



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:08 AM UTC

PDB ID : 6Q81 / pdb_00006q81
EMDB ID : EMD-4391
Title : Structure of P-glycoprotein(ABCB1) in the post-hydrolytic state
Authors : Ford, R.C.; Thonghin, N.; Collins, R.F.; Barbieri, A.; Shafi, T.; Siebert, A.
Deposited on : 2018-12-13
Resolution : 7.90 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

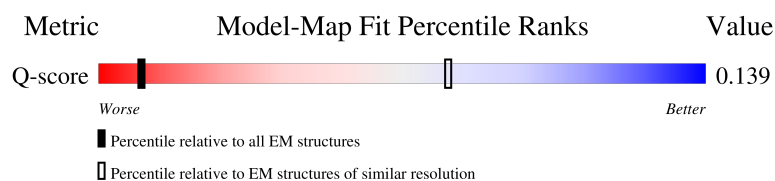
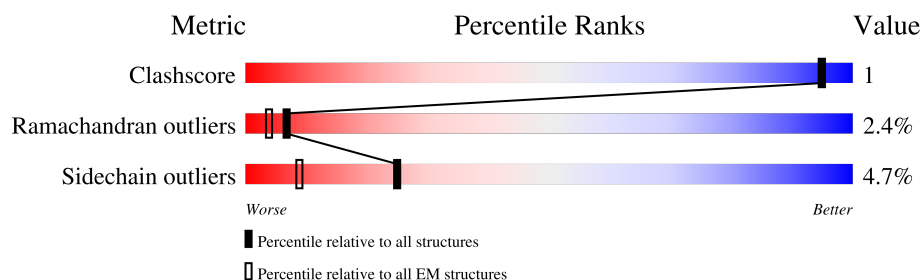
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 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	366 (7.40 - 8.40)

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	1276	

2 Entry composition [i](#)

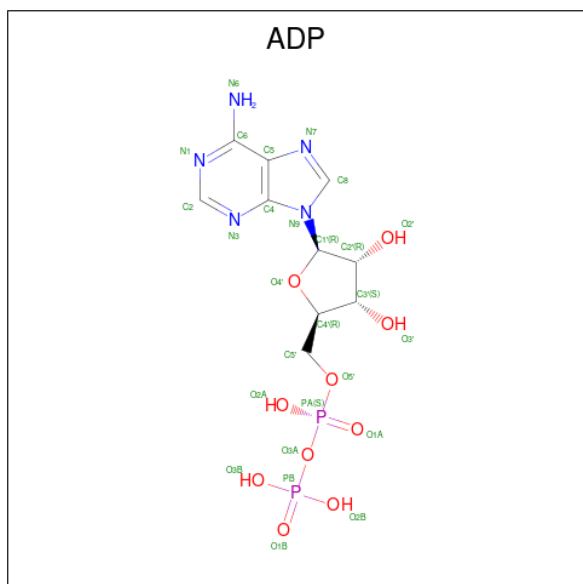
There are 2 unique types of molecules in this entry. The entry contains 9225 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P-glycoprotein (ABCB1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1182	9171	5895	1552	1686	38	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

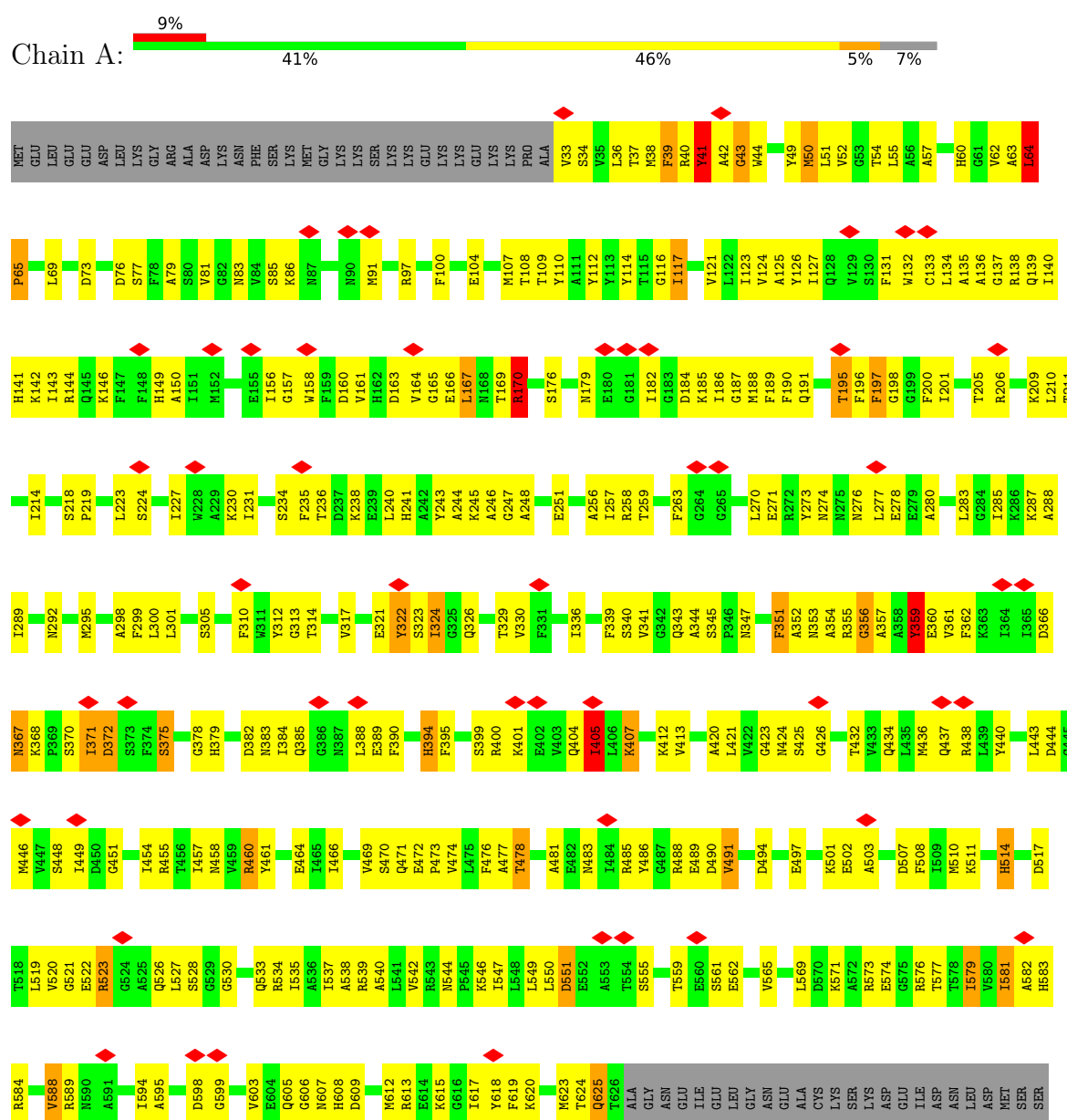


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

3 Residue-property plots

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

• Molecule 1: P-glycoprotein (ABCB1)



L1224	L1157	F1091	S1016	K930	L853	T781	N717	LYS
V1225	P1158	L1092	Y1017	A931	T854	K782	G718	ASP
I1226	D1159	K1095	S1018	H932	L855	R783	G719	SER
A1227	K1160	E1096	K1023	I936	A859	W785	Q721	GLY
H1228	T1163	I1097	P1024	T937	I860	W786		SER
R1229	R1164	K1098	N1025	F938	P861	W788	F724	LEU
L1230	V1165	Q1099	M1026	S939	V862	F789	S725	ILE
S1231	G1166	L1100	L1027	P940	I863	K790	W726	ARG
T1232	G1167	N1101	E1028	A943	I864		F727	ARG
H1233	D1167	Q1102	G1029	Y946	A865	L793	F728	SER
Q1234	K1168	W1103	N1030		G868	R794	S729	THR
N1235	G1169	A1107	Q1032	Y949	E871	Q795	K730	ARG
A1236	T1170	Q1108	F1033	A950		D796	V731	LYS
D1237	G1174	L1109	S1034	A951	L875	D797	V732	SER
L1238	G1175	G1110	G1035	C952	S876	S798	G733	ILE
V1239	K1176	I1111	V1037	F953	G877	W799	V734	CYS
I1240	K1177	I1112	P1043	R954		F800	F735	GLY
V1241	Q1178	S1113	Y1040	F955	L880	D801	T736	PRO
I1242	R1179	Q1114	P1041	G956	K881	D802	N737	HIS
Q1243	R1180	E1115	T1042	A957	D882	P803	G738	ASP
N1244	A1181		R1043	Y958	L886	N805	P740	ASP
G1245	I1182	F1119	P1044	L959	E887	T806	P741	ARG
K1246	A1183	D1120	S1045	V960	G888	T807		LYS
V1247	A1184	C1121	I1046	Q963	S889	G808	Q744	LEU
K1248	A1185		P1047	F967	G890	A809	Q746	THR
E1249	A1186	A1124	V1048	E968	T894	R813	N747	LYS
H1250	A1187	I1127	L1049	N969	I897	A815	L750	GLU
Q1251	V1187	Y1129	Q1050	V970	E898	N816	F751	ALA
G1252	R1188	G1130	G1051	K1057	N999	Q820	S752	
H1253	Q1189	D1131	K1058	S975	F900	V821	D885	
Q1254	L1191	N1132	G1059	A976	R901	G823	E886	
L1255	I1192	S1133	T1061	I977	V903	A824	D887	
T1256	L1193	V1135	G1066		V904	T825	V688	
G1257	D1196	W1136	S1067	A981	S905	G826	P689	
A1258	E1197	S1137	S1068	M982	L906	S827	S892	
Q1259	L1198	Y1138	G1069	A983	T907	R828	F693	
L1260	D1199	E1139	C1070	V984	R908	V831	W694	
G1261	T1199	E1140	G1071	S989	E913	Q834	R695	
I1262	T1199	I1141	K1072	F990	T914	N835	L697	
Y1263	S1200	V1142	S1073	A991		I836	W700	
F1264	A1201	R1143	T1074	P992	A917	A837	S701	
S1265	L1202	A1144	V1075	D993	L920	N838	T702	
M1266	D1203		E1080	S1002	Q921	L839	P705	
V1267	T1204		R1081	H1003	I922	T843	Y706	
S1268			F1082	R1006	P923	I844	F707	
V1269	K1208		N1149	I1007	N926	I845	V708	
Q1270	V1209		D1084	I1008	N927	I848	V709	
A1271	V1210		P1085	E1013	A928	G777	G710	
GLY			M1086		W928	E778	I711	
ALA			A1087		R929	I779	F712	
LYS			S1088				G713	
ARG			V1089				A714	
SER								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.220	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	165.35999, 165.35999, 165.35999	wwPDB
Map dimensions	156, 156, 156	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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

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	2.27	339/9339 (3.6%)	2.52	667/12626 (5.3%)

