



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 06:51 PM UTC

PDB ID : 7JPL / pdb_00007jpl
EMDB ID : EMD-22415
Title : Rabbit Cav1.1 in the presence of 10 micromolar (S)-(-)-Bay K8644 in nanodiscs at 3.4 Angstrom resolution
Authors : Yan, N.; Gao, S.
Deposited on : 2020-08-09
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

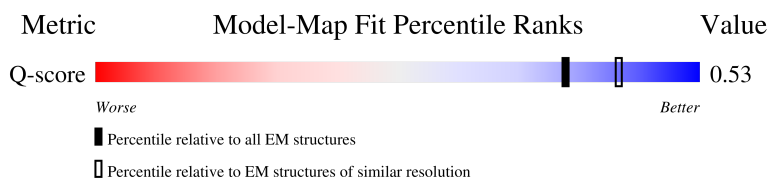
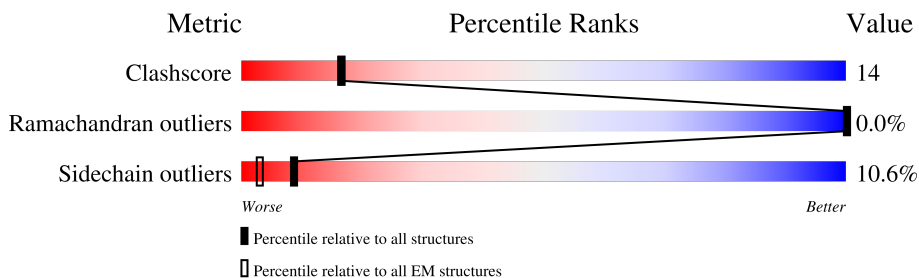
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1873	
2	E	222	
3	F	1105	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18565 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1114	Total	C	N	O	S	0	0
			8998	5970	1433	1536	59		

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	169	Total	C	N	O	S	0	0
			1326	872	216	220	18		

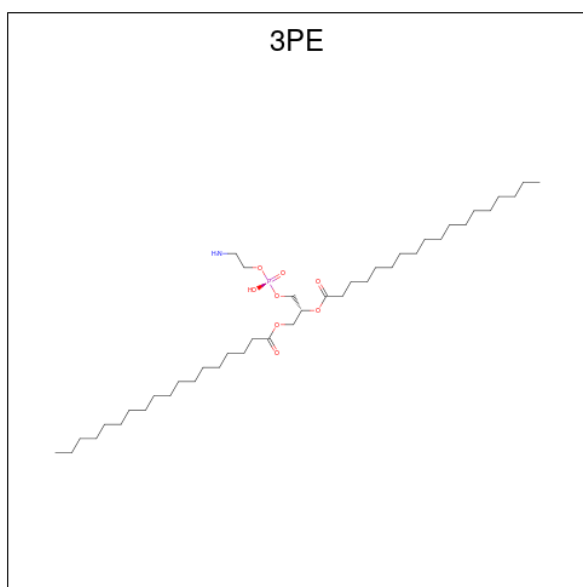
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	973	Total	C	N	O	S	1	0
			7804	4942	1320	1510	32		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

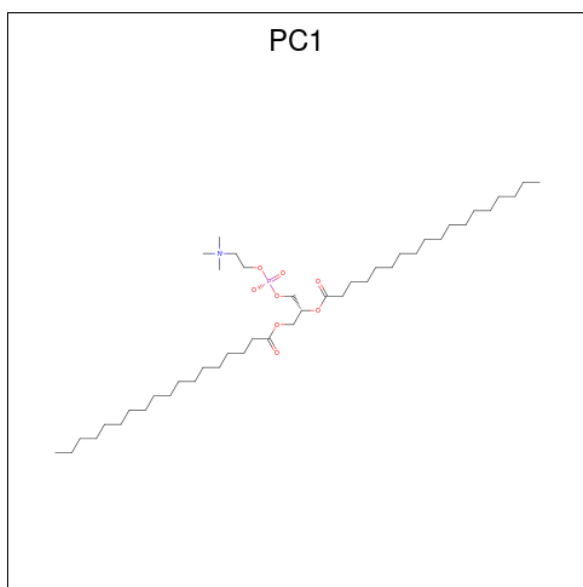
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



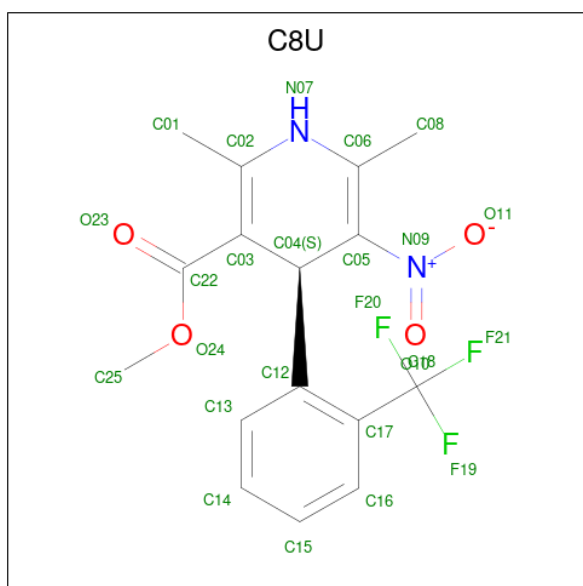
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
5	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

