



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 03:48 PM EDT

PDB ID : 3J15 / pdb_00003j15
EMDB ID : EMD-2009
Title : Model of ribosome-bound archaeal Pelota and ABCE1
Authors : Becker, T.; Franckenberg, S.; Wickles, S.; Shoemaker, C.J.; Anger, A.M.; Armache, J.-P.; Sieber, H.; Ungewickell, C.; Berninghausen, O.; Daberkow, I.; Karcher, A.; Thomm, M.; Hopfner, K.-P.; Green, R.; Beckmann, R.
Deposited on : 2011-12-12
Resolution : 6.60 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.dev133
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) : 2.50

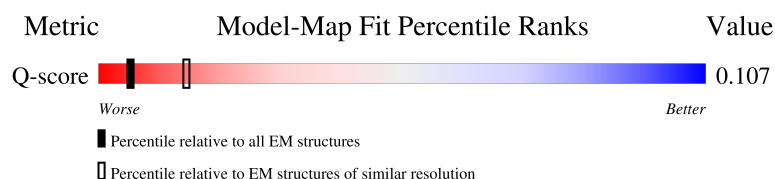
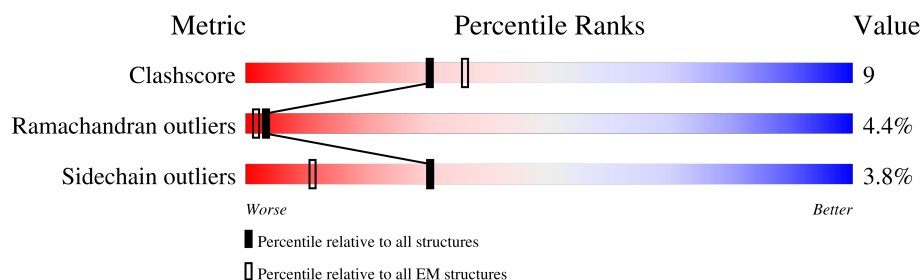
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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	531 (6.10 - 7.10)

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	357	
2	B	593	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	601	-	-	X	-
3	ADP	B	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein pelota.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	357	Total	C	N	O	S	0	0
			2861	1818	503	533	7		

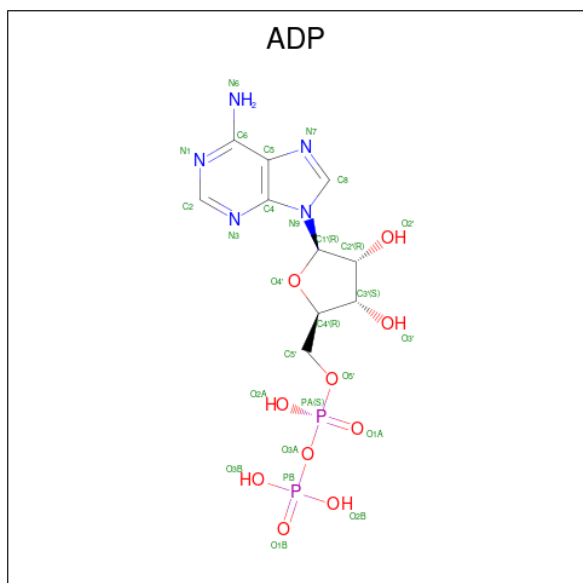
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLN	conflict	UNP Q5JIB9

- Molecule 2 is a protein called ABC transporter ATP-binding protein.

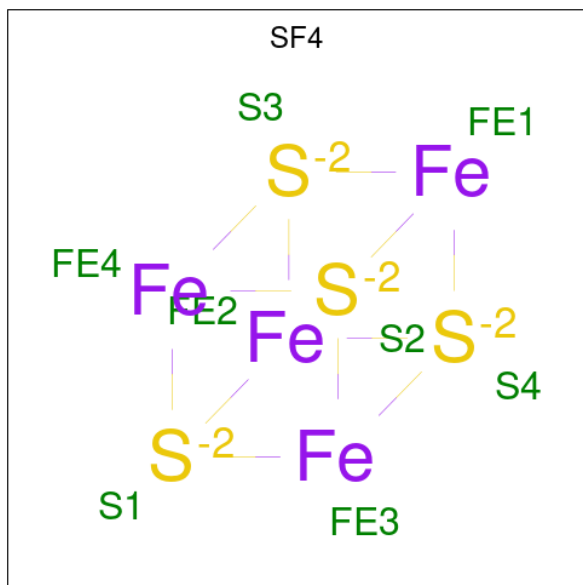
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	593	Total	C	N	O	S	0	0
			4729	3003	826	880	20		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

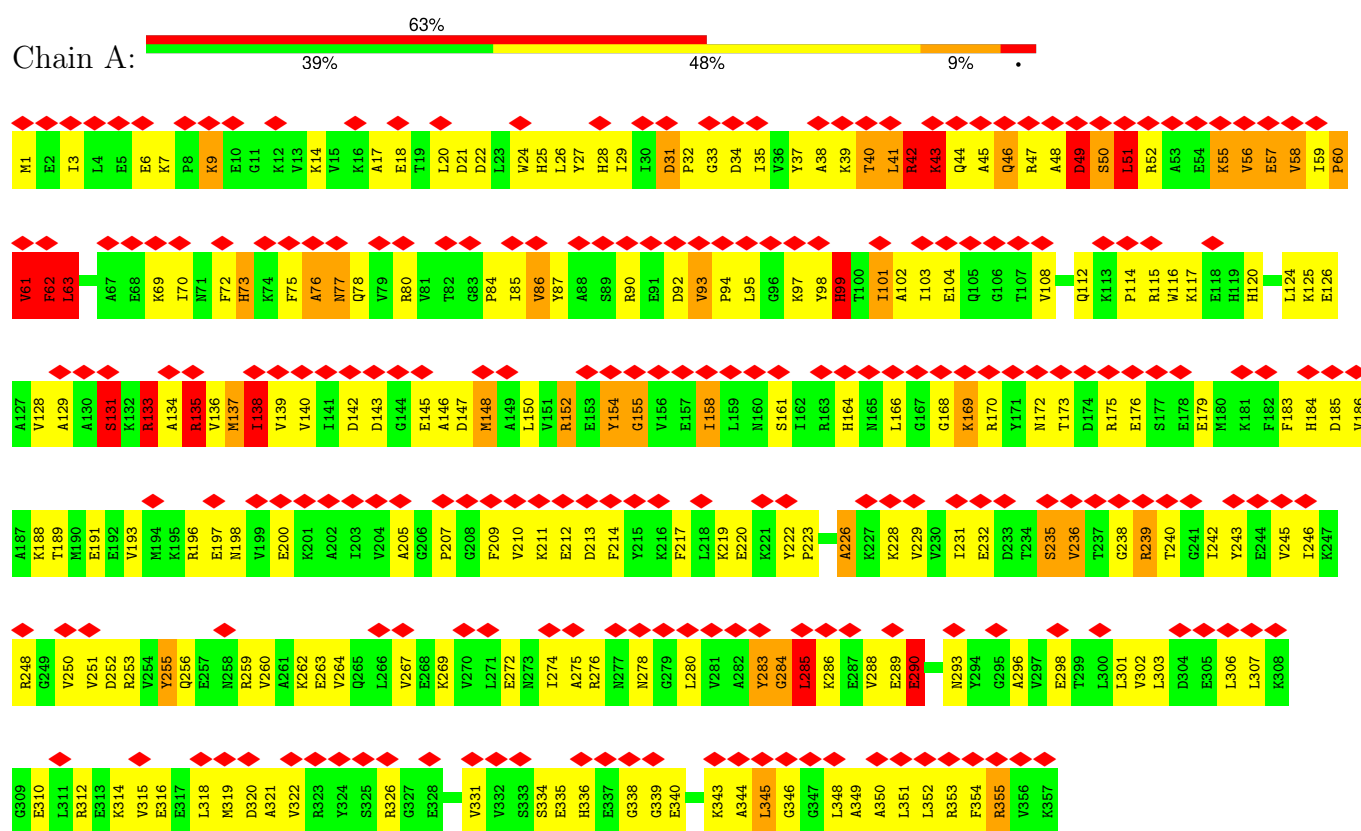


Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	Fe	S	0
			8	4	4	
4	B	1	Total	Fe	S	0
			8	4	4	

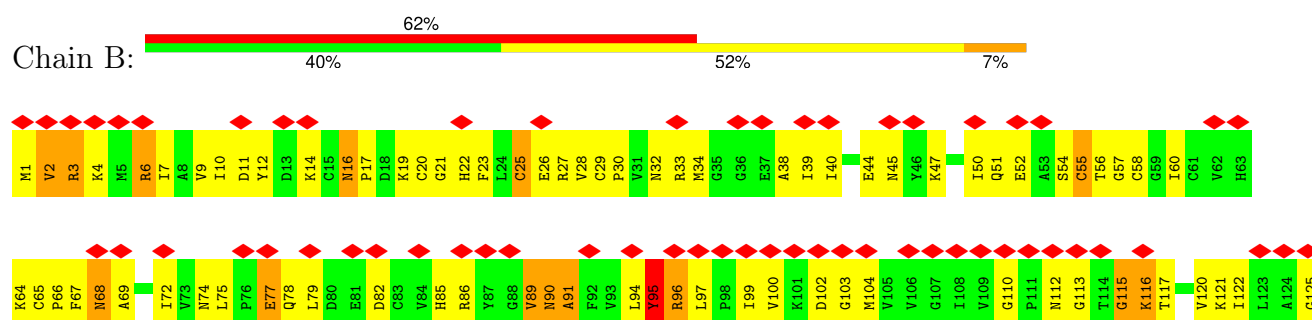
3 Residue-property plots

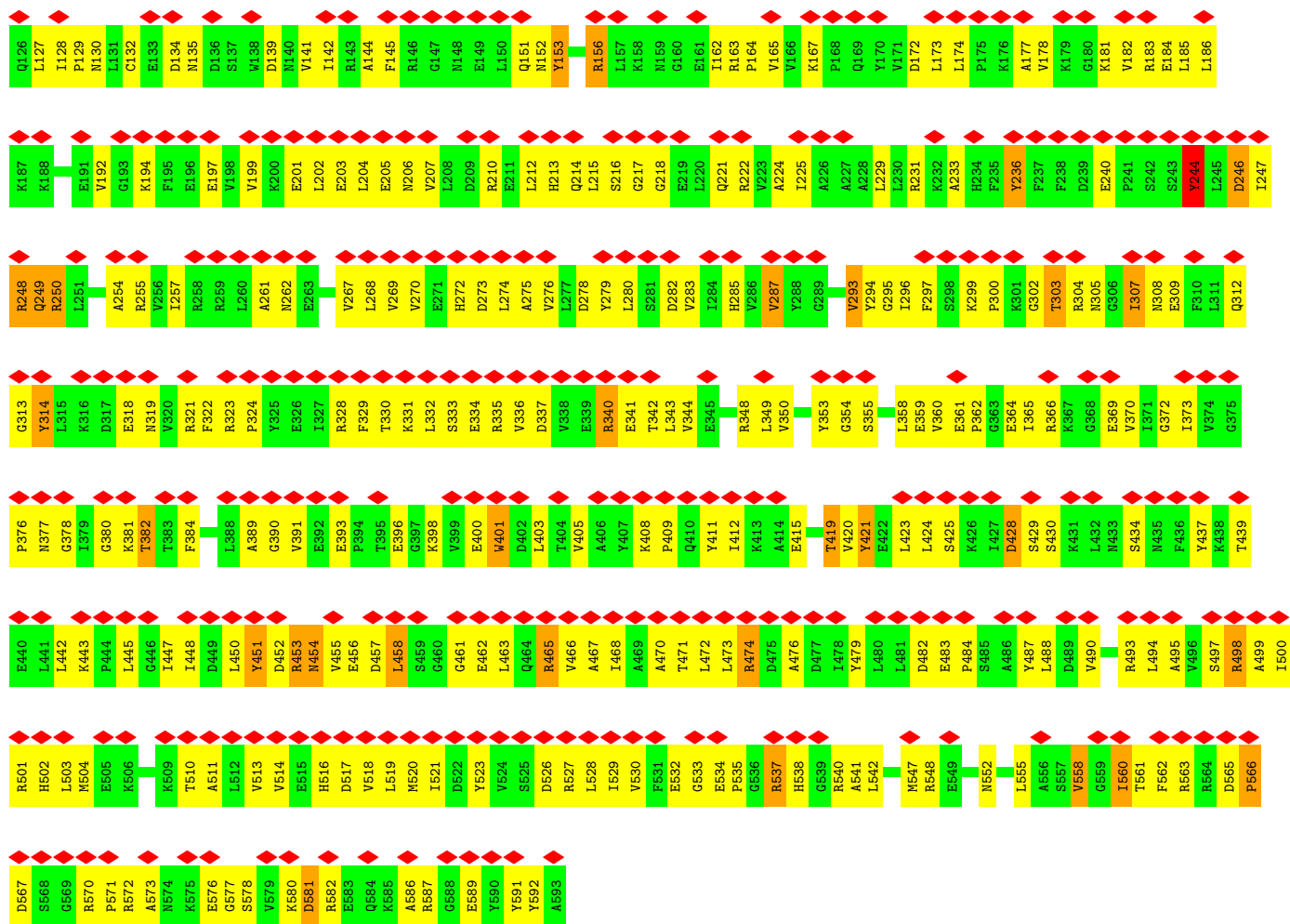
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Protein pelota



• Molecule 2: ABC transporter ATP-binding protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51000	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	75000	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	0.745	Depositor
Minimum map value	-0.497	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.28	102/2903 (3.5%)	2.51	216/3904 (5.5%)
2	B	2.14	167/4815 (3.5%)	2.37	295/6499 (4.5%)
All	All	2.20	269/7718 (3.5%)	2.42	511/10403 (4.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
2	B	0	19
All	All	0	30