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	25

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	VAL	CA-C	-11.56	1.38	1.52
1	A	782	LYS	N-CA	-10.48	1.35	1.46
1	A	709	VAL	C-N	10.44	1.46	1.33
1	A	1023	LYS	CA-C	10.14	1.64	1.53
1	A	1246	LYS	CA-C	-9.79	1.40	1.52
1	A	344	ALA	CA-C	-9.60	1.40	1.52
1	A	413	VAL	CA-CB	-9.54	1.42	1.54
1	A	778	GLU	C-N	9.37	1.45	1.33
1	A	362	PHE	C-N	9.05	1.45	1.33
1	A	946	TYR	CA-C	-8.78	1.41	1.52
1	A	1188	ARG	CD-NE	8.77	1.58	1.46
1	A	561	SER	N-CA	8.75	1.57	1.46
1	A	954	ARG	CD-NE	8.70	1.58	1.46
1	A	324	ILE	N-CA	8.65	1.54	1.46
1	A	615	LYS	N-CA	-8.56	1.35	1.46
1	A	238	LYS	C-N	8.36	1.44	1.33
1	A	330	VAL	CA-CB	8.29	1.65	1.54
1	A	523	ARG	NE-CZ	8.22	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	ASN	CA-C	-8.14	1.42	1.52
1	A	954	ARG	CA-C	-7.97	1.42	1.52
1	A	390	PHE	N-CA	-7.97	1.36	1.46
1	A	717	ASN	C-N	7.96	1.42	1.33
1	A	1155	ASP	CA-C	-7.94	1.43	1.52
1	A	244	ALA	N-CA	-7.90	1.36	1.46
1	A	1201	ALA	C-N	7.77	1.44	1.33
1	A	474	VAL	CA-CB	-7.77	1.45	1.54
1	A	1091	PHE	CA-C	-7.74	1.43	1.52
1	A	783	ARG	N-CA	-7.72	1.36	1.46
1	A	1081	ARG	CD-NE	7.67	1.56	1.46
1	A	796	ASP	N-CA	-7.65	1.37	1.46
1	A	1095	LYS	CA-CB	7.63	1.64	1.53
1	A	733	GLY	CA-C	-7.62	1.43	1.52
1	A	235	PHE	C-N	7.54	1.43	1.33
1	A	163	ASP	CA-C	-7.48	1.43	1.52
1	A	926	ASN	CA-C	-7.45	1.42	1.52
1	A	740	PRO	CA-C	7.36	1.59	1.52
1	A	757	ILE	N-CA	-7.24	1.37	1.46
1	A	142	LYS	CA-C	-7.23	1.43	1.52
1	A	582	ALA	N-CA	-7.22	1.37	1.46
1	A	143	ILE	C-N	7.19	1.43	1.33
1	A	477	ALA	CA-C	-7.16	1.46	1.53
1	A	612	MET	N-CA	-7.16	1.37	1.46
1	A	378	GLY	N-CA	7.16	1.51	1.45
1	A	356	GLY	CA-C	-7.13	1.44	1.52
1	A	697	LEU	N-CA	-7.12	1.37	1.46
1	A	619	PHE	C-N	7.08	1.43	1.33
1	A	827	SER	C-N	7.06	1.42	1.33
1	A	205	THR	CA-C	7.05	1.61	1.52
1	A	780	LEU	CA-CB	7.03	1.64	1.53
1	A	785	ARG	N-CA	-7.03	1.37	1.46
1	A	263	PHE	C-N	7.00	1.42	1.33
1	A	1036	VAL	CA-C	-6.99	1.44	1.52
1	A	849	TYR	CA-CB	6.99	1.63	1.53
1	A	473	PRO	CA-CB	6.94	1.63	1.53
1	A	1037	VAL	CA-C	-6.93	1.44	1.52
1	A	1265	SER	CA-C	6.92	1.61	1.52
1	A	806	THR	CA-C	6.90	1.61	1.52
1	A	379	HIS	CA-C	-6.89	1.43	1.52
1	A	127	ILE	N-CA	-6.88	1.38	1.46
1	A	114	TYR	C-N	6.88	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	TRP	CA-CB	6.83	1.64	1.53
1	A	800	PHE	N-CA	-6.83	1.36	1.46
1	A	133	CYS	CA-C	-6.82	1.48	1.52
1	A	444	ASP	N-CA	-6.75	1.37	1.45
1	A	60	HIS	ND1-CE1	6.74	1.39	1.32
1	A	425	SER	C-N	6.74	1.41	1.33
1	A	164	VAL	CA-CB	-6.73	1.47	1.54
1	A	1132	ASN	CA-C	-6.73	1.43	1.52
1	A	238	LYS	CA-CB	6.70	1.63	1.53
1	A	853	LEU	CA-CB	6.68	1.63	1.53
1	A	1221	ARG	C-N	6.67	1.42	1.33
1	A	140	ILE	CA-C	-6.67	1.44	1.52
1	A	992	PRO	CA-CB	6.66	1.63	1.53
1	A	759	GLY	CA-C	-6.66	1.44	1.51
1	A	330	VAL	C-N	6.60	1.43	1.34
1	A	1241	VAL	C-N	6.59	1.42	1.33
1	A	247	GLY	CA-C	-6.57	1.44	1.52
1	A	1090	VAL	N-CA	-6.54	1.38	1.46
1	A	990	PHE	CA-C	-6.54	1.43	1.52
1	A	1152	GLN	CA-CB	6.53	1.63	1.53
1	A	956	GLY	C-N	6.52	1.42	1.33
1	A	940	PHE	C-N	6.50	1.42	1.33
1	A	186	ILE	N-CA	-6.49	1.38	1.46
1	A	107	MET	N-CA	-6.49	1.38	1.46
1	A	258	ARG	CA-C	-6.47	1.44	1.52
1	A	345	SER	CA-CB	6.46	1.61	1.53
1	A	389	GLU	CA-C	-6.44	1.44	1.52
1	A	1191	HIS	C-N	6.44	1.41	1.33
1	A	144	ARG	CD-NE	6.43	1.55	1.46
1	A	211	THR	N-CA	6.43	1.54	1.46
1	A	625	GLN	CA-C	-6.42	1.43	1.52
1	A	550	LEU	N-CA	6.42	1.54	1.46
1	A	533	GLN	CA-C	-6.39	1.44	1.52
1	A	788	VAL	CA-CB	-6.39	1.45	1.54
1	A	1112	VAL	N-CA	-6.37	1.38	1.46
1	A	1032	GLN	CA-C	-6.37	1.44	1.52
1	A	607	ASN	C-N	6.36	1.42	1.33
1	A	761	ILE	C-N	6.36	1.42	1.33
1	A	1120	ASP	C-N	6.36	1.41	1.33
1	A	494	ASP	CA-C	-6.35	1.44	1.52
1	A	589	ARG	CD-NE	6.33	1.55	1.46
1	A	141	HIS	ND1-CE1	6.32	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	CA-C	-6.31	1.43	1.52
1	A	321	GLU	CA-CB	6.29	1.63	1.53
1	A	1219	GLU	C-N	6.29	1.42	1.33
1	A	379	HIS	ND1-CE1	6.28	1.38	1.32
1	A	1193	LEU	CA-C	-6.28	1.45	1.52
1	A	814	LEU	CA-CB	6.27	1.63	1.53
1	A	565	VAL	C-N	6.26	1.41	1.33
1	A	141	HIS	CD2-NE2	6.26	1.44	1.37
1	A	1246	LYS	C-N	6.26	1.41	1.33
1	A	454	ILE	C-N	6.25	1.41	1.33
1	A	1145	ALA	C-N	6.24	1.41	1.33
1	A	1270	GLN	CA-CB	6.23	1.63	1.53
1	A	1002	SER	CA-C	-6.21	1.44	1.52
1	A	780	LEU	CA-C	-6.20	1.44	1.52
1	A	1218	ARG	CZ-NH2	6.19	1.41	1.33
1	A	124	VAL	C-N	6.18	1.42	1.33
1	A	1230	LEU	CA-C	-6.18	1.43	1.52
1	A	388	LEU	N-CA	-6.18	1.38	1.46
1	A	827	SER	CA-CB	6.17	1.63	1.53
1	A	1028	GLU	CA-C	-6.14	1.44	1.52
1	A	245	LYS	CA-C	-6.12	1.45	1.52
1	A	384	ILE	N-CA	-6.11	1.37	1.46
1	A	1072	LYS	CA-C	-6.10	1.44	1.52
1	A	1003	HIS	CE1-NE2	-6.09	1.26	1.32
1	A	248	ALA	N-CA	6.09	1.53	1.46
1	A	1149	ASN	C-N	6.09	1.40	1.34
1	A	1080	GLU	CA-C	-6.08	1.44	1.52
1	A	1108	GLN	N-CA	-6.07	1.39	1.46
1	A	609	ASP	N-CA	-6.07	1.39	1.46
1	A	688	VAL	C-O	-6.06	1.16	1.24
1	A	1188	ARG	NE-CZ	6.05	1.39	1.33
1	A	943	ALA	CA-C	-6.04	1.44	1.52
1	A	848	ILE	C-N	6.04	1.41	1.33
1	A	946	TYR	CA-CB	6.03	1.62	1.53
1	A	73	ASP	CA-CB	6.01	1.62	1.53
1	A	981	ALA	N-CA	-5.98	1.38	1.46
1	A	109	THR	CA-C	5.97	1.60	1.52
1	A	1024	PRO	CA-C	-5.97	1.44	1.52
1	A	523	ARG	C-N	5.96	1.42	1.33
1	A	757	ILE	C-N	5.95	1.42	1.33
1	A	1256	LEU	CA-C	-5.95	1.45	1.52
1	A	257	ILE	C-N	5.95	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1134	ARG	NE-CZ	5.94	1.39	1.33
1	A	1046	ILE	CA-CB	-5.94	1.46	1.54
1	A	744	GLN	C-N	5.93	1.41	1.33
1	A	605	GLN	CA-C	5.93	1.60	1.52
1	A	582	ALA	CA-CB	5.93	1.63	1.53
1	A	711	ILE	CA-C	-5.92	1.45	1.52
1	A	1017	TYR	CA-C	-5.89	1.45	1.52
1	A	1089	SER	C-N	5.89	1.41	1.33
1	A	125	ALA	N-CA	-5.87	1.39	1.46
1	A	767	PHE	C-N	5.86	1.41	1.33
1	A	52	VAL	CA-C	-5.85	1.45	1.52
1	A	1240	VAL	N-CA	-5.85	1.39	1.46
1	A	263	PHE	CA-C	-5.83	1.44	1.52
1	A	1255	GLN	CA-CB	5.83	1.62	1.53
1	A	728	PHE	C-N	5.82	1.41	1.34
1	A	1042	THR	CA-C	5.82	1.60	1.52
1	A	1142	VAL	CA-CB	-5.81	1.47	1.54
1	A	753	LEU	C-N	5.81	1.42	1.34
1	A	573	ARG	CD-NE	5.80	1.54	1.46
1	A	871	GLU	CA-C	-5.80	1.45	1.52
1	A	491	VAL	N-CA	5.79	1.53	1.46
1	A	519	LEU	C-N	5.79	1.39	1.33
1	A	108	THR	C-N	5.79	1.41	1.33
1	A	1208	LYS	CA-C	-5.79	1.45	1.52
1	A	745	ARG	CA-CB	5.78	1.62	1.53
1	A	733	GLY	N-CA	-5.78	1.38	1.45
1	A	1192	ILE	N-CA	-5.77	1.39	1.46
1	A	839	LEU	CA-C	-5.77	1.45	1.52
1	A	555	SER	CA-C	5.76	1.59	1.52
1	A	44	TRP	CA-CB	5.76	1.62	1.53
1	A	809	ALA	CA-C	-5.75	1.44	1.52
1	A	1221	ARG	C-O	-5.75	1.17	1.23
1	A	280	ALA	C-N	5.75	1.42	1.33
1	A	443	LEU	C-N	5.75	1.41	1.33
1	A	731	VAL	CA-C	-5.74	1.45	1.52
1	A	64	LEU	N-CA	-5.74	1.41	1.46
1	A	1129	TYR	N-CA	-5.73	1.39	1.46
1	A	77	SER	C-N	5.73	1.41	1.33
1	A	460	ARG	CZ-NH2	5.72	1.40	1.33
1	A	583	HIS	ND1-CE1	5.71	1.38	1.32
1	A	584	ARG	N-CA	-5.71	1.39	1.46
1	A	160	ASP	CA-C	-5.70	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	ASP	C-N	5.70	1.41	1.33
1	A	839	LEU	C-N	5.70	1.41	1.33
1	A	603	VAL	CA-CB	-5.69	1.48	1.55
1	A	521	GLY	N-CA	5.69	1.52	1.45
1	A	724	PHE	CA-CB	5.68	1.62	1.53
1	A	323	SER	CA-CB	5.68	1.64	1.53
1	A	623	MET	C-N	5.67	1.41	1.33
1	A	1250	HIS	CD2-NE2	5.67	1.44	1.37
1	A	963	GLN	CA-C	-5.67	1.45	1.52
1	A	747	ASN	C-N	5.66	1.41	1.33
1	A	517	ASP	CA-CB	5.66	1.63	1.53
1	A	1049	LEU	N-CA	-5.66	1.39	1.46
1	A	1229	ARG	N-CA	-5.64	1.39	1.46
1	A	520	VAL	C-O	-5.63	1.18	1.23
1	A	134	LEU	N-CA	-5.63	1.39	1.46
1	A	813	ARG	CZ-NH1	5.62	1.40	1.32
1	A	160	ASP	CA-CB	5.62	1.62	1.53
1	A	188	MET	CA-C	-5.61	1.45	1.52
1	A	347	ASN	CA-C	-5.60	1.45	1.52
1	A	1087	ALA	CA-C	-5.60	1.45	1.52
1	A	507	ASP	C-N	5.60	1.41	1.34
1	A	125	ALA	CA-CB	5.59	1.62	1.53
1	A	1244	ASN	CA-C	-5.58	1.46	1.53
1	A	455	ARG	CD-NE	5.58	1.54	1.46
1	A	687	ASP	CA-CB	5.57	1.60	1.53
1	A	457	ILE	N-CA	-5.56	1.36	1.45
1	A	1232	THR	C-N	5.56	1.41	1.33
1	A	1138	TYR	N-CA	5.56	1.52	1.46
1	A	132	TRP	CA-C	-5.55	1.45	1.52
1	A	54	THR	CA-C	5.55	1.59	1.52
1	A	472	GLU	N-CA	-5.55	1.38	1.46
1	A	1137	SER	C-O	5.55	1.30	1.23
1	A	1112	VAL	C-N	5.54	1.41	1.33
1	A	91	MET	N-CA	-5.54	1.39	1.46
1	A	326	GLN	CA-C	-5.54	1.46	1.52
1	A	274	ASN	N-CA	-5.54	1.39	1.46
1	A	458	ASN	C-N	5.53	1.40	1.33
1	A	156	ILE	N-CA	-5.52	1.40	1.46
1	A	1087	ALA	N-CA	-5.50	1.39	1.45
1	A	710	GLY	CA-C	-5.50	1.46	1.52
1	A	753	LEU	CB-CG	5.49	1.64	1.53
1	A	1196	ASP	CA-CB	5.49	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	PHE	N-CA	-5.48	1.39	1.46
1	A	314	THR	CB-OG1	5.48	1.52	1.43
1	A	370	SER	CA-C	5.48	1.60	1.52
1	A	1254	GLN	CA-CB	5.48	1.62	1.53
1	A	1200	SER	C-N	5.47	1.41	1.33
1	A	1137	SER	CA-C	-5.47	1.46	1.52
1	A	855	LEU	C-O	5.46	1.30	1.24
1	A	1191	HIS	ND1-CE1	5.45	1.38	1.32
1	A	576	ARG	C-N	5.45	1.41	1.33
1	A	218	SER	N-CA	-5.45	1.41	1.46
1	A	1164	ARG	CD-NE	5.44	1.53	1.46
1	A	43	GLY	N-CA	5.42	1.53	1.45
1	A	930	LYS	CA-C	-5.41	1.45	1.52
1	A	243	TYR	CA-C	-5.40	1.45	1.52
1	A	1042	THR	C-O	-5.40	1.17	1.24
1	A	176	SER	CA-CB	5.40	1.61	1.53
1	A	813	ARG	N-CA	-5.39	1.40	1.46
1	A	1121	CYS	C-N	5.39	1.40	1.33
1	A	1151	HIS	C-N	5.38	1.40	1.33
1	A	1222	THR	C-N	5.38	1.41	1.33
1	A	1006	ARG	C-N	5.37	1.40	1.33
1	A	712	PHE	CA-CB	5.36	1.61	1.53
1	A	1154	ILE	C-N	5.36	1.40	1.33
1	A	1147	GLU	CA-C	-5.36	1.45	1.52
1	A	617	ILE	N-CA	-5.35	1.40	1.46
1	A	1176	GLN	N-CA	-5.35	1.40	1.46
1	A	231	ILE	N-CA	-5.34	1.40	1.46
1	A	816	ASN	N-CA	-5.34	1.40	1.46
1	A	1256	LEU	N-CA	-5.34	1.39	1.46
1	A	97	ARG	CD-NE	5.34	1.53	1.46
1	A	55	LEU	C-N	5.33	1.41	1.34
1	A	1057	LYS	CA-C	-5.33	1.46	1.52
1	A	718	GLY	N-CA	-5.33	1.39	1.45
1	A	808	GLY	N-CA	-5.33	1.39	1.45
1	A	138	ARG	C-N	5.32	1.41	1.33
1	A	845	ILE	CA-CB	-5.32	1.47	1.54
1	A	42	ALA	N-CA	-5.31	1.39	1.46
1	A	41	TYR	N-CA	-5.30	1.39	1.46
1	A	460	ARG	CA-C	-5.30	1.45	1.52
1	A	697	LEU	C-N	5.30	1.40	1.33
1	A	1073	SER	C-N	5.30	1.40	1.33
1	A	768	LEU	N-CA	5.29	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	799	TRP	NE1-CE2	-5.28	1.31	1.37
1	A	608	HIS	CG-ND1	-5.26	1.32	1.38
1	A	831	VAL	C-N	5.25	1.40	1.33
1	A	375	SER	CA-C	-5.25	1.45	1.52
1	A	1119	PHE	N-CA	-5.24	1.39	1.45
1	A	469	VAL	C-N	5.24	1.40	1.33
1	A	407	LYS	CA-C	-5.24	1.45	1.52
1	A	274	ASN	C-N	-5.22	1.26	1.33
1	A	813	ARG	C-N	5.22	1.41	1.34
1	A	370	SER	C-N	5.22	1.40	1.33
1	A	502	GLU	C-N	5.22	1.41	1.33
1	A	859	ALA	N-CA	-5.21	1.39	1.46
1	A	720	LEU	C-N	5.21	1.40	1.33
1	A	1098	LYS	C-N	5.20	1.41	1.33
1	A	571	LYS	C-N	5.20	1.41	1.33
1	A	1032	GLN	N-CA	5.19	1.52	1.46
1	A	562	GLU	C-O	-5.18	1.18	1.24
1	A	481	ALA	C-N	5.18	1.41	1.33
1	A	1066	GLY	CA-C	-5.18	1.44	1.51
1	A	201	ILE	N-CA	5.18	1.52	1.46
1	A	706	TYR	C-N	5.18	1.41	1.33
1	A	576	ARG	NE-CZ	5.17	1.38	1.33
1	A	57	ALA	C-N	5.17	1.40	1.33
1	A	470	SER	N-CA	-5.17	1.39	1.46
1	A	1168	LYS	N-CA	-5.17	1.39	1.46
1	A	1222	THR	CA-C	-5.17	1.46	1.52
1	A	488	ARG	CA-C	-5.16	1.46	1.52
1	A	685	ASP	N-CA	-5.16	1.39	1.46
1	A	39	PHE	CA-CB	5.14	1.61	1.53
1	A	581	ILE	N-CA	-5.14	1.40	1.46
1	A	1024	PRO	C-N	5.14	1.42	1.34
1	A	39	PHE	N-CA	-5.12	1.40	1.46
1	A	305	SER	C-N	5.12	1.40	1.33
1	A	1033	PHE	C-O	-5.12	1.18	1.24
1	A	1151	HIS	CG-ND1	5.12	1.43	1.38
1	A	730	LYS	CA-CB	5.12	1.61	1.53
1	A	412	LYS	CA-C	-5.11	1.46	1.52
1	A	283	LEU	N-CA	5.10	1.52	1.46
1	A	379	HIS	CD2-NE2	5.10	1.43	1.37
1	A	508	PHE	CA-CB	5.10	1.61	1.53
1	A	527	LEU	N-CA	-5.10	1.39	1.46
1	A	603	VAL	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1260	LYS	C-N	5.09	1.41	1.33
1	A	100	PHE	C-N	5.08	1.40	1.33
1	A	573	ARG	C-O	-5.08	1.17	1.23
1	A	753	LEU	C-O	-5.08	1.18	1.24
1	A	744	GLN	CA-CB	5.08	1.61	1.53
1	A	784	LEU	CA-CB	5.08	1.61	1.53
1	A	1154	ILE	CA-C	5.08	1.59	1.52
1	A	737	ASN	N-CA	-5.07	1.39	1.45
1	A	785	ARG	NE-CZ	5.07	1.38	1.33
1	A	982	MET	C-N	5.07	1.40	1.33
1	A	219	PRO	CA-C	5.07	1.59	1.52
1	A	400	ARG	CA-CB	5.07	1.59	1.53
1	A	160	ASP	N-CA	-5.06	1.40	1.46
1	A	209	LYS	CA-C	-5.06	1.46	1.52
1	A	526	GLN	CA-C	5.06	1.59	1.52
1	A	1085	PRO	CA-C	-5.04	1.46	1.52
1	A	538	ALA	CA-C	-5.03	1.46	1.52
1	A	613	ARG	CZ-NH1	5.03	1.39	1.32
1	A	514	HIS	C-N	5.02	1.40	1.33
1	A	1238	LEU	CA-CB	5.02	1.61	1.53
1	A	826	GLY	N-CA	-5.02	1.39	1.45
1	A	1127	ILE	CA-CB	5.02	1.60	1.54
1	A	1209	VAL	N-CA	-5.02	1.39	1.46
1	A	278	GLU	CA-CB	-5.01	1.45	1.53
1	A	494	ASP	CA-CB	5.01	1.61	1.53
1	A	794	ARG	CA-C	-5.01	1.45	1.52
1	A	1075	VAL	CA-CB	5.00	1.59	1.54

