET:N	2.36	0.41
9:P:168:ASP:HB3	9:P:169:PRO:HD3	2.03	0.41
12:T:891:UNK:CG	12:T:892:UNK:N	2.83	0.41
9:q:381:ASN:O	9:q:385:VAL:HG23	2.21	0.41
14:s:1143:LEU:HB3	14:s:1144:PRO:CD	2.50	0.41
1:B:2260:ALA:N	1:B:2261:PRO:HD2	2.36	0.41
3:J:35:PRO:HB2	3:J:37:CYS:SG	2.61	0.41
6:M:171:LEU:N	6:M:172:PRO:HD2	2.36	0.41
9:P:168:ASP:HB3	9:P:169:PRO:CD	2.50	0.41
9:P:168:ASP:N	9:P:169:PRO:HD2	2.36	0.41
10:r:48:SER:OG	10:r:49:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD12	1:C:310:PHE:HA	2.03	0.41
1:E:357:TRP:HD1	1:E:357:TRP:O	2.04	0.41
2:H:253:GLU:OE1	2:H:253:GLU:N	2.43	0.41
3:J:24:PHE:CZ	3:J:55:VAL:HB	2.55	0.41
3:J:57:TYR:O	3:J:58:ASN:C	2.64	0.41
3:J:71:PHE:O	3:J:74:ILE:HB	2.21	0.41
3:J:314:GLY:O	3:J:315:PHE:O	2.38	0.41
5:L:105:GLY:N	5:L:122:LEU:O	2.51	0.41
11:S:1166:THR:HG22	11:S:1170:ASP:OD2	2.21	0.41
9:q:103:TYR:OH	9:q:157:LEU:HD23	2.21	0.41
1:E:154:THR:O	1:E:297:ASN:ND2	2.54	0.41
2:H:59:GLN:O	2:H:62:ARG:HG3	2.21	0.41
2:H:370:VAL:HG13	2:H:371:HIS:N	2.36	0.41
1:I:275:ILE:HG23	1:I:276:HIS:N	2.36	0.41
3:J:133:ILE:HG22	3:J:135:SER:H	1.86	0.41
3:J:391:ASN:O	3:J:393:PRO:N	2.53	0.41
9:Q:313:TYR:C	9:Q:313:TYR:CD1	2.95	0.41
1:F:48:MET:HG3	2:H:168:GLY:HA2	2.02	0.40
2:H:142:LEU:HB3	2:H:147:ARG:O	2.20	0.40
11:S:1226:PHE:HB2	11:S:1227:PRO:CD	2.50	0.40
14:s:1143:LEU:HB3	14:s:1144:PRO:HD3	2.02	0.40
3:J:295:THR:O	3:J:299:LEU:HD13	2.21	0.40
10:R:35:ASP:OD2	10:R:39:LYS:NZ	2.54	0.40
12:T:911:UNK:HG2	12:T:912:UNK:N	2.35	0.40
1:C:148:TYR:CE1	1:C:347:LEU:HD13	2.56	0.40
1:F:363:TYR:O	1:F:367:GLY:N	2.54	0.40
3:J:55:VAL:C	3:J:56:GLN:N	2.79	0.40
3:J:329:LYS:CB	3:J:330:PRO:HD2	2.45	0.40
12:T:842:UNK:O	12:T:845:UNK:HG3	2.20	0.40
3:J:72:ILE:O	3:J:73:HIS:O	2.39	0.40
3:J:240:PRO:O	3:J:241:SER:C	2.61	0.40
12:T:887:UNK:O	12:T:890:UNK:HG3	2.22	0.40
13:U:830:UNK:O	13:U:833:UNK:HG3	2.22	0.40
1:E:128:PHE:O	1:E:132:PHE:O	2.40	0.40
1:F:20:VAL:O	1:F:20:VAL:HG23	2.21	0.40
3:J:18:ILE:O	3:J:20:LEU:HG	2.22	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%)	356 (97%)	12 (3%)	0	100	100
1	B	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	C	373/376 (99%)	364 (98%)	9 (2%)	0	100	100
1	D	368/376 (98%)	358 (97%)	10 (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%)	359 (98%)	9 (2%)	0	100	100
1	I	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
2	H	368/375 (98%)	356 (97%)	12 (3%)	0	100	100
3	J	379/417 (91%)	358 (94%)	18 (5%)	3 (1%)	16	49
4	K	349/460 (76%)	343 (98%)	6 (2%)	0	100	100
5	L	180/182 (99%)	176 (98%)	4 (2%)	0	100	100
6	M	152/190 (80%)	144 (95%)	8 (5%)	0	100	100
7	N	282/286 (99%)	278 (99%)	4 (1%)	0	100	100
8	O	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
9	P	329/401 (82%)	312 (95%)	13 (4%)	4 (1%)	10	41
9	Q	268/401 (67%)	261 (97%)	6 (2%)	1 (0%)	30	62
9	p	320/401 (80%)	309 (97%)	10 (3%)	1 (0%)	36	67
9	q	329/401 (82%)	309 (94%)	18 (6%)	2 (1%)	21	54
10	R	177/186 (95%)	167 (94%)	9 (5%)	1 (1%)	21	54
10	r	168/186 (90%)	163 (97%)	4 (2%)	1 (1%)	21	54
11	S	146/1278 (11%)	140 (96%)	6 (4%)	0	100	100
14	s	187/1278 (15%)	180 (96%)	6 (3%)	1 (0%)	24	57
All	All	6850/9722 (70%)	6617 (97%)	219 (3%)	14 (0%)	44	74

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	283	LEU
9	P	213	PRO
9	p	25	LEU
9	q	202	SER
9	Q	161	ASP
10	R	69	ASP
3	J	23	ALA
3	J	145	GLU
9	q	199	PRO
10	r	69	ASP
14	s	1140	GLY
9	P	10	PRO
9	P	268	VAL
9	P	212	ARG

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	132/164 (80%)	132 (100%)	0	100	100
7	N	251/252 (100%)	251 (100%)	0	100	100
8	O	238/241 (99%)	238 (100%)	0	100	100
9	P	298/343 (87%)	298 (100%)	0	100	100
9	Q	245/343 (71%)	245 (100%)	0	100	100
9	p	281/343 (82%)	281 (100%)	0	100	100
9	q	298/343 (87%)	298 (100%)	0	100	100
10	R	154/160 (96%)	154 (100%)	0	100	100
10	r	149/160 (93%)	149 (100%)	0	100	100
11	S	137/1080 (13%)	137 (100%)	0	100	100
14	s	164/1080 (15%)	164 (100%)	0	100	100
All	All	6041/8357 (72%)	6041 (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 (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	98	GLN
1	A	133	ASN
1	B	2135	ASN
1	D	44	HIS
1	D	65	HIS
1	D	133	ASN
1	E	91	GLN
1	E	284	GLN
1	F	65	HIS
1	F	116	ASN
1	F	120	ASN
1	F	284	GLN
1	G	120	ASN
2	H	40	HIS
2	H	101	HIS
2	H	246	GLN
2	H	296	ASN
1	I	178	HIS
1	I	284	GLN

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Mol	Chain	Res	Type
3	J	73	HIS
3	J	178	GLN
3	J	344	HIS
4	K	81	HIS
4	K	251	GLN
4	K	266	HIS
5	L	86	HIS
6	M	153	GLN
7	N	203	ASN
7	N	205	GLN
8	O	77	ASN
8	O	178	GLN
8	O	180	ASN
8	O	188	ASN
8	O	196	GLN
9	P	296	HIS
9	P	311	GLN
9	P	352	HIS
9	P	375	GLN
9	Q	278	GLN
9	Q	358	GLN
10	R	97	GLN
10	R	105	ASN
10	R	115	HIS
10	R	122	HIS
11	S	1161	GLN
9	q	352	HIS
10	r	115	HIS
14	s	1108	GLN
14	s	1266	GLN
14	s	1270	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
15	ADP	E	800	-	28,29,29	0.44	0	43,45,45	0.44	0
15	ADP	D	800	-	28,29,29	0.45	0	43,45,45	0.44	0
15	ADP	I	800	-	28,29,29	0.47	0	43,45,45	0.44	0
15	ADP	F	800	-	28,29,29	0.45	0	43,45,45	0.44	0
15	ADP	C	800	-	28,29,29	0.47	0	43,45,45	0.44	0
15	ADP	B	2401	-	28,29,29	0.46	0	43,45,45	0.44	0
16	ANP	H	401	-	33,33,33	1.94	9 (27%)	45,52,52	1.99	15 (33%)
15	ADP	A	800	-	28,29,29	0.44	0	43,45,45	0.43	0
15	ADP	G	800	-	28,29,29	0.43	0	43,45,45	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	E	800	-	-	4/16/32/32	0/3/3/3
15	ADP	D	800	-	-	4/16/32/32	0/3/3/3
15	ADP	I	800	-	-	4/16/32/32	0/3/3/3
15	ADP	F	800	-	-	4/16/32/32	0/3/3/3
15	ADP	C	800	-	-	4/16/32/32	0/3/3/3
15	ADP	B	2401	-	-	3/16/32/32	0/3/3/3
16	ANP	H	401	-	-	6/18/38/38	0/3/3/3
15	ADP	A	800	-	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	G	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)
16	H	401	ANP	C5-C4	5.00	1.48	1.39
16	H	401	ANP	PG-N3B	4.37	1.74	1.63
16	H	401	ANP	PG-O1G	3.96	1.52	1.46
16	H	401	ANP	PB-N3B	3.56	1.72	1.63
16	H	401	ANP	PB-O1B	3.39	1.51	1.46
16	H	401	ANP	C8-N7	2.72	1.36	1.31
16	H	401	ANP	C5-C6	2.65	1.48	1.41
16	H	401	ANP	PB-O2B	-2.38	1.50	1.56
16	H	401	ANP	C4-N9	-2.33	1.32	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	401	ANP	C5-C4-N3	-5.13	119.66	126.72
16	H	401	ANP	N3-C4-N9	4.54	134.89	127.17
16	H	401	ANP	C4-N9-C8	3.92	109.86	105.74
16	H	401	ANP	C2-N3-C4	3.75	120.99	111.83
16	H	401	ANP	N3-C2-N1	-3.61	123.12	128.58
16	H	401	ANP	O1B-PB-N3B	-3.47	106.67	111.77
16	H	401	ANP	O1G-PG-N3B	-2.76	107.71	111.77
16	H	401	ANP	C4-C5-N7	-2.70	107.50	110.58
16	H	401	ANP	O2B-PB-O1B	2.65	115.55	109.87
16	H	401	ANP	O2A-PA-O1A	2.64	124.73	112.44
16	H	401	ANP	N9-C8-N7	-2.40	110.53	113.94
16	H	401	ANP	O3A-PB-N3B	2.22	112.75	106.59
16	H	401	ANP	C6-C5-N7	2.21	136.35	132.09
16	H	401	ANP	O2G-PG-O3G	2.05	113.09	107.59
16	H	401	ANP	C5-N7-C8	2.04	106.66	103.45