All (269) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLN	CA-C	-11.79	1.47	1.53
2	B	213	HIS	ND1-CE1	10.29	1.42	1.32
1	A	135	ARG	CD-NE	10.02	1.60	1.46
2	B	269	VAL	CA-C	-9.98	1.40	1.52
2	B	400	GLU	CA-CB	9.84	1.65	1.52
1	A	21	ASP	N-CA	-9.62	1.33	1.46
2	B	484	PRO	CA-C	-9.42	1.40	1.52
2	B	453	ARG	NE-CZ	9.36	1.43	1.33
2	B	360	VAL	CA-CB	-9.32	1.42	1.54
1	A	49	ASP	CA-C	-9.08	1.40	1.52
1	A	164	HIS	CE1-NE2	-8.85	1.23	1.32
2	B	95	TYR	CA-C	-8.63	1.42	1.52
2	B	563	ARG	CD-NE	8.56	1.58	1.46
1	A	38	ALA	CA-C	-8.55	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	ALA	N-CA	-8.33	1.35	1.46
2	B	488	LEU	CA-C	-8.01	1.43	1.52
2	B	540	ARG	NE-CZ	8.00	1.41	1.33
2	B	372	GLY	CA-C	-7.99	1.46	1.52
1	A	37	TYR	N-CA	-7.98	1.35	1.45
2	B	343	LEU	CA-C	-7.84	1.42	1.53
2	B	562	PHE	CA-C	-7.78	1.42	1.52
1	A	14	LYS	N-CA	-7.60	1.37	1.46
2	B	353	TYR	CA-C	-7.60	1.43	1.52
2	B	490	VAL	CA-C	-7.58	1.43	1.52
2	B	302	GLY	C-N	7.58	1.43	1.33
1	A	99	HIS	ND1-CE1	7.51	1.40	1.32
1	A	73	HIS	CG-CD2	7.38	1.44	1.35
1	A	75	PHE	CA-CB	7.34	1.64	1.53
1	A	3	ILE	CA-C	-7.34	1.43	1.52
1	A	290	GLU	CA-C	7.34	1.62	1.52
1	A	259	ARG	CD-NE	7.31	1.56	1.46
1	A	58	VAL	C-N	7.31	1.41	1.33
1	A	6	GLU	CA-C	-7.29	1.43	1.52
2	B	270	VAL	C-N	7.26	1.43	1.33
2	B	203	GLU	C-N	7.25	1.43	1.33
1	A	253	ARG	CD-NE	7.25	1.56	1.46
2	B	207	VAL	C-N	7.21	1.43	1.33
2	B	322	PHE	CA-C	-7.19	1.44	1.53
1	A	117	LYS	N-CA	-7.19	1.36	1.45
2	B	526	ASP	CA-C	-7.12	1.43	1.52
2	B	537	ARG	NE-CZ	7.09	1.40	1.33
2	B	582	ARG	NE-CZ	7.02	1.40	1.33
2	B	328	ARG	NE-CZ	6.93	1.40	1.33
2	B	90	ASN	CA-CB	6.91	1.63	1.53
1	A	352	LEU	CA-C	-6.90	1.43	1.52
2	B	483	GLU	C-N	6.90	1.40	1.34
1	A	321	ALA	CA-C	-6.90	1.44	1.52
2	B	513	VAL	CA-C	-6.89	1.43	1.52
2	B	165	VAL	CA-C	-6.88	1.43	1.52
2	B	334	GLU	CA-CB	6.84	1.62	1.53
1	A	50	SER	N-CA	-6.83	1.37	1.46
2	B	297	PHE	CA-C	6.76	1.61	1.52
2	B	244	TYR	C-N	6.76	1.42	1.33
2	B	194	LYS	N-CA	-6.75	1.38	1.46
1	A	3	ILE	CA-CB	6.73	1.62	1.54
1	A	353	ARG	CZ-NH2	6.72	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	534	GLU	C-O	-6.72	1.18	1.25
1	A	253	ARG	CZ-NH2	6.62	1.42	1.33
2	B	523	TYR	CA-CB	6.58	1.63	1.53
1	A	3	ILE	C-N	-6.58	1.24	1.33
1	A	326	ARG	N-CA	-6.57	1.36	1.46
2	B	201	GLU	C-O	-6.56	1.16	1.24
2	B	589	GLU	CA-CB	6.53	1.64	1.53
2	B	465	ARG	NE-CZ	6.51	1.40	1.33
2	B	467	ALA	C-N	6.51	1.42	1.33
2	B	145	PHE	CA-C	-6.49	1.42	1.52
1	A	301	LEU	CA-C	-6.48	1.45	1.52
2	B	537	ARG	CD-NE	6.48	1.55	1.46
2	B	183	ARG	CA-C	-6.47	1.44	1.52
1	A	120	HIS	CE1-NE2	-6.46	1.26	1.32
1	A	207	PRO	N-CA	-6.46	1.39	1.47
2	B	519	LEU	CA-C	-6.45	1.44	1.52
2	B	358	LEU	N-CA	-6.43	1.38	1.46
1	A	99	HIS	CA-C	-6.40	1.44	1.52
1	A	318	LEU	C-N	6.39	1.42	1.33
1	A	97	LYS	N-CA	-6.38	1.38	1.46
1	A	101	ILE	CA-CB	6.37	1.60	1.55
1	A	60	PRO	C-N	6.34	1.42	1.33
2	B	304	ARG	NE-CZ	6.34	1.40	1.33
2	B	96	ARG	C-N	6.33	1.40	1.33
2	B	502	HIS	ND1-CE1	6.33	1.38	1.32
1	A	154	TYR	C-N	6.32	1.39	1.32
2	B	184	GLU	C-N	6.31	1.41	1.33
2	B	153	TYR	CA-CB	6.30	1.63	1.53
2	B	112	ASN	CA-C	-6.29	1.44	1.52
2	B	453	ARG	CZ-NH1	6.28	1.41	1.32
2	B	452	ASP	CA-CB	6.28	1.64	1.53
2	B	566	PRO	CA-C	6.27	1.61	1.52
2	B	91	ALA	C-N	6.27	1.41	1.33
2	B	463	LEU	CA-C	6.26	1.61	1.52
2	B	350	VAL	N-CA	-6.24	1.38	1.46
1	A	49	ASP	CA-CB	6.20	1.64	1.53
2	B	177	ALA	N-CA	-6.17	1.38	1.46
2	B	285	HIS	CA-C	-6.17	1.45	1.52
2	B	229	LEU	CB-CG	6.16	1.65	1.53
2	B	401	TRP	CA-CB	6.12	1.62	1.53
1	A	236	VAL	CA-CB	-6.12	1.49	1.55
2	B	156	ARG	CD-NE	6.12	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	GLU	CA-CB	6.11	1.62	1.53
2	B	86	ARG	NE-CZ	6.09	1.39	1.33
1	A	170	ARG	NE-CZ	6.07	1.39	1.33
2	B	373	ILE	CA-C	-6.06	1.45	1.52
1	A	25	HIS	ND1-CE1	6.05	1.38	1.32
2	B	128	ILE	CA-C	-6.04	1.46	1.52
2	B	349	LEU	CA-C	-6.04	1.45	1.52
2	B	365	ILE	CA-C	-6.04	1.45	1.52
1	A	243	TYR	C-N	6.04	1.42	1.33
1	A	166	LEU	N-CA	-6.04	1.39	1.46
1	A	267	VAL	CA-CB	-6.04	1.47	1.54
1	A	312	ARG	CZ-NH1	6.01	1.41	1.32
1	A	298	GLU	N-CA	-6.00	1.38	1.46
2	B	369	GLU	C-N	6.00	1.41	1.33
1	A	63	LEU	N-CA	5.99	1.53	1.46
2	B	313	GLY	C-N	5.98	1.42	1.33
2	B	185	LEU	CA-CB	5.98	1.62	1.53
1	A	252	ASP	CA-C	-5.97	1.45	1.52
2	B	500	ILE	N-CA	-5.96	1.39	1.46
1	A	184	HIS	CA-C	-5.94	1.45	1.52
2	B	377	ASN	C-O	-5.94	1.16	1.23
2	B	493	ARG	CD-NE	5.93	1.54	1.46
1	A	63	LEU	C-N	5.90	1.40	1.33
1	A	248	ARG	CD-NE	5.89	1.54	1.46
2	B	430	SER	CA-CB	5.88	1.62	1.53
1	A	262	LYS	CA-C	-5.88	1.45	1.52
2	B	532	GLU	C-N	5.88	1.40	1.33
2	B	405	VAL	CA-C	-5.87	1.45	1.52
1	A	198	ASN	CA-CB	5.86	1.62	1.53
2	B	419	THR	N-CA	-5.85	1.38	1.45
2	B	215	LEU	CA-CB	5.84	1.63	1.53
2	B	194	LYS	CA-CB	5.84	1.61	1.53
2	B	229	LEU	C-N	5.83	1.42	1.33
1	A	140	VAL	N-CA	-5.83	1.39	1.46
2	B	591	TYR	CA-CB	5.82	1.63	1.53
2	B	272	HIS	ND1-CE1	5.81	1.38	1.32
2	B	570	ARG	NE-CZ	5.81	1.39	1.33
2	B	102	ASP	CA-C	-5.80	1.45	1.52
2	B	511	ALA	N-CA	-5.80	1.38	1.45
2	B	77	GLU	N-CA	5.78	1.53	1.46
2	B	33	ARG	CD-NE	5.77	1.54	1.46
2	B	589	GLU	CA-C	-5.77	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	PRO	CA-C	5.76	1.60	1.52
1	A	315	VAL	N-CA	-5.76	1.39	1.46
2	B	224	ALA	C-N	5.75	1.41	1.33
2	B	461	GLY	C-N	5.73	1.41	1.33
1	A	211	LYS	CA-C	-5.72	1.45	1.52
2	B	240	GLU	C-N	-5.72	1.27	1.34
2	B	247	ILE	CA-CB	-5.72	1.48	1.54
1	A	99	HIS	CA-CB	5.72	1.63	1.53
2	B	274	LEU	CA-CB	-5.72	1.44	1.53
2	B	186	LEU	C-N	5.72	1.41	1.33
2	B	527	ARG	NE-CZ	5.70	1.39	1.33
1	A	296	ALA	CA-C	-5.69	1.45	1.52
1	A	184	HIS	ND1-CE1	5.68	1.38	1.32
2	B	285	HIS	CE1-NE2	-5.68	1.26	1.32
2	B	471	THR	CA-C	5.67	1.60	1.52
2	B	498	ARG	CA-CB	5.67	1.62	1.53
2	B	398	LYS	CA-C	-5.66	1.45	1.52
1	A	179	GLU	CA-C	-5.66	1.45	1.52
2	B	517	ASP	N-CA	-5.65	1.39	1.46
2	B	204	LEU	N-CA	-5.65	1.39	1.46
2	B	424	LEU	C-N	5.64	1.41	1.33
2	B	473	LEU	CA-C	-5.64	1.44	1.52
2	B	458	LEU	N-CA	-5.64	1.39	1.45
1	A	205	ALA	N-CA	-5.63	1.38	1.45
1	A	95	LEU	CA-CB	5.62	1.62	1.53
2	B	335	ARG	CZ-NH2	5.61	1.40	1.33
2	B	340	ARG	CZ-NH1	5.61	1.40	1.32
2	B	482	ASP	CA-C	-5.59	1.45	1.53
2	B	275	ALA	C-N	5.59	1.41	1.33
1	A	344	ALA	C-O	-5.58	1.17	1.24
1	A	238	GLY	CA-C	-5.58	1.43	1.52
2	B	563	ARG	NE-CZ	5.57	1.39	1.33
1	A	250	VAL	C-N	5.57	1.41	1.33
1	A	124	LEU	CA-CB	5.56	1.62	1.53
1	A	77	ASN	CA-C	-5.55	1.46	1.53
2	B	586	ALA	C-N	5.55	1.40	1.33
2	B	321	ARG	NE-CZ	5.55	1.39	1.33
1	A	37	TYR	C-N	-5.54	1.25	1.33
2	B	398	LYS	N-CA	-5.54	1.39	1.46
1	A	200	GLU	C-N	5.53	1.40	1.33
2	B	323	ARG	CZ-NH2	5.53	1.40	1.33
2	B	269	VAL	C-O	-5.52	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	LYS	C-N	5.50	1.38	1.32
1	A	335	GLU	CA-C	-5.50	1.45	1.52
2	B	201	GLU	CA-CB	5.49	1.61	1.53
2	B	501	ARG	NE-CZ	5.47	1.39	1.33
1	A	283	TYR	CA-CB	5.47	1.62	1.53
2	B	100	VAL	CA-C	5.46	1.58	1.52
1	A	276	ARG	NE-CZ	5.45	1.39	1.33
2	B	120	VAL	CA-C	-5.44	1.46	1.52
1	A	260	VAL	CA-CB	-5.44	1.47	1.54
2	B	323	ARG	CZ-NH1	5.42	1.40	1.32
2	B	558	VAL	CA-C	5.42	1.58	1.52
2	B	233	ALA	CA-C	-5.41	1.45	1.52
2	B	283	VAL	N-CA	5.41	1.52	1.46
2	B	222	ARG	CZ-NH1	5.41	1.40	1.32
2	B	541	ALA	CA-CB	-5.40	1.45	1.53
1	A	191	GLU	CA-C	-5.39	1.45	1.52
1	A	334	SER	N-CA	5.39	1.53	1.46
1	A	101	ILE	CA-C	-5.38	1.46	1.52
1	A	284	GLY	CA-C	-5.38	1.44	1.51
2	B	197	GLU	C-N	5.38	1.40	1.33
2	B	33	ARG	N-CA	-5.38	1.39	1.46
1	A	152	ARG	NE-CZ	5.37	1.39	1.33
1	A	343	LYS	C-N	5.36	1.41	1.33
1	A	35	ILE	N-CA	-5.35	1.39	1.46
2	B	267	VAL	CA-CB	-5.35	1.47	1.54
2	B	474	ARG	NE-CZ	5.35	1.39	1.33
2	B	482	ASP	CA-CB	5.34	1.59	1.53
2	B	409	PRO	N-CA	5.34	1.53	1.47
2	B	573	ALA	CA-C	-5.33	1.46	1.52
2	B	493	ARG	NE-CZ	5.33	1.39	1.33
1	A	217	PHE	C-N	5.32	1.41	1.33
2	B	250	ARG	CD-NE	5.32	1.53	1.46
1	A	87	TYR	C-N	5.32	1.40	1.33
2	B	577	GLY	C-N	5.31	1.40	1.33
1	A	34	ASP	C-N	5.30	1.40	1.33
2	B	448	ILE	N-CA	-5.28	1.40	1.46
2	B	552	ASN	N-CA	5.28	1.52	1.46
1	A	185	ASP	C-N	5.27	1.40	1.33
2	B	294	TYR	CZ-OH	5.26	1.49	1.38
2	B	272	HIS	C-O	5.24	1.31	1.24
1	A	170	ARG	CD-NE	5.24	1.53	1.46
2	B	250	ARG	NE-CZ	5.23	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	309	GLU	N-CA	-5.23	1.40	1.46
2	B	510	THR	CA-C	-5.22	1.46	1.52
2	B	164	PRO	CA-CB	-5.21	1.46	1.53
2	B	359	GLU	C-O	-5.21	1.18	1.24
1	A	114	PRO	N-CA	-5.21	1.40	1.47
2	B	494	LEU	C-N	5.20	1.40	1.33
2	B	555	LEU	CA-C	-5.18	1.45	1.52
2	B	96	ARG	CZ-NH1	5.17	1.40	1.32
2	B	336	VAL	N-CA	-5.17	1.40	1.46
1	A	196	ARG	NE-CZ	5.17	1.38	1.33
1	A	339	GLY	C-N	5.17	1.41	1.33
1	A	80	ARG	CZ-NH2	5.17	1.40	1.33
1	A	353	ARG	CD-NE	5.16	1.53	1.46
2	B	210	ARG	NE-CZ	5.16	1.38	1.33
2	B	533	GLY	CA-C	-5.15	1.45	1.52
2	B	389	ALA	CA-C	-5.14	1.45	1.52
2	B	328	ARG	N-CA	-5.13	1.39	1.45
1	A	302	VAL	CA-C	-5.13	1.46	1.52
1	A	307	LEU	C-N	5.13	1.39	1.33
1	A	319	MET	C-N	5.12	1.40	1.33
2	B	580	LYS	CA-C	5.12	1.59	1.52
2	B	212	LEU	CB-CG	5.12	1.63	1.53
2	B	210	ARG	CD-NE	5.12	1.53	1.46
2	B	384	PHE	CA-CB	5.12	1.61	1.53
2	B	174	LEU	C-N	5.11	1.41	1.33
2	B	214	GLN	C-N	5.11	1.40	1.33
1	A	248	ARG	NE-CZ	5.10	1.38	1.33
2	B	319	ASN	C-N	5.10	1.40	1.33
2	B	329	PHE	N-CA	5.08	1.52	1.45
2	B	99	ILE	N-CA	-5.08	1.40	1.46
1	A	350	ALA	C-N	5.08	1.40	1.33
1	A	131	SER	CA-CB	5.07	1.62	1.53
1	A	312	ARG	CZ-NH2	5.07	1.40	1.33
2	B	592	TYR	CA-C	5.07	1.58	1.52
2	B	381	LYS	N-CA	-5.07	1.40	1.46
2	B	295	GLY	C-N	5.05	1.40	1.33
1	A	128	VAL	C-N	5.05	1.40	1.33
2	B	504	MET	CA-CB	-5.05	1.45	1.53
2	B	303	THR	CA-CB	-5.05	1.45	1.53
2	B	122	ILE	CA-CB	5.05	1.60	1.54
1	A	70	ILE	CA-CB	5.04	1.60	1.54
1	A	51	LEU	N-CA	-5.04	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ILE	C-N	5.01	1.40	1.33
2	B	348	ARG	NE-CZ	5.01	1.38	1.33
2	B	255	ARG	NE-CZ	5.00	1.38	1.33