All (667) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	906	LEU	N-CA-C	-11.77	101.20	114.62
1	A	835	ASN	CA-CB-CG	11.67	124.27	112.60
1	A	816	ASN	CA-CB-CG	-10.73	101.87	112.60
1	A	240	LEU	N-CA-C	10.47	122.69	111.28
1	A	1200	SER	N-CA-C	-10.46	99.22	114.39
1	A	1120	ASP	CA-CB-CG	10.17	122.77	112.60
1	A	696	ILE	CA-C-N	9.94	134.59	120.28
1	A	696	ILE	C-N-CA	9.94	134.59	120.28
1	A	747	ASN	OD1-CG-ND2	9.76	132.36	122.60
1	A	1260	LYS	N-CA-C	-9.57	100.92	112.59
1	A	83	ASN	CA-C-O	-9.47	110.51	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1124	ALA	N-CA-C	9.25	121.36	111.28
1	A	579	ILE	N-CA-C	-9.02	95.00	108.17
1	A	1250	HIS	ND1-CE1-NE2	8.96	117.36	108.40
1	A	60	HIS	CA-CB-CG	8.91	122.72	113.80
1	A	984	VAL	CA-C-N	8.87	129.78	119.94
1	A	984	VAL	C-N-CA	8.87	129.78	119.94
1	A	469	VAL	CA-C-N	8.85	134.11	120.75
1	A	469	VAL	C-N-CA	8.85	134.11	120.75
1	A	581	ILE	N-CA-C	-8.83	95.75	108.11
1	A	288	ALA	CA-C-N	8.81	131.71	120.70
1	A	288	ALA	C-N-CA	8.81	131.71	120.70
1	A	353	ASN	CA-CB-CG	-8.81	103.79	112.60
1	A	76	ASP	CA-CB-CG	8.70	121.30	112.60
1	A	860	ILE	CA-C-N	8.70	128.78	120.43
1	A	860	ILE	C-N-CA	8.70	128.78	120.43
1	A	1115	GLU	CA-C-O	-8.66	112.66	121.32
1	A	179	ASN	CA-CB-CG	-8.65	103.95	112.60
1	A	368	LYS	N-CA-C	-8.57	98.88	110.36
1	A	583	HIS	CA-CB-CG	-8.56	105.24	113.80
1	A	1114	GLN	N-CA-C	-8.36	102.64	113.17
1	A	837	ALA	N-CA-C	8.34	120.36	111.28
1	A	1102	VAL	O-C-N	8.33	129.95	121.87
1	A	881	LYS	CA-C-N	8.33	131.27	120.44
1	A	881	LYS	C-N-CA	8.33	131.27	120.44
1	A	283	LEU	CA-C-N	8.30	128.99	119.94
1	A	283	LEU	C-N-CA	8.30	128.99	119.94
1	A	815	ALA	CA-C-N	8.27	131.19	120.44
1	A	815	ALA	C-N-CA	8.27	131.19	120.44
1	A	461	TYR	CA-C-N	8.26	131.35	120.28
1	A	461	TYR	C-N-CA	8.26	131.35	120.28
1	A	201	ILE	N-CA-C	8.26	119.03	110.36
1	A	1124	ALA	CA-C-N	8.26	135.60	121.14
1	A	1124	ALA	C-N-CA	8.26	135.60	121.14
1	A	544	ASN	OD1-CG-ND2	8.23	130.83	122.60
1	A	813	ARG	O-C-N	-8.22	113.60	122.07
1	A	769	GLN	CA-C-N	8.21	129.09	119.98
1	A	769	GLN	C-N-CA	8.21	129.09	119.98
1	A	1057	LYS	N-CA-C	-8.20	97.43	110.14
1	A	466	ILE	CA-C-N	8.19	130.14	121.45
1	A	466	ILE	C-N-CA	8.19	130.14	121.45
1	A	807	THR	CA-C-N	8.19	129.07	119.98
1	A	807	THR	C-N-CA	8.19	129.07	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	PHE	CA-C-N	8.17	131.23	120.28
1	A	131	PHE	C-N-CA	8.17	131.23	120.28
1	A	758	LEU	CA-C-N	8.13	129.18	119.99
1	A	758	LEU	C-N-CA	8.13	129.18	119.99
1	A	538	ALA	CA-C-N	8.10	131.13	120.28
1	A	538	ALA	C-N-CA	8.10	131.13	120.28
1	A	501	LYS	N-CA-C	8.09	120.17	111.36
1	A	1250	HIS	CE1-NE2-CD2	-8.05	100.95	109.00
1	A	969	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	731	VAL	CA-C-N	8.01	133.93	120.64
1	A	731	VAL	C-N-CA	8.01	133.93	120.64
1	A	608	HIS	CE1-NE2-CD2	-7.98	101.02	109.00
1	A	1204	THR	N-CA-C	7.93	120.36	108.31
1	A	1164	ARG	NE-CZ-NH2	-7.89	112.10	119.20
1	A	551	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	806	THR	CA-C-N	7.82	131.10	120.54
1	A	806	THR	C-N-CA	7.82	131.10	120.54
1	A	117	ILE	N-CA-C	-7.79	102.50	111.00
1	A	962	GLN	N-CA-C	7.74	119.36	111.07
1	A	206	ARG	NE-CZ-NH2	7.66	126.09	119.20
1	A	81	VAL	N-CA-C	7.65	117.72	110.53
1	A	733	GLY	N-CA-C	7.64	121.36	112.50
1	A	189	PHE	CA-CB-CG	-7.63	106.17	113.80
1	A	149	HIS	ND1-CE1-NE2	7.61	116.01	108.40
1	A	197	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	1114	GLN	CA-C-N	7.59	128.96	122.28
1	A	1114	GLN	C-N-CA	7.59	128.96	122.28
1	A	546	LYS	N-CA-C	-7.58	103.86	113.72
1	A	803	PRO	CA-C-O	-7.55	113.15	121.23
1	A	196	PHE	CA-C-N	7.54	130.38	120.28
1	A	196	PHE	C-N-CA	7.54	130.38	120.28
1	A	514	HIS	ND1-CE1-NE2	7.53	115.93	108.40
1	A	1174	GLY	CA-C-N	7.53	128.34	119.98
1	A	1174	GLY	C-N-CA	7.53	128.34	119.98
1	A	190	PHE	CA-C-N	7.52	130.35	120.28
1	A	190	PHE	C-N-CA	7.52	130.35	120.28
1	A	687	ASP	N-CA-C	-7.50	94.71	107.99
1	A	164	VAL	N-CA-C	7.47	120.38	109.63
1	A	354	ALA	CA-C-N	7.46	130.14	120.44
1	A	354	ALA	C-N-CA	7.46	130.14	120.44
1	A	813	ARG	NH1-CZ-NH2	-7.45	109.62	119.30
1	A	351	PHE	CA-CB-CG	7.43	121.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LYS	N-CA-CB	7.38	120.71	110.01
1	A	740	PRO	N-CA-C	7.37	119.69	110.70
1	A	336	ILE	CA-C-N	7.34	129.54	120.22
1	A	336	ILE	C-N-CA	7.34	129.54	120.22
1	A	959	LEU	CA-C-N	7.34	130.84	120.42
1	A	959	LEU	C-N-CA	7.34	130.84	120.42
1	A	107	MET	O-C-N	-7.33	113.65	122.22
1	A	341	VAL	CA-C-N	7.33	129.52	120.22
1	A	341	VAL	C-N-CA	7.33	129.52	120.22
1	A	156	ILE	CA-C-O	-7.32	113.44	121.05
1	A	1240	VAL	N-CA-C	-7.32	97.87	108.11
1	A	588	VAL	N-CA-C	-7.31	104.39	112.80
1	A	189	PHE	CB-CA-C	7.31	122.45	110.90
1	A	321	GLU	CA-C-O	7.27	128.06	119.56
1	A	1185	ALA	O-C-N	7.25	129.86	122.03
1	A	740	PRO	CA-C-O	-7.24	110.06	120.56
1	A	51	LEU	CA-C-O	-7.23	112.21	120.24
1	A	423	GLY	CA-C-O	7.23	128.95	121.21
1	A	551	ASP	CA-C-N	7.22	132.61	122.36
1	A	551	ASP	C-N-CA	7.22	132.61	122.36
1	A	738	GLY	N-CA-C	-7.21	102.52	112.18
1	A	946	TYR	CA-C-N	7.20	130.65	120.28
1	A	946	TYR	C-N-CA	7.20	130.65	120.28
1	A	219	PRO	CA-C-N	7.19	129.76	120.56
1	A	219	PRO	C-N-CA	7.19	129.76	120.56
1	A	1151	HIS	CA-CB-CG	7.13	120.93	113.80
1	A	797	VAL	N-CA-CB	7.12	122.98	111.23
1	A	932	HIS	CA-C-N	7.11	129.66	120.56
1	A	932	HIS	C-N-CA	7.11	129.66	120.56
1	A	517	ASP	CA-CB-CG	-7.09	105.51	112.60
1	A	825	THR	CA-C-N	7.09	129.22	120.22
1	A	825	THR	C-N-CA	7.09	129.22	120.22
1	A	889	SER	O-C-N	-7.07	114.09	122.15
1	A	149	HIS	CE1-NE2-CD2	-7.07	101.93	109.00
1	A	273	TYR	CA-C-N	7.07	131.05	120.31
1	A	273	TYR	C-N-CA	7.07	131.05	120.31
1	A	908	ARG	NE-CZ-NH2	7.05	125.54	119.20
1	A	695	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	A	726	VAL	N-CA-C	-7.01	103.36	111.00
1	A	339	PHE	CA-C-N	6.99	130.93	120.31
1	A	339	PHE	C-N-CA	6.99	130.93	120.31
1	A	1203	ASP	CA-CB-CG	6.96	119.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	SER	CA-C-O	-6.95	112.24	118.63
1	A	702	THR	N-CA-C	6.95	118.85	111.28
1	A	1084	ASP	CA-C-N	6.95	126.93	119.78
1	A	1084	ASP	C-N-CA	6.95	126.93	119.78
1	A	285	ILE	N-CA-C	6.93	117.72	110.72
1	A	805	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	478	THR	N-CA-C	-6.89	98.69	108.96
1	A	530	GLY	O-C-N	6.89	128.87	122.19
1	A	140	ILE	O-C-N	6.88	128.55	121.87
1	A	745	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	569	LEU	N-CA-CB	6.87	120.22	110.12
1	A	473	PRO	N-CD-CG	6.87	113.50	103.20
1	A	594	ILE	N-CA-C	-6.86	98.60	108.48
1	A	887	GLU	CA-C-O	-6.86	113.79	121.00
1	A	717	ASN	CA-C-N	6.86	127.41	119.94
1	A	717	ASN	C-N-CA	6.86	127.41	119.94
1	A	785	ARG	CA-C-N	6.85	129.69	120.65
1	A	785	ARG	C-N-CA	6.85	129.69	120.65
1	A	1252	THR	CA-C-N	6.84	130.30	120.79
1	A	1252	THR	C-N-CA	6.84	130.30	120.79
1	A	1213	ALA	N-CA-CB	6.84	120.17	110.12
1	A	882	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	890	GLY	N-CA-C	6.83	122.52	113.37
1	A	160	ASP	CA-C-O	6.82	127.98	120.82
1	A	779	ILE	CA-C-N	6.82	129.42	120.28
1	A	779	ILE	C-N-CA	6.82	129.42	120.28
1	A	741	PRO	CA-C-O	-6.82	114.11	121.27
1	A	977	ILE	N-CA-CB	6.81	118.52	110.55
1	A	685	ASP	N-CA-C	-6.79	104.56	112.92
1	A	976	ALA	CA-C-N	6.78	129.10	120.56
1	A	976	ALA	C-N-CA	6.78	129.10	120.56
1	A	950	ALA	N-CA-CB	6.75	121.89	110.49
1	A	764	ILE	O-C-N	6.75	128.89	121.94
1	A	379	HIS	CA-CB-CG	6.74	120.54	113.80
1	A	276	ASN	CA-C-N	6.73	129.84	120.29
1	A	276	ASN	C-N-CA	6.73	129.84	120.29
1	A	368	LYS	CA-C-O	-6.73	113.63	120.96
1	A	478	THR	CA-C-N	6.72	130.70	120.82
1	A	478	THR	C-N-CA	6.72	130.70	120.82
1	A	299	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	1101	ASN	CA-C-N	6.71	129.66	120.46
1	A	1101	ASN	C-N-CA	6.71	129.66	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	903	VAL	CA-C-N	6.69	129.93	120.42
1	A	903	VAL	C-N-CA	6.69	129.93	120.42
1	A	1043	ARG	NE-CZ-NH1	-6.69	114.81	121.50
1	A	510	MET	CA-C-N	6.68	129.53	120.38
1	A	510	MET	C-N-CA	6.68	129.53	120.38
1	A	523	ARG	N-CA-C	-6.68	104.44	112.59
1	A	534	ARG	NE-CZ-NH2	6.66	125.19	119.20
1	A	107	MET	CA-C-O	6.63	127.59	120.10
1	A	540	ALA	N-CA-C	-6.62	104.68	112.89
1	A	962	GLN	OE1-CD-NE2	6.62	129.22	122.60
1	A	379	HIS	CA-C-O	-6.62	114.35	121.56
1	A	503	ALA	N-CA-CB	6.62	120.06	110.47
1	A	821	VAL	O-C-N	6.61	128.55	121.87
1	A	1157	LEU	N-CA-CB	6.61	122.13	110.37
1	A	843	ILE	CA-C-N	6.59	128.87	120.56
1	A	843	ILE	C-N-CA	6.59	128.87	120.56
1	A	132	TRP	N-CA-C	6.59	118.46	111.28
1	A	39	PHE	CA-CB-CG	-6.59	107.21	113.80
1	A	244	ALA	N-CA-C	6.59	118.46	111.28
1	A	1138	TYR	CA-C-O	6.58	127.73	120.82
1	A	949	TYR	CA-C-N	6.57	134.08	121.54
1	A	949	TYR	C-N-CA	6.57	134.08	121.54
1	A	606	GLY	N-CA-C	-6.54	101.09	110.38
1	A	236	THR	O-C-N	-6.54	115.34	122.07
1	A	1170	THR	N-CA-C	-6.53	104.94	113.17
1	A	150	ALA	CA-C-O	-6.53	113.50	120.42
1	A	299	PHE	N-CA-CB	6.53	120.40	110.28
1	A	974	PHE	CA-C-N	6.52	129.02	120.28
1	A	974	PHE	C-N-CA	6.52	129.02	120.28
1	A	494	ASP	N-CA-C	6.51	118.38	111.28
1	A	434	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	1144	ALA	N-CA-C	6.50	118.03	111.07
1	A	195	THR	N-CA-CB	6.50	120.35	110.28
1	A	1132	ASN	N-CA-C	-6.48	104.61	113.30
1	A	1270	GLN	O-C-N	6.48	129.54	122.15
1	A	1214	LEU	N-CA-C	6.48	118.34	111.28
1	A	497	GLU	CA-C-N	6.47	128.95	120.28
1	A	497	GLU	C-N-CA	6.47	128.95	120.28
1	A	359	TYR	N-CA-CB	6.44	120.27	110.28
1	A	405	ILE	N-CA-C	-6.43	102.82	111.44
1	A	901	ARG	CB-CG-CD	6.42	126.07	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	GLU	CA-C-N	6.41	128.87	120.28
1	A	321	GLU	C-N-CA	6.41	128.87	120.28
1	A	104	GLU	CA-C-N	6.40	128.85	120.28
1	A	104	GLU	C-N-CA	6.40	128.85	120.28
1	A	1003	HIS	CA-C-O	6.39	127.29	120.70
1	A	1127	ILE	N-CA-CB	6.38	118.02	110.55
1	A	476	PHE	N-CA-CB	6.38	119.56	110.44
1	A	437	GLN	N-CA-C	-6.38	104.55	112.90
1	A	786	TYR	N-CA-CB	6.38	119.22	109.91
1	A	756	LEU	CA-C-N	6.37	129.47	120.42
1	A	756	LEU	C-N-CA	6.37	129.47	120.42
1	A	1240	VAL	N-CA-CB	6.37	120.20	111.41
1	A	312	TYR	CA-C-N	6.36	128.30	120.22
1	A	312	TYR	C-N-CA	6.36	128.30	120.22
1	A	366	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	165	GLY	CA-C-O	-6.33	112.94	119.20
1	A	289	ILE	CA-C-O	-6.32	114.53	121.29
1	A	125	ALA	O-C-N	6.32	128.91	122.09
1	A	472	GLU	CA-C-O	6.30	125.60	119.55
1	A	784	LEU	N-CA-CB	6.29	119.09	109.91
1	A	123	ILE	CB-CA-C	-6.29	103.78	112.02
1	A	1007	ILE	N-CA-C	-6.28	104.37	110.72
1	A	241	HIS	CA-CB-CG	6.27	120.07	113.80
1	A	426	GLY	N-CA-C	-6.26	106.12	114.95
1	A	813	ARG	CA-C-N	6.24	129.27	120.28
1	A	813	ARG	C-N-CA	6.24	129.27	120.28
1	A	372	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	871	GLU	CA-C-N	6.24	128.64	120.28
1	A	871	GLU	C-N-CA	6.24	128.64	120.28
1	A	1198	ALA	CA-C-O	6.24	126.95	119.59
1	A	773	PHE	CA-CB-CG	6.21	120.02	113.80
1	A	1095	LYS	N-CA-C	-6.21	99.11	109.24
1	A	707	PHE	N-CA-CB	6.21	120.99	110.49
1	A	689	PRO	CA-C-O	-6.20	111.56	120.56
1	A	1229	ARG	N-CA-C	-6.19	97.03	107.99
1	A	1134	ARG	O-C-N	-6.18	116.20	123.25
1	A	169	THR	CA-C-N	6.18	128.56	120.28
1	A	169	THR	C-N-CA	6.18	128.56	120.28
1	A	187	GLY	CA-C-N	6.18	128.56	120.28
1	A	187	GLY	C-N-CA	6.18	128.56	120.28
1	A	1131	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	694	TRP	CA-C-N	6.15	130.99	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	TRP	C-N-CA	6.15	130.99	120.72
1	A	1226	ILE	N-CA-C	-6.14	106.75	112.83
1	A	292	ASN	CA-C-N	6.13	129.12	120.42
1	A	292	ASN	C-N-CA	6.13	129.12	120.42
1	A	156	ILE	O-C-N	6.12	127.89	121.89
1	A	1003	HIS	ND1-CE1-NE2	6.12	114.52	108.40
1	A	401	LYS	N-CA-C	-6.11	105.48	113.12
1	A	100	PHE	CA-C-O	-6.09	112.61	119.79
1	A	310	PHE	CA-C-N	6.09	128.35	120.44
1	A	310	PHE	C-N-CA	6.09	128.35	120.44
1	A	517	ASP	N-CA-C	-6.09	105.72	113.02
1	A	595	ALA	CA-C-N	6.09	126.75	120.60
1	A	595	ALA	C-N-CA	6.09	126.75	120.60
1	A	823	GLY	CA-C-N	6.07	128.42	120.28
1	A	823	GLY	C-N-CA	6.07	128.42	120.28
1	A	1164	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	A	360	GLU	CA-C-O	-6.06	114.00	120.42
1	A	1003	HIS	O-C-N	-6.05	115.55	122.09
1	A	1025	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	A	191	GLN	O-C-N	6.05	128.53	122.12
1	A	544	ASN	CA-C-O	-6.05	116.30	120.47
1	A	295	MET	CA-C-N	6.05	126.65	119.94
1	A	295	MET	C-N-CA	6.05	126.65	119.94
1	A	244	ALA	CA-C-N	6.04	128.30	120.44
1	A	244	ALA	C-N-CA	6.04	128.30	120.44
1	A	887	GLU	O-C-N	6.04	128.32	122.03
1	A	1018	SER	CA-C-N	6.03	133.05	121.54
1	A	1018	SER	C-N-CA	6.03	133.05	121.54
1	A	845	ILE	CA-C-N	6.02	128.96	120.28
1	A	845	ILE	C-N-CA	6.02	128.96	120.28
1	A	197	PHE	CA-C-N	6.02	127.87	120.22
1	A	197	PHE	C-N-CA	6.02	127.87	120.22
1	A	287	LYS	O-C-N	6.02	128.27	122.07
1	A	1252	THR	CA-C-O	-6.00	114.72	121.81
1	A	1141	ILE	O-C-N	6.00	128.58	121.80
1	A	984	VAL	N-CA-CB	6.00	117.17	110.51
1	A	224	SER	N-CA-C	5.99	117.81	111.28
1	A	802	ASP	CA-C-N	5.99	126.30	119.83
1	A	802	ASP	C-N-CA	5.99	126.30	119.83
1	A	861	VAL	CA-C-O	-5.97	114.17	118.71
1	A	950	ALA	CA-C-N	5.97	128.88	120.28
1	A	950	ALA	C-N-CA	5.97	128.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	N-CA-C	5.97	117.79	111.28
1	A	1008	ILE	CA-C-N	5.96	128.27	120.28
1	A	1008	ILE	C-N-CA	5.96	128.27	120.28
1	A	928	MET	CA-C-N	5.96	128.54	120.44
1	A	928	MET	C-N-CA	5.96	128.54	120.44
1	A	1165	VAL	N-CA-C	-5.95	105.05	110.82
1	A	313	GLY	CA-C-N	5.95	128.74	120.29
1	A	313	GLY	C-N-CA	5.95	128.74	120.29
1	A	54	THR	CA-C-N	5.95	128.57	120.54
1	A	54	THR	C-N-CA	5.95	128.57	120.54
1	A	270	LEU	N-CA-CB	5.95	118.63	110.01
1	A	865	ALA	N-CA-C	5.94	117.42	111.07
1	A	1085	PRO	N-CA-C	5.94	120.65	111.21
1	A	50	MET	CA-C-N	5.93	130.72	120.58
1	A	50	MET	C-N-CA	5.93	130.72	120.58
1	A	1033	PHE	N-CA-C	-5.93	98.73	108.76
1	A	745	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	790	LYS	CA-C-N	5.92	128.80	120.28
1	A	790	LYS	C-N-CA	5.92	128.80	120.28
1	A	41	TYR	CA-C-N	5.92	130.30	121.72
1	A	41	TYR	C-N-CA	5.92	130.30	121.72
1	A	461	TYR	CA-C-O	5.92	126.69	120.42
1	A	1253	HIS	ND1-CE1-NE2	5.91	114.31	108.40
1	A	277	LEU	N-CA-CB	5.91	118.90	110.16
1	A	689	PRO	N-CA-C	5.90	117.90	110.70
1	A	489	GLU	N-CA-C	-5.90	102.48	110.68
1	A	405	ILE	CA-CB-CG1	5.90	120.42	110.40
1	A	200	PHE	CA-C-O	-5.90	113.44	120.10
1	A	361	VAL	CA-C-N	5.89	128.18	120.28
1	A	361	VAL	C-N-CA	5.89	128.18	120.28