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	800	ADP	PA-O3A-PB-O2B
15	A	800	ADP	PA-O3A-PB-O3B
15	A	800	ADP	C5'-O5'-PA-O1A

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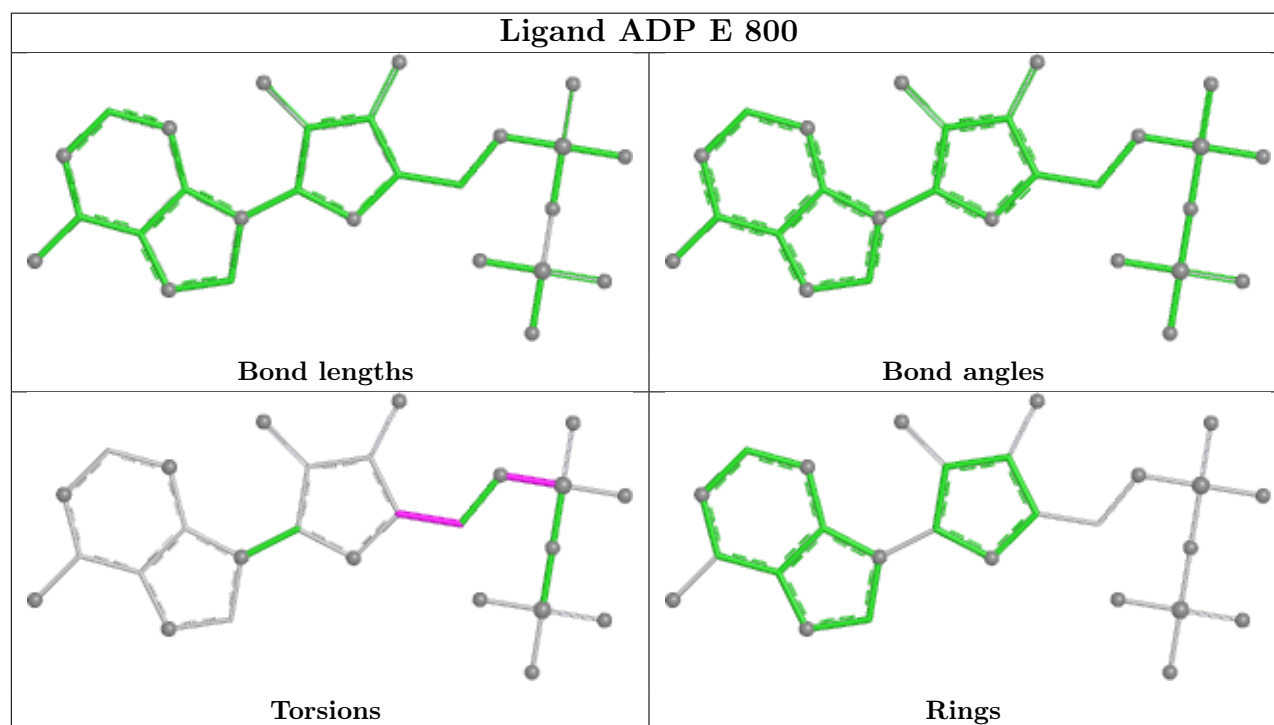
Mol	Chain	Res	Type	Atoms
15	C	800	ADP	C5'-O5'-PA-O1A
15	C	800	ADP	C5'-O5'-PA-O3A
15	D	800	ADP	C5'-O5'-PA-O3A
15	E	800	ADP	C5'-O5'-PA-O1A
15	E	800	ADP	C5'-O5'-PA-O3A
15	F	800	ADP	C5'-O5'-PA-O1A
15	G	800	ADP	C5'-O5'-PA-O3A
15	I	800	ADP	C5'-O5'-PA-O1A
15	I	800	ADP	C5'-O5'-PA-O3A
16	H	401	ANP	PB-N3B-PG-O1G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

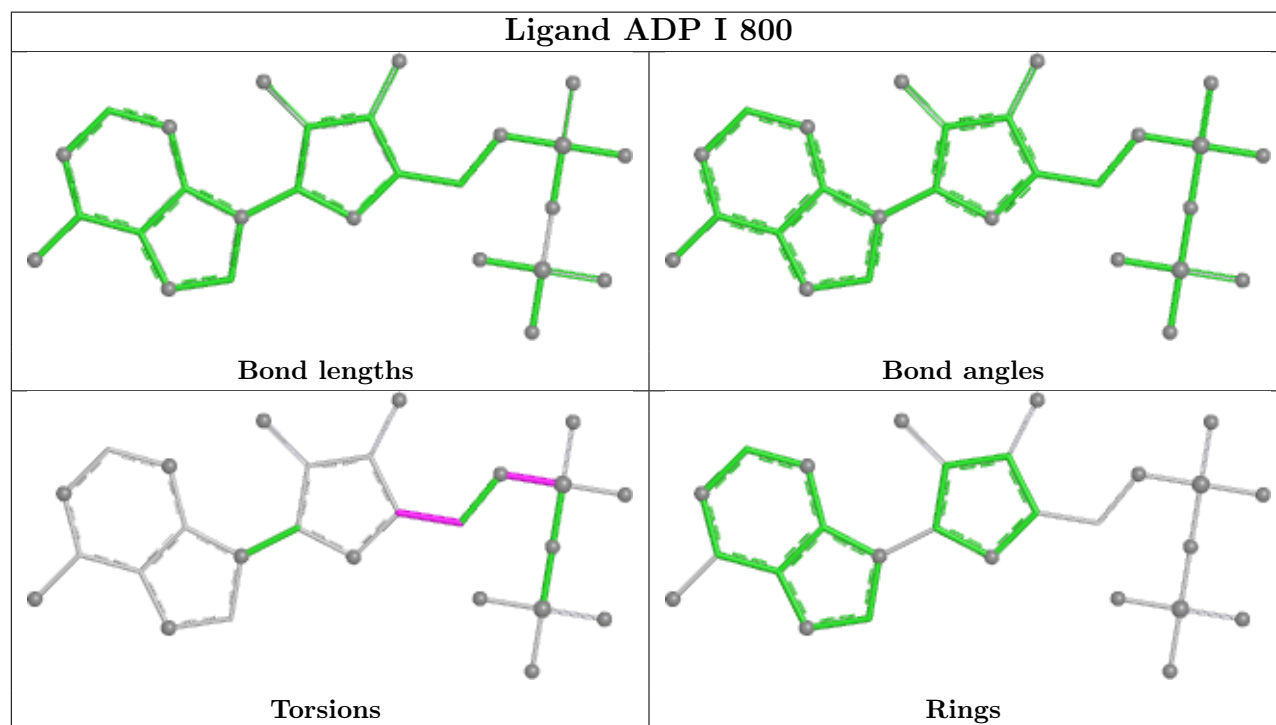
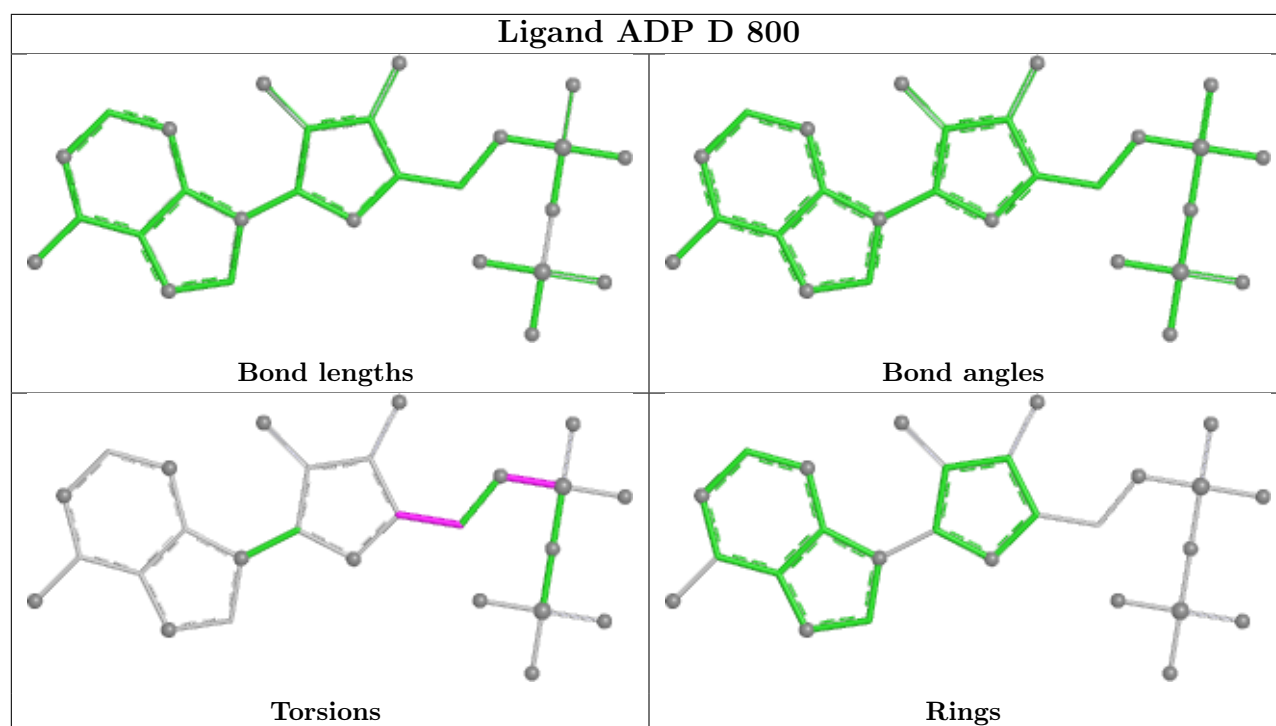
There are no ring outliers.