All (511) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	GLY	N-CA-C	-12.89	98.54	111.56
1	A	31	ASP	CA-C-N	11.55	131.68	119.90
1	A	31	ASP	C-N-CA	11.55	131.68	119.90
1	A	183	PHE	CA-CB-CG	10.87	124.67	113.80
2	B	565	ASP	CA-C-O	-10.75	108.98	120.70
1	A	235	SER	CA-C-N	10.75	134.15	122.11
1	A	235	SER	C-N-CA	10.75	134.15	122.11
1	A	92	ASP	N-CA-C	-10.32	101.74	114.75
1	A	314	LYS	CA-C-N	9.98	133.14	120.56
1	A	314	LYS	C-N-CA	9.98	133.14	120.56
1	A	50	SER	N-CA-C	-9.95	99.87	112.90
2	B	526	ASP	N-CA-C	-9.81	101.08	113.43
2	B	425	SER	N-CA-C	9.53	122.86	111.33
2	B	362	PRO	N-CA-CB	9.46	111.57	103.25
2	B	182	VAL	N-CA-C	-9.42	101.21	110.72
2	B	381	LYS	CA-C-N	9.30	132.53	120.44
2	B	381	LYS	C-N-CA	9.30	132.53	120.44
2	B	558	VAL	N-CA-C	-9.21	104.17	113.47
2	B	442	LEU	N-CA-C	8.96	120.66	111.07
1	A	103	ILE	CB-CA-C	8.95	122.78	111.15
1	A	179	GLU	N-CA-C	-8.93	102.18	113.43
2	B	77	GLU	N-CA-CB	8.79	125.35	110.49
1	A	239	ARG	NE-CZ-NH1	-8.79	112.71	121.50
2	B	337	ASP	CA-CB-CG	-8.64	103.96	112.60
2	B	476	ALA	CA-C-N	8.64	132.56	120.29
2	B	476	ALA	C-N-CA	8.64	132.56	120.29
1	A	338	GLY	CA-C-N	8.63	129.56	119.98
1	A	338	GLY	C-N-CA	8.63	129.56	119.98
2	B	373	ILE	N-CA-CB	8.62	122.98	111.25
2	B	225	ILE	N-CA-CB	8.55	120.00	110.51
2	B	453	ARG	NE-CZ-NH1	-8.55	112.95	121.50
2	B	197	GLU	CA-C-N	8.54	131.38	120.70
2	B	197	GLU	C-N-CA	8.54	131.38	120.70
2	B	86	ARG	NE-CZ-NH1	-8.54	112.97	121.50
1	A	336	HIS	CA-C-N	8.53	134.25	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	HIS	C-N-CA	8.53	134.25	120.60
2	B	213	HIS	CG-CD2-NE2	8.51	115.71	107.20
2	B	181	LYS	CA-C-N	8.47	132.44	120.42
2	B	181	LYS	C-N-CA	8.47	132.44	120.42
1	A	37	TYR	N-CA-C	-8.46	96.87	109.81
1	A	155	GLY	CA-C-O	-8.32	113.73	122.05
1	A	26	LEU	CA-C-N	8.28	131.21	120.44
1	A	26	LEU	C-N-CA	8.28	131.21	120.44
2	B	462	GLU	CA-C-N	8.27	131.71	120.38
2	B	462	GLU	C-N-CA	8.27	131.71	120.38
2	B	206	ASN	N-CA-C	-8.18	103.44	113.50
1	A	275	ALA	CA-C-N	8.05	131.07	120.28
1	A	275	ALA	C-N-CA	8.05	131.07	120.28
2	B	273	ASP	CA-C-N	8.04	131.39	120.38
2	B	273	ASP	C-N-CA	8.04	131.39	120.38
2	B	257	ILE	CB-CA-C	8.04	122.55	112.02
2	B	412	ILE	CA-C-O	7.97	128.81	120.36
2	B	443	LYS	N-CA-CB	7.89	124.42	110.37
2	B	542	LEU	CA-C-N	7.85	128.47	120.38
2	B	542	LEU	C-N-CA	7.85	128.47	120.38
1	A	284	GLY	N-CA-C	7.83	131.73	113.18
1	A	322	VAL	CA-C-N	7.80	130.58	120.44
1	A	322	VAL	C-N-CA	7.80	130.58	120.44
2	B	466	VAL	CA-C-O	-7.73	112.65	120.85
2	B	581	ASP	CA-C-N	7.73	130.95	120.44
2	B	581	ASP	C-N-CA	7.73	130.95	120.44
2	B	354	GLY	CA-C-N	7.69	133.23	120.70
2	B	354	GLY	C-N-CA	7.69	133.23	120.70
2	B	467	ALA	O-C-N	7.68	129.99	122.07
2	B	498	ARG	CA-C-N	7.68	130.88	120.44
2	B	498	ARG	C-N-CA	7.68	130.88	120.44
1	A	69	LYS	N-CA-C	-7.63	97.11	108.79
1	A	284	GLY	CA-C-N	7.63	136.12	121.54
1	A	284	GLY	C-N-CA	7.63	136.12	121.54
1	A	226	ALA	N-CA-CB	7.63	123.39	110.49
1	A	173	THR	N-CA-C	-7.62	104.21	113.97
1	A	169	LYS	N-CA-CB	7.62	123.37	110.49
1	A	146	ALA	N-CA-C	-7.58	96.58	109.24
1	A	57	GLU	CB-CA-C	-7.49	96.94	111.78
2	B	82	ASP	CA-C-N	7.49	131.43	120.95
2	B	82	ASP	C-N-CA	7.49	131.43	120.95
1	A	154	TYR	N-CA-C	-7.47	103.75	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	LYS	CA-C-N	7.47	127.48	119.78
2	B	167	LYS	C-N-CA	7.47	127.48	119.78
2	B	343	LEU	N-CA-C	-7.41	101.37	112.04
1	A	21	ASP	CA-CB-CG	-7.39	105.21	112.60
2	B	261	ALA	CA-C-N	7.35	129.99	120.44
2	B	261	ALA	C-N-CA	7.35	129.99	120.44
1	A	142	ASP	N-CA-C	-7.34	98.75	109.18
1	A	175	ARG	N-CA-C	-7.27	101.52	111.56
1	A	229	VAL	CA-C-O	7.27	128.35	120.57
2	B	333	SER	CA-C-N	7.20	134.40	122.66
2	B	333	SER	C-N-CA	7.20	134.40	122.66
2	B	248	ARG	NE-CZ-NH1	-7.19	114.31	121.50
2	B	448	ILE	N-CA-C	-7.17	103.86	110.82
1	A	255	TYR	CA-C-N	7.15	129.86	120.28
1	A	255	TYR	C-N-CA	7.15	129.86	120.28
2	B	85	HIS	CA-C-O	-7.14	112.24	120.31
1	A	293	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	316	GLU	CA-C-O	-7.13	112.99	120.55
2	B	213	HIS	CA-CB-CG	7.12	120.92	113.80
1	A	239	ARG	NE-CZ-NH2	7.12	125.61	119.20
2	B	255	ARG	CA-C-N	7.07	129.47	120.56
2	B	255	ARG	C-N-CA	7.07	129.47	120.56
2	B	152	ASN	CA-C-O	-7.07	112.93	120.42
2	B	110	GLY	CA-C-N	7.06	127.05	119.78
2	B	110	GLY	C-N-CA	7.06	127.05	119.78
1	A	93	VAL	N-CA-CB	7.03	121.05	111.21
2	B	323	ARG	CA-C-O	-7.02	110.55	120.16
2	B	152	ASN	N-CA-C	-7.01	103.72	111.36
1	A	319	MET	N-CA-CB	7.00	120.53	110.16
2	B	135	ASN	OD1-CG-ND2	7.00	129.60	122.60
1	A	289	GLU	N-CA-C	-6.97	103.68	111.28
2	B	254	ALA	CA-C-O	-6.97	113.16	120.55
2	B	530	VAL	N-CA-C	-6.96	98.33	108.71
1	A	186	VAL	N-CA-CB	6.95	118.68	110.55
2	B	282	ASP	N-CA-C	-6.90	105.80	114.56
2	B	552	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	210	VAL	N-CA-C	6.83	118.40	110.62
2	B	497	SER	CA-C-N	6.80	129.39	120.28
2	B	497	SER	C-N-CA	6.80	129.39	120.28
1	A	335	GLU	CA-C-N	6.78	130.99	120.75
1	A	335	GLU	C-N-CA	6.78	130.99	120.75
2	B	370	VAL	CA-C-O	6.77	126.95	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	ALA	CA-C-O	6.77	127.75	120.10
1	A	353	ARG	NE-CZ-NH1	6.77	128.27	121.50
2	B	361	GLU	CA-C-N	6.71	126.75	119.90
2	B	361	GLU	C-N-CA	6.71	126.75	119.90
2	B	293	VAL	N-CA-CB	-6.67	104.08	111.41
2	B	79	LEU	CA-C-N	6.65	131.24	120.60
2	B	79	LEU	C-N-CA	6.65	131.24	120.60
2	B	305	ASN	CA-CB-CG	-6.64	105.96	112.60
2	B	262	ASN	CA-CB-CG	-6.63	105.97	112.60
1	A	246	ILE	N-CA-C	6.62	117.41	110.72
1	A	126	GLU	CA-C-N	6.62	130.15	120.82
1	A	126	GLU	C-N-CA	6.62	130.15	120.82
2	B	116	LYS	N-CA-CB	6.62	119.88	109.82
1	A	61	VAL	CA-C-N	6.60	134.15	121.54
1	A	61	VAL	C-N-CA	6.60	134.15	121.54
2	B	493	ARG	NE-CZ-NH1	-6.60	114.90	121.50
2	B	494	LEU	N-CA-C	6.59	118.47	111.28
1	A	290	GLU	N-CA-CB	-6.59	100.41	110.16
2	B	428	ASP	CA-C-N	6.58	129.40	120.38
2	B	428	ASP	C-N-CA	6.58	129.40	120.38
2	B	341	GLU	CA-C-N	6.58	130.91	121.50
2	B	341	GLU	C-N-CA	6.58	130.91	121.50
1	A	63	LEU	CA-C-N	6.57	127.70	121.46
1	A	63	LEU	C-N-CA	6.57	127.70	121.46
1	A	104	GLU	CA-C-N	6.57	130.47	120.82
1	A	104	GLU	C-N-CA	6.57	130.47	120.82
1	A	253	ARG	NE-CZ-NH1	6.57	128.07	121.50
2	B	142	ILE	CA-CB-CG2	6.56	121.65	110.50
2	B	314	TYR	CA-C-O	6.56	128.20	120.66
2	B	487	TYR	CB-CA-C	-6.55	102.12	111.95
1	A	189	THR	N-CA-CB	6.55	119.75	110.12
2	B	523	TYR	N-CA-C	6.55	118.22	111.14
2	B	279	TYR	N-CA-C	6.54	118.07	111.07
2	B	451	TYR	CA-C-O	-6.53	112.89	120.20
2	B	523	TYR	O-C-N	6.53	129.14	122.09
2	B	408	LYS	CA-C-N	6.51	126.89	119.92
2	B	408	LYS	C-N-CA	6.51	126.89	119.92
2	B	340	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	98	TYR	CB-CG-CD1	6.49	130.53	120.80
1	A	183	PHE	N-CA-CB	6.48	119.65	110.12
2	B	429	SER	O-C-N	6.47	128.98	122.12
2	B	565	ASP	O-C-N	6.47	128.65	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	581	ASP	O-C-N	-6.47	115.26	122.12
2	B	415	GLU	CA-C-O	6.47	125.57	118.65
2	B	547	MET	O-C-N	6.46	128.81	122.09
1	A	148	MET	N-CA-CB	6.46	121.40	110.49
1	A	158	ILE	CA-C-O	6.46	128.76	120.95
2	B	437	TYR	N-CA-CB	6.43	120.25	110.28
2	B	571	PRO	CA-C-O	-6.42	113.41	120.92
2	B	589	GLU	N-CA-C	-6.42	97.81	108.34
1	A	90	ARG	N-CA-CB	6.37	120.53	110.84
2	B	499	ALA	CA-C-O	-6.35	114.16	120.70
2	B	192	VAL	N-CA-C	-6.35	105.99	113.42
2	B	493	ARG	N-CA-CB	6.34	119.26	110.07
2	B	520	MET	N-CA-C	-6.33	104.30	111.14
2	B	393	GLU	N-CA-C	-6.33	99.76	109.64
1	A	46	GLN	CA-CB-CG	6.33	126.76	114.10
1	A	263	GLU	N-CA-C	6.32	118.17	111.28
1	A	27	TYR	CA-C-N	6.31	129.91	120.31
1	A	27	TYR	C-N-CA	6.31	129.91	120.31
2	B	548	ARG	CA-C-N	6.31	129.37	120.28
2	B	548	ARG	C-N-CA	6.31	129.37	120.28
1	A	112	GLN	OE1-CD-NE2	6.30	128.90	122.60
1	A	238	GLY	CA-C-O	-6.29	114.56	122.74
1	A	220	GLU	CA-C-N	6.29	128.95	120.65
1	A	220	GLU	C-N-CA	6.29	128.95	120.65
1	A	285	LEU	N-CA-CB	6.27	121.08	110.49
2	B	548	ARG	N-CA-CB	6.27	119.16	110.07
1	A	214	PHE	N-CA-C	6.25	118.09	111.28
2	B	97	LEU	O-C-N	-6.25	117.71	121.71
2	B	527	ARG	N-CA-CB	6.23	121.41	111.56
1	A	90	ARG	N-CA-C	-6.22	96.95	108.02
2	B	217	GLY	O-C-N	6.21	130.78	122.70
1	A	38	ALA	N-CA-C	-6.21	97.58	110.80
1	A	145	GLU	CB-CA-C	-6.19	99.05	111.17
1	A	126	GLU	CA-C-O	-6.18	114.33	120.70
2	B	523	TYR	CA-C-O	-6.17	114.34	120.70
2	B	465	ARG	CA-C-N	6.16	129.16	120.42
2	B	465	ARG	C-N-CA	6.16	129.16	120.42
1	A	139	VAL	CA-CB-CG2	6.15	120.86	110.40
2	B	273	ASP	N-CA-C	-6.15	97.07	108.02
2	B	450	LEU	CA-C-N	6.15	129.36	120.38
2	B	450	LEU	C-N-CA	6.15	129.36	120.38
1	A	22	ASP	N-CA-CB	6.15	119.16	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	VAL	N-CA-C	-6.14	99.53	108.87
1	A	264	VAL	N-CA-CB	6.14	117.73	110.55
1	A	29	ILE	N-CA-CB	6.11	119.32	110.52
2	B	552	ASN	CB-CA-C	-6.11	100.46	110.85
2	B	216	SER	N-CA-C	-6.11	100.95	110.17
2	B	538	HIS	CA-CB-CG	-6.10	107.70	113.80
2	B	533	GLY	CA-C-N	6.10	131.69	122.42
2	B	533	GLY	C-N-CA	6.10	131.69	122.42
2	B	365	ILE	CA-C-N	6.09	132.99	122.64
2	B	365	ILE	C-N-CA	6.09	132.99	122.64
2	B	254	ALA	O-C-N	6.08	128.57	122.12
2	B	224	ALA	CA-C-O	-6.07	114.44	120.70
1	A	283	TYR	CA-CB-CG	6.06	124.82	113.90
2	B	534	GLU	CA-C-O	-6.06	113.92	119.62
2	B	116	LYS	CA-C-N	6.06	130.84	120.72
2	B	116	LYS	C-N-CA	6.06	130.84	120.72
2	B	538	HIS	CB-CG-CD2	-6.06	123.33	131.20
2	B	560	ILE	CA-C-O	6.04	126.76	120.36
1	A	62	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	117	LYS	CA-C-N	6.02	128.84	120.29
1	A	117	LYS	C-N-CA	6.02	128.84	120.29
1	A	272	GLU	CB-CG-CD	-6.02	102.37	112.60
1	A	280	LEU	N-CA-C	-6.00	106.28	113.97
2	B	307	ILE	N-CA-C	-6.00	104.66	110.72
2	B	173	LEU	N-CA-C	-5.99	104.72	112.68
2	B	555	LEU	N-CA-CB	5.98	119.42	110.22
2	B	128	ILE	CA-C-N	5.97	125.91	119.76
2	B	128	ILE	C-N-CA	5.97	125.91	119.76
1	A	219	LYS	N-CA-C	-5.95	104.88	111.36
2	B	437	TYR	N-CA-C	-5.95	104.92	111.82
1	A	166	LEU	N-CA-C	-5.94	99.11	108.14
1	A	17	ALA	N-CA-C	-5.94	97.79	108.48
1	A	191	GLU	CA-C-N	5.93	128.51	120.44
1	A	191	GLU	C-N-CA	5.93	128.51	120.44
1	A	214	PHE	CB-CG-CD1	5.93	130.79	120.70
2	B	97	LEU	CA-C-N	5.93	125.87	119.76
2	B	97	LEU	C-N-CA	5.93	125.87	119.76
2	B	276	VAL	CA-C-N	5.91	128.68	120.29
2	B	276	VAL	C-N-CA	5.91	128.68	120.29
1	A	150	LEU	CA-C-O	5.91	126.60	120.40
2	B	194	LYS	CA-C-N	5.90	128.47	120.38
2	B	194	LYS	C-N-CA	5.90	128.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	589	GLU	CA-C-O	5.89	126.48	120.24
1	A	278	ASN	OD1-CG-ND2	5.89	128.49	122.60
2	B	576	GLU	CA-C-O	5.87	127.61	120.62
1	A	84	PRO	CA-C-O	-5.87	114.79	122.19
1	A	260	VAL	O-C-N	5.87	127.88	121.83
1	A	242	ILE	N-CA-CB	5.87	117.41	110.55
2	B	318	GLU	CA-C-N	5.87	130.98	122.36
2	B	318	GLU	C-N-CA	5.87	130.98	122.36
2	B	380	GLY	CA-C-N	5.87	128.07	120.44
2	B	380	GLY	C-N-CA	5.87	128.07	120.44
2	B	246	ASP	CA-C-N	5.86	128.16	120.60
2	B	246	ASP	C-N-CA	5.86	128.16	120.60