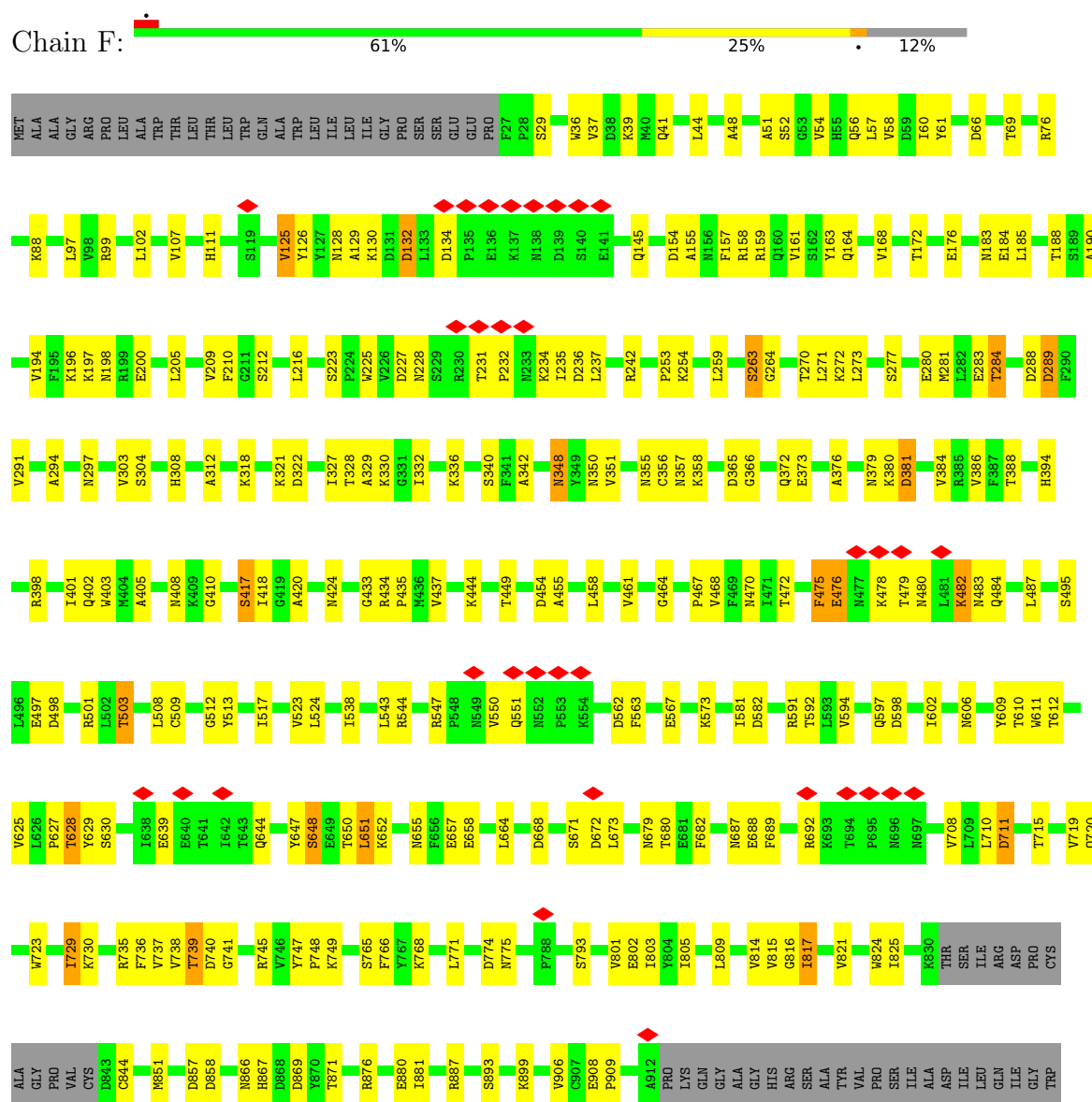
- Molecule 7 is methyl (4 {S})-2,6-dimethyl-5-nitro-4-[2-(trifluoromethyl)phenyl]-1,4-dihydropyridine-3-carboxylate (CCD ID: C8U) (formula: $C_{16}H_{15}F_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).