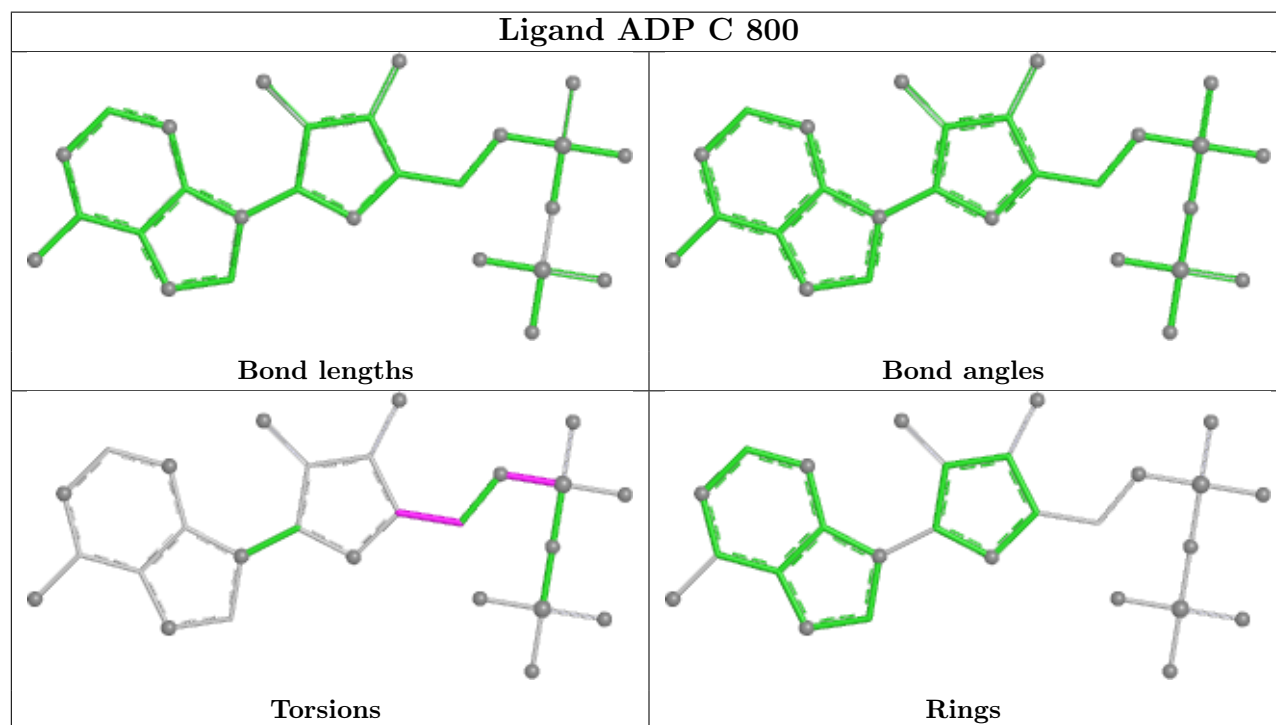
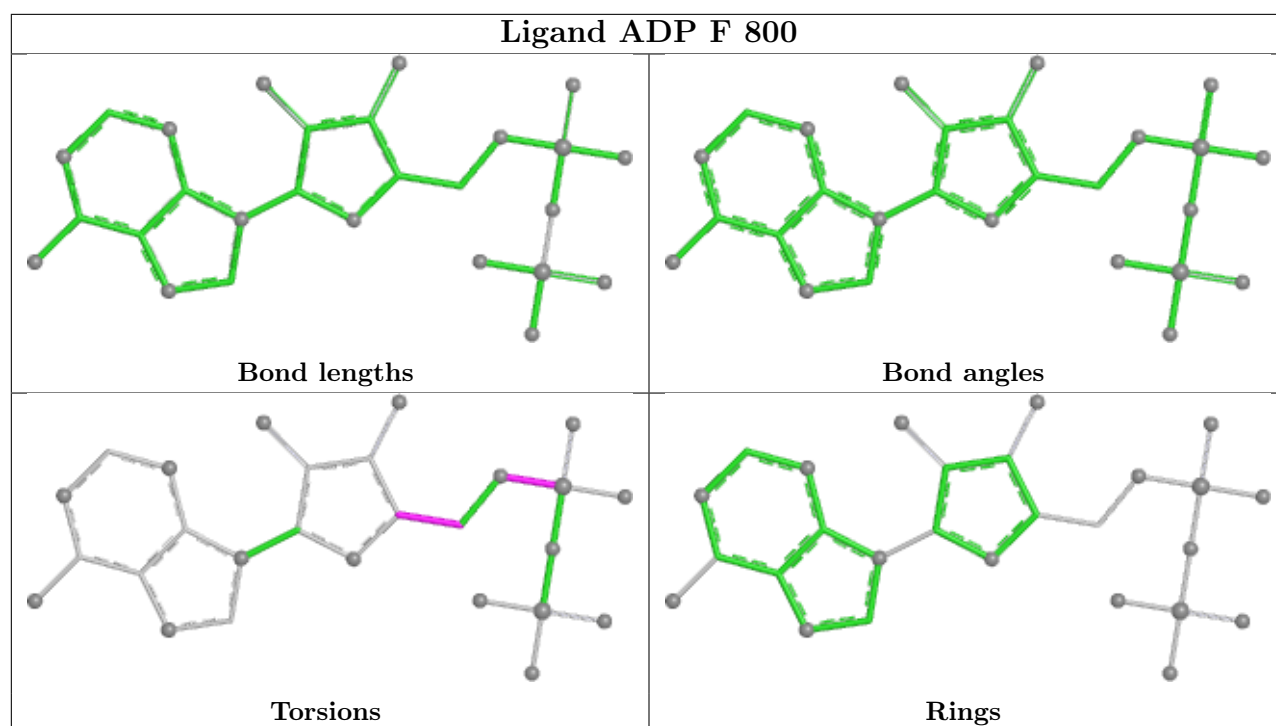
1 monomer is involved in 1 short contact:

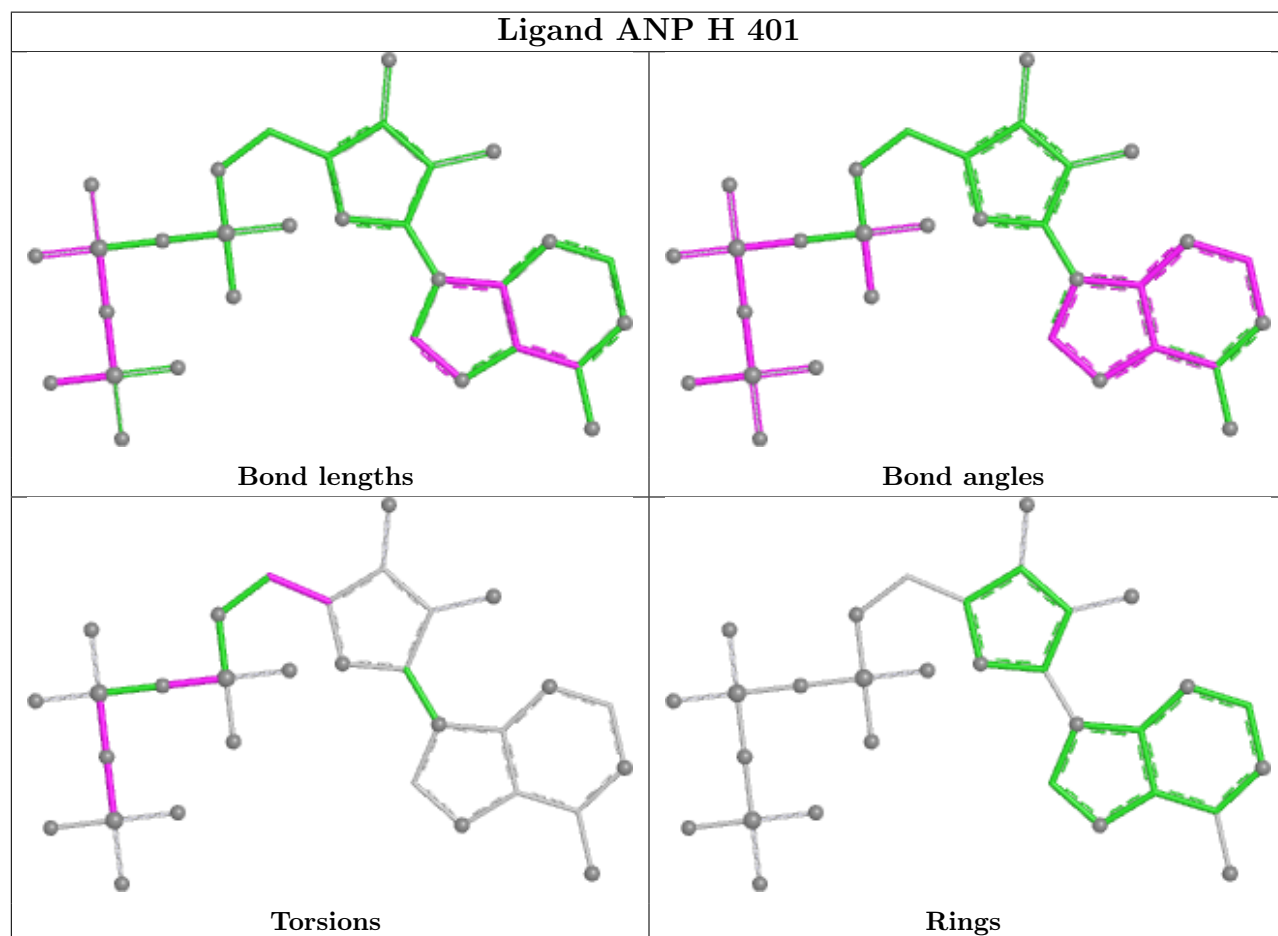
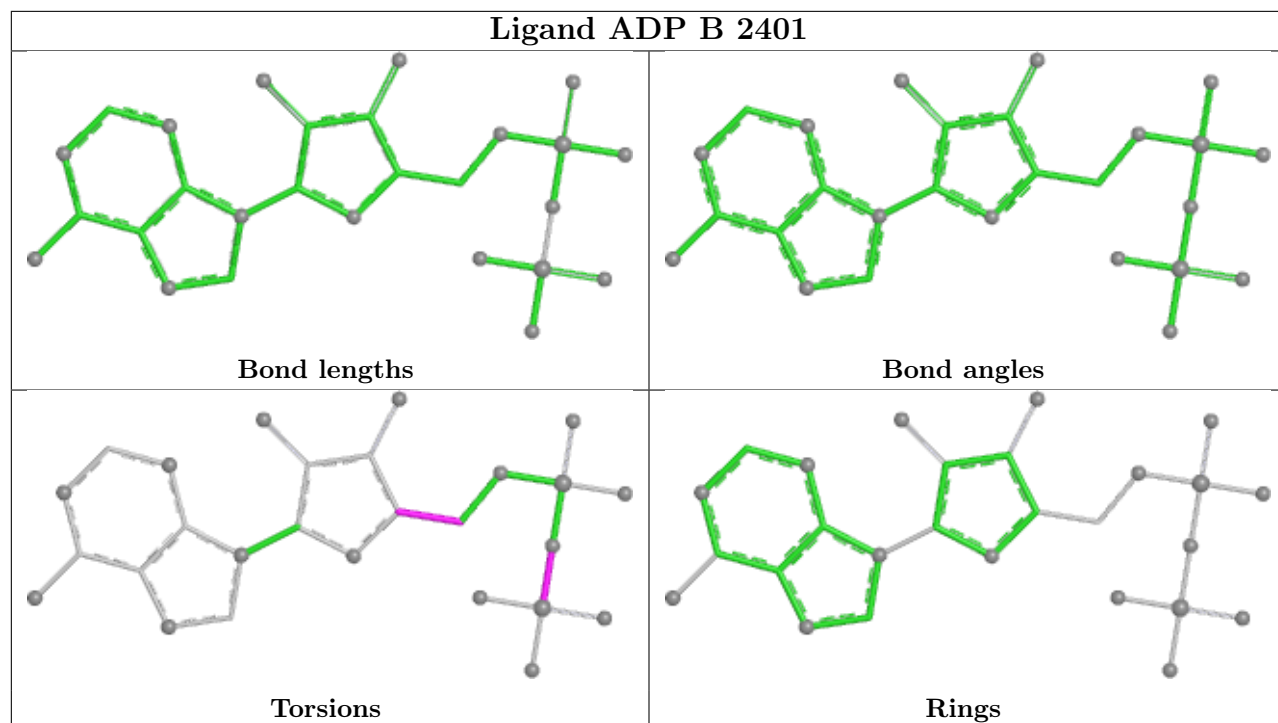
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	401	ANP	1	0

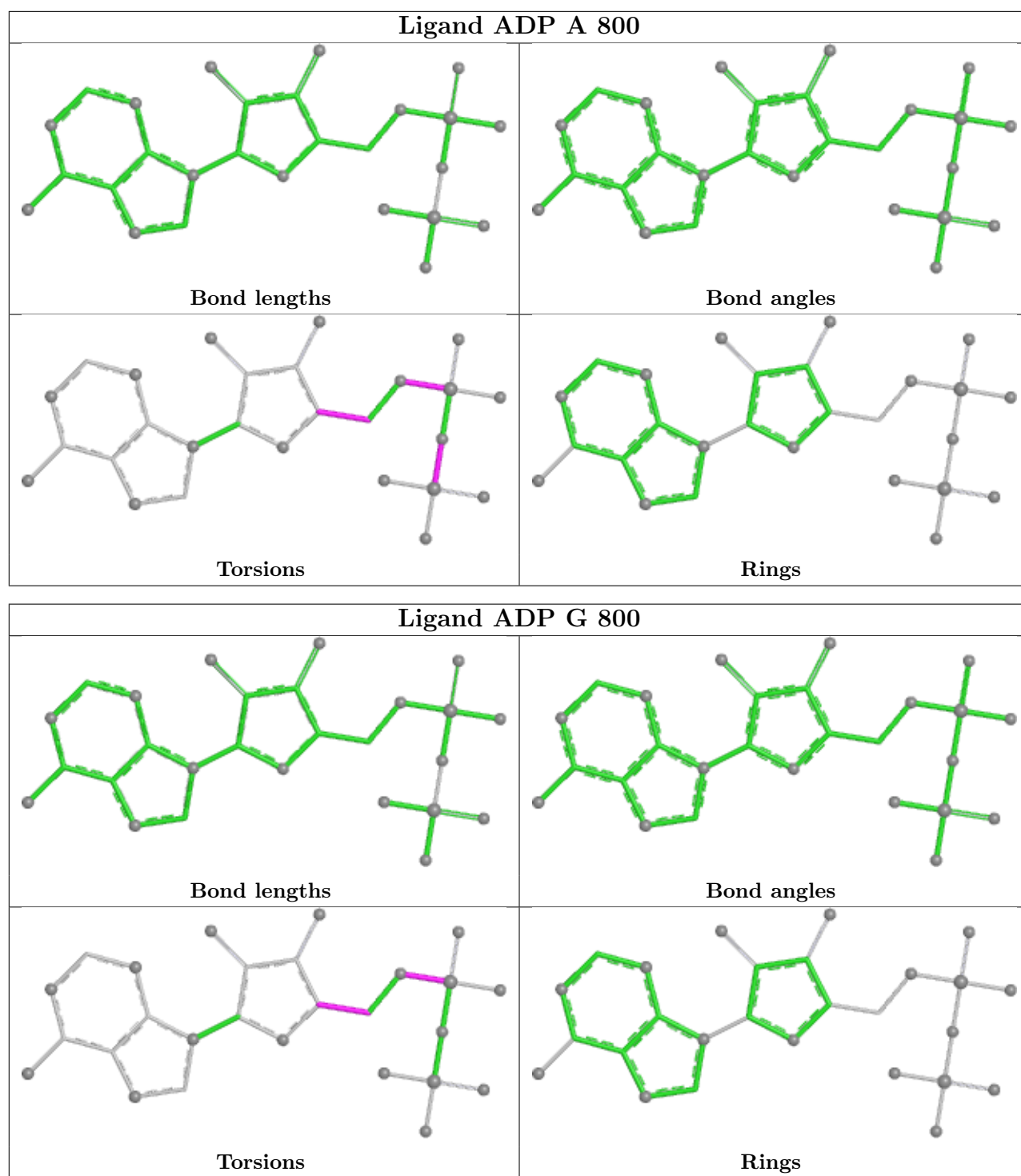
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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
11	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	1243:VAL	C	1252:TYR	N	35.42
1	J	94:SER	C	95:VAL	N	3.81
1	J	116:PRO	C	117:SER	N	2.93
1	J	55:VAL	C	56:GLN	N	2.79
1	J	89:VAL	C	90:VAL	N	1.20
1	J	329:LYS	C	330:PRO	N	1.20
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	1.17

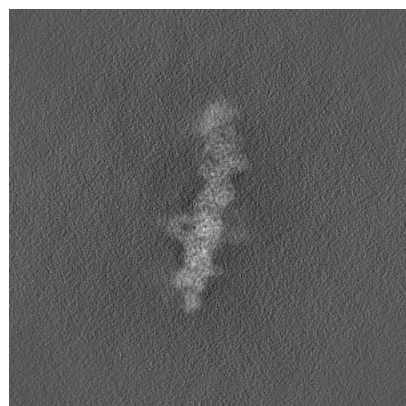
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44306. These allow visual inspection of the internal detail of the map and identification of artifacts.