1	A	260	VAL	CA-C-N	5.85	128.11	120.28
1	A	260	VAL	C-N-CA	5.85	128.11	120.28
1	A	99	HIS	CE1-NE2-CD2	-5.84	103.16	109.00
2	B	45	ASN	N-CA-C	-5.84	106.13	113.20
2	B	497	SER	CB-CA-C	-5.84	101.67	110.90
2	B	86	ARG	N-CA-C	-5.83	99.15	109.06
2	B	429	SER	CA-C-N	5.82	128.00	120.44
2	B	429	SER	C-N-CA	5.82	128.00	120.44
1	A	222	TYR	CB-CA-C	-5.82	100.96	109.97
2	B	328	ARG	CG-CD-NE	-5.81	99.21	112.00
2	B	129	PRO	N-CA-CB	5.80	108.48	103.31
2	B	312	GLN	OE1-CD-NE2	5.80	128.40	122.60
2	B	365	ILE	N-CA-C	-5.80	100.00	108.11
1	A	209	PHE	N-CA-CB	5.79	118.73	110.16
2	B	273	ASP	N-CA-CB	5.79	119.64	110.84
1	A	336	HIS	CE1-NE2-CD2	-5.79	103.22	109.00
1	A	128	VAL	N-CA-CB	-5.78	104.42	110.72
2	B	202	LEU	CB-CA-C	-5.78	100.09	110.37
2	B	521	ILE	CB-CA-C	-5.76	104.36	112.14
1	A	283	TYR	N-CA-CB	5.75	120.21	110.49
2	B	236	TYR	N-CA-CB	5.75	119.79	110.77
2	B	581	ASP	CA-C-O	5.75	126.64	120.55
2	B	490	VAL	CA-C-N	5.74	128.45	120.29
2	B	490	VAL	C-N-CA	5.74	128.45	120.29
2	B	425	SER	N-CA-CB	5.74	118.67	110.06
1	A	269	LYS	CA-C-N	5.72	128.30	120.46
1	A	269	LYS	C-N-CA	5.72	128.30	120.46
2	B	340	ARG	CA-C-N	5.72	132.47	121.54
2	B	340	ARG	C-N-CA	5.72	132.47	121.54
2	B	381	LYS	CB-CA-C	-5.71	101.91	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	O-C-N	5.71	128.37	122.54
2	B	308	ASN	CA-C-N	5.71	127.93	120.28
2	B	308	ASN	C-N-CA	5.71	127.93	120.28
2	B	89	VAL	CA-C-O	-5.70	115.13	121.23
2	B	318	GLU	N-CA-C	-5.70	106.96	114.31
2	B	359	GLU	CB-CA-C	5.70	120.02	109.70
2	B	587	ARG	N-CA-CB	5.69	119.55	110.73
2	B	163	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	86	VAL	N-CA-CB	5.67	120.58	111.23
2	B	535	PRO	N-CA-C	5.66	120.11	111.11
2	B	529	ILE	N-CA-C	-5.66	99.40	107.77
1	A	6	GLU	CA-C-O	5.66	125.27	119.05
1	A	228	LYS	CA-C-O	5.65	127.62	121.06
1	A	229	VAL	CB-CA-C	-5.65	103.15	110.84
2	B	128	ILE	N-CA-CB	5.65	119.12	111.21
2	B	434	SER	CA-C-N	5.65	128.90	120.31
2	B	434	SER	C-N-CA	5.65	128.90	120.31
1	A	284	GLY	CA-C-O	-5.64	110.75	120.57
1	A	303	LEU	N-CA-CB	5.64	118.27	109.97
1	A	41	LEU	CD1-CG-CD2	5.64	123.21	110.80
1	A	274	ILE	CB-CA-C	5.64	121.40	112.26
2	B	503	LEU	CA-C-N	5.64	128.30	120.29
2	B	503	LEU	C-N-CA	5.64	128.30	120.29
1	A	25	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
1	A	133	ARG	N-CA-CB	5.64	120.01	110.49
2	B	487	TYR	N-CA-C	5.64	118.97	111.30
1	A	161	SER	N-CA-C	-5.63	104.03	112.54
1	A	198	ASN	CB-CA-C	-5.63	101.86	111.26
2	B	366	ARG	CA-C-N	5.62	130.41	122.09
2	B	366	ARG	C-N-CA	5.62	130.41	122.09
1	A	339	GLY	CA-C-N	5.61	128.26	120.29
1	A	339	GLY	C-N-CA	5.61	128.26	120.29
2	B	104	MET	CA-C-O	-5.61	115.06	121.40
2	B	130	ASN	N-CA-CB	5.60	118.87	110.53
1	A	24	TRP	CD2-CE2-CZ2	-5.59	116.81	122.40
2	B	382	THR	CA-C-O	-5.59	114.95	120.82
1	A	108	VAL	N-CA-C	-5.59	100.61	108.27
1	A	158	ILE	O-C-N	-5.59	116.24	122.66
2	B	213	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
2	B	249	GLN	CA-C-N	5.58	127.76	120.28
2	B	249	GLN	C-N-CA	5.58	127.76	120.28
1	A	210	VAL	CA-C-N	5.58	127.69	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	VAL	C-N-CA	5.58	127.69	120.44
2	B	162	ILE	O-C-N	-5.58	117.03	123.00
2	B	419	THR	N-CA-CB	5.57	118.41	110.44
2	B	511	ALA	N-CA-C	-5.57	100.24	108.99
1	A	316	GLU	O-C-N	5.57	128.02	122.12
2	B	121	LYS	CA-C-N	5.57	127.69	120.56
2	B	121	LYS	C-N-CA	5.57	127.69	120.56
1	A	256	GLN	CB-CG-CD	5.56	122.06	112.60
2	B	350	VAL	CB-CA-C	-5.55	102.19	111.29
1	A	212	GLU	CA-C-N	5.55	127.65	120.44
1	A	212	GLU	C-N-CA	5.55	127.65	120.44
1	A	170	ARG	N-CA-CB	5.54	118.64	110.33
2	B	468	ILE	N-CA-CB	5.54	117.03	110.55
2	B	409	PRO	CA-C-N	5.54	128.15	120.29
2	B	409	PRO	C-N-CA	5.54	128.15	120.29
2	B	487	TYR	CB-CG-CD2	-5.53	112.50	120.80
2	B	139	ASP	N-CA-C	5.53	117.30	111.28
1	A	42	ARG	N-CA-C	5.52	117.40	108.34
1	A	248	ARG	N-CA-C	-5.52	106.31	113.16
1	A	124	LEU	N-CA-CB	5.52	118.20	109.82
2	B	231	ARG	N-CA-CB	5.52	118.08	109.97
2	B	428	ASP	N-CA-C	-5.52	99.05	110.80
2	B	21	GLY	N-CA-C	-5.51	104.67	111.45
2	B	420	VAL	O-C-N	-5.51	116.51	121.91
1	A	336	HIS	ND1-CE1-NE2	5.51	113.91	108.40
2	B	324	PRO	N-CD-CG	5.50	111.45	103.20
1	A	245	VAL	N-CA-CB	5.50	118.02	110.54
1	A	59	ILE	N-CA-CB	5.50	118.91	111.21
2	B	167	LYS	CB-CA-C	5.49	116.40	110.08
2	B	210	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	345	LEU	CA-C-O	5.49	126.34	120.20
2	B	204	LEU	N-CA-C	-5.49	105.90	112.59
2	B	139	ASP	CB-CA-C	-5.48	101.69	110.79
2	B	141	VAL	CA-C-N	5.47	127.96	120.46
2	B	141	VAL	C-N-CA	5.47	127.96	120.46
1	A	158	ILE	CA-C-N	5.47	127.88	120.44
1	A	158	ILE	C-N-CA	5.47	127.88	120.44
2	B	127	LEU	N-CA-CB	5.46	119.78	110.71
2	B	278	ASP	CA-C-O	5.46	126.55	120.82
2	B	542	LEU	N-CA-C	-5.45	102.77	110.29
1	A	256	GLN	N-CA-C	-5.45	105.34	111.28
1	A	349	ALA	N-CA-CB	5.45	119.96	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	351	LEU	CB-CA-C	-5.44	101.38	110.19
2	B	100	VAL	CB-CA-C	-5.44	103.98	111.49
1	A	188	LYS	CA-C-N	5.43	127.56	120.28
1	A	188	LYS	C-N-CA	5.43	127.56	120.28
2	B	502	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
2	B	141	VAL	N-CA-CB	5.42	117.51	110.57
1	A	251	VAL	CA-C-N	5.42	127.80	120.65
1	A	251	VAL	C-N-CA	5.42	127.80	120.65
1	A	138	ILE	CA-CB-CG1	5.42	119.61	110.40
1	A	319	MET	CA-C-N	5.41	127.97	120.29
1	A	319	MET	C-N-CA	5.41	127.97	120.29
2	B	205	GLU	N-CA-C	5.41	119.50	113.01
2	B	94	LEU	CA-C-N	5.41	131.05	122.94
2	B	94	LEU	C-N-CA	5.41	131.05	122.94
2	B	163	ARG	N-CA-CB	5.41	123.36	111.25
2	B	445	LEU	N-CA-C	-5.39	105.92	112.88
2	B	430	SER	CA-C-N	5.39	127.50	120.28
2	B	430	SER	C-N-CA	5.39	127.50	120.28
1	A	213	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	75	PHE	CB-CA-C	-5.37	104.66	111.86
2	B	249	GLN	CB-CG-CD	5.37	121.73	112.60
2	B	330	THR	CA-C-O	-5.37	114.56	120.36
1	A	72	PHE	N-CA-C	-5.36	99.20	108.69
2	B	421	TYR	CA-C-N	5.36	127.40	120.44
2	B	421	TYR	C-N-CA	5.36	127.40	120.44
1	A	240	THR	CA-C-N	5.35	125.77	119.94
1	A	240	THR	C-N-CA	5.35	125.77	119.94
2	B	184	GLU	CA-C-N	5.35	127.76	120.54
2	B	184	GLU	C-N-CA	5.35	127.76	120.54
2	B	424	LEU	O-C-N	5.34	128.24	122.15
2	B	456	GLU	CA-C-N	5.34	131.52	122.65
2	B	456	GLU	C-N-CA	5.34	131.52	122.65
2	B	135	ASN	CA-C-O	5.34	127.38	121.56
2	B	563	ARG	CA-C-N	5.34	130.44	122.86
2	B	563	ARG	C-N-CA	5.34	130.44	122.86
1	A	307	LEU	CD1-CG-CD2	5.33	122.53	110.80
1	A	288	VAL	CB-CA-C	-5.33	104.87	112.22
1	A	320	ASP	CA-C-N	5.33	127.85	120.29
1	A	320	ASP	C-N-CA	5.33	127.85	120.29
1	A	168	GLY	O-C-N	5.32	129.62	122.70
1	A	322	VAL	CA-C-O	-5.32	115.21	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	578	SER	N-CA-C	-5.31	101.21	108.38
2	B	16	ASN	CA-C-N	5.30	125.62	119.47
2	B	16	ASN	C-N-CA	5.30	125.62	119.47
2	B	268	LEU	N-CA-C	-5.29	99.82	108.76
2	B	151	GLN	OE1-CD-NE2	5.29	127.89	122.60
2	B	299	LYS	CA-C-O	-5.28	114.97	120.88
1	A	21	ASP	CB-CA-C	-5.28	100.53	110.67
2	B	421	TYR	N-CA-C	5.28	117.78	111.71
1	A	102	ALA	CA-C-O	-5.27	114.67	120.36
1	A	193	VAL	CB-CA-C	-5.27	105.03	112.14
2	B	302	GLY	O-C-N	5.26	127.52	122.99
1	A	42	ARG	CB-CA-C	-5.26	101.72	110.14
2	B	566	PRO	N-CA-C	-5.24	101.67	112.47
1	A	183	PHE	CA-C-O	-5.24	115.00	120.55
1	A	94	PRO	CA-C-N	5.23	129.16	120.94
1	A	94	PRO	C-N-CA	5.23	129.16	120.94
2	B	376	PRO	CB-CA-C	-5.23	103.15	110.63
1	A	306	LEU	N-CA-C	5.23	117.72	111.71
2	B	287	VAL	CB-CA-C	-5.22	103.36	110.77
2	B	470	ALA	N-CA-C	5.22	116.66	111.07
2	B	91	ALA	N-CA-CB	5.21	119.90	111.21
1	A	223	PRO	N-CA-CB	5.20	108.18	103.34
2	B	222	ARG	CA-C-N	5.20	128.83	120.30
2	B	222	ARG	C-N-CA	5.20	128.83	120.30
1	A	196	ARG	CB-CA-C	-5.19	102.69	110.90
2	B	419	THR	CA-C-N	5.19	127.09	120.56
2	B	419	THR	C-N-CA	5.19	127.09	120.56
2	B	178	VAL	N-CA-C	-5.18	100.06	107.78
1	A	150	LEU	CB-CA-C	-5.18	102.40	110.74
1	A	32	PRO	CA-C-O	-5.18	115.51	121.36
2	B	132	CYS	CB-CA-C	-5.18	104.54	111.89
2	B	299	LYS	CA-CB-CG	5.17	124.45	114.10
2	B	103	GLY	O-C-N	5.17	128.73	122.32
2	B	353	TYR	CB-CA-C	-5.17	102.06	110.85
2	B	472	LEU	N-CA-C	5.17	119.21	113.01
2	B	300	PRO	CA-C-O	-5.16	115.12	121.31
1	A	209	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	186	VAL	CA-C-N	5.15	127.19	120.28
1	A	186	VAL	C-N-CA	5.15	127.19	120.28
1	A	314	LYS	O-C-N	5.15	127.45	122.09
1	A	33	GLY	O-C-N	5.14	127.79	122.54
2	B	518	VAL	CA-C-N	5.14	128.13	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	518	VAL	C-N-CA	5.14	128.13	120.31
2	B	221	GLN	OE1-CD-NE2	5.14	127.74	122.60
2	B	125	GLY	N-CA-C	-5.12	108.55	115.21
2	B	391	VAL	O-C-N	5.12	126.82	122.16
2	B	495	ALA	N-CA-C	5.12	116.86	111.28
1	A	340	GLU	CB-CG-CD	-5.12	103.89	112.60
1	A	129	ALA	O-C-N	5.12	127.99	122.15
2	B	567	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	143	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	285	LEU	CA-C-N	5.11	127.09	120.44
1	A	285	LEU	C-N-CA	5.11	127.09	120.44
1	A	229	VAL	N-CA-CB	5.11	117.12	110.99
2	B	199	VAL	CA-C-N	5.11	129.24	120.71
2	B	199	VAL	C-N-CA	5.11	129.24	120.71
2	B	450	LEU	N-CA-CB	5.11	117.93	110.88
2	B	130	ASN	CA-C-N	5.10	129.37	122.07
2	B	130	ASN	C-N-CA	5.10	129.37	122.07
1	A	319	MET	CG-SD-CE	-5.10	89.68	100.90
1	A	314	LYS	CA-C-O	-5.09	115.46	120.90
2	B	439	THR	CA-C-O	5.09	125.79	119.79
1	A	344	ALA	CA-C-N	5.08	127.80	120.38
1	A	344	ALA	C-N-CA	5.08	127.80	120.38
1	A	348	LEU	N-CA-CB	5.08	119.67	110.83
2	B	244	TYR	N-CA-C	5.08	121.61	110.80
1	A	28	HIS	CB-CG-CD2	-5.08	124.60	131.20
2	B	194	LYS	N-CA-CB	-5.07	102.81	110.92
1	A	152	ARG	N-CA-C	-5.07	102.69	110.14
1	A	355	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	A	97	LYS	CA-C-N	5.06	132.63	123.27
1	A	97	LYS	C-N-CA	5.06	132.63	123.27
1	A	33	GLY	CA-C-O	-5.06	114.05	119.82
2	B	296	ILE	CB-CA-C	-5.06	102.94	110.33
1	A	352	LEU	CB-CA-C	-5.06	101.46	109.80
2	B	519	LEU	CB-CA-C	-5.05	100.97	110.67
2	B	390	GLY	O-C-N	5.05	128.21	122.55
2	B	454	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	146	ALA	CA-C-N	5.05	130.43	122.36
1	A	146	ALA	C-N-CA	5.05	130.43	122.36
2	B	255	ARG	N-CA-CB	5.03	117.52	110.12
2	B	139	ASP	CA-C-N	5.03	127.96	120.31
2	B	139	ASP	C-N-CA	5.03	127.96	120.31
1	A	186	VAL	CB-CA-C	-5.03	105.54	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	521	ILE	N-CA-CB	5.02	117.37	110.54
1	A	34	ASP	N-CA-C	-5.02	101.74	109.52
2	B	203	GLU	CA-C-O	-5.02	115.92	122.14
1	A	116	TRP	N-CA-C	5.02	117.17	110.35
1	A	269	LYS	CA-C-O	5.02	125.87	120.55
1	A	306	LEU	CA-C-N	5.02	127.00	120.28
1	A	306	LEU	C-N-CA	5.02	127.00	120.28
1	A	9	LYS	CA-C-N	5.01	129.31	122.34
1	A	9	LYS	C-N-CA	5.01	129.31	122.34
1	A	18	GLU	CB-CA-C	-5.01	100.45	110.42
1	A	125	LYS	N-CA-CB	5.01	119.24	110.42
2	B	396	GLU	CB-CA-C	-5.01	98.44	109.56
1	A	164	HIS	ND1-CE1-NE2	5.00	113.40	108.40
2	B	225	ILE	N-CA-C	-5.00	105.11	110.36