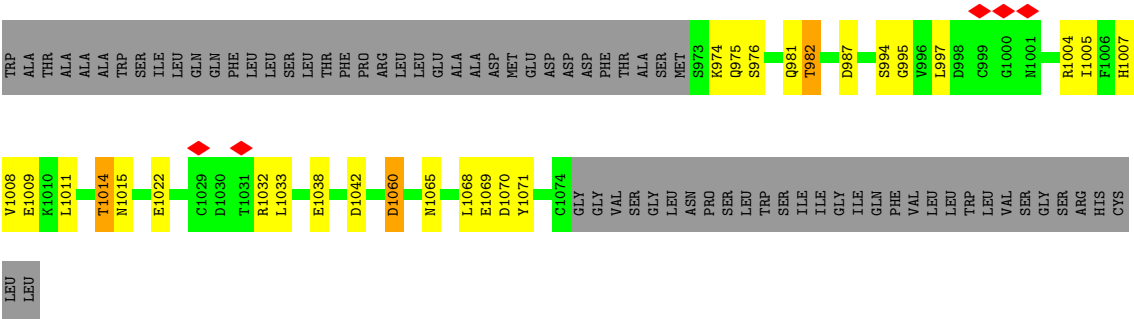


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			25	16	3	2	4	

LEU	LYS	GLY	PRO	THR	MET	PHE	THR	E1412	Q1299	GLY	M124	V1039	G929	LYS	ARG
ALA	SER	GLY	HIS	ALA	GLU	ARG	ALA	A1413	I1300	CYS	F1125	E1040	N930	GLY	ILE
ARG	PRO	THR	SER	LEU	GLU	LYS	LEU	K1414	N1301	ASN		M1041	I931	SER	
GLY	PRO	ARG	LYS	ILE	ILE	LYS	THR		R1302	VAL	M129	I1043	L933	CYS	
VAL	ALA	ARG	ALA	THR	PHE	ARG	THR	I1417	N1303	ASP	I1133	F1044	V934	ARG	
PRO	ALA	ARG	ALA	GLN	THR	GLN	GLY	K1418	N1304	PRO		F1045	T935	ASN	
GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	H1419	Q1307	ASP	H1141	I1047	T936		
LEU	LEU	THR	LEU	THR	GLY	GLY	THR	L1420	T1308	SER	GLN	I1048	L937		
ALA	ASN	ALA	ASN	PHE	GLY	THR	PHE	L1421	F1309	ALA	SER	I1049	Q939		
GLY	ALA	GLY	ALA	GLN	GLY	THR	GLN	D1421	P1310	ARG	GLU	I1049	F940		
LEU	ASN	PHE	ASN	ALA	PHE	THR	ALA	V1423	V1313	ILE	GLU		M941		
VAL	ASN	GLY	ASN	ALA	GLY	TYR	ALA	T1424		SER	MET	N1058	F942		
ILE	ASN	VAL	ASN	GLN	GLN	TYR	ASN	L1425	R1318	ASN	ASN	I1059	A943		
PRO	ALA	VAL	VAL	GLU	VAL	PRO	GLU			F1234	I1148		Q944		
GLY	PRO	GLY	ALA	LEU	THR	LYS	LEU	L1426	E1323	GLY	I1149	V1064	I945		
MET	GLY	THR	TYR	ARG	ASP	THR	ARG	R1427	A1324	ARG	I1152	E1070	Q946		
PRO	PRO	GLY	GLY	ALA	LEU	THR	ALA	R1428	W1325	ALA	L1153	G1071	Q948		
ILE	ASN	VAL	ILE	ILE	LEU	VAL	ILE	I1429	Y1344	THR	N1154	G1072			
GLY	ASN	THR	GLN	ILE	GLU	VAL	LYS	Q1430	E1348	LYS	T1158	GLU	K951		
LEU	ASN	ASP	LYS	ILE	ARG	GLY	LYS	P1431		L1243		THR	G952		
ASP	ASN	THR	ASN	ILE	LEU	GLY	TRP	G1434	T1351	L1246	T1162	GLU	K953		
THR	GLN	LEU	GLN	ALA	PRO	LEU	ALA		C1352	L1247	L1163	GLY			
ALA	PRO	PRO	ALA	GLY	ARG	ARG	ARG	PHE	G1353	S1248	E1164	TYR	S961		
VAL	ALA	VAL	ALA	THR	THR	THR	THR	LYS	T1354	S1249		LYS	Y973		
ASP	GLY	ILE	ILE	ILE	ILE	ILE	MET	PHE		R1249	L1167	CYS	V974		
ALA	GLY	THR	THR	THR	THR	THR	THR	CYS	Y1359	A1250	K1168	GLU			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO		E1251	L1169	LEU	D977		
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	HIS	F1361	T1255	A1171	Q1085	M983		
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	ARG	G1362	L1256	K1172	R1086	E984		
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	VAL	S1363	L1257	K1173	THR	L985		
THR	THR	THR	THR	THR	THR	THR	THR	ALA		W1258	A1174	ILE			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	CYS	M1366	T1259	R1175	V1039	I991		
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LYS	F1370		L1093	L1093	D994		
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	PRO	L1371	S1263	L1188	Q1099			
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	PRO	I1372	F1264	I1189	Y1107			
THR	THR	THR	THR	THR	THR	THR	THR	VAL	I1373	Q1265		C1100			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	MET	N1374	V1270	D1196	Y1101			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASN			V1197		S1002		
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	MET	V1377	Y1275	I1198	K1104			
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASN	M1381	W1276	I1202	N1105	M1005		
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	PRO		L1277	D1203	P1106			
THR	THR	THR	THR	THR	THR	THR	THR	LEU	F1384	F1279	L1206	Y1107	T1009		
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL		I1280	ALA	Q1108			
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	T1388	Y1281	SER	Y1109	S1011		
THR	THR	THR	THR	THR	THR	THR	THR	GLY	R1389		GLY	Q1110	T1012		
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL		T1284	ALA	W1111	F1013		
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL	S1392		SER	W1112			
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR	I1393	Q1287	GLY	Y1113	W1016		
THR	THR	THR	THR	THR	THR	THR	THR	PHE	L1394		LEU	Y1114	P1017		
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASN		M1288	TYR	T1115	S1026		
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	ALA	H1397	F1289	CYS	T1116	N1027		
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	THR	E1408	G1290	LEU	S1117	E1028		
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	LEU			GLY	S1118	E1029		
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU		D1296	GLY	Y1119	D1030		
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL							
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG							

- Molecule 2: Voltage-dependent calcium channel gamma-1 subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.159	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.114, 1.114, 1.114	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: PC1, C8U, 3PE, CA

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	0.31	0/9222	0.49	2/12520 (0.0%)
2	E	0.20	0/1358	0.43	0/1832
3	F	0.38	0/7974	0.44	0/10816
All	All	0.34	0/18554	0.47	2/25168 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	VAL	N-CA-C	-6.08	107.94	113.71
1	A	1046	ILE	N-CA-C	-5.62	108.03	113.53

There are no chirality outliers.

There are no planarity outliers.

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	8998	0	9133	279	0
2	E	1326	0	1345	36	0
3	F	7804	0	7617	166	0
4	A	1	0	0	0	0
5	A	357	0	508	113	0
6	A	54	0	88	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	25	0	0	6	0
All	All	18565	0	18691	524	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 14.