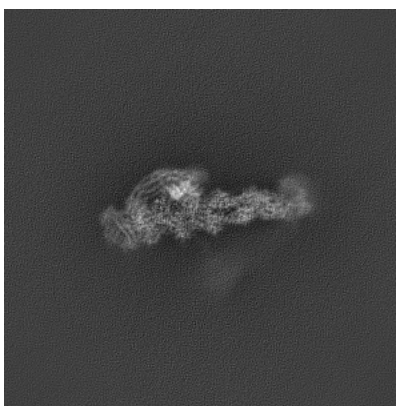
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

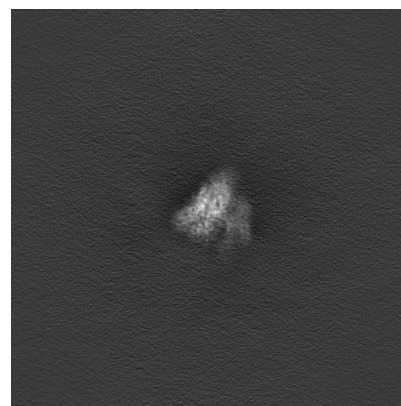
6.1.1 Primary map



X

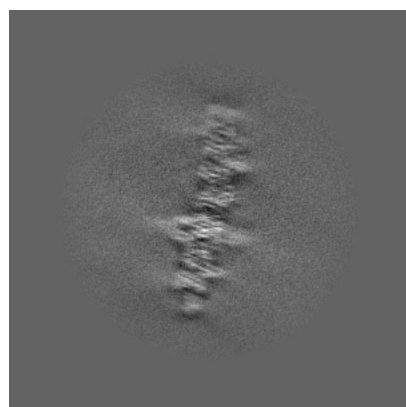


Y

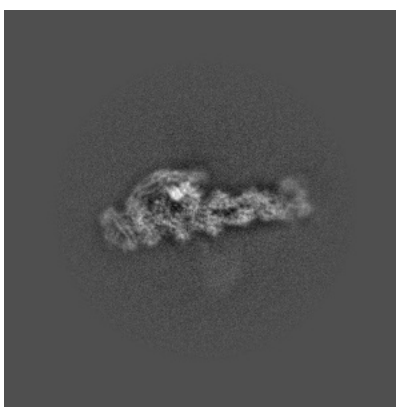


Z

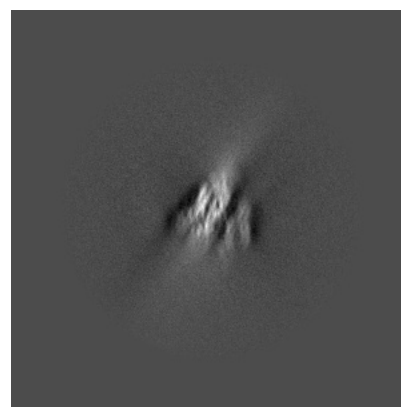
6.1.2 Raw map



X



Y

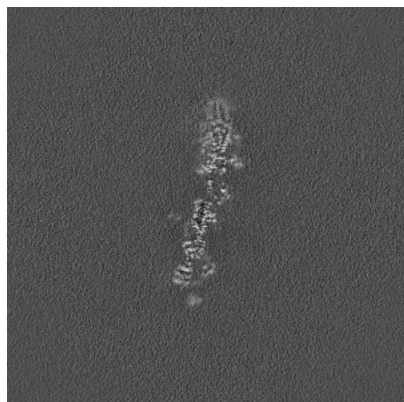


Z

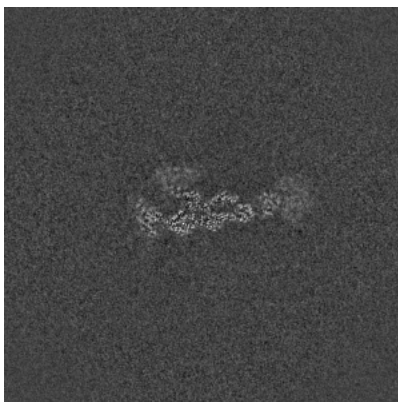
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 432

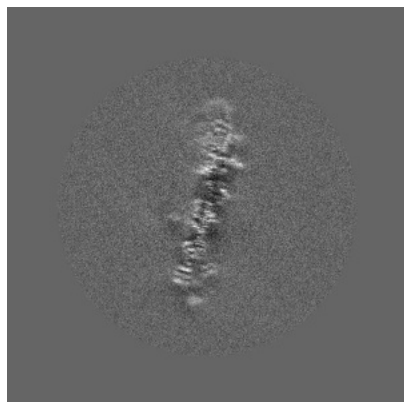


Y Index: 432

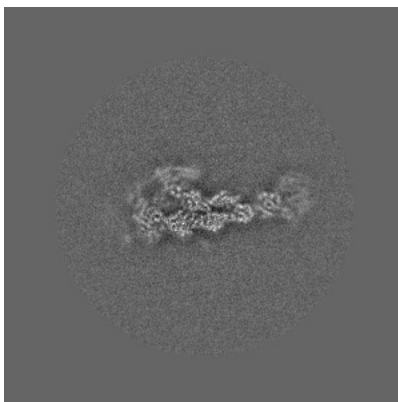


Z Index: 432

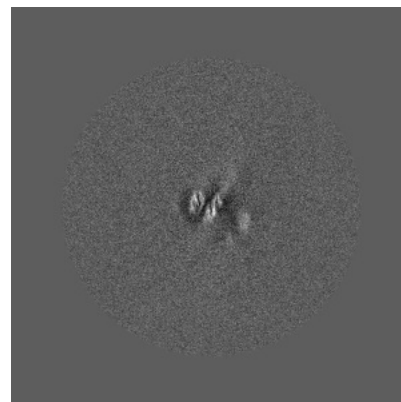
6.2.2 Raw map



X Index: 432



Y Index: 432

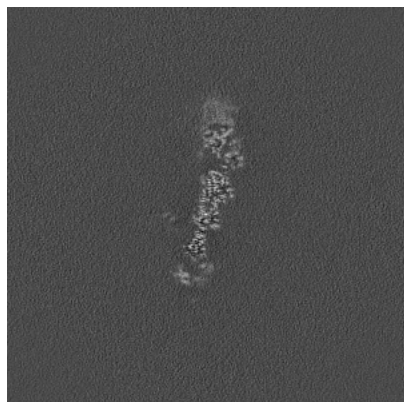


Z Index: 432

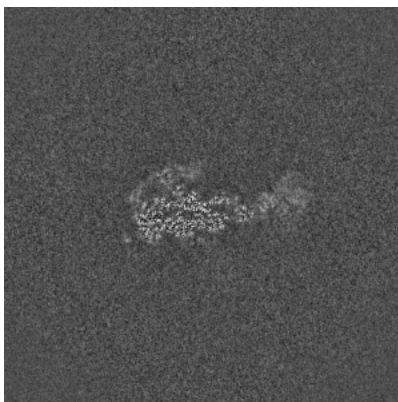
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

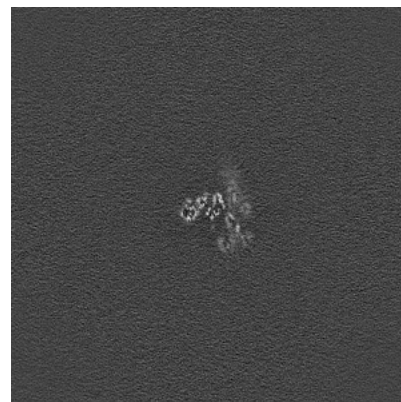
6.3.1 Primary map



X Index: 441

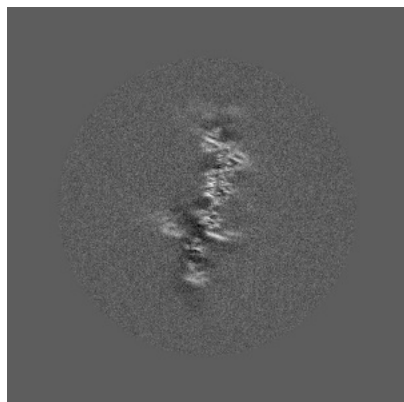


Y Index: 426

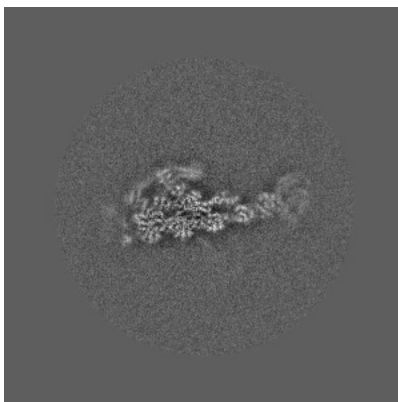


Z Index: 392

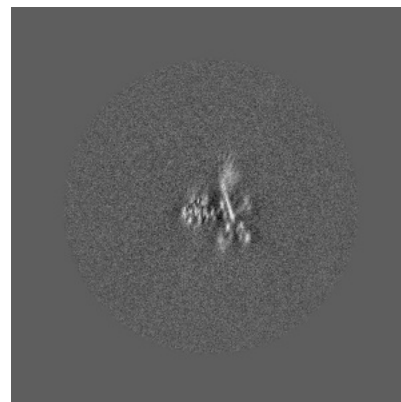
6.3.2 Raw map



X Index: 454



Y Index: 426

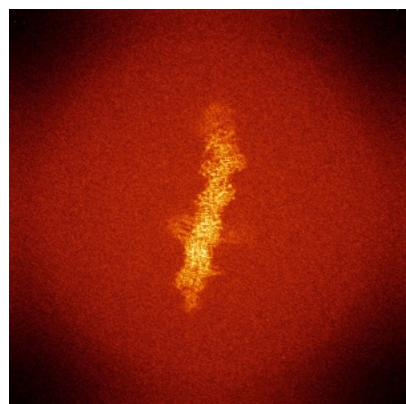


Z Index: 376

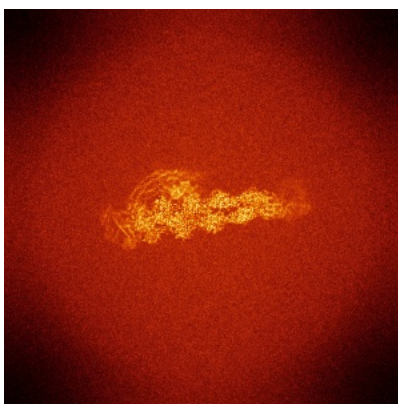
The images above show the largest variance slices of the map in three orthogonal directions.