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	147	ASP	Peptide
1	A	154	TYR	Sidechain
1	A	155	GLY	Peptide
1	A	239	ARG	Sidechain
1	A	284	GLY	Peptide
1	A	31	ASP	Peptide
1	A	310	GLU	Peptide
1	A	354	PHE	Sidechain
1	A	355	ARG	Sidechain
1	A	73	HIS	Sidechain
2	B	153	TYR	Sidechain
2	B	156	ARG	Sidechain
2	B	236	TYR	Sidechain
2	B	244	TYR	Sidechain
2	B	248	ARG	Sidechain
2	B	250	ARG	Sidechain
2	B	280	LEU	Peptide
2	B	314	TYR	Sidechain
2	B	340	ARG	Sidechain
2	B	411	TYR	Sidechain
2	B	421	TYR	Sidechain
2	B	451	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	465	ARG	Sidechain
2	B	474	ARG	Sidechain
2	B	479	TYR	Sidechain
2	B	498	ARG	Sidechain
2	B	537	ARG	Sidechain
2	B	572	ARG	Sidechain
2	B	95	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2947	48	0
2	B	4729	0	4777	97	0
3	B	54	0	24	27	0
4	B	16	0	0	1	0
All	All	7660	0	7748	138	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 9.

All (138) 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)
1:A:42:ARG:HB2	1:A:99:HIS:NE2	1.21	1.46
2:B:355:SER:OG	3:B:601:ADP:N3	1.65	1.26
1:A:40:THR:OG1	1:A:101:ILE:HD11	1.38	1.23
2:B:355:SER:OG	3:B:601:ADP:C2	1.92	1.21
1:A:42:ARG:HB2	1:A:99:HIS:CE1	1.76	1.20
1:A:42:ARG:HD2	1:A:99:HIS:CG	1.79	1.17
1:A:40:THR:OG1	1:A:101:ILE:CD1	1.92	1.16
2:B:113:GLY:C	3:B:602:ADP:H5'2	1.72	1.15
1:A:42:ARG:HD2	1:A:99:HIS:ND1	1.60	1.15
1:A:42:ARG:CB	1:A:99:HIS:NE2	2.11	1.14
2:B:113:GLY:H	3:B:602:ADP:PB	1.76	1.09
1:A:42:ARG:HD2	1:A:99:HIS:CE1	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG1	1:A:101:ILE:HD11	0.95	1.02
2:B:113:GLY:N	3:B:602:ADP:O1B	1.95	0.99
1:A:346:GLY:HA3	2:B:34:MET:CE	1.95	0.97
2:B:22:HIS:H	2:B:27:ARG:NH1	1.67	0.92
2:B:6:ARG:NH2	2:B:74:ASN:HD21	1.69	0.90
1:A:42:ARG:HB2	1:A:99:HIS:HE2	1.33	0.89
1:A:42:ARG:CD	1:A:99:HIS:CE1	2.55	0.89
2:B:115:GLY:HA2	3:B:602:ADP:O2A	1.71	0.89
1:A:42:ARG:HD2	1:A:99:HIS:CD2	2.10	0.87
1:A:42:ARG:HB2	1:A:99:HIS:CD2	2.10	0.85
1:A:346:GLY:HA3	2:B:34:MET:HE1	1.59	0.85
1:A:40:THR:OG1	1:A:101:ILE:HD12	1.76	0.83
2:B:4:LYS:HG3	2:B:75:LEU:O	1.78	0.83
2:B:113:GLY:N	3:B:602:ADP:PB	2.50	0.82
1:A:40:THR:HG21	1:A:101:ILE:HG13	1.66	0.77
2:B:113:GLY:CA	3:B:602:ADP:H5'2	2.15	0.77
2:B:2:VAL:O	2:B:3:ARG:HB2	1.84	0.75
1:A:42:ARG:CB	1:A:99:HIS:CD2	2.69	0.74
1:A:42:ARG:CD	1:A:99:HIS:ND1	2.47	0.74
2:B:25:CYS:HB3	2:B:39:ILE:HD13	1.68	0.73
2:B:113:GLY:O	3:B:602:ADP:H5'2	1.88	0.73
2:B:6:ARG:CZ	2:B:74:ASN:HD21	2.01	0.72
1:A:42:ARG:CB	1:A:99:HIS:CE1	2.67	0.72
1:A:43:LYS:HB3	1:A:58:VAL:HA	1.73	0.70
1:A:346:GLY:CA	2:B:34:MET:HE1	2.22	0.69
1:A:137:MET:H	1:A:138:ILE:HD12	1.55	0.69
2:B:22:HIS:H	2:B:27:ARG:HH12	1.40	0.69
2:B:7:ILE:HD13	2:B:95:TYR:OH	1.94	0.68
1:A:61:VAL:HG12	1:A:62:PHE:H	1.59	0.66
2:B:30:PRO:HD2	4:B:603:SF4:S2	2.36	0.66
2:B:113:GLY:C	3:B:602:ADP:C5'	2.62	0.64
2:B:113:GLY:O	3:B:602:ADP:C5'	2.46	0.63
1:A:345:LEU:O	2:B:30:PRO:HB2	1.99	0.63
2:B:67:PHE:O	2:B:68:ASN:HB2	1.99	0.62
2:B:113:GLY:HA2	3:B:602:ADP:H5'2	1.80	0.62
1:A:39:LYS:HA	1:A:62:PHE:HA	1.80	0.62
2:B:54:SER:O	2:B:55:CYS:C	2.44	0.61
2:B:378:GLY:N	3:B:601:ADP:O2B	2.34	0.60
2:B:6:ARG:HD2	2:B:55:CYS:O	2.00	0.60
2:B:378:GLY:H	3:B:601:ADP:PB	2.24	0.59
1:A:42:ARG:NE	1:A:99:HIS:CE1	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LYS:HE2	2:B:74:ASN:HB3	1.85	0.58
2:B:19:LYS:HD3	2:B:67:PHE:HZ	1.66	0.58
2:B:9:VAL:HG21	2:B:293:VAL:O	2.03	0.57
2:B:10:ILE:HG23	2:B:69:ALA:O	2.05	0.57
2:B:22:HIS:H	2:B:27:ARG:HH11	1.50	0.57
2:B:378:GLY:HA2	3:B:601:ADP:PB	2.45	0.57
2:B:115:GLY:N	3:B:602:ADP:H5'1	2.18	0.56
2:B:16:ASN:C	2:B:16:ASN:HD22	2.13	0.56
2:B:115:GLY:H	3:B:602:ADP:C5'	2.19	0.56
2:B:355:SER:OG	3:B:601:ADP:H2	1.78	0.55
2:B:40:ILE:HD12	2:B:51:GLN:OE1	2.06	0.55
1:A:43:LYS:HG2	1:A:58:VAL:HG22	1.88	0.54
2:B:6:ARG:NH2	2:B:74:ASN:ND2	2.49	0.54
2:B:6:ARG:CZ	2:B:74:ASN:ND2	2.70	0.54
2:B:115:GLY:CA	3:B:602:ADP:O2A	2.52	0.53
2:B:28:VAL:CG1	2:B:60:ILE:HG22	2.40	0.52
2:B:38:ALA:HA	2:B:54:SER:HB2	1.90	0.52
1:A:56:VAL:HG12	1:A:57:GLU:H	1.75	0.52
2:B:26:GLU:CG	2:B:32:ASN:HD22	2.23	0.51
1:A:42:ARG:CD	1:A:99:HIS:CG	2.73	0.50
2:B:4:LYS:HA	2:B:75:LEU:O	2.13	0.48
2:B:4:LYS:CG	2:B:75:LEU:O	2.57	0.48
2:B:453:ARG:HH21	2:B:457:ASP:HB3	1.77	0.48
1:A:346:GLY:HA3	2:B:34:MET:SD	2.53	0.48
2:B:58:CYS:SG	2:B:60:ILE:HG13	2.53	0.48
2:B:9:VAL:HG11	2:B:293:VAL:HA	1.95	0.48
2:B:382:THR:OG1	3:B:601:ADP:O1B	2.29	0.48
1:A:20:LEU:HD13	1:A:77:ASN:HD22	1.78	0.48
1:A:42:ARG:CD	1:A:99:HIS:CD2	2.91	0.48
1:A:285:LEU:HD12	1:A:286:LYS:N	2.29	0.48
2:B:12:TYR:HE1	2:B:90:ASN:O	1.96	0.47
2:B:344:VAL:HG21	2:B:401:TRP:CE3	2.49	0.47
2:B:54:SER:O	2:B:55:CYS:O	2.33	0.47
2:B:423:LEU:HD22	2:B:455:VAL:HG21	1.97	0.47
1:A:43:LYS:H	1:A:43:LYS:HG3	1.41	0.47
2:B:39:ILE:HG12	2:B:50:ILE:HG12	1.97	0.47
2:B:64:LYS:O	2:B:65:CYS:C	2.57	0.46
2:B:558:VAL:O	2:B:560:ILE:HG12	2.15	0.46
2:B:26:GLU:HG3	2:B:32:ASN:HD22	1.80	0.46
1:A:346:GLY:CA	2:B:34:MET:CE	2.80	0.46
2:B:12:TYR:C	2:B:14:LYS:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:CYS:HB3	2:B:66:PRO:HG3	1.97	0.46
1:A:346:GLY:C	2:B:34:MET:SD	2.99	0.46
2:B:115:GLY:H	3:B:602:ADP:H5'1	1.79	0.46
2:B:113:GLY:O	3:B:602:ADP:C4'	2.63	0.46
2:B:378:GLY:HA2	3:B:601:ADP:O3A	2.16	0.46
1:A:76:ALA:HB1	1:A:78:GLN:HE21	1.80	0.46
2:B:7:ILE:CD1	2:B:95:TYR:OH	2.64	0.45
1:A:41:LEU:HD21	1:A:58:VAL:HG13	1.99	0.45
2:B:9:VAL:HG22	2:B:91:ALA:O	2.16	0.45
2:B:116:LYS:HB2	3:B:602:ADP:O3B	2.16	0.45
2:B:419:THR:HA	2:B:454:ASN:HA	1.98	0.45
1:A:135:ARG:HH21	1:A:255:TYR:HB3	1.82	0.44
1:A:133:ARG:HE	1:A:197:GLU:HG3	1.81	0.44
2:B:12:TYR:C	2:B:14:LYS:N	2.74	0.44
2:B:12:TYR:CE1	2:B:90:ASN:O	2.71	0.43
2:B:342:THR:HG23	2:B:364:GLU:HG3	2.01	0.43
2:B:378:GLY:CA	3:B:601:ADP:O2B	2.67	0.43
1:A:7:LYS:HG3	1:A:9:LYS:H	1.85	0.42
2:B:11:ASP:CG	2:B:14:LYS:HE2	2.43	0.42
2:B:561:THR:OG1	2:B:581:ASP:HA	2.20	0.42
2:B:28:VAL:HG12	2:B:60:ILE:HG22	2.01	0.42
2:B:65:CYS:HA	2:B:66:PRO:HD2	1.83	0.42
2:B:218:GLY:CA	2:B:249:GLN:HE22	2.32	0.42
2:B:11:ASP:OD1	2:B:14:LYS:HE2	2.19	0.42
2:B:344:VAL:HG21	2:B:401:TRP:CD2	2.55	0.42
2:B:10:ILE:CD1	2:B:90:ASN:OD1	2.68	0.42
1:A:47:ARG:CG	1:A:48:ALA:H	2.33	0.41
1:A:131:SER:HA	1:A:152:ARG:HG2	2.02	0.41
2:B:17:PRO:HB3	2:B:23:PHE:CE1	2.54	0.41
2:B:218:GLY:HA3	2:B:249:GLN:HE22	1.86	0.41
2:B:29:CYS:HB2	2:B:39:ILE:HD12	2.02	0.41
2:B:16:ASN:C	2:B:16:ASN:ND2	2.78	0.41
2:B:28:VAL:HG11	2:B:64:LYS:HG2	2.01	0.41
2:B:378:GLY:CA	3:B:601:ADP:PB	3.08	0.41
2:B:6:ARG:NH2	2:B:56:THR:O	2.54	0.41
2:B:1:MET:O	2:B:2:VAL:HG13	2.20	0.41
2:B:113:GLY:O	3:B:602:ADP:H4'	2.20	0.41
1:A:42:ARG:CB	1:A:99:HIS:HE2	2.07	0.41
1:A:286:LYS:O	1:A:290:GLU:HB3	2.21	0.41
1:A:50:SER:C	1:A:51:LEU:HD22	2.46	0.41
2:B:10:ILE:HA	2:B:69:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:THR:O	2:B:307:ILE:HG13	2.21	0.40
2:B:57:GLY:HA2	2:B:72:ILE:HG21	2.03	0.40
1:A:42:ARG:HH11	1:A:42:ARG:HD3	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	355/357 (99%)	293 (82%)	36 (10%)	26 (7%)	1	10
2	B	591/593 (100%)	524 (89%)	51 (9%)	16 (3%)	4	25
All	All	946/950 (100%)	817 (86%)	87 (9%)	42 (4%)	3	17