1	A	298	ALA	N-CA-C	5.89	117.70	111.28
1	A	989	SER	CB-CA-C	5.89	120.86	110.85
1	A	1253	HIS	CE1-NE2-CD2	-5.89	103.11	109.00
1	A	844	ILE	CA-C-O	5.88	127.40	121.17
1	A	764	ILE	CA-C-O	-5.88	115.00	121.29
1	A	288	ALA	CA-C-O	-5.88	114.32	120.55
1	A	1086	MET	CB-CA-C	-5.87	101.05	110.79
1	A	146	LYS	N-CA-C	-5.87	104.97	111.36
1	A	271	GLU	CA-C-N	5.85	128.12	120.28
1	A	271	GLU	C-N-CA	5.85	128.12	120.28
1	A	394	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	A	1023	LYS	N-CA-CB	5.85	119.26	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	N-CA-C	5.84	119.74	112.73
1	A	595	ALA	O-C-N	-5.84	116.44	123.27
1	A	38	MET	O-C-N	5.84	128.80	122.15
1	A	157	GLY	O-C-N	5.83	127.83	122.17
1	A	899	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	1199	THR	CA-C-O	5.83	125.09	119.08
1	A	514	HIS	CA-CB-CG	5.83	119.63	113.80
1	A	357	ALA	CA-C-N	5.82	128.35	120.44
1	A	357	ALA	C-N-CA	5.82	128.35	120.44
1	A	107	MET	CG-SD-CE	-5.81	88.11	100.90
1	A	166	GLU	N-CA-C	-5.81	104.91	112.23
1	A	1089	SER	O-C-N	-5.79	116.16	123.17
1	A	146	LYS	N-CA-CB	5.79	118.73	110.16
1	A	1100	LEU	CA-C-N	5.79	130.69	121.66
1	A	1100	LEU	C-N-CA	5.79	130.69	121.66
1	A	371	ILE	CB-CA-C	5.79	120.78	111.29
1	A	952	CYS	CA-C-O	-5.79	114.92	121.00
1	A	121	VAL	CA-C-N	5.78	128.31	120.44
1	A	121	VAL	C-N-CA	5.78	128.31	120.44
1	A	144	ARG	O-C-N	5.78	128.02	122.07
1	A	274	ASN	N-CA-CB	5.78	119.24	110.28
1	A	347	ASN	CA-C-N	5.78	127.96	120.56
1	A	347	ASN	C-N-CA	5.78	127.96	120.56
1	A	65	PRO	CB-CA-C	-5.78	103.68	112.11
1	A	1189	GLN	CA-C-N	5.77	127.06	119.84
1	A	1189	GLN	C-N-CA	5.77	127.06	119.84
1	A	620	LYS	N-CA-CB	5.77	118.61	110.12
1	A	1149	ASN	OD1-CG-ND2	5.77	128.37	122.60
1	A	926	ASN	CA-C-N	5.77	128.01	120.28
1	A	926	ASN	C-N-CA	5.77	128.01	120.28
1	A	241	HIS	CE1-NE2-CD2	-5.76	103.23	109.00
1	A	831	VAL	CA-C-O	-5.76	115.06	121.17
1	A	205	THR	CA-C-O	-5.76	114.45	120.55
1	A	1269	VAL	CG1-CB-CG2	5.75	123.45	110.80
1	A	1177	LYS	N-CA-C	5.74	117.21	111.07
1	A	763	PHE	CA-C-N	5.72	127.85	120.70
1	A	763	PHE	C-N-CA	5.72	127.85	120.70
1	A	782	LYS	O-C-N	5.71	128.85	122.11
1	A	744	GLN	N-CA-CB	5.71	118.61	110.16
1	A	135	ALA	CA-C-O	-5.70	114.38	120.42
1	A	707	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	1254	GLN	CA-C-N	5.70	128.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1254	GLN	C-N-CA	5.70	128.19	120.44
1	A	1182	ILE	CA-C-N	5.69	128.47	120.28
1	A	1182	ILE	C-N-CA	5.69	128.47	120.28
1	A	37	THR	N-CA-C	-5.68	104.55	112.45
1	A	379	HIS	CE1-NE2-CD2	-5.68	103.31	109.00
1	A	139	GLN	CA-C-N	5.68	128.24	120.46
1	A	139	GLN	C-N-CA	5.68	128.24	120.46
1	A	547	ILE	N-CA-C	-5.68	99.95	108.12
1	A	1191	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	917	ALA	CA-C-N	5.67	128.92	120.31
1	A	917	ALA	C-N-CA	5.67	128.92	120.31
1	A	1196	ASP	CA-C-N	5.66	132.35	121.54
1	A	1196	ASP	C-N-CA	5.66	132.35	121.54
1	A	107	MET	N-CA-C	5.66	118.22	111.71
1	A	448	SER	CA-C-N	5.66	129.72	121.80
1	A	448	SER	C-N-CA	5.66	129.72	121.80
1	A	782	LYS	CB-CA-C	5.65	120.38	111.39
1	A	549	LEU	N-CA-C	-5.64	98.00	107.99
1	A	1262	ILE	N-CA-C	5.64	116.28	110.36
1	A	1167	ASP	CA-C-N	5.64	132.09	123.47
1	A	1167	ASP	C-N-CA	5.64	132.09	123.47
1	A	561	SER	CA-C-N	5.63	127.76	120.44
1	A	561	SER	C-N-CA	5.63	127.76	120.44
1	A	583	HIS	ND1-CE1-NE2	5.63	114.03	108.40
1	A	834	GLN	CA-CB-CG	5.63	125.36	114.10
1	A	1097	ILE	CA-C-N	5.63	128.09	120.38
1	A	1097	ILE	C-N-CA	5.63	128.09	120.38
1	A	185	LYS	CA-C-N	5.62	128.16	120.46
1	A	185	LYS	C-N-CA	5.62	128.16	120.46
1	A	588	VAL	CA-CB-CG2	-5.62	100.84	110.40
1	A	1191	HIS	CA-C-O	5.62	124.87	119.08
1	A	494	ASP	O-C-N	5.62	128.08	122.12
1	A	245	LYS	CA-C-N	5.62	127.81	120.28
1	A	245	LYS	C-N-CA	5.62	127.81	120.28
1	A	729	SER	CA-C-O	-5.62	113.75	120.10
1	A	1061	THR	CA-C-O	5.61	126.71	120.43
1	A	953	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	317	VAL	O-C-N	5.60	126.10	121.85
1	A	449	ILE	CA-C-N	5.59	130.50	122.40
1	A	449	ILE	C-N-CA	5.59	130.50	122.40
1	A	583	HIS	N-CA-C	-5.59	106.51	113.38
1	A	727	ILE	CB-CA-C	5.59	119.12	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	SER	CA-C-N	5.58	128.11	120.46
1	A	340	SER	C-N-CA	5.58	128.11	120.46
1	A	1013	GLU	CA-C-O	-5.58	115.48	121.56
1	A	79	ALA	N-CA-CB	5.58	118.16	110.07
1	A	241	HIS	ND1-CE1-NE2	5.58	113.98	108.40
1	A	432	THR	N-CA-CB	5.58	118.81	110.22
1	A	993	ASP	N-CA-C	5.57	117.36	111.28
1	A	868	GLY	O-C-N	5.57	128.75	122.34
1	A	51	LEU	O-C-N	5.57	129.47	122.23
1	A	913	GLU	CA-C-N	5.57	127.68	120.44
1	A	913	GLU	C-N-CA	5.57	127.68	120.44
1	A	761	ILE	CA-C-N	5.56	127.73	120.28
1	A	761	ILE	C-N-CA	5.56	127.73	120.28
1	A	109	THR	CA-C-O	-5.55	114.53	120.42
1	A	330	VAL	N-CA-CB	5.55	118.90	110.58
1	A	877	GLY	CA-C-N	5.54	130.06	120.58
1	A	877	GLY	C-N-CA	5.54	130.06	120.58
1	A	752	SER	CA-C-N	5.53	127.69	120.28
1	A	752	SER	C-N-CA	5.53	127.69	120.28
1	A	821	VAL	N-CA-C	5.51	117.94	111.05
1	A	1262	ILE	O-C-N	-5.51	116.43	121.94
1	A	388	LEU	N-CA-CB	5.50	119.24	110.65
1	A	1150	ILE	N-CA-C	-5.50	106.47	112.80
1	A	1266	MET	N-CA-C	5.50	117.28	111.28
1	A	62	VAL	CA-CB-CG2	-5.49	101.06	110.40
1	A	685	ASP	CB-CA-C	5.48	119.83	110.56
1	A	146	LYS	CA-C-N	5.48	127.89	120.65
1	A	146	LYS	C-N-CA	5.48	127.89	120.65
1	A	711	ILE	O-C-N	-5.47	116.19	121.83
1	A	251	GLU	N-CA-CB	5.47	118.00	110.07
1	A	227	ILE	N-CA-CB	5.47	118.78	110.58
1	A	783	ARG	N-CA-CB	5.46	118.25	110.06
1	A	1073	SER	N-CA-CB	5.46	118.63	110.22
1	A	692	SER	N-CA-C	5.46	117.33	110.24
1	A	425	SER	O-C-N	-5.46	116.31	123.02
1	A	551	ASP	CA-C-O	-5.45	114.62	120.46
1	A	708	VAL	N-CA-C	-5.45	106.51	113.22
1	A	1025	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	170	ARG	NE-CZ-NH2	-5.45	114.30	119.20
1	A	485	ARG	N-CA-C	5.45	119.02	112.38
1	A	537	ILE	O-C-N	5.45	127.15	121.87
1	A	776	ALA	CA-C-N	5.44	127.13	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	776	ALA	C-N-CA	5.44	127.13	120.22
1	A	1112	VAL	N-CA-C	-5.44	100.22	108.17
1	A	511	LYS	CA-C-N	5.44	127.96	120.67
1	A	511	LYS	C-N-CA	5.44	127.96	120.67
1	A	244	ALA	N-CA-CB	5.44	118.11	110.12
1	A	292	ASN	N-CA-C	5.43	117.20	111.28
1	A	528	SER	N-CA-CB	5.43	118.81	110.49
1	A	329	THR	CA-CB-OG1	5.43	117.75	109.60
1	A	1188	ARG	N-CA-CB	5.43	119.40	110.39
1	A	137	GLY	CA-C-N	5.42	128.55	120.31
1	A	137	GLY	C-N-CA	5.42	128.55	120.31
1	A	436	MET	O-C-N	-5.42	115.88	122.22
1	A	1153	PHE	N-CA-C	5.42	118.11	111.82
1	A	595	ALA	CA-C-O	5.42	125.98	120.24
1	A	1182	ILE	N-CA-C	5.42	116.14	110.62
1	A	922	ILE	CA-C-N	5.41	124.93	119.19
1	A	922	ILE	C-N-CA	5.41	124.93	119.19
1	A	158	TRP	CA-C-O	5.41	126.19	119.97
1	A	1249	GLU	N-CA-C	-5.41	101.06	109.72
1	A	126	TYR	CA-C-N	5.40	127.47	120.56
1	A	126	TYR	C-N-CA	5.40	127.47	120.56
1	A	1095	LYS	N-CA-CB	5.40	119.23	110.43
1	A	1199	THR	O-C-N	-5.40	114.75	122.04
1	A	1191	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	A	1268	SER	N-CA-CB	5.40	118.06	110.12
1	A	1058	LYS	N-CA-CB	5.40	117.94	110.17
1	A	539	ARG	CA-C-O	-5.40	114.83	120.55
1	A	305	SER	O-C-N	5.39	127.83	122.12
1	A	1158	PRO	CA-C-O	-5.39	115.29	121.86
1	A	85	SER	CB-CA-C	-5.38	101.70	110.85
1	A	223	LEU	N-CA-C	-5.38	105.49	111.36
1	A	399	SER	N-CA-CB	5.38	117.96	109.83
1	A	1168	LYS	N-CA-CB	5.38	121.30	112.63
1	A	733	GLY	CA-C-O	5.37	126.80	121.00
1	A	752	SER	N-CA-C	5.37	117.13	111.28
1	A	863	ILE	N-CA-C	5.36	115.57	110.42
1	A	1034	SER	CA-C-N	5.36	128.20	120.11
1	A	1034	SER	C-N-CA	5.36	128.20	120.11
1	A	1204	THR	CA-CB-OG1	5.36	117.64	109.60
1	A	1107	ALA	CB-CA-C	-5.36	102.40	111.02
1	A	970	VAL	CB-CA-C	-5.35	105.19	111.94
1	A	514	HIS	CE1-NE2-CD2	-5.35	103.65	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	464	GLU	CB-CG-CD	-5.33	103.53	112.60
1	A	136	ALA	CA-C-N	5.33	126.02	119.99
1	A	136	ALA	C-N-CA	5.33	126.02	119.99
1	A	478	THR	CA-CB-CG2	-5.33	101.44	110.50
1	A	1184	ARG	CA-C-N	5.33	127.88	120.63
1	A	1184	ARG	C-N-CA	5.33	127.88	120.63
1	A	838	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	A	619	PHE	CA-C-N	5.32	127.40	120.28
1	A	619	PHE	C-N-CA	5.32	127.40	120.28
1	A	322	TYR	O-C-N	-5.31	116.50	122.12
1	A	520	VAL	O-C-N	5.31	128.58	122.64
1	A	405	ILE	CA-CB-CG2	-5.30	101.48	110.50
1	A	1048	VAL	CA-C-O	-5.30	114.74	120.47
1	A	123	ILE	N-CA-CB	5.30	117.36	110.57
1	A	923	PRO	N-CA-CB	5.30	109.14	103.52
1	A	594	ILE	CA-C-O	5.30	126.87	120.67
1	A	1124	ALA	CA-C-O	5.29	126.15	120.55
1	A	382	ASP	CA-C-O	-5.29	114.65	120.36
1	A	1081	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	184	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	446	MET	CG-SD-CE	-5.27	89.30	100.90
1	A	751	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	914	THR	CA-C-N	5.26	127.33	120.28
1	A	914	THR	C-N-CA	5.26	127.33	120.28
1	A	209	LYS	N-CA-C	-5.26	104.98	111.40
1	A	782	LYS	CA-C-N	5.26	127.59	120.38
1	A	782	LYS	C-N-CA	5.26	127.59	120.38
1	A	1003	HIS	CA-C-N	5.26	128.93	120.30
1	A	1003	HIS	C-N-CA	5.26	128.93	120.30
1	A	528	SER	N-CA-C	-5.26	102.21	110.36
1	A	1181	ALA	N-CA-CB	5.25	117.84	110.12
1	A	864	ILE	O-C-N	-5.24	115.88	121.80
1	A	489	GLU	CB-CG-CD	-5.24	103.69	112.60
1	A	301	LEU	CA-C-N	5.24	127.26	120.56
1	A	301	LEU	C-N-CA	5.24	127.26	120.56
1	A	712	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	880	LEU	N-CA-C	5.23	116.79	111.14
1	A	936	ILE	CA-C-O	-5.23	114.83	120.47
1	A	1130	GLY	O-C-N	-5.22	118.32	122.81
1	A	977	ILE	N-CA-C	-5.22	105.41	110.42
1	A	124	VAL	CA-C-N	5.22	127.54	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	VAL	C-N-CA	5.22	127.54	120.44
1	A	1051	GLY	CA-C-N	-5.22	115.80	123.00
1	A	1051	GLY	C-N-CA	-5.22	115.80	123.00
1	A	123	ILE	CA-C-N	5.22	129.57	120.86
1	A	123	ILE	C-N-CA	5.22	129.57	120.86
1	A	312	TYR	N-CA-CB	5.21	118.90	110.40
1	A	535	ILE	N-CA-C	-5.21	105.63	110.53
1	A	582	ALA	CA-C-N	5.21	131.28	122.26
1	A	582	ALA	C-N-CA	5.21	131.28	122.26
1	A	856	LEU	CA-C-O	5.21	126.07	120.55
1	A	1111	ILE	CA-CB-CG1	5.21	119.26	110.40
1	A	768	LEU	N-CA-CB	5.21	117.78	110.12
1	A	52	VAL	CA-C-N	5.21	125.72	119.94
1	A	52	VAL	C-N-CA	5.21	125.72	119.94
1	A	256	ALA	CA-C-N	5.20	127.87	120.53
1	A	256	ALA	C-N-CA	5.20	127.87	120.53
1	A	1187	VAL	CA-C-N	5.20	129.40	120.72
1	A	1187	VAL	C-N-CA	5.20	129.40	120.72
1	A	714	ALA	CA-C-N	5.19	127.21	120.56
1	A	714	ALA	C-N-CA	5.19	127.21	120.56
1	A	126	TYR	N-CA-C	5.19	116.93	111.28
1	A	721	GLN	CA-C-O	-5.18	113.86	118.63
1	A	1036	VAL	CA-CB-CG2	-5.18	101.59	110.40
1	A	161	VAL	N-CA-CB	5.18	116.90	111.00
1	A	367	ASN	N-CA-CB	5.18	119.24	110.49
1	A	494	ASP	CA-C-O	-5.18	115.06	120.55
1	A	1202	LEU	N-CA-C	-5.18	101.43	109.14
1	A	483	ASN	N-CA-C	5.17	116.92	111.28
1	A	1067	SER	CA-C-N	5.17	128.06	120.71
1	A	1067	SER	C-N-CA	5.17	128.06	120.71
1	A	141	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	1175	GLY	CA-C-N	5.17	127.16	120.44
1	A	1175	GLY	C-N-CA	5.17	127.16	120.44
1	A	750	LEU	CA-C-N	5.17	127.16	120.44
1	A	750	LEU	C-N-CA	5.17	127.16	120.44
1	A	615	LYS	N-CA-CB	5.17	119.22	110.49
1	A	383	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	A	182	ILE	N-CA-C	-5.16	106.86	112.80
1	A	1163	THR	N-CA-CB	5.16	117.65	109.71
1	A	246	ALA	N-CA-CB	5.16	117.70	110.12
1	A	534	ARG	N-CA-C	5.15	116.89	111.28
1	A	198	GLY	CA-C-N	5.14	125.55	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLY	C-N-CA	5.14	125.55	119.94
1	A	69	LEU	N-CA-C	-5.14	105.75	111.36
1	A	839	LEU	N-CA-C	5.14	116.57	111.07
1	A	231	ILE	CB-CA-C	5.14	118.75	112.02
1	A	886	LEU	CA-C-N	5.13	127.43	120.65
1	A	886	LEU	C-N-CA	5.13	127.43	120.65
1	A	156	ILE	N-CA-CB	5.13	116.88	110.47
1	A	932	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	1242	ILE	CA-CB-CG2	5.13	119.22	110.50
1	A	522	GLU	N-CA-C	5.13	116.10	108.31
1	A	807	THR	N-CA-CB	5.12	117.58	109.94
1	A	343	GLN	OE1-CD-NE2	5.12	127.72	122.60
1	A	1075	VAL	N-CA-C	5.12	115.73	110.36
1	A	394	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	A	143	ILE	N-CA-C	5.11	115.33	110.42
1	A	1191	HIS	ND1-CE1-NE2	5.11	113.51	108.40
1	A	477	ALA	CA-C-N	5.11	130.25	121.87
1	A	477	ALA	C-N-CA	5.11	130.25	121.87
1	A	1003	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	A	1245	GLY	N-CA-C	-5.11	108.28	114.92
1	A	370	SER	CA-CB-OG	5.10	121.31	111.10
1	A	1111	ILE	O-C-N	-5.10	117.22	122.63
1	A	1136	VAL	CB-CA-C	5.09	118.84	110.69
1	A	424	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	983	ALA	CA-C-N	5.09	127.16	120.60
1	A	983	ALA	C-N-CA	5.09	127.16	120.60
1	A	317	VAL	CA-C-N	5.08	127.06	120.70
1	A	317	VAL	C-N-CA	5.08	127.06	120.70
1	A	700	ASN	CA-C-N	5.08	127.60	120.28
1	A	700	ASN	C-N-CA	5.08	127.60	120.28
1	A	1224	ILE	CA-CB-CG1	5.08	119.04	110.40
1	A	1255	GLN	OE1-CD-NE2	5.08	127.68	122.60
1	A	608	HIS	CA-C-O	-5.08	115.49	120.82
1	A	702	THR	O-C-N	-5.08	116.73	122.12
1	A	875	LEU	O-C-N	-5.08	116.75	122.03
1	A	1027	LEU	CA-C-N	5.08	131.24	121.54
1	A	1027	LEU	C-N-CA	5.08	131.24	121.54
1	A	1143	ARG	N-CA-C	5.07	116.81	111.28
1	A	451	GLY	O-C-N	5.07	128.53	122.34
1	A	182	ILE	CA-C-N	5.07	131.34	121.41
1	A	182	ILE	C-N-CA	5.07	131.34	121.41
1	A	828	ARG	N-CA-CB	5.06	117.30	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	CA-C-O	5.06	126.31	120.90
1	A	401	LYS	CA-C-N	5.06	130.04	122.86
1	A	401	LYS	C-N-CA	5.06	130.04	122.86
1	A	903	VAL	O-C-N	-5.06	115.14	122.12
1	A	943	ALA	N-CA-CB	5.05	118.11	110.28
1	A	83	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	881	LYS	N-CA-C	5.05	117.51	111.71
1	A	1049	LEU	N-CA-CB	5.04	118.64	110.42
1	A	1103	GLN	CA-C-N	5.04	127.97	120.31
1	A	1103	GLN	C-N-CA	5.04	127.97	120.31
1	A	877	GLY	O-C-N	-5.04	117.36	122.19
1	A	466	ILE	CB-CA-C	5.03	117.53	110.99
1	A	503	ALA	CB-CA-C	-5.03	101.41	110.37
1	A	967	PHE	CA-C-O	5.02	125.87	120.55
1	A	728	PHE	CA-C-O	-5.02	115.23	120.55
1	A	569	LEU	CA-C-N	5.02	127.00	120.28
1	A	569	LEU	C-N-CA	5.02	127.00	120.28
1	A	292	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	A	214	ILE	CB-CG1-CD1	5.01	124.33	113.80
1	A	234	SER	N-CA-C	5.01	116.55	111.14
1	A	289	ILE	O-C-N	5.01	127.10	121.94
1	A	287	LYS	CA-C-O	-5.01	115.56	120.82
1	A	814	LEU	N-CA-CB	5.01	117.93	110.22
1	A	1082	PHE	O-C-N	5.01	130.20	123.34
1	A	735	PHE	CZ-CE2-CD2	-5.00	110.99	120.00
1	A	820	GLN	O-C-N	5.00	127.85	122.15