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

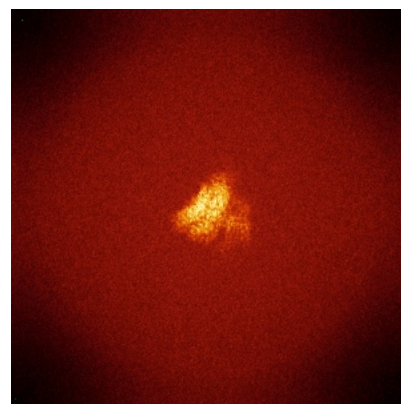
6.4.1 Primary map



X

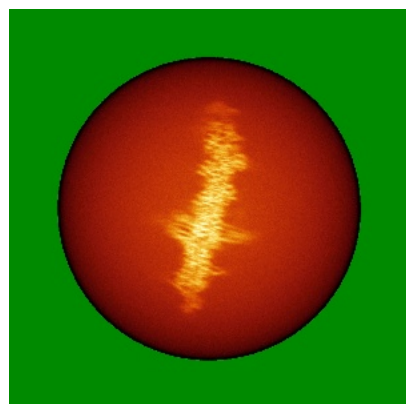


Y

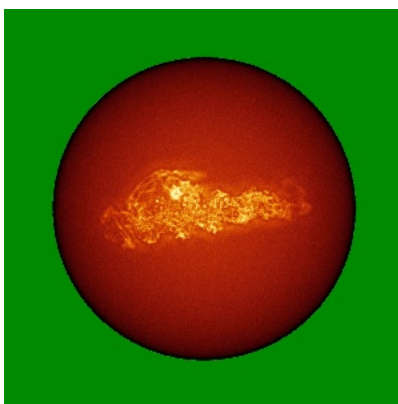


Z

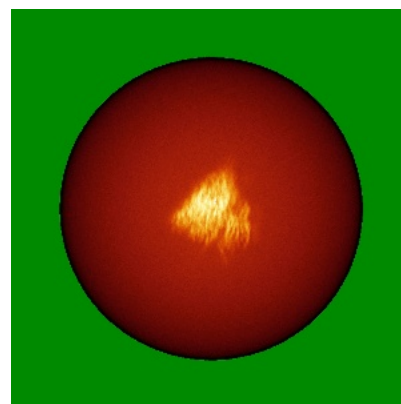
6.4.2 Raw map



X



Y

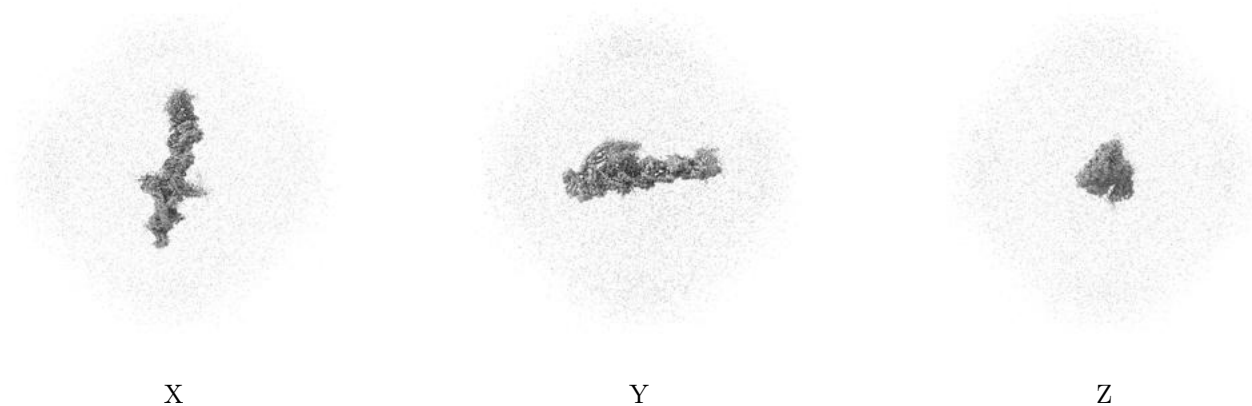


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

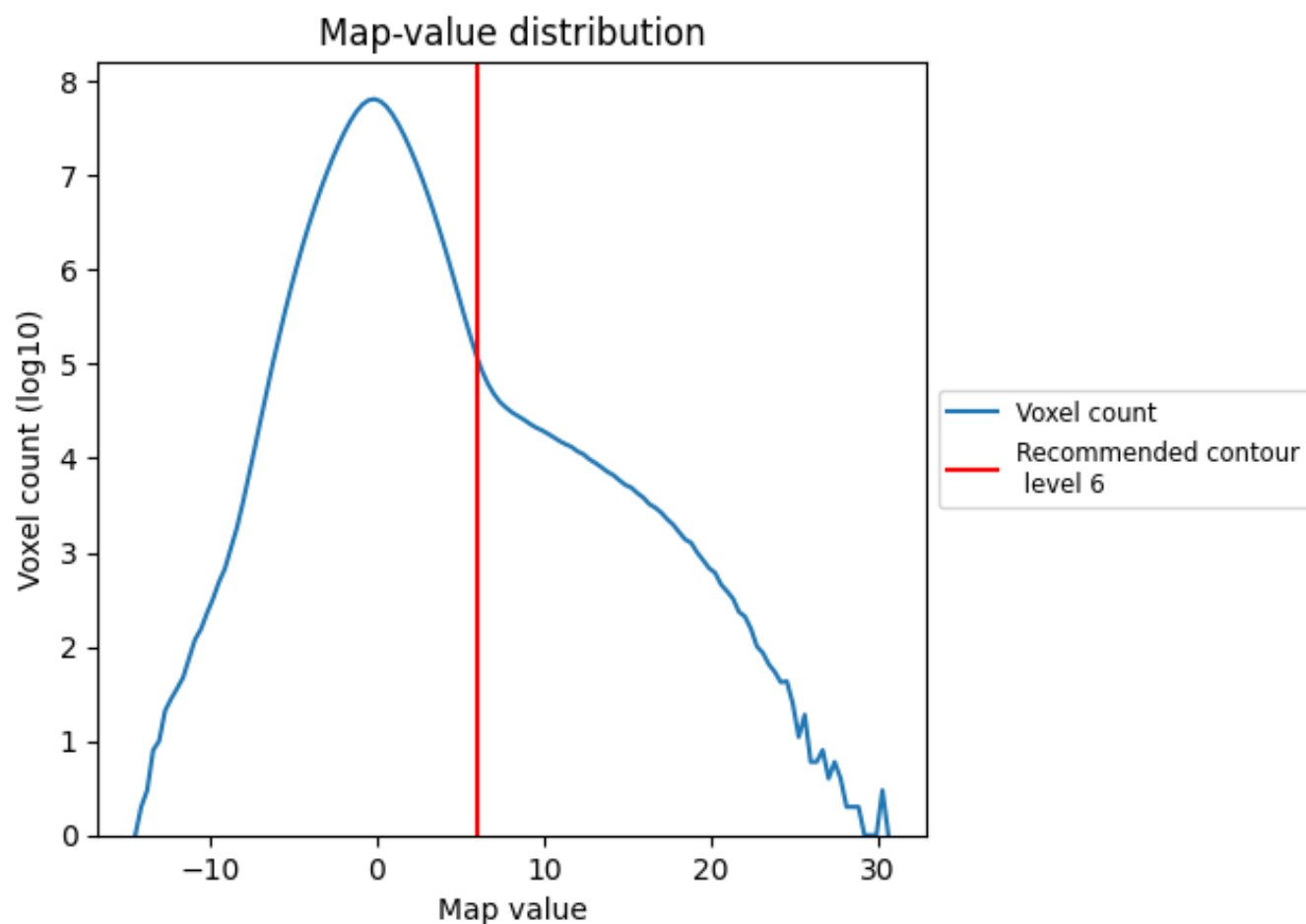
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

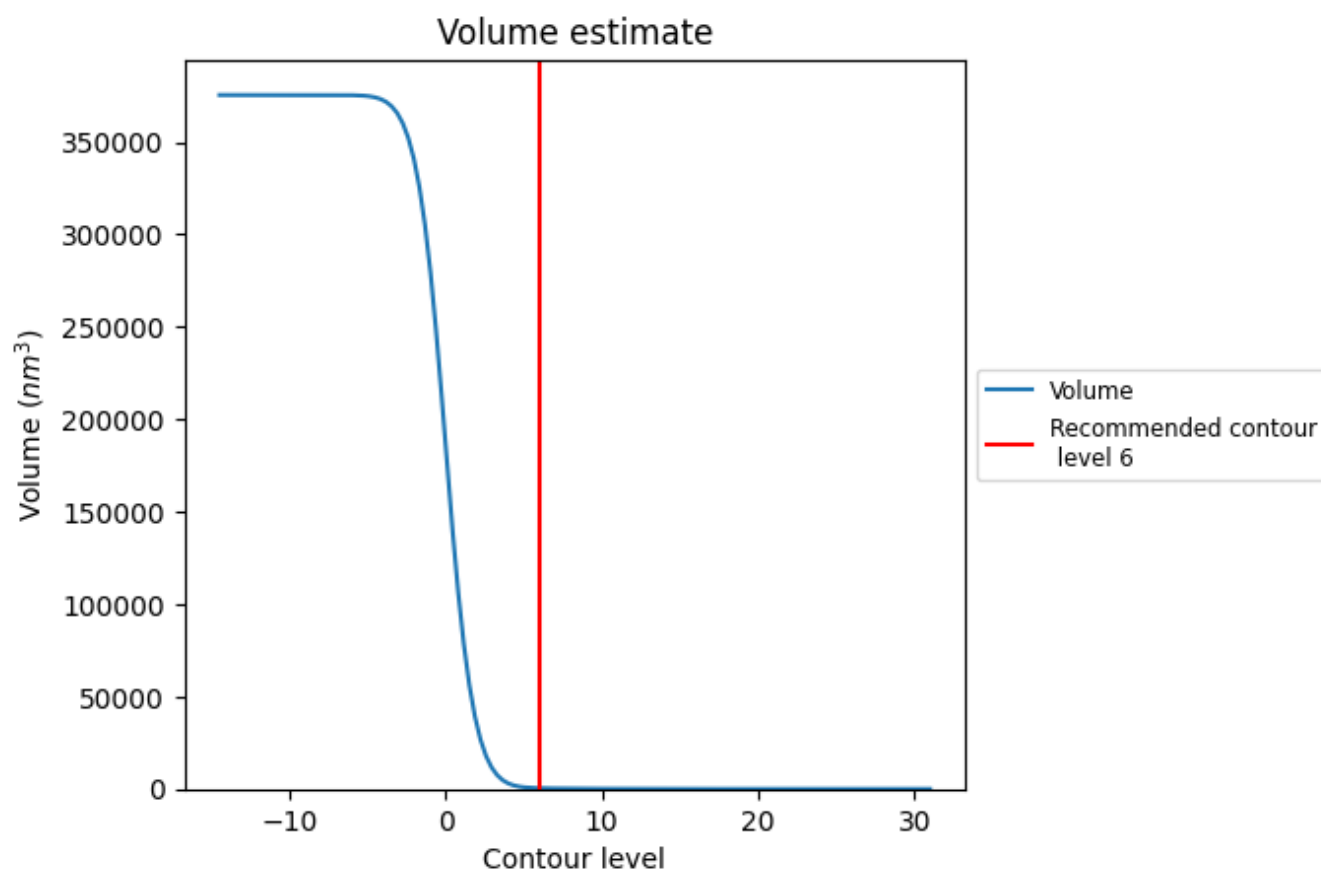
This section contains the results of statistical analysis of the map.