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	55	LYS
1	A	60	PRO
1	A	61	VAL
1	A	63	LEU
1	A	131	SER
1	A	137	MET
1	A	148	MET
1	A	176	GLU
1	A	232	GLU
1	A	235	SER
1	A	285	LEU
2	B	3	ARG
2	B	55	CYS
2	B	68	ASN

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Mol	Chain	Res	Type
1	A	45	ALA
1	A	76	ALA
1	A	86	VAL
1	A	99	HIS
1	A	226	ALA
2	B	134	ASP
1	A	49	ASP
1	A	62	PHE
1	A	135	ARG
1	A	169	LYS
1	A	172	ASN
2	B	44	GLU
2	B	428	ASP
1	A	115	ARG
1	A	133	ARG
2	B	25	CYS
2	B	96	ARG
2	B	331	LYS
1	A	134	ALA
2	B	78	GLN
2	B	516	HIS
1	A	136	VAL
2	B	52	GLU
2	B	172	ASP
2	B	244	TYR
2	B	332	LEU
2	B	566	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/305 (100%)	286 (94%)	19 (6%)	16	38
2	B	512/512 (100%)	500 (98%)	12 (2%)	44	64
All	All	817/817 (100%)	786 (96%)	31 (4%)	30	50

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	THR
1	A	42	ARG
1	A	43	LYS
1	A	49	ASP
1	A	51	LEU
1	A	52	ARG
1	A	55	LYS
1	A	56	VAL
1	A	62	PHE
1	A	63	LEU
1	A	85	ILE
1	A	93	VAL
1	A	138	ILE
1	A	158	ILE
1	A	236	VAL
1	A	283	TYR
1	A	290	GLU
1	A	331	VAL
2	B	2	VAL
2	B	6	ARG
2	B	47	LYS
2	B	77	GLU
2	B	89	VAL
2	B	117	THR
2	B	246	ASP
2	B	287	VAL
2	B	403	LEU
2	B	447	ILE
2	B	458	LEU
2	B	528	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	28	HIS
1	A	73	HIS
1	A	77	ASN
1	A	78	GLN
1	A	164	HIS

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Mol	Chain	Res	Type
1	A	277	ASN
2	B	16	ASN
2	B	74	ASN
2	B	85	HIS
2	B	135	ASN
2	B	249	GLN
2	B	305	ASN
2	B	507	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
4	SF4	B	604	2	0,12,12	-	-	-		
3	ADP	B	601	-	28,29,29	1.01	3 (10%)	43,45,45	0.98	2 (4%)
4	SF4	B	603	2	0,12,12	-	-	-		
3	ADP	B	602	-	28,29,29	1.27	3 (10%)	43,45,45	1.02	3 (6%)

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
4	SF4	B	604	2	-	-	0/6/5/5
3	ADP	B	601	-	-	4/16/32/32	0/3/3/3
4	SF4	B	603	2	-	-	0/6/5/5
3	ADP	B	602	-	-	5/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	PB-O1B	4.31	1.63	1.50
3	B	602	ADP	C4-N3	2.95	1.39	1.34
3	B	601	ADP	PB-O3B	2.72	1.64	1.54
3	B	601	ADP	C4-N3	2.49	1.39	1.34
3	B	602	ADP	PB-O2B	-2.08	1.47	1.54
3	B	601	ADP	PB-O2B	-2.02	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ADP	O3B-PB-O2B	2.87	118.55	107.80
3	B	601	ADP	O2B-PB-O3A	2.82	114.11	104.64
3	B	602	ADP	C3'-C2'-C1'	2.41	106.03	101.46
3	B	602	ADP	O2B-PB-O3A	2.36	112.56	104.64
3	B	601	ADP	O4'-C1'-C2'	-2.12	102.07	106.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

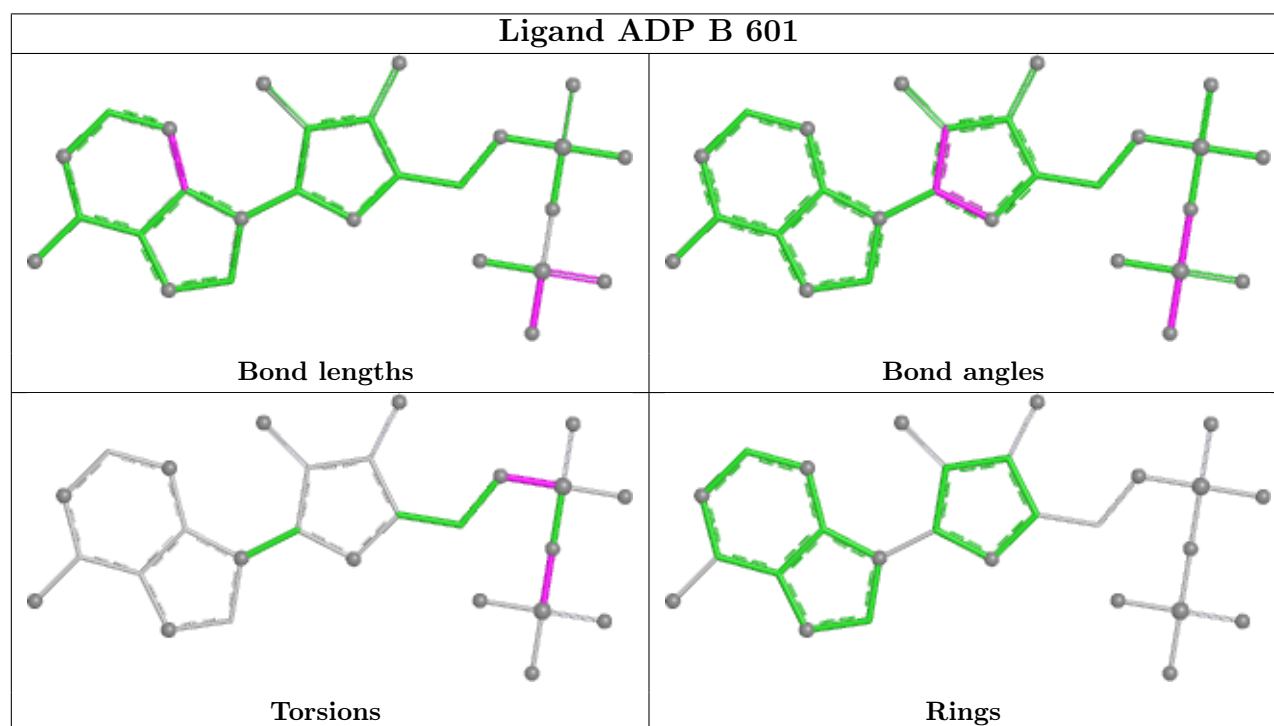
Mol	Chain	Res	Type	Atoms
3	B	601	ADP	C5'-O5'-PA-O1A
3	B	601	ADP	C5'-O5'-PA-O3A
3	B	602	ADP	PA-O3A-PB-O3B
3	B	602	ADP	C5'-O5'-PA-O2A
3	B	602	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	C5'-O5'-PA-O3A
3	B	601	ADP	PA-O3A-PB-O2B
3	B	601	ADP	PA-O3A-PB-O3B
3	B	602	ADP	PA-O3A-PB-O2B