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	112	TYR	Sidechain
1	A	1138	TYR	Sidechain
1	A	1179	ARG	Sidechain
1	A	1218	ARG	Sidechain
1	A	1263	TYR	Sidechain
1	A	1264	PHE	Sidechain
1	A	170	ARG	Sidechain
1	A	197	PHE	Sidechain
1	A	322	TYR	Sidechain
1	A	359	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	39	PHE	Sidechain
1	A	41	TYR	Sidechain
1	A	440	TYR	Sidechain
1	A	460	ARG	Sidechain
1	A	486	TYR	Sidechain
1	A	49	TYR	Sidechain
1	A	523	ARG	Sidechain
1	A	618	TYR	Sidechain
1	A	693	PHE	Sidechain
1	A	706	TYR	Sidechain
1	A	783	ARG	Sidechain
1	A	849	TYR	Sidechain
1	A	938	PHE	Sidechain
1	A	958	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9171	0	9344	21	0
2	A	54	0	24	0	0
All	All	9225	0	9368	21	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 1.

All (21) 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:33:VAL:HG23	1:A:34:SER:H	1.66	0.60
1:A:405:ILE:HD13	1:A:405:ILE:H	1.69	0.58
1:A:64:LEU:HD22	1:A:64:LEU:H	1.68	0.57
1:A:421:LEU:HD12	1:A:581:ILE:HG12	1.93	0.50
1:A:395:PHE:O	1:A:404:GLN:HA	2.15	0.47
1:A:813:ARG:HA	1:A:813:ARG:HE	1.80	0.46
1:A:167:LEU:HD23	1:A:170:ARG:HH21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:PHE:CZ	1:A:775:LYS:HD2	2.51	0.46
1:A:1084:ASP:HB3	1:A:1085:PRO:HD2	1.98	0.46
1:A:36:LEU:HD23	1:A:36:LEU:H	1.82	0.45
1:A:356:GLY:HA2	1:A:359:TYR:CZ	2.51	0.45
1:A:894:THR:HA	1:A:897:ILE:HG12	1.99	0.44
1:A:352:ALA:HA	1:A:355:ARG:HH21	1.81	0.44
1:A:1037:VAL:HG22	1:A:1087:ALA:HB3	2.00	0.43
1:A:696:ILE:HD12	1:A:696:ILE:H	1.85	0.41
1:A:624:THR:HB	1:A:625:GLN:HE21	1.86	0.41
1:A:63:ALA:HB1	1:A:117:ILE:HG23	2.03	0.41
1:A:394:HIS:HB3	1:A:404:GLN:HE22	1.85	0.41
1:A:1071:GLY:O	1:A:1075:VAL:HG23	2.21	0.41
1:A:40:ARG:HH12	1:A:351:PHE:HZ	1.69	0.41
1:A:420:ALA:CB	1:A:588:VAL:HG13	2.51	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	1178/1276 (92%)	1079 (92%)	71 (6%)	28 (2%)	4 27