All (524) 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:536:PHE:CE1	1:A:941:MET:HE1	1.35	1.59
1:A:646:VAL:CG1	5:A:1905:3PE:H3F1	1.37	1.50
1:A:536:PHE:HE1	1:A:941:MET:CE	1.20	1.50
5:A:1904:3PE:H371	7:A:1912:C8U:C25	1.50	1.41
1:A:536:PHE:CE1	1:A:941:MET:CE	1.99	1.33
1:A:282:MET:CE	5:A:1903:3PE:H371	1.74	1.16
1:A:646:VAL:HG12	5:A:1905:3PE:C3F	1.74	1.16
1:A:646:VAL:CG1	5:A:1905:3PE:C3F	2.24	1.15
5:A:1904:3PE:C37	7:A:1912:C8U:C25	2.25	1.14
1:A:282:MET:HE3	5:A:1903:3PE:H371	1.35	1.06
1:A:536:PHE:CD1	1:A:941:MET:HE1	1.95	1.01
1:A:646:VAL:HG12	5:A:1905:3PE:H3F1	1.00	1.00
5:A:1911:3PE:H2I1	5:A:1911:3PE:C3A	1.90	0.99
5:A:1911:3PE:H3A1	5:A:1911:3PE:C2I	1.93	0.98
1:A:163:ALA:CB	5:A:1906:3PE:H321	1.94	0.98
5:A:1911:3PE:H2I1	5:A:1911:3PE:H3A1	0.98	0.96
1:A:282:MET:HE1	5:A:1903:3PE:H382	1.47	0.93
3:F:386:VAL:O	3:F:410:GLY:HA3	1.67	0.93
5:A:1903:3PE:H391	5:A:1905:3PE:H372	1.51	0.92
1:A:567:PHE:HE1	5:A:1908:3PE:C29	1.83	0.91
5:A:1904:3PE:H221	5:A:1904:3PE:H31	1.53	0.90
1:A:536:PHE:CE1	1:A:941:MET:HE3	2.07	0.89
1:A:584:ARG:NH1	5:A:1906:3PE:O12	2.05	0.88
1:A:70:VAL:HG12	5:A:1907:3PE:H11	1.56	0.88
5:A:1903:3PE:H352	5:A:1905:3PE:H341	1.55	0.87
1:A:1366:MET:HE1	5:A:1904:3PE:H391	1.58	0.85
1:A:536:PHE:CD1	1:A:941:MET:CE	2.55	0.85
3:F:688:GLU:O	3:F:692:ARG:HB2	1.76	0.85
1:A:567:PHE:HZ	5:A:1907:3PE:H361	1.42	0.84
1:A:163:ALA:HB2	5:A:1906:3PE:H321	1.58	0.84
1:A:1044:PHE:HD1	5:A:1910:3PE:H221	1.42	0.84
1:A:536:PHE:HE1	1:A:941:MET:HE2	1.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:PHE:CE1	5:A:1908:3PE:C29	2.61	0.83
1:A:646:VAL:HG13	5:A:1905:3PE:H3F1	1.59	0.83
5:A:1904:3PE:H382	7:A:1912:C8U:C25	2.08	0.83
1:A:282:MET:HE1	5:A:1903:3PE:C38	2.08	0.82
1:A:1420:LEU:O	1:A:1423:VAL:N	2.12	0.82
1:A:282:MET:HE1	5:A:1903:3PE:H371	1.59	0.82
5:A:1904:3PE:C38	7:A:1912:C8U:C25	2.57	0.81
1:A:1046:ILE:CD1	5:A:1908:3PE:H262	2.11	0.81
5:A:1904:3PE:H31	5:A:1904:3PE:C22	2.08	0.81
1:A:646:VAL:HG11	5:A:1905:3PE:H3E2	1.63	0.80
1:A:646:VAL:HG11	5:A:1905:3PE:H3F1	1.56	0.80
1:A:163:ALA:HB1	5:A:1906:3PE:H321	1.63	0.78
1:A:112:PHE:O	1:A:113:HIS:ND1	2.16	0.78
1:A:567:PHE:CZ	5:A:1907:3PE:H361	2.18	0.78
1:A:282:MET:HE1	5:A:1903:3PE:C37	2.14	0.77
1:A:282:MET:CE	5:A:1903:3PE:C37	2.59	0.77
1:A:1370:PHE:HB2	5:A:1904:3PE:H2H1	1.66	0.76
1:A:510:GLU:HB3	1:A:527:LEU:HD12	1.68	0.75
1:A:646:VAL:HG11	5:A:1905:3PE:C3E	2.15	0.75
1:A:245:CYS:SG	1:A:246:ALA:N	2.58	0.75
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.68	0.75
3:F:235:ILE:H	3:F:551:GLN:HG3	1.52	0.75
1:A:646:VAL:HG11	5:A:1905:3PE:C3F	2.15	0.74
5:A:1903:3PE:C39	5:A:1905:3PE:H372	2.18	0.73
5:A:1906:3PE:H122	5:A:1906:3PE:O14	1.89	0.72
3:F:711:ASP:OD2	3:F:739:THR:OG1	2.04	0.72
1:A:58:LEU:HD11	1:A:178:GLY:HA3	1.72	0.72
3:F:858:ASP:OD1	3:F:1015:ASN:ND2	2.19	0.72
1:A:571:ILE:HD13	5:A:1907:3PE:H262	1.71	0.71
5:A:1910:3PE:O14	5:A:1910:3PE:H32	1.90	0.71
1:A:45:ILE:HD11	1:A:106:ILE:HG22	1.72	0.71
1:A:309:TRP:CE3	6:A:1909:PC1:H252	2.26	0.70
3:F:164:GLN:O	3:F:196:LYS:NZ	2.24	0.70
1:A:1359:TYR:CD2	5:A:1904:3PE:H231	2.27	0.69
3:F:37:VAL:HG21	3:F:1009:GLU:HG2	1.75	0.69
1:A:449:ILE:HG21	1:A:535:LEU:HD11	1.76	0.68
1:A:1275:VAL:HG13	5:A:1911:3PE:H2G2	1.74	0.68
1:A:510:GLU:OE1	1:A:531:ARG:NH1	2.26	0.68
1:A:1046:ILE:HD13	5:A:1908:3PE:H262	1.76	0.68
1:A:341:ARG:NH2	1:A:661:VAL:O	2.26	0.68
1:A:601:PRO:HB3	5:A:1908:3PE:O22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:MET:HE1	2:E:132:LYS:H	1.59	0.67
1:A:1046:ILE:HD12	5:A:1908:3PE:H262	1.75	0.67
3:F:184:GLU:O	3:F:188:THR:OG1	2.08	0.67
3:F:644:GLN:O	3:F:648:SER:OG	2.13	0.67
1:A:232:ASP:OD2	3:F:544:ARG:NH1	2.28	0.66
3:F:739:THR:OG1	3:F:740:ASP:N	2.27	0.66