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.

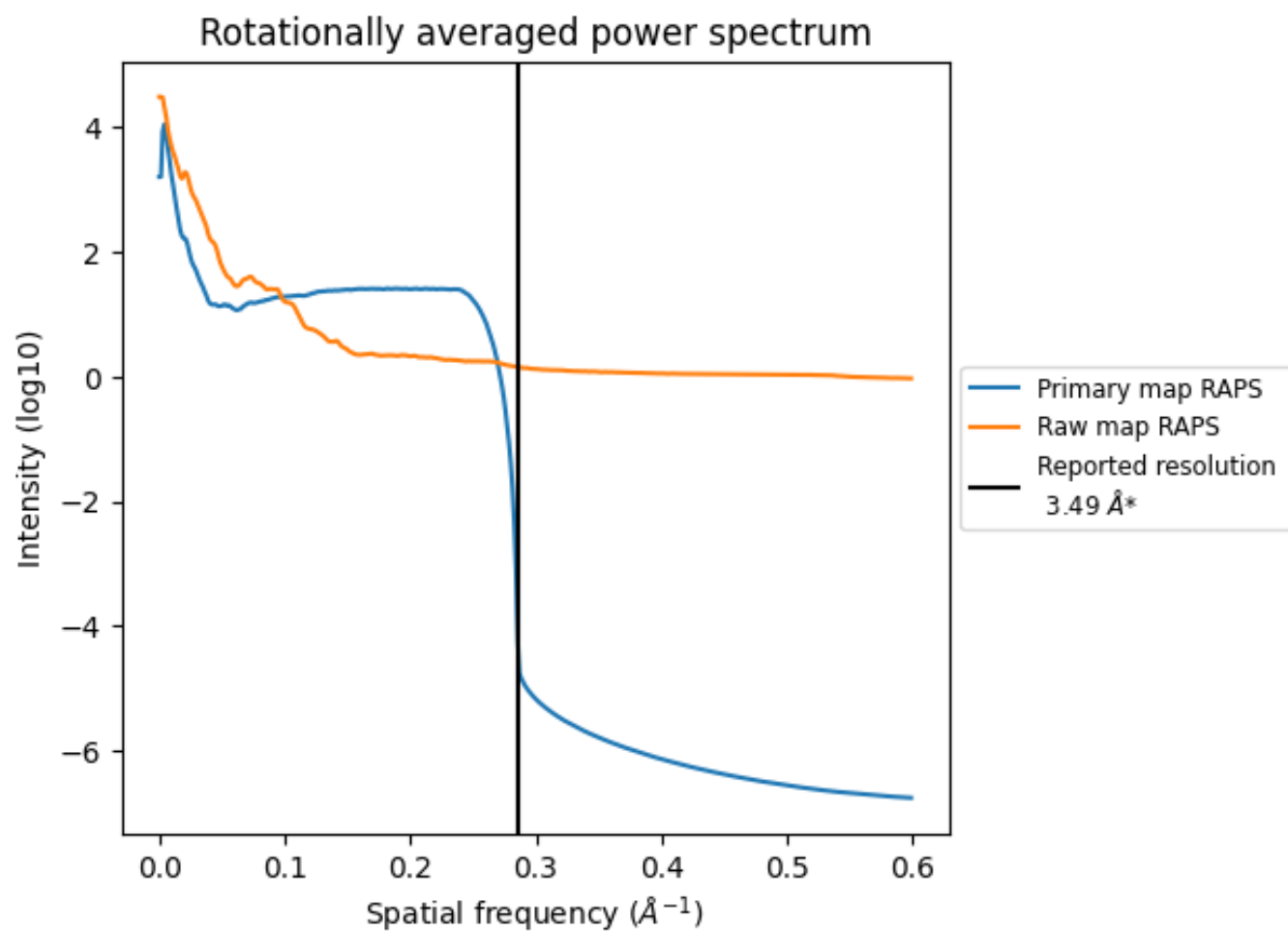
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 417 nm^3 ; this corresponds to an approximate mass of 376 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 ⓘ

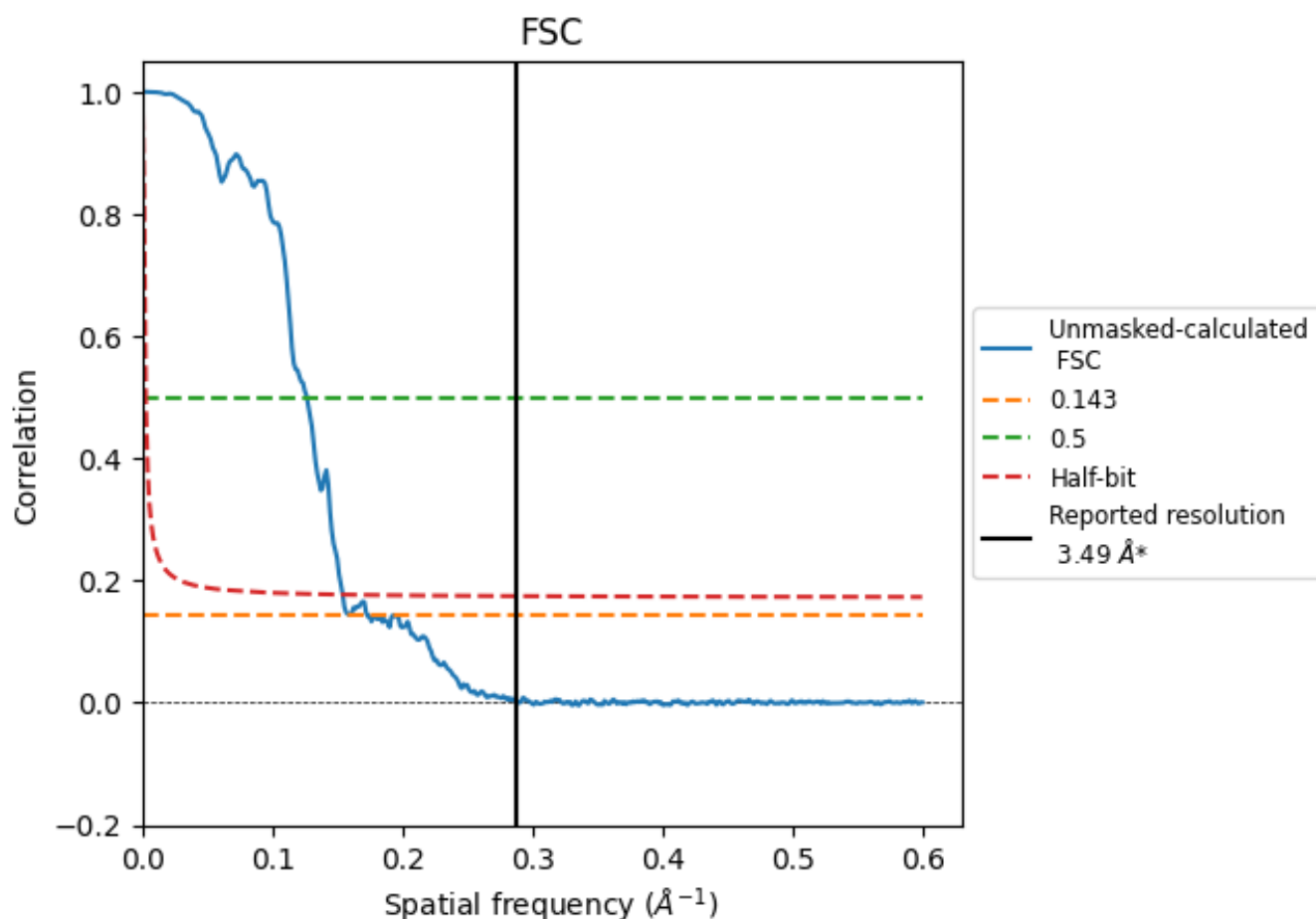


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 $0.287 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