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	TYR
1	A	514	HIS
1	A	705	PRO
1	A	707	PHE
1	A	1016	SER
1	A	1028	GLU
1	A	43	GLY

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Mol	Chain	Res	Type
1	A	372	ASP
1	A	375	SER
1	A	797	VAL
1	A	1045	SER
1	A	1131	ASP
1	A	1197	GLU
1	A	1234	GLN
1	A	367	ASN
1	A	438	ARG
1	A	490	ASP
1	A	574	GLU
1	A	599	GLY
1	A	1046	ILE
1	A	1157	LEU
1	A	1159	ASP
1	A	802	ASP
1	A	957	ALA
1	A	1092	LEU
1	A	1040	TYR
1	A	371	ILE
1	A	1024	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	976/1057 (92%)	930 (95%)	46 (5%)	23	45

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	MET
1	A	64	LEU
1	A	65	PRO
1	A	86	LYS
1	A	167	LEU

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Mol	Chain	Res	Type
1	A	195	THR
1	A	210	LEU
1	A	230	LYS
1	A	259	THR
1	A	300	LEU
1	A	324	ILE
1	A	405	ILE
1	A	407	LYS
1	A	471	GLN
1	A	478	THR
1	A	491	VAL
1	A	542	VAL
1	A	551	ASP
1	A	559	THR
1	A	577	THR
1	A	579	ILE
1	A	598	ASP
1	A	706	TYR
1	A	744	GLN
1	A	834	GLN
1	A	894	THR
1	A	903	VAL
1	A	904	VAL
1	A	906	LEU
1	A	920	LEU
1	A	937	THR
1	A	961	THR
1	A	968	GLU
1	A	1095	LYS
1	A	1104	TRP
1	A	1114	GLN
1	A	1160	LYS
1	A	1164	ARG
1	A	1186	LEU
1	A	1187	VAL
1	A	1192	ILE
1	A	1210	VAL
1	A	1234	GLN
1	A	1239	ILE
1	A	1247	VAL
1	A	1255	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	90	ASN
1	A	128	GLN
1	A	145	GLN
1	A	162	HIS
1	A	168	ASN
1	A	179	ASN
1	A	292	ASN
1	A	392	ASN
1	A	404	GLN
1	A	504	ASN
1	A	515	GLN
1	A	526	GLN
1	A	608	HIS
1	A	717	ASN
1	A	737	ASN
1	A	747	ASN
1	A	805	ASN
1	A	834	GLN
1	A	852	GLN
1	A	910	GLN
1	A	921	GLN
1	A	926	ASN
1	A	962	GLN
1	A	986	GLN
1	A	1020	GLN
1	A	1025	ASN
1	A	1101	ASN
1	A	1108	GLN
1	A	1149	ASN
1	A	1151	HIS
1	A	1191	HIS
1	A	1211	GLN
1	A	1259	GLN

5.3.3 RNA ⓘ

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](#)

2 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$
2	ADP	A	2001	-	28,29,29	1.64	3 (10%)	43,45,45	1.28	6 (13%)
2	ADP	A	2000	-	28,29,29	2.09	4 (14%)	43,45,45	1.24	4 (9%)

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
2	ADP	A	2001	-	-	2/16/32/32	0/3/3/3
2	ADP	A	2000	-	-	10/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	ADP	PA-O3A	8.70	1.68	1.59
2	A	2001	ADP	PA-O3A	5.29	1.65	1.59
2	A	2001	ADP	C5-C4	2.88	1.44	1.39
2	A	2000	ADP	PB-O1B	2.40	1.57	1.50
2	A	2000	ADP	PB-O3B	-2.33	1.46	1.54
2	A	2001	ADP	C2'-C1'	2.21	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	ADP	C5-N7	-2.08	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	ADP	C5-N7-C8	2.95	108.09	103.45
2	A	2001	ADP	N6-C6-N1	2.72	124.44	118.38
2	A	2000	ADP	C6-C5-N7	-2.48	127.32	132.09
2	A	2001	ADP	C2-N1-C6	2.38	122.64	118.73
2	A	2000	ADP	C1'-N9-C8	2.38	132.38	127.09
2	A	2001	ADP	O4'-C4'-C5'	2.24	116.50	109.33
2	A	2001	ADP	C4-C5-N7	-2.23	108.03	110.58
2	A	2000	ADP	C2'-C3'-C4'	-2.04	98.67	102.61
2	A	2001	ADP	N3-C2-N1	-2.02	125.52	128.58
2	A	2000	ADP	O5'-C5'-C4'	2.02	115.86	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

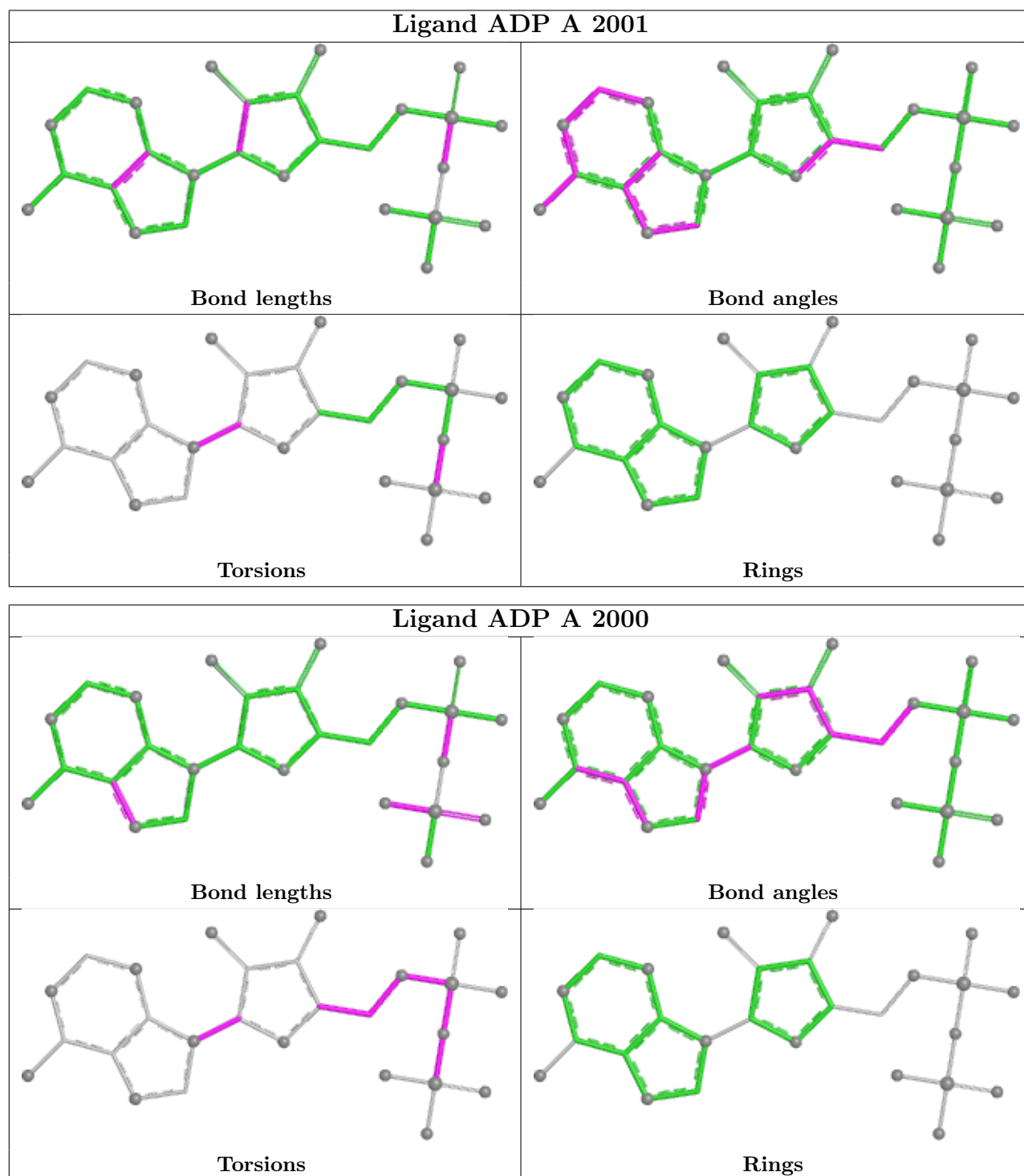
Mol	Chain	Res	Type	Atoms
2	A	2000	ADP	PA-O3A-PB-O2B
2	A	2000	ADP	C5'-O5'-PA-O1A
2	A	2000	ADP	C2'-C1'-N9-C8
2	A	2000	ADP	O4'-C4'-C5'-O5'
2	A	2000	ADP	C2'-C1'-N9-C4
2	A	2000	ADP	C3'-C4'-C5'-O5'
2	A	2000	ADP	C5'-O5'-PA-O2A
2	A	2000	ADP	C5'-O5'-PA-O3A
2	A	2000	ADP	C4'-C5'-O5'-PA
2	A	2001	ADP	PA-O3A-PB-O2B
2	A	2001	ADP	C2'-C1'-N9-C8
2	A	2000	ADP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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.