1:A:542:TRP:HB3	1:A:545:LEU:HB2	1.78	0.66
1:A:78:ASP:OD1	1:A:79:ASN:N	2.28	0.66
3:F:658:GLU:O	3:F:720:GLN:NE2	2.28	0.65
1:A:1277:LEU:HD22	1:A:1371:LEU:HD12	1.78	0.65
5:A:1910:3PE:H32	5:A:1910:3PE:P	2.36	0.65
3:F:994:SER:HB3	3:F:1007:HIS:HD2	1.61	0.65
3:F:283:GLU:OE2	3:F:321:LYS:NZ	2.24	0.65
1:A:1313:VAL:HG12	5:A:1911:3PE:H362	1.79	0.64
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.79	0.64
1:A:338:THR:O	1:A:342:GLU:HG2	1.96	0.64
3:F:981:GLN:HG2	3:F:1038:GLU:HG3	1.79	0.64
1:A:529:CYS:O	5:A:1910:3PE:H352	1.98	0.64
3:F:472:THR:H	3:F:483:ASN:HD21	1.46	0.63
3:F:242:ARG:NH2	3:F:280:GLU:O	2.32	0.63
1:A:817:ALA:HB2	1:A:1279:PHE:HE1	1.63	0.63
1:A:112:PHE:HD2	1:A:115:ASP:H	1.46	0.63
3:F:273:LEU:O	3:F:277:SER:OG	2.14	0.63
1:A:64:ASN:OD1	1:A:171:ARG:NH1	2.29	0.62
3:F:228:ASN:HB2	3:F:232:PRO:HD3	1.81	0.62
3:F:652:LYS:O	3:F:655:ASN:ND2	2.32	0.62
1:A:307:ASN:OD1	5:A:1911:3PE:H12	2.00	0.62
5:A:1906:3PE:H112	5:A:1906:3PE:H12	1.82	0.62
1:A:633:PRO:CB	5:A:1906:3PE:H222	2.29	0.62
5:A:1910:3PE:O22	5:A:1910:3PE:H242	1.99	0.62
3:F:318:LYS:NZ	3:F:322:ASP:OD2	2.32	0.62
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.18	0.62
1:A:1255:THR:O	1:A:1259:THR:HG23	2.00	0.62
1:A:132:LEU:O	1:A:136:THR:HG23	2.00	0.61
3:F:154:ASP:OD2	3:F:163:TYR:OH	2.17	0.61
3:F:651:LEU:O	3:F:687:ASN:ND2	2.32	0.61
3:F:227:ASP:HB2	3:F:236:ASP:HB3	1.80	0.61
1:A:1039:VAL:CG1	5:A:1908:3PE:O12	2.47	0.61
1:A:114:GLN:HG3	1:A:116:ALA:HB2	1.82	0.61
1:A:116:ALA:O	1:A:120:SER:OG	2.18	0.61
3:F:444:LYS:NZ	3:F:467:PRO:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ILE:HG22	1:A:928:ILE:O	2.01	0.60
3:F:365:ASP:OD1	3:F:366:GLY:N	2.35	0.60
1:A:215:LEU:O	1:A:219:LYS:HB2	2.01	0.60
1:A:1039:VAL:HG13	5:A:1908:3PE:O12	2.01	0.60
1:A:62:PHE:CE1	5:A:1907:3PE:H281	2.37	0.60
1:A:448:SER:O	1:A:464:GLN:NE2	2.35	0.59
5:A:1903:3PE:H3A2	5:A:1905:3PE:H392	1.84	0.59
3:F:597:GLN:OE1	3:F:768:LYS:NZ	2.31	0.59
1:A:932:VAL:HG12	1:A:932:VAL:O	2.02	0.59
3:F:259:LEU:HD13	3:F:342:ALA:HB2	1.83	0.59
3:F:498:ASP:OD1	3:F:501:ARG:NH2	2.35	0.59
2:E:37:PRO:HA	2:E:174:ILE:HA	1.85	0.59
3:F:373:GLU:H	3:F:373:GLU:CD	2.11	0.59
3:F:503:THR:O	3:F:503:THR:OG1	2.21	0.58
1:A:999:ASN:HD22	1:A:1002:SER:H	1.52	0.58
1:A:1323:GLU:O	1:A:1325:TRP:N	2.35	0.58
1:A:909:ASN:HB3	1:A:910:ARG:HH11	1.67	0.58
3:F:281:MET:O	3:F:284:THR:OG1	2.21	0.58
1:A:527:LEU:HD13	1:A:530:ILE:HD11	1.86	0.57
1:A:115:ASP:HB3	1:A:119:ARG:HB2	1.84	0.57
1:A:532:LEU:HD11	1:A:945:ILE:HG12	1.85	0.57
1:A:473:SER:HA	1:A:476:THR:HG22	1.86	0.57
3:F:51:ALA:HB3	3:F:817:ILE:HD11	1.85	0.57
1:A:1290:GLY:O	1:A:1307:GLN:NE2	2.38	0.57
1:A:625:MET:HE2	1:A:629:GLY:HA2	1.86	0.57
3:F:365:ASP:HB2	3:F:394:HIS:CD2	2.40	0.57
1:A:633:PRO:HB3	5:A:1906:3PE:C22	2.35	0.57
1:A:1275:VAL:HG13	5:A:1911:3PE:C2G	2.34	0.57
3:F:1014:THR:OG1	3:F:1015:ASN:N	2.38	0.57
1:A:210:TYR:O	1:A:313:TYR:OH	2.21	0.56
3:F:381:ASP:OD1	3:F:381:ASP:N	2.36	0.56
3:F:582:ASP:OD1	3:F:582:ASP:N	2.34	0.56
3:F:562:ASP:OD1	3:F:563:PHE:N	2.38	0.56
1:A:999:ASN:ND2	1:A:1002:SER:OG	2.37	0.56
1:A:309:TRP:C	6:A:1909:PC1:O32	2.48	0.56
1:A:552:LEU:HA	1:A:555:SER:HB2	1.88	0.56
2:E:55:ARG:HA	2:E:81:SER:O	2.06	0.56
3:F:480:ASN:HA	3:F:483:ASN:HB2	1.88	0.56
5:A:1903:3PE:O32	5:A:1903:3PE:H341	2.05	0.56
1:A:536:PHE:CD1	1:A:941:MET:HE3	2.35	0.55
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:ARG:NH2	3:F:611:TRP:O	2.39	0.55
3:F:715:THR:HB	3:F:745:ARG:HH21	1.71	0.55
1:A:947:VAL:O	1:A:951:LYS:HB2	2.06	0.55
3:F:297:ASN:ND2	3:F:330:LYS:O	2.38	0.55
3:F:1060:ASP:OD1	3:F:1060:ASP:N	2.32	0.55
1:A:280:PHE:O	1:A:284:THR:HG22	2.07	0.55
1:A:1133:ILE:HG12	5:A:1903:3PE:H282	1.89	0.55