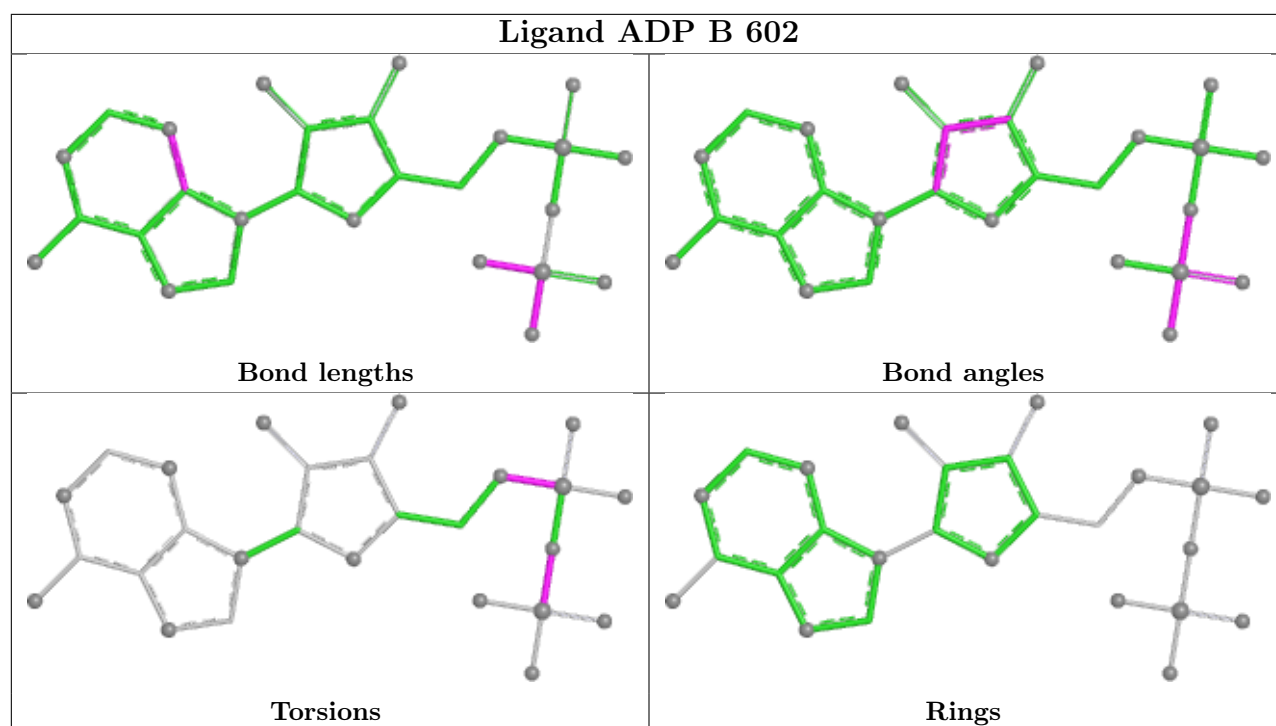
There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	10	0
4	B	603	SF4	1	0
3	B	602	ADP	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

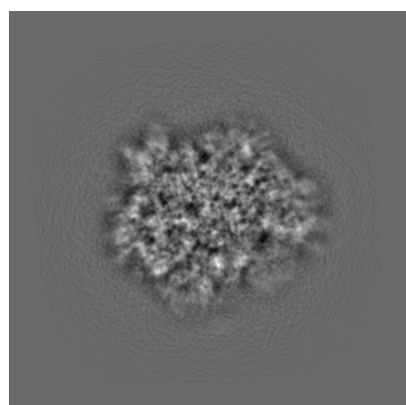
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2009. These allow visual inspection of the internal detail of the map and identification of artifacts.

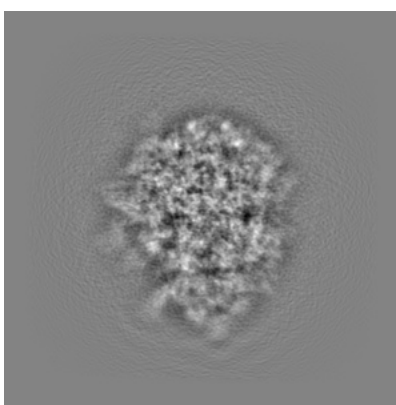
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

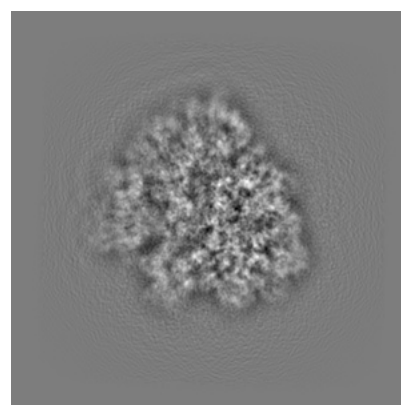
6.1.1 Primary map



X



Y

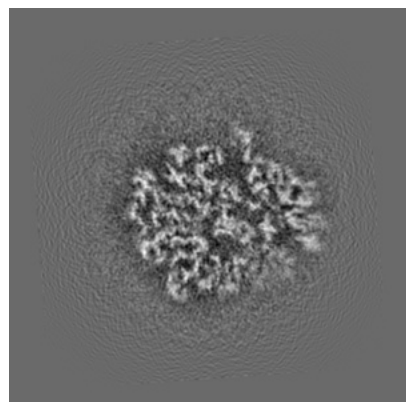


Z

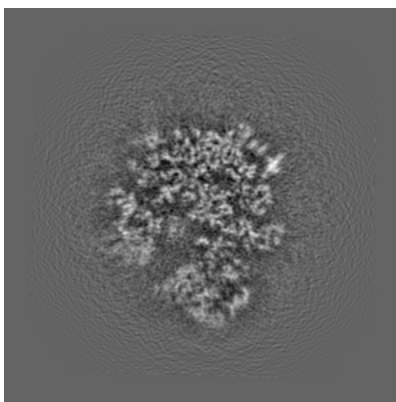
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

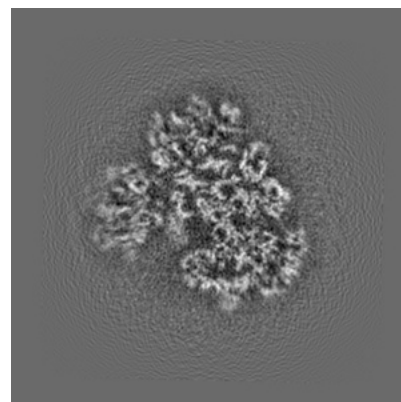
6.2.1 Primary map



X Index: 184



Y Index: 184

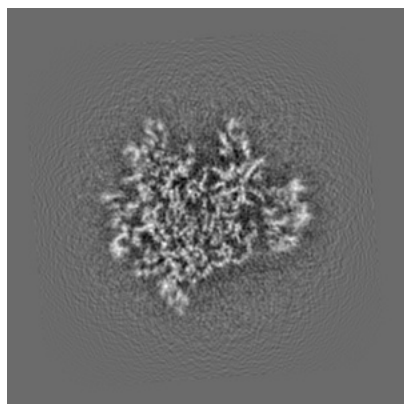


Z Index: 184

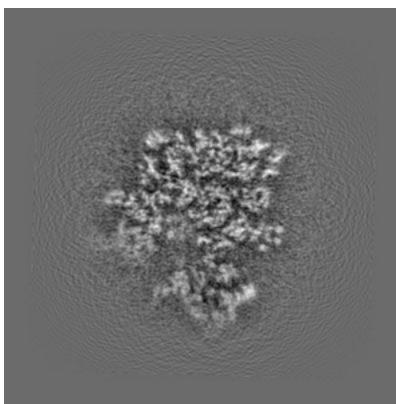
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

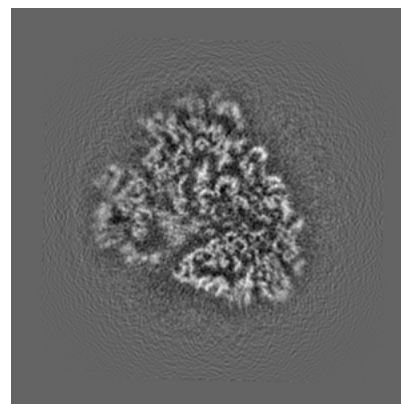
6.3.1 Primary map



X Index: 207



Y Index: 187

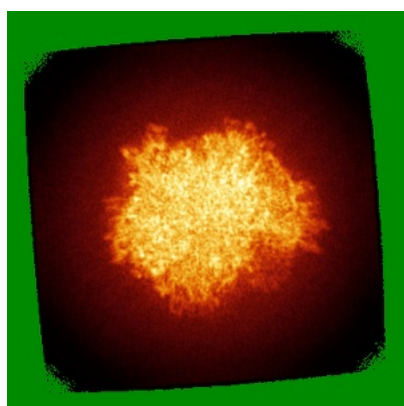


Z Index: 178

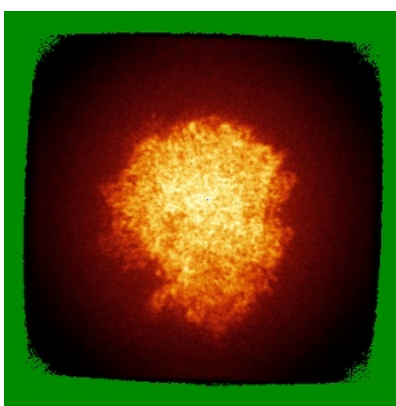
The images above show the largest variance slices of the map in three orthogonal directions.

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

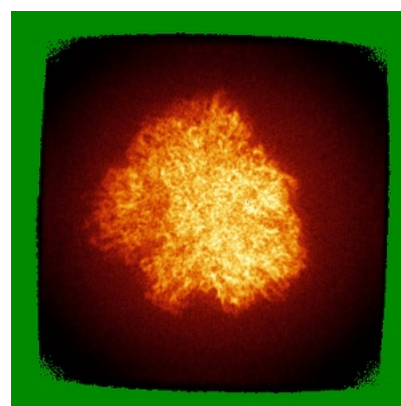
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

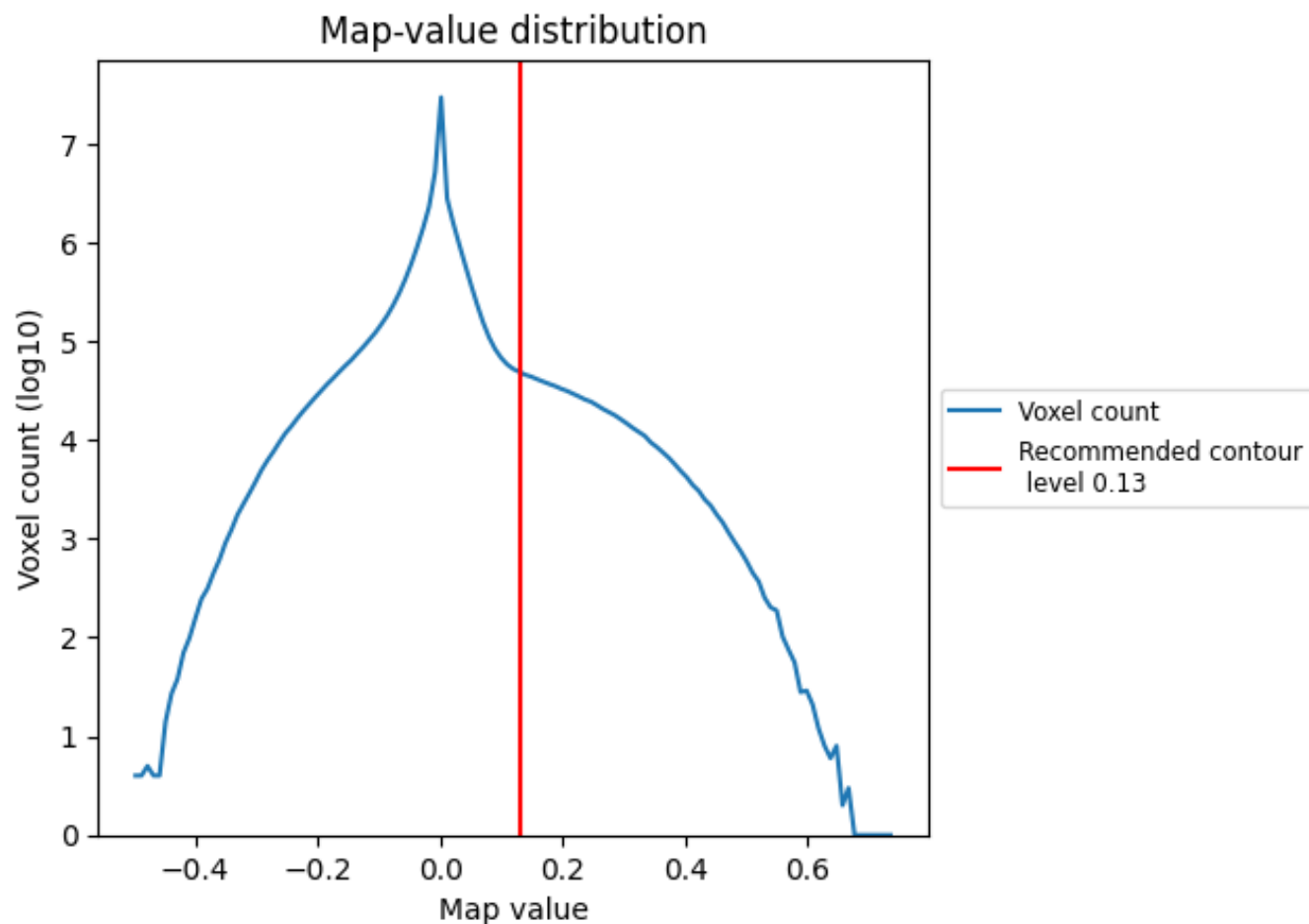
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

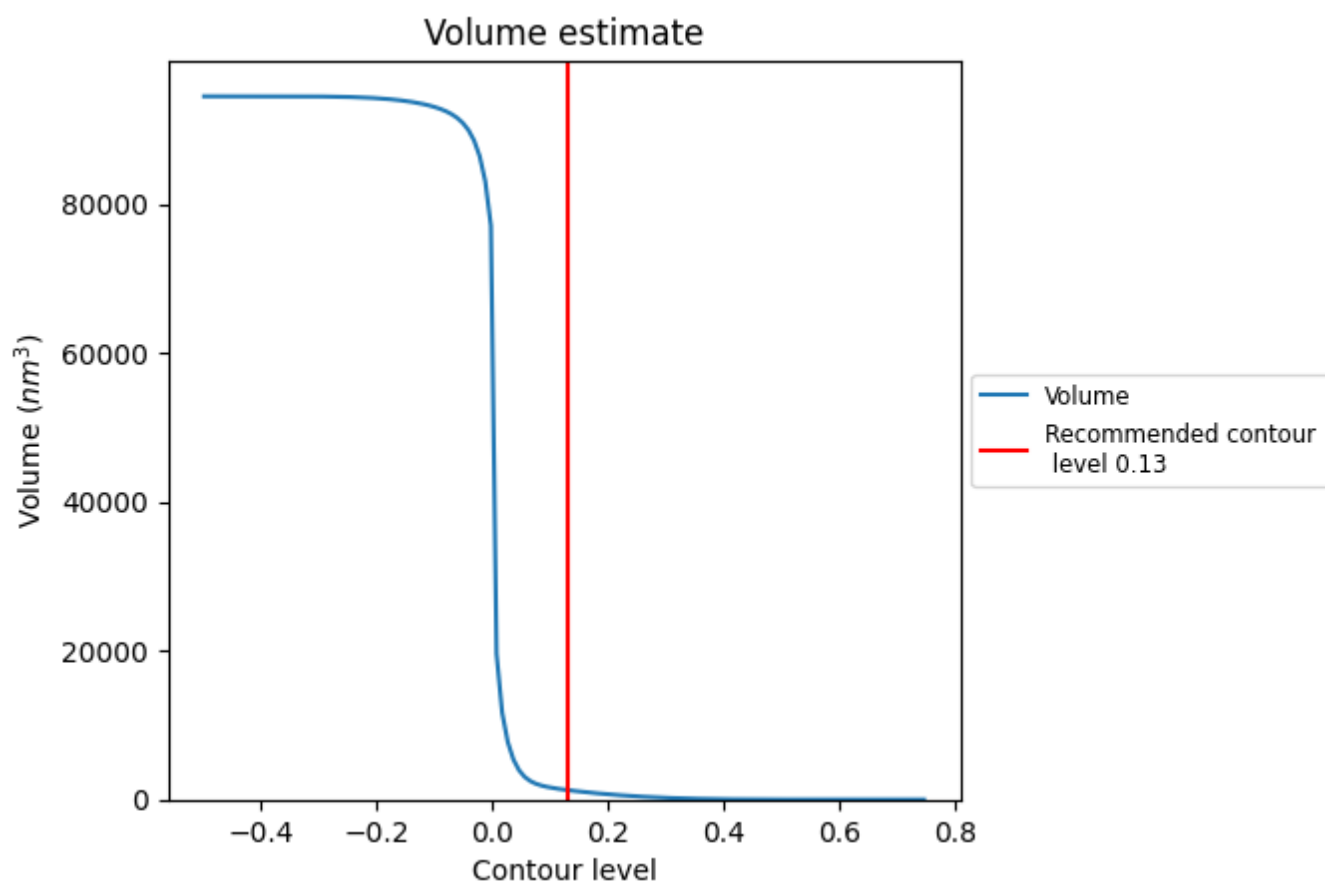
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