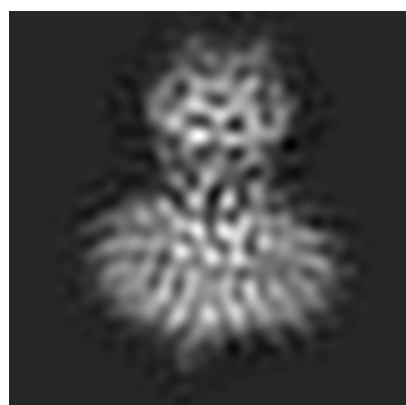
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4391. These allow visual inspection of the internal detail of the map and identification of artifacts.

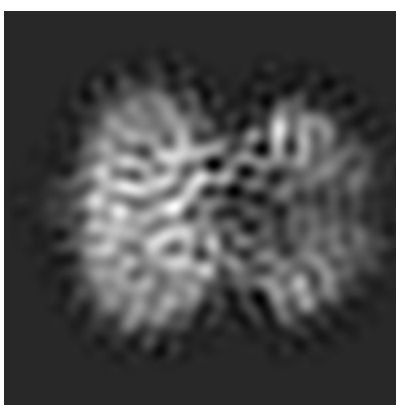
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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](#)

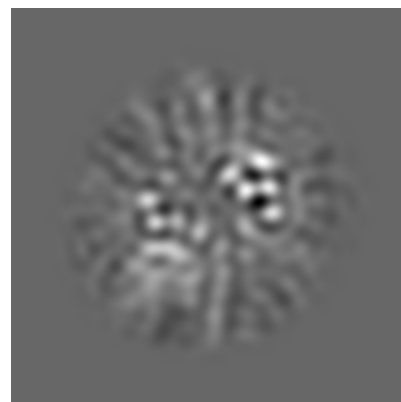
6.2.1 Primary map



X Index: 78



Y Index: 78



Z Index: 78

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: 99



Y Index: 85



Z Index: 106

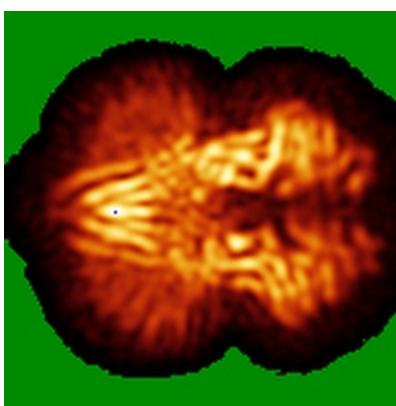
The images above show the largest variance slices of the map in three orthogonal directions.

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

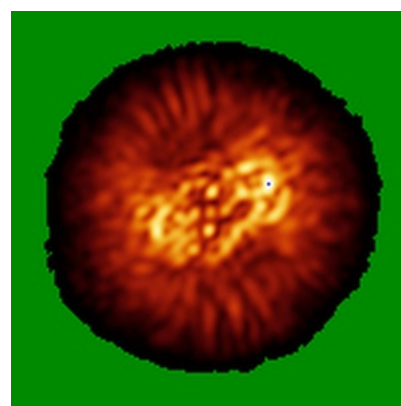
6.4.1 Primary map



X



Y

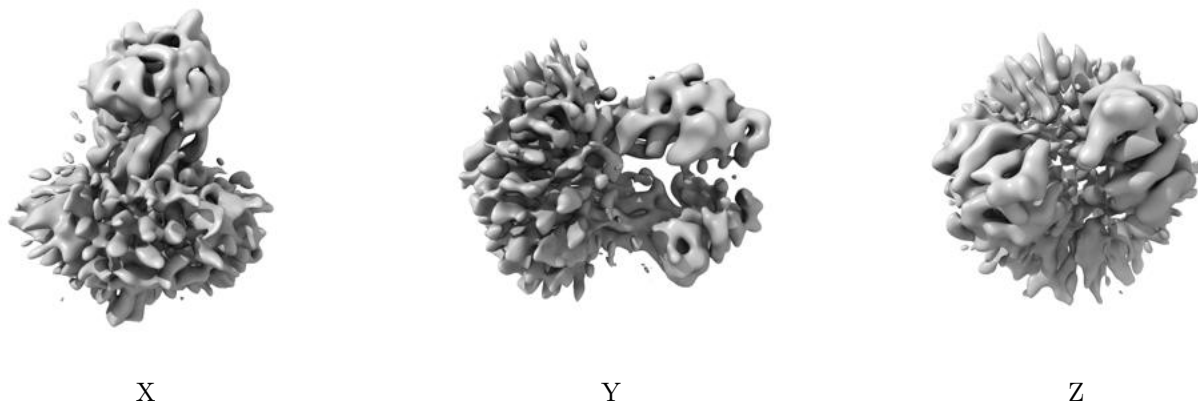


Z

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

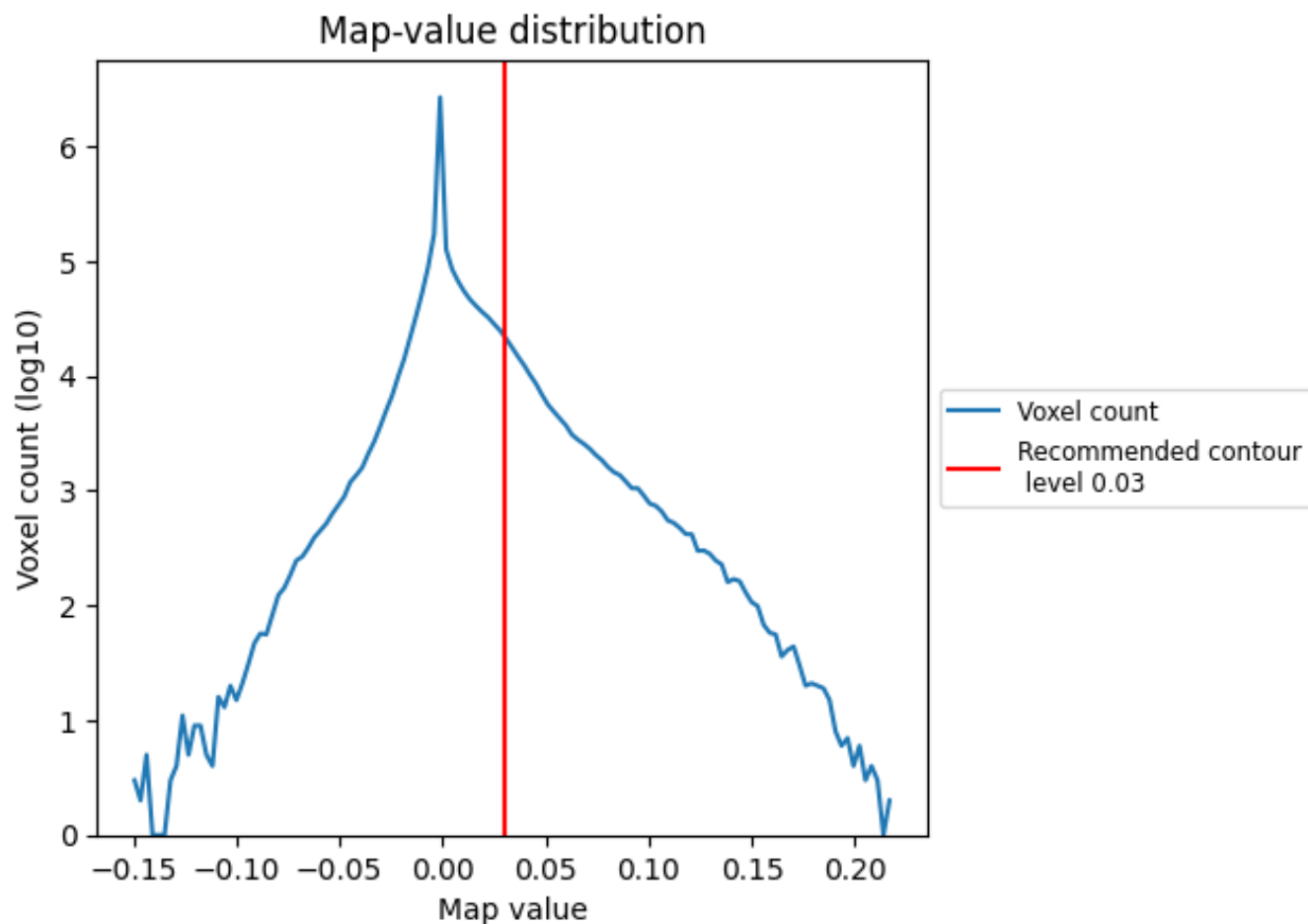
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

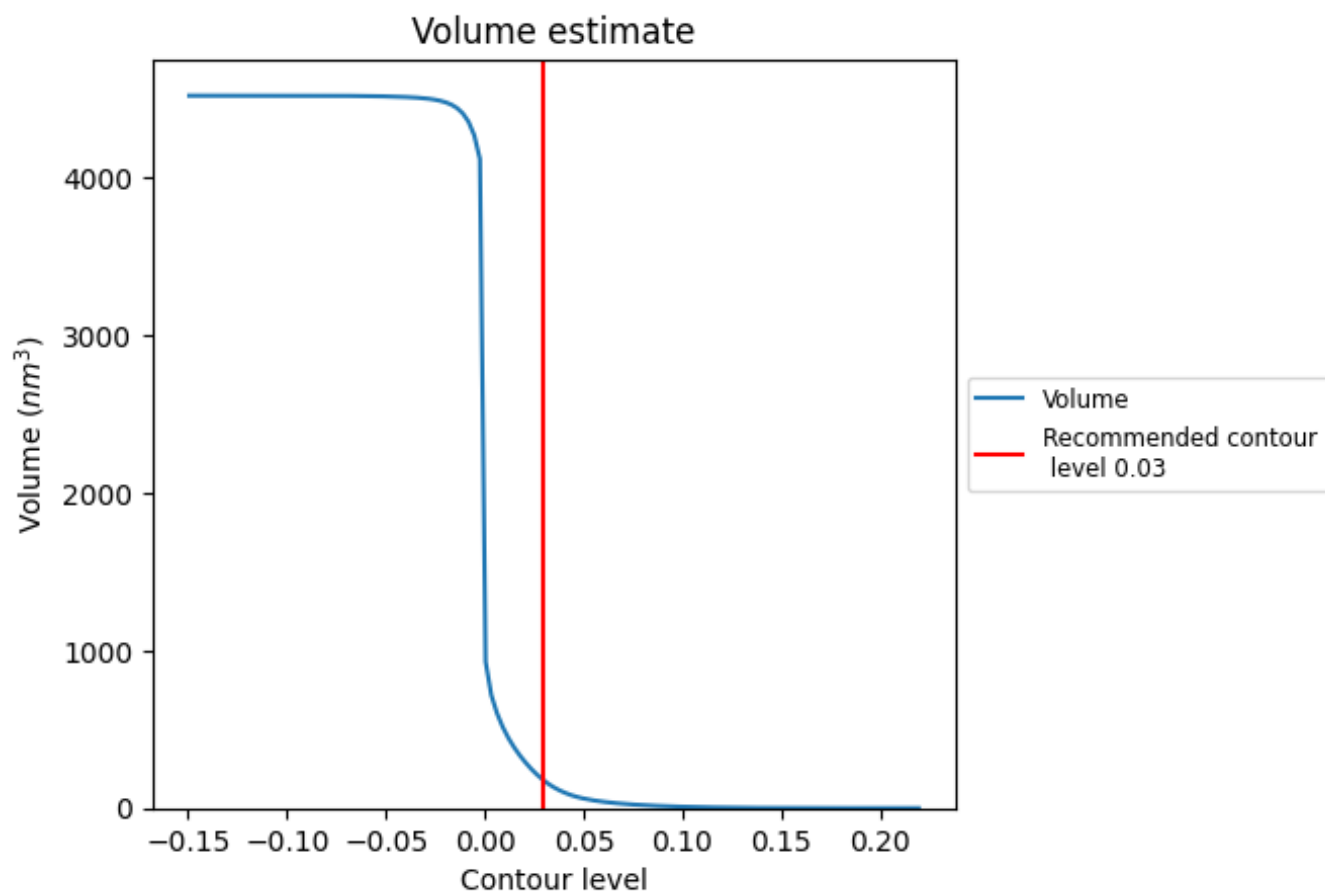
This section contains the results of statistical analysis of the map.

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.