5:A:1907:3PE:C2C	5:A:1907:3PE:H271	2.37	0.55
3:F:672:ASP:HB2	3:F:689:PHE:HE1	1.72	0.55
5:A:1910:3PE:P	5:A:1910:3PE:C3	2.94	0.55
3:F:99:ARG:NH1	3:F:198:ASN:OD1	2.37	0.55
3:F:597:GLN:HB3	3:F:765:SER:HB2	1.89	0.55
1:A:932:VAL:HG22	7:A:1912:C8U:F21	1.98	0.54
1:A:627:TYR:CD2	5:A:1906:3PE:H232	2.42	0.54
1:A:1005:MET:SD	1:A:1362:ILE:HD11	2.47	0.54
1:A:880:LEU:HD22	1:A:883:MET:HA	1.89	0.54
1:A:43:ALA:HB1	1:A:46:SER:OG	2.08	0.54
1:A:224:LYS:HA	1:A:263:GLY:HA2	1.90	0.54
1:A:662:ASP:C	1:A:663:ASN:HD22	2.16	0.54
1:A:939:GLN:HG3	1:A:939:GLN:O	2.07	0.54
5:A:1907:3PE:C2C	5:A:1907:3PE:C27	2.86	0.54
3:F:379:ASN:HD21	3:F:408:ASN:HD22	1.53	0.54
5:A:1904:3PE:H3I3	5:A:1904:3PE:H272	1.90	0.54
2:E:178:TYR:HB3	2:E:182:PHE:CG	2.43	0.54
1:A:486:LEU:HD22	1:A:491:TYR:HB2	1.89	0.54
5:A:1907:3PE:C2C	5:A:1907:3PE:C28	2.86	0.54
3:F:358:LYS:HB3	3:F:384:VAL:HG22	1.89	0.53
1:A:1418:LYS:NZ	1:A:1420:LEU:H	2.07	0.53
1:A:1175:ARG:HH21	2:E:133:ARG:HH11	1.57	0.53
3:F:168:VAL:HG11	3:F:185:LEU:HD21	1.90	0.53
5:A:1911:3PE:C2G	5:A:1911:3PE:C2C	2.85	0.53
3:F:538:ILE:HG13	3:F:1042:ASP:HB3	1.90	0.53
1:A:309:TRP:CE3	6:A:1909:PC1:C25	2.91	0.52
1:A:928:ILE:CD1	1:A:1064:VAL:HG22	2.39	0.52
1:A:186:LEU:HD13	1:A:565:LEU:HD11	1.90	0.52
1:A:1418:LYS:HZ2	1:A:1420:LEU:H	1.57	0.52
5:A:1902:3PE:O22	5:A:1902:3PE:H252	2.09	0.52
3:F:107:VAL:HG11	3:F:190:ALA:HB3	1.90	0.52
3:F:475:PHE:HD1	3:F:476:GLU:HG3	1.74	0.52
1:A:1373:ILE:O	1:A:1377:VAL:HG23	2.09	0.52
1:A:1041:MET:SD	5:A:1910:3PE:O12	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:HIS:HB2	1:A:625:MET:HE3	1.91	0.52
1:A:112:PHE:HB2	1:A:115:ASP:HA	1.91	0.52
1:A:1234:PHE:HB3	6:A:1909:PC1:H221	1.91	0.52
2:E:133:ARG:HD2	2:E:135:TYR:HE1	1.75	0.52
1:A:295:THR:HG21	1:A:1318:ARG:HG3	1.92	0.52
1:A:490:GLN:HA	1:A:493:MET:HE3	1.91	0.52
3:F:513:TYR:OH	3:F:567:GLU:OE1	2.26	0.52
3:F:130:LYS:HB2	3:F:228:ASN:HA	1.92	0.52
1:A:1085:GLN:O	1:A:1089:VAL:HG22	2.10	0.52
1:A:636:LEU:HD21	5:A:1905:3PE:H321	1.92	0.51
5:A:1903:3PE:H321	5:A:1903:3PE:H222	1.92	0.51
1:A:452:GLU:OE1	1:A:948:GLN:NE2	2.34	0.51
3:F:176:GLU:OE1	3:F:176:GLU:N	2.41	0.51
1:A:61:ILE:HD11	1:A:171:ARG:HB3	1.92	0.51
1:A:232:ASP:OD1	1:A:262:ARG:NH1	2.41	0.51
1:A:627:TYR:CE2	5:A:1906:3PE:H232	2.45	0.51
3:F:461:VAL:HG12	3:F:495:SER:HA	1.91	0.51
1:A:834:TYR:O	1:A:837:ILE:HG13	2.09	0.51
1:A:939:GLN:NE2	1:A:1048:TYR:OH	2.43	0.51
3:F:1042:ASP:OD1	3:F:1042:ASP:N	2.42	0.51
1:A:932:VAL:HA	1:A:935:THR:HG22	1.91	0.51
1:A:309:TRP:HB3	6:A:1909:PC1:O32	2.11	0.51
1:A:920:CYS:HA	1:A:923:VAL:HG12	1.92	0.51
1:A:1099:ARG:NH1	2:E:219:GLU:OE1	2.34	0.51
3:F:57:LEU:HD23	3:F:801:VAL:HG21	1.91	0.51
3:F:893:SER:O	3:F:893:SER:OG	2.22	0.51
7:A:1912:C8U:O11	7:A:1912:C8U:F19	2.18	0.51
1:A:1348:GLU:HB3	1:A:1351:THR:HG21	1.93	0.51
5:A:1904:3PE:H221	5:A:1904:3PE:C3	2.28	0.51
3:F:509:CYS:SG	3:F:630:SER:HB2	2.50	0.51
1:A:917:VAL:O	1:A:921:VAL:HG13	2.11	0.51
3:F:194:VAL:HA	3:F:197:LYS:HG2	1.93	0.51
5:A:1911:3PE:C2G	5:A:1911:3PE:H2C1	2.39	0.51
1:A:874:LEU:O	1:A:878:VAL:HG22	2.10	0.50
1:A:916:HIS:O	1:A:916:HIS:ND1	2.44	0.50
3:F:56:GLN:O	3:F:60:ILE:HG23	2.11	0.50
3:F:291:VAL:HG12	3:F:312:ALA:HB2	1.94	0.50
3:F:908:GLU:HG3	3:F:974:LYS:HD3	1.93	0.50
1:A:61:ILE:HG12	1:A:174:ARG:HB2	1.93	0.50
1:A:1071:GLN:N	1:A:1071:GLN:OE1	2.44	0.50
3:F:398:ARG:O	3:F:402:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TRP:O	6:A:1909:PC1:O32	2.30	0.50
3:F:995:GLY:O	3:F:1005:ILE:HG13	2.12	0.50
3:F:155:ALA:C	3:F:157:PHE:H	2.20	0.50
3:F:729:ILE:HG22	3:F:730:LYS:H	1.77	0.50
1:A:848:VAL:O	1:A:852:THR:N	2.45	0.50
2:E:36:SER:HB2	2:E:175:GLU:HB2	1.94	0.49
3:F:48:ALA:O	3:F:52:SER:OG	2.28	0.49