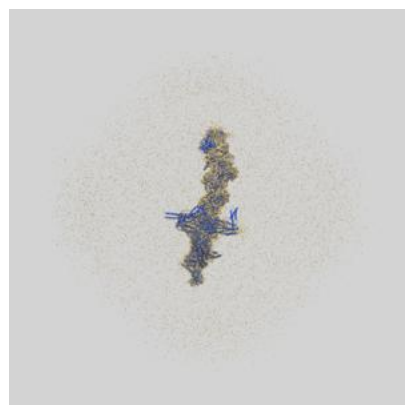
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.79	7.91	6.50

*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 5.79 differs from the reported value 3.49 by more than 10 %

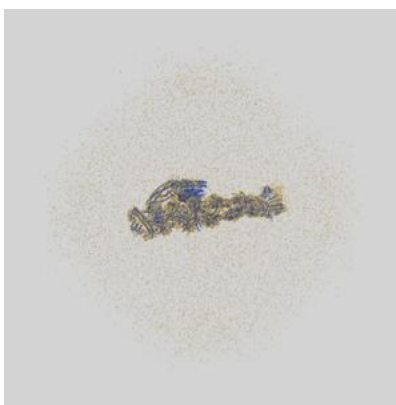
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44306 and PDB model 9B7J. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

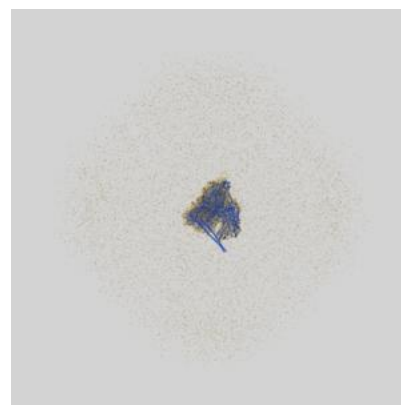
9.1 Map-model overlay [i](#)



X



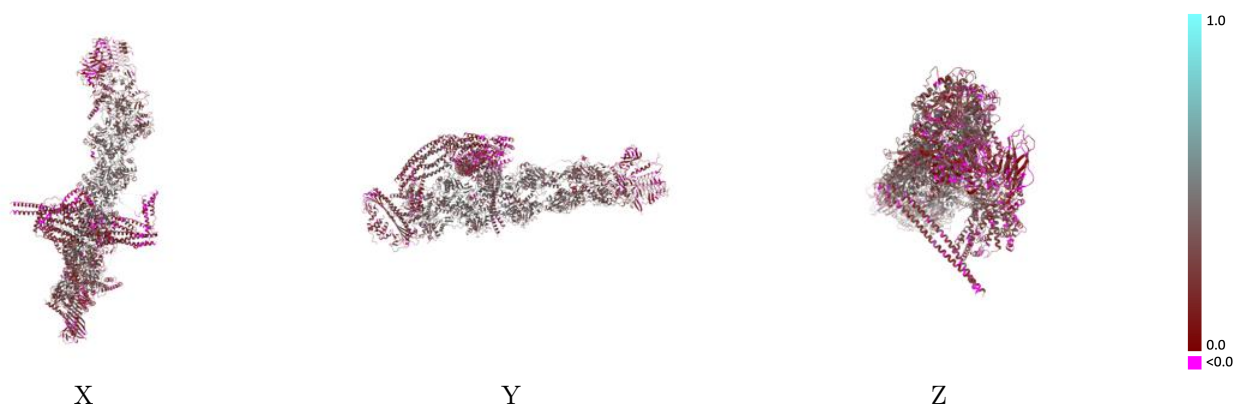
Y



Z

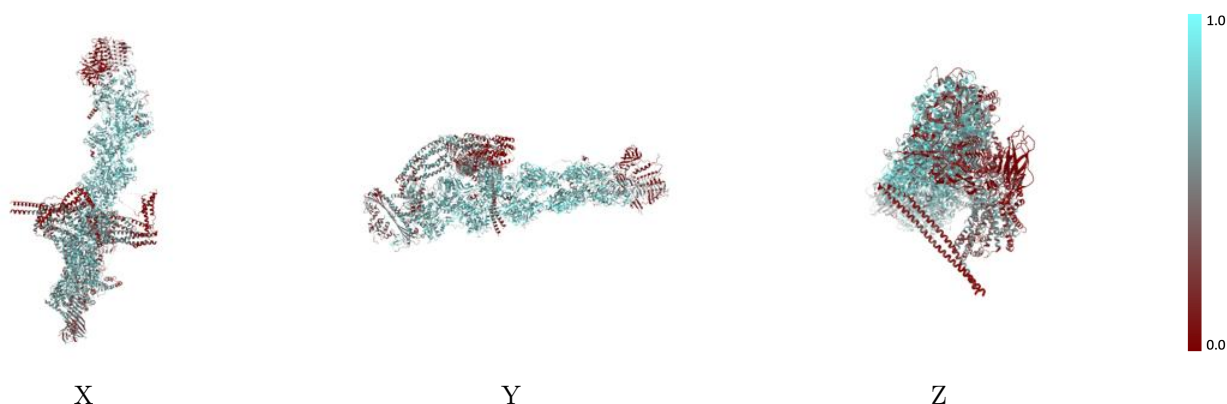
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



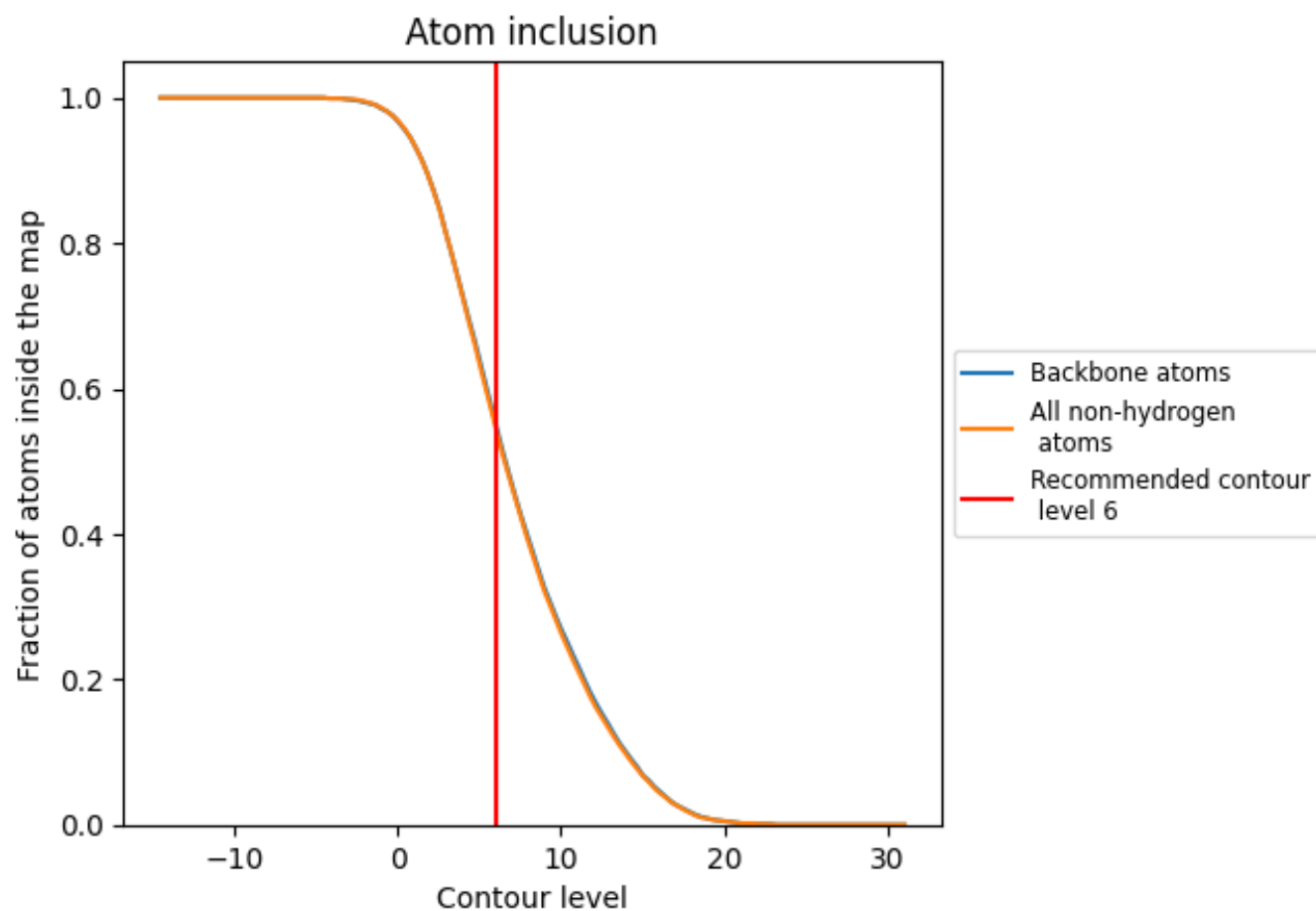
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5480	 0.2800
A	 0.6440	 0.3200
B	 0.7130	 0.3640
C	 0.7460	 0.4090
D	 0.7500	 0.3870
E	 0.7460	 0.3880
F	 0.7650	 0.3890
G	 0.7540	 0.3930
H	 0.7480	 0.3770
I	 0.6800	 0.3300
J	 0.6380	 0.2850
K	 0.2430	 0.1450
L	 0.1820	 0.1210
M	 0.2770	 0.1510
N	 0.4240	 0.1870
O	 0.5190	 0.2220
P	 0.3840	 0.1820
Q	 0.3310	 0.1580
R	 0.3610	 0.1770
S	 0.3390	 0.1490
T	 0.0980	 0.1550
U	 0.0900	 0.1450
p	 0.4950	 0.2340
q	 0.4520	 0.2180
r	 0.3930	 0.1830
s	 0.5030	 0.2650