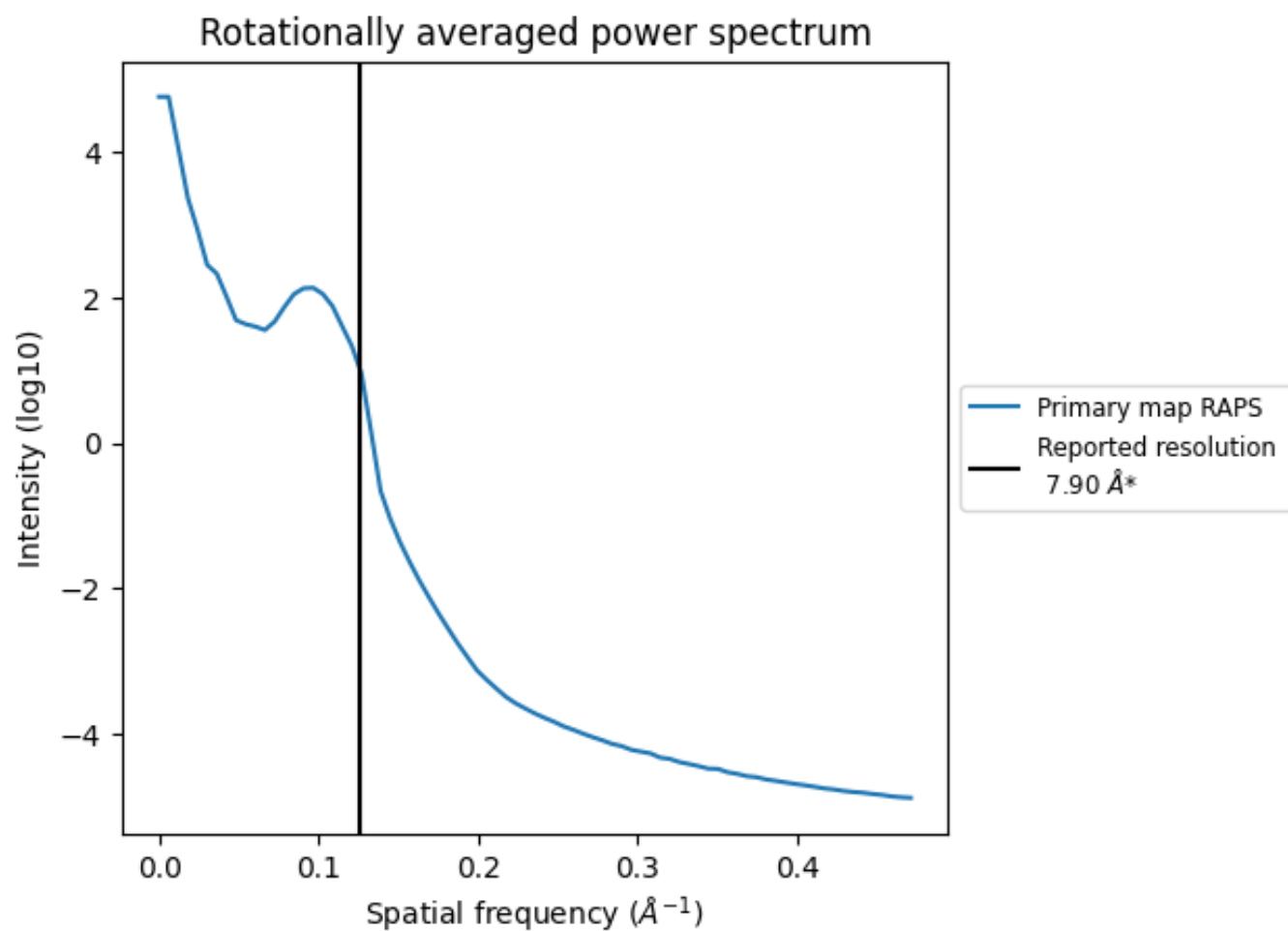
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 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 ⓘ

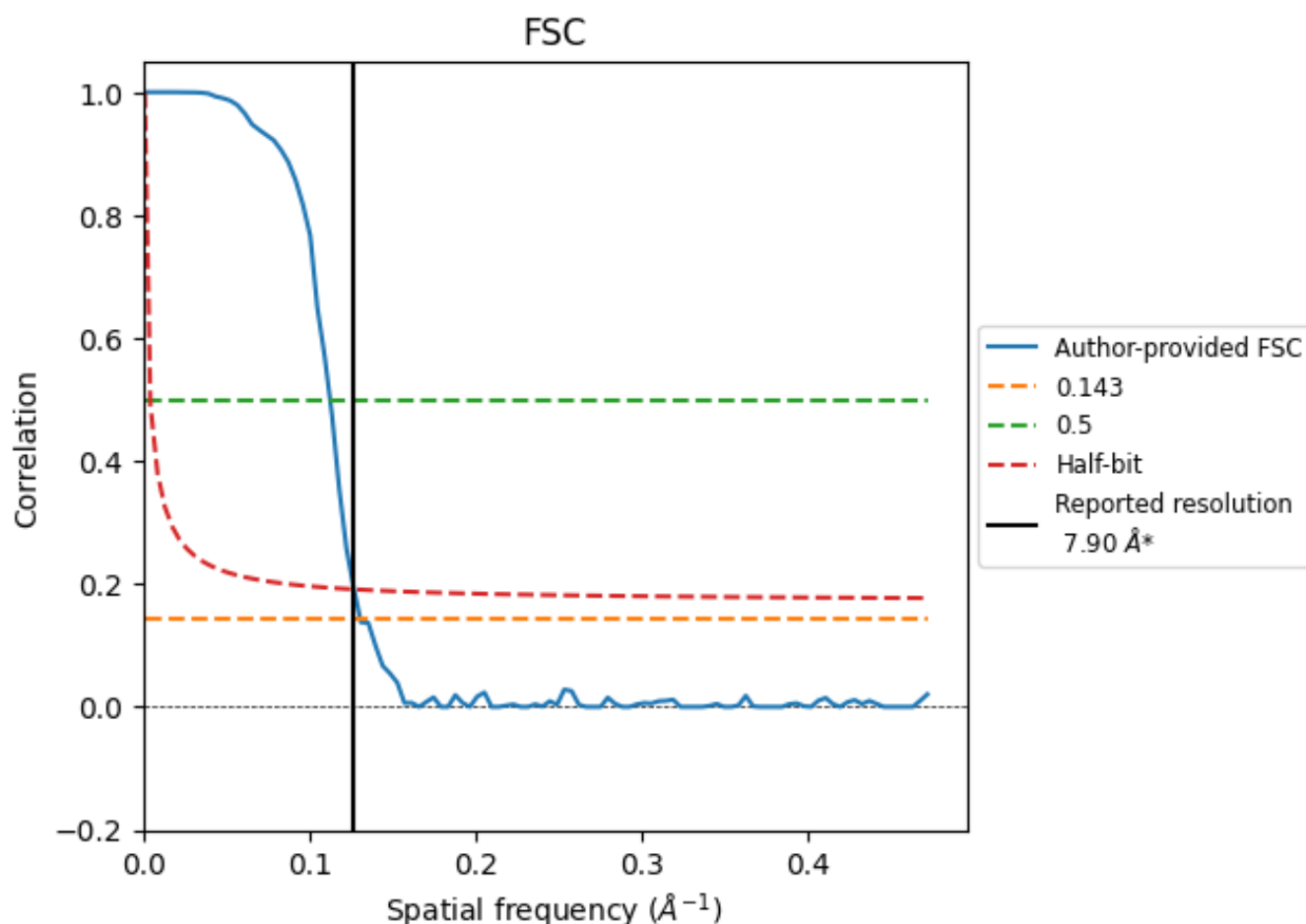


*Reported resolution corresponds to spatial frequency of 0.127 $\text{\AA}^{-1}$

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 0.127 Å⁻¹

8.2 Resolution estimates [i](#)

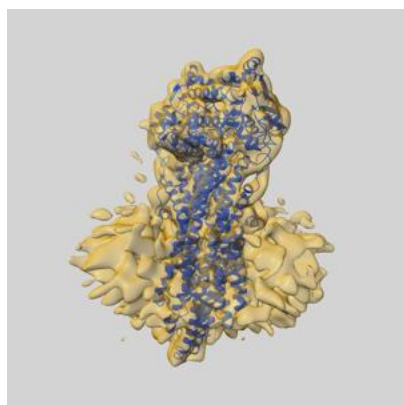
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.66	8.90	7.89
Unmasked-calculated*	-	-	-

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

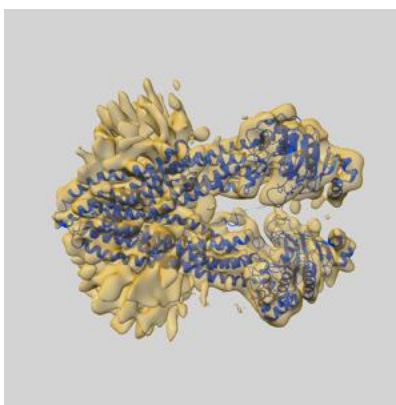
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4391 and PDB model 6Q81. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

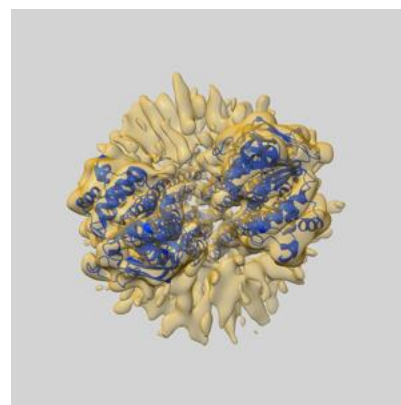
9.1 Map-model overlay [i](#)



X



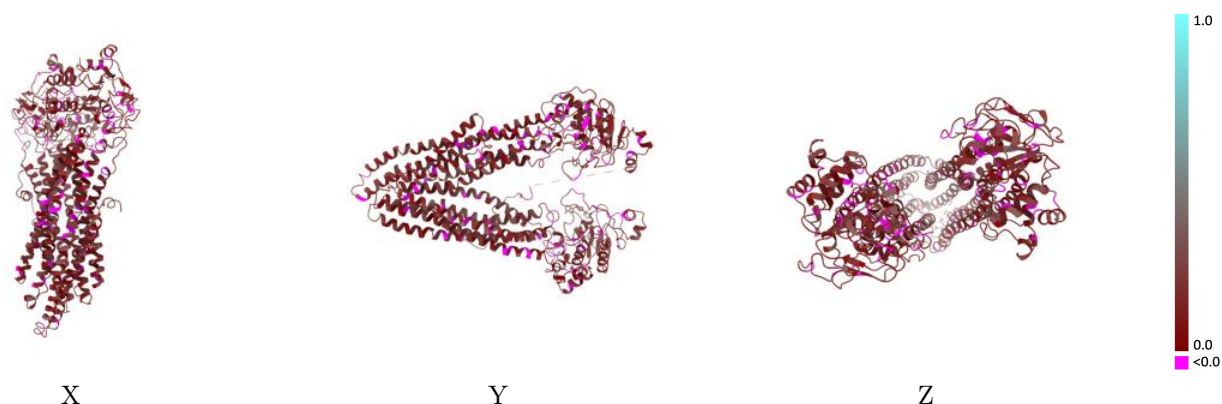
Y



Z

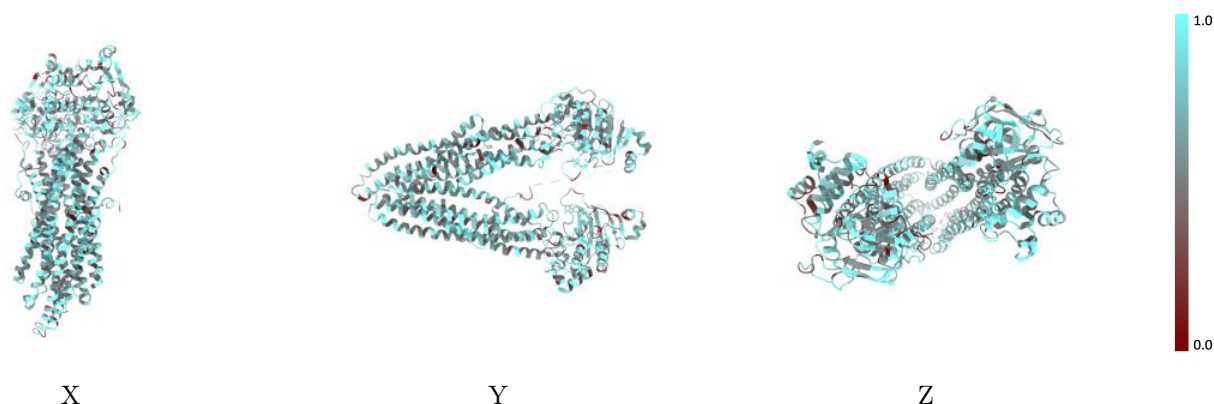
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



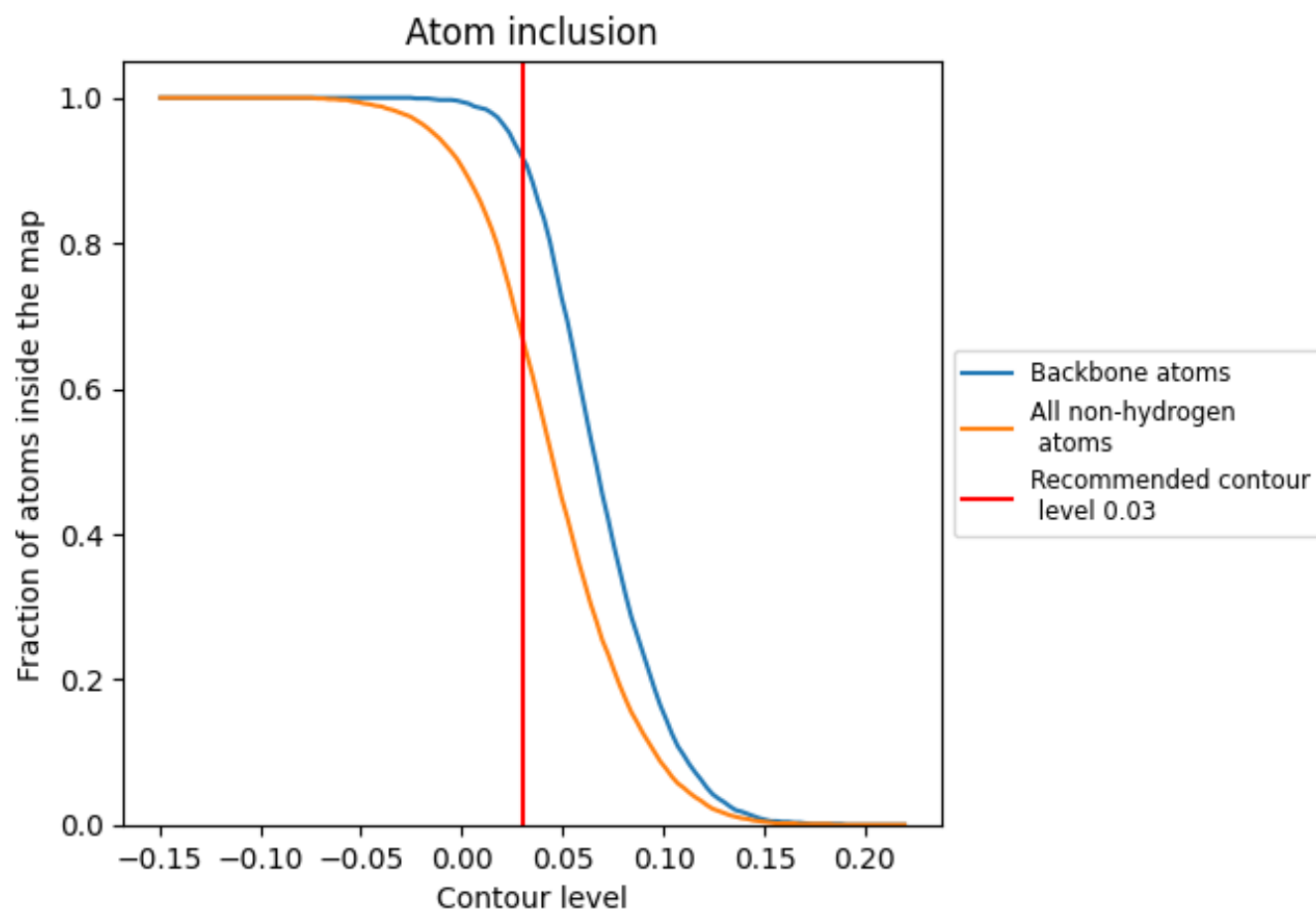
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 67% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6710	0.1390
A	0.6710	0.1390