1:A:646:VAL:HG12	5:A:1905:3PE:H3F2	1.84	0.49
3:F:738:VAL:HG21	3:F:766:PHE:HZ	1.78	0.49
2:E:32:TRP:HB2	2:E:182:PHE:N	2.28	0.49
1:A:39:PRO:HG2	1:A:41:ARG:HE	1.78	0.49
1:A:921:VAL:HG12	1:A:1374:ASN:HD21	1.78	0.49
1:A:128:ILE:O	1:A:132:LEU:HD12	2.13	0.49
3:F:657:GLU:HG3	3:F:749:LYS:CD	2.43	0.49
1:A:1112:TRP:HA	1:A:1171:ALA:HB1	1.93	0.49
1:A:1158:THR:O	1:A:1162:THR:OG1	2.28	0.49
3:F:111:HIS:NE2	3:F:183:ASN:OD1	2.32	0.48
3:F:736:PHE:CZ	3:F:816:GLY:HA3	2.48	0.48
1:A:633:PRO:HB3	5:A:1906:3PE:H222	1.93	0.48
1:A:828:ARG:O	1:A:832:LEU:HG	2.13	0.48
1:A:932:VAL:HA	1:A:935:THR:CG2	2.43	0.48
5:A:1907:3PE:H2	5:A:1907:3PE:O12	2.12	0.48
3:F:125:VAL:HA	3:F:145:GLN:O	2.14	0.48
3:F:417:SER:OG	3:F:418:ILE:N	2.44	0.48
1:A:582:GLY:HA2	1:A:597:PHE:O	2.14	0.48
1:A:479:MET:HE3	1:A:479:MET:HB3	1.74	0.48
5:A:1907:3PE:O32	5:A:1907:3PE:H342	2.11	0.48
2:E:16:ILE:O	2:E:20:ILE:HG13	2.14	0.48
2:E:164:ARG:HG3	2:E:165:MET:HG2	1.93	0.48
3:F:259:LEU:HD12	3:F:294:ALA:HB3	1.96	0.48
1:A:1039:VAL:HG11	5:A:1908:3PE:O12	2.13	0.48
1:A:163:ALA:HB2	5:A:1906:3PE:C32	2.37	0.48
3:F:58:VAL:HG13	3:F:803:ILE:HG22	1.96	0.48
3:F:484:GLN:HE22	3:F:1070:ASP:N	2.11	0.48
1:A:1393:ILE:HG13	1:A:1394:LEU:H	1.79	0.48
3:F:591:ARG:NH2	3:F:606:ASN:OD1	2.47	0.48
1:A:842:VAL:O	1:A:845:VAL:HG22	2.14	0.48
1:A:1359:TYR:CE2	5:A:1904:3PE:H231	2.48	0.47
1:A:1363:SER:HA	5:A:1904:3PE:H291	1.96	0.47
3:F:176:GLU:O	3:F:176:GLU:HG2	2.14	0.47
3:F:547:ARG:HB2	3:F:550:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:HE2	1:A:1246:LEU:HD11	1.80	0.47
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.96	0.47
1:A:809:ILE:HD12	1:A:810:LEU:N	2.29	0.47
1:A:1414:LYS:HD2	1:A:1414:LYS:HA	1.73	0.47
1:A:1418:LYS:HE3	1:A:1420:LEU:HB3	1.97	0.47
3:F:36:TRP:O	3:F:39:LYS:HG3	2.13	0.47
3:F:876:ARG:NE	3:F:880:GLU:OE2	2.48	0.47
1:A:1040:GLU:OE2	5:A:1910:3PE:H112	2.13	0.47
5:A:1902:3PE:H221	5:A:1902:3PE:H2	1.79	0.47
1:A:45:ILE:HD12	1:A:46:SER:N	2.29	0.47
3:F:253:PRO:O	3:F:356:CYS:HB3	2.15	0.47
1:A:897:ARG:O	1:A:900:ARG:HG2	2.15	0.47
5:A:1907:3PE:H281	5:A:1907:3PE:C2C	2.39	0.47
5:A:1907:3PE:H111	5:A:1908:3PE:H112	1.97	0.47
6:A:1909:PC1:H131	2:E:160:GLN:HE22	1.79	0.47
1:A:39:PRO:HG2	1:A:41:ARG:HG3	1.97	0.47
1:A:660:ALA:HB1	1:A:1059:ILE:HA	1.96	0.47
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.50	0.47
2:E:144:TYR:O	2:E:147:ALA:HB3	2.15	0.47
2:E:194:LEU:O	2:E:198:SER:OG	2.25	0.47
1:A:1412:GLU:HB3	1:A:1414:LYS:HD3	1.97	0.47
3:F:263:SER:OG	3:F:264:GLY:N	2.48	0.47
3:F:210:PHE:CE2	3:F:212:SER:HB3	2.50	0.46
3:F:497:GLU:O	3:F:501:ARG:HG3	2.15	0.46
3:F:647:TYR:O	3:F:650:THR:OG1	2.30	0.46
1:A:124:VAL:O	1:A:128:ILE:HG13	2.15	0.46
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.77	0.46
5:A:1910:3PE:H252	5:A:1910:3PE:H282	1.84	0.46
3:F:336:LYS:O	3:F:340:SER:OG	2.27	0.46
1:A:928:ILE:HD12	1:A:1064:VAL:CG2	2.45	0.46
3:F:857:ASP:OD1	3:F:857:ASP:N	2.46	0.46
1:A:817:ALA:HB2	1:A:1279:PHE:CE1	2.47	0.46
3:F:434:ARG:HB2	3:F:435:PRO:HD3	1.98	0.46
1:A:1417:ILE:HD12	1:A:1418:LYS:O	2.15	0.46
5:A:1904:3PE:H2I3	5:A:1904:3PE:H2F2	1.64	0.46
3:F:373:GLU:OE1	3:F:373:GLU:N	2.36	0.46
3:F:909:PRO:HG3	3:F:975:GLN:HG2	1.98	0.46
3:F:630:SER:O	3:F:630:SER:OG	2.29	0.46
2:E:115:LEU:O	2:E:119:ILE:HG13	2.16	0.46
3:F:887:ARG:NH2	3:F:1032:ARG:O	2.26	0.46
1:A:49:GLU:OE2	1:A:103:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:MET:HE1	1:A:289:ILE:HD11	1.97	0.45
1:A:1149:ILE:O	1:A:1153:LEU:HD12	2.16	0.45
3:F:271:LEU:HD22	3:F:329:ALA:HB2	1.98	0.45
3:F:899:LYS:HG2	3:F:982:THR:HG23	1.98	0.45
1:A:194:LEU:N	1:A:195:PRO:HD2	2.31	0.45
1:A:559:ILE:O	1:A:559:ILE:HG22	2.16	0.45
3:F:475:PHE:CD1	3:F:476:GLU:HG3	2.52	0.45