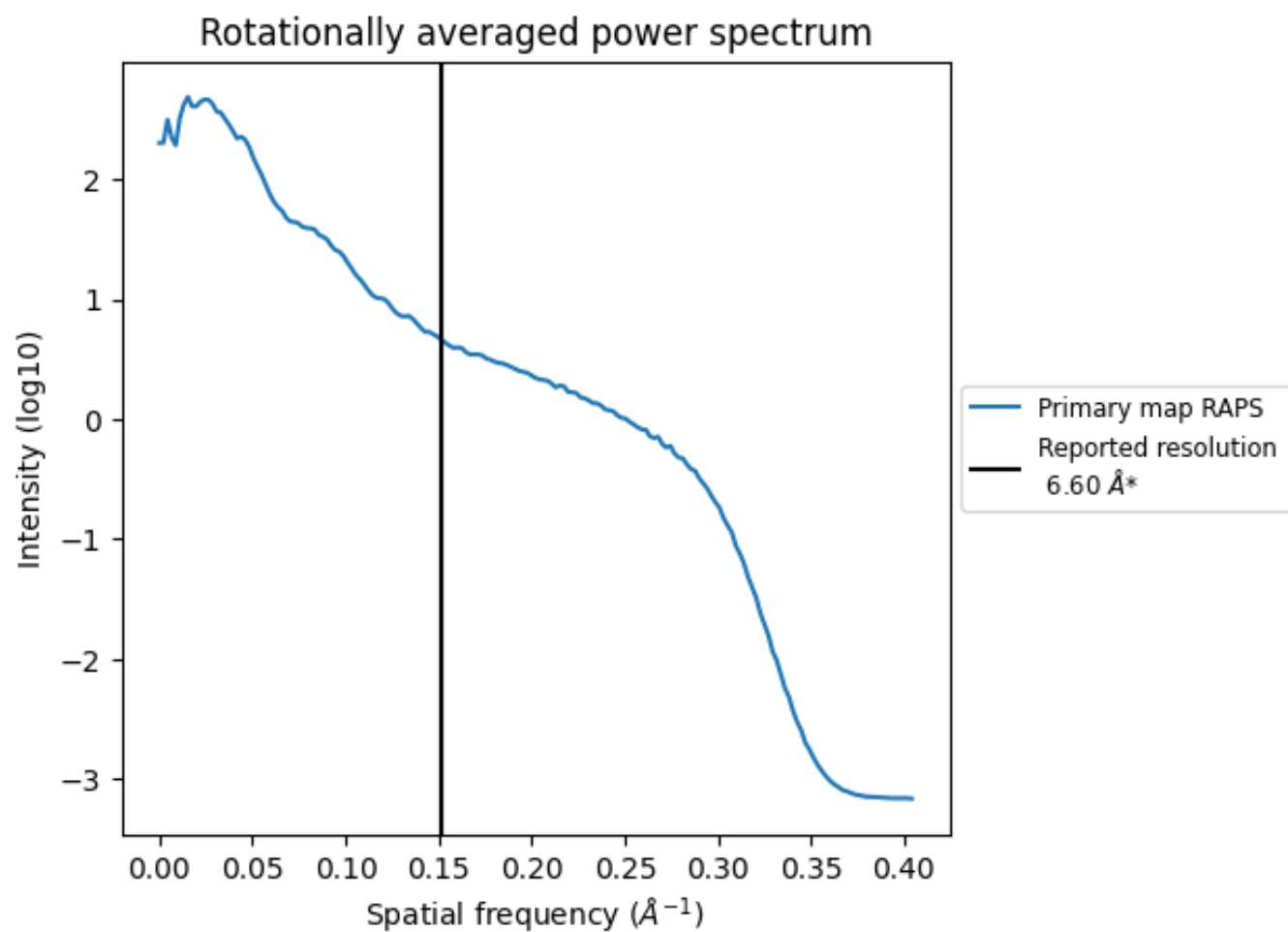
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1275 nm³; this corresponds to an approximate mass of 1152 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 0.152 Å⁻¹

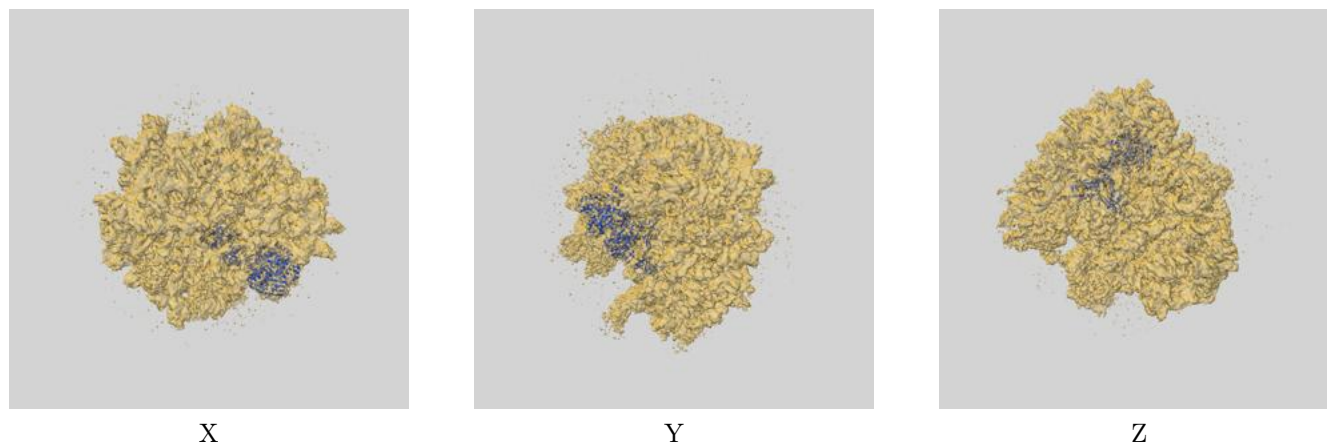
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

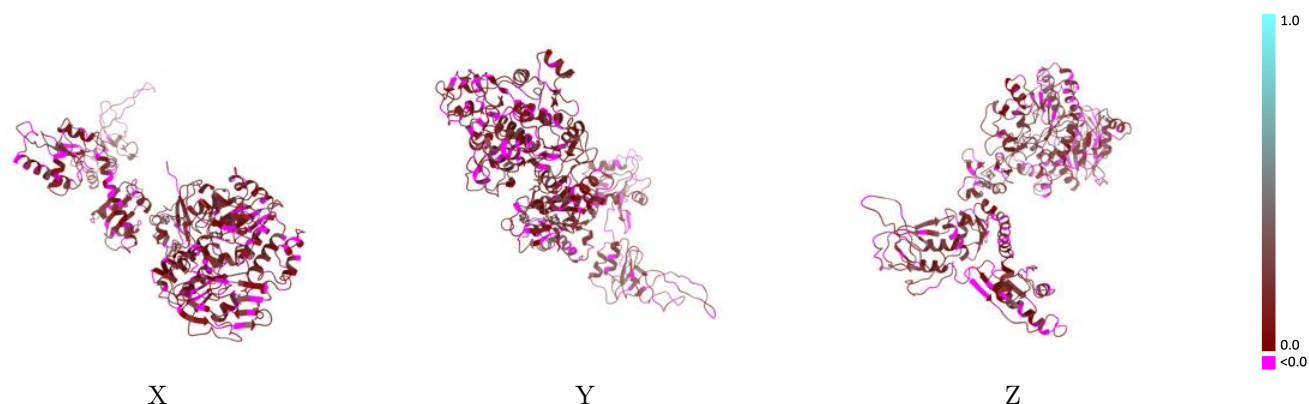
This section contains information regarding the fit between EMDB map EMD-2009 and PDB model 3J15. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



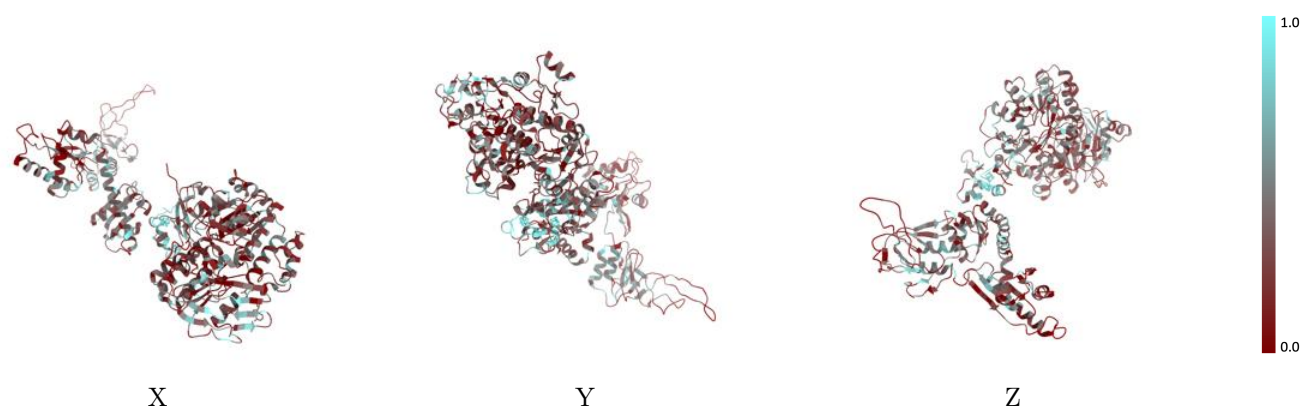
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



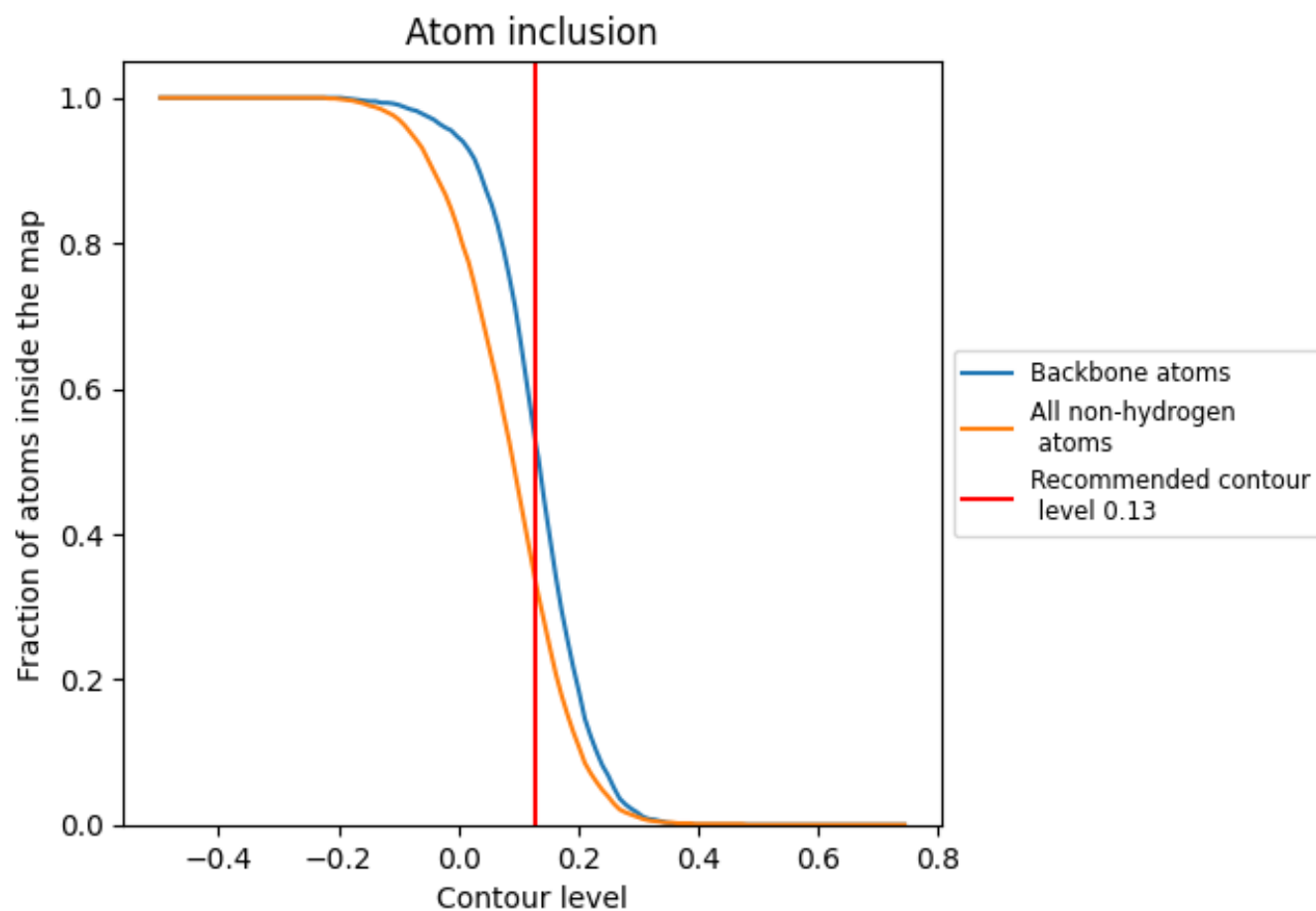
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 33% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3310	0.1070
A	0.3170	0.1090
B	0.3400	0.1050