3:F:821:VAL:O	3:F:825:ILE:HG13	2.16	0.45
1:A:1430:GLN:HB3	1:A:1431:PRO:CD	2.46	0.45
2:E:53:LEU:HA	2:E:158:MET:HE2	1.97	0.45
3:F:657:GLU:HG3	3:F:749:LYS:HD3	1.97	0.45
1:A:278:PHE:CE2	5:A:1903:3PE:H261	2.51	0.45
1:A:631:SER:O	1:A:635:VAL:HG22	2.16	0.45
1:A:1381:MET:HA	1:A:1384:PHE:CD2	2.51	0.45
3:F:254:LYS:HA	3:F:357:ASN:HB2	1.97	0.45
1:A:656:PHE:CB	1:A:1058:ASN:HD22	2.30	0.45
2:E:54:TRP:CH2	2:E:108:ALA:HB1	2.51	0.45
1:A:657:LEU:O	1:A:661:VAL:HG22	2.17	0.45
1:A:554:ASN:O	1:A:558:SER:HB2	2.15	0.45
5:A:1903:3PE:H322	5:A:1903:3PE:H31	1.78	0.45
5:A:1911:3PE:H2A1	5:A:1911:3PE:H2D2	1.74	0.45
2:E:150:CYS:O	2:E:153:VAL:HG22	2.17	0.45
1:A:509:LEU:O	1:A:513:LEU:HB2	2.17	0.45
1:A:656:PHE:HB3	1:A:1058:ASN:HD22	1.82	0.45
2:E:122:THR:HG23	2:E:123:ILE:HD13	1.99	0.45
1:A:877:ALA:O	1:A:881:ILE:HG23	2.17	0.45
3:F:129:ALA:O	3:F:130:LYS:HG2	2.17	0.45
1:A:69:ALA:CB	5:A:1907:3PE:O22	2.66	0.44
1:A:1196:ASP:HB2	1:A:1235:PHE:HB3	2.00	0.44
2:E:14:PHE:O	2:E:18:VAL:HG23	2.17	0.44
1:A:837:ILE:HG21	1:A:883:MET:HE3	1.99	0.44
1:A:869:ASN:OD1	1:A:869:ASN:N	2.37	0.44
1:A:163:ALA:CB	5:A:1906:3PE:C32	2.83	0.44
1:A:233:ILE:HD13	3:F:547:ARG:HG2	2.00	0.44
1:A:1366:MET:HE3	5:A:1904:3PE:C2A	2.48	0.44
3:F:270:THR:HG21	3:F:365:ASP:HB3	1.98	0.44
1:A:1120:PHE:O	1:A:1124:MET:HG2	2.17	0.44
3:F:479:THR:OG1	3:F:480:ASN:N	2.49	0.44
1:A:254:CYS:SG	1:A:261:CYS:HB2	2.58	0.44
1:A:1013:PHE:HE1	1:A:1049:ILE:HG23	1.83	0.44
2:E:8:LYS:O	2:E:12:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:141:SER:OG	2:E:196:GLY:O	2.35	0.44
3:F:627:PRO:O	3:F:630:SER:HB3	2.18	0.44
3:F:673:LEU:H	3:F:673:LEU:HD23	1.82	0.44
1:A:1188:LEU:HD12	2:E:146:PHE:CE2	2.53	0.44
1:A:1359:TYR:HD2	5:A:1904:3PE:H252	1.81	0.44
3:F:159:ARG:HH11	3:F:223:SER:HB3	1.83	0.44
3:F:844:CYS:HB3	3:F:866:ASN:ND2	2.33	0.44
1:A:260:GLU:OE2	1:A:262:ARG:HD3	2.17	0.44
1:A:892:VAL:HG12	1:A:893:VAL:H	1.82	0.44
1:A:1082:ASP:O	1:A:1086:ARG:NH2	2.51	0.44
1:A:440:LEU:O	1:A:444:LEU:HG	2.17	0.44
1:A:808:PHE:O	1:A:812:SER:OG	2.27	0.44
1:A:836:ASP:OD2	1:A:903:ARG:NH1	2.51	0.44
3:F:512:GLY:HA2	3:F:625:VAL:O	2.18	0.44
1:A:1299:GLN:O	1:A:1304:ASN:ND2	2.49	0.44
3:F:197:LYS:HA	3:F:200:GLU:HG2	2.00	0.44
1:A:1251:GLU:H	1:A:1251:GLU:HG2	1.66	0.43
3:F:232:PRO:HB2	3:F:234:LYS:HD3	2.00	0.43
3:F:1004:ARG:HB3	3:F:1022:GLU:HB2	2.00	0.43
1:A:177:SER:HA	1:A:183:GLN:HE21	1.82	0.43
1:A:1251:GLU:O	1:A:1255:THR:HG22	2.18	0.43
3:F:308:HIS:CD2	3:F:351:VAL:HG11	2.53	0.43
3:F:454:ASP:OD1	3:F:455:ALA:N	2.51	0.43
3:F:478:LYS:HB2	3:F:478:LYS:HE2	1.73	0.43
1:A:953:LYS:HG2	1:A:1028:GLU:O	2.17	0.43
3:F:44:LEU:HD11	3:F:824:TRP:CZ2	2.54	0.43
1:A:480:LEU:HA	1:A:483:MET:HG2	2.01	0.43
5:A:1911:3PE:C2C	5:A:1911:3PE:H2G1	2.48	0.43
3:F:372:GLN:HG3	3:F:403:TRP:CH2	2.53	0.43
1:A:39:PRO:HD2	1:A:41:ARG:HH11	1.84	0.43
3:F:719:VAL:HG22	3:F:723:TRP:CE3	2.54	0.43
1:A:172:PRO:HA	1:A:175:LEU:HD12	2.00	0.43
1:A:939:GLN:HE21	1:A:939:GLN:HB2	1.49	0.43
1:A:953:LYS:HB3	1:A:1026:SER:HB2	1.99	0.43
2:E:118:LEU:HD21	2:E:192:LEU:HD11	2.01	0.43
1:A:1430:GLN:HB3	1:A:1431:PRO:HD2	1.99	0.43
3:F:130:LYS:HB3	3:F:225:TRP:HB3	2.01	0.43
3:F:484:GLN:HE22	3:F:1070:ASP:HB2	1.84	0.43
3:F:802:GLU:HG3	3:F:809:LEU:HD11	2.01	0.43
1:A:62:PHE:HE1	5:A:1907:3PE:H281	1.79	0.43
1:A:555:SER:HA	1:A:663:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:MET:HE3	1:A:983:MET:HB3	1.78	0.43
1:A:1108:GLN:HE21	1:A:1108:GLN:C	2.27	0.43
2:E:7:PRO:O	2:E:11:VAL:HG13	2.19	0.43
2:E:134:ASP:OD1	2:E:134:ASP:N	2.47	0.43
3:F:154:ASP:HB2	3:F:161:VAL:HG22	2.01	0.43
1:A:580:LEU:O	1:A:584:ARG:HD2	2.19	0.43
1:A:636:LEU:HD21	5:A:1905:3PE:C32	2.48	0.43
1:A:1148:HIS:O	1:A:1152:ILE:HG12	2.19	0.43
1:A:1189:ILE:HG21	1:A:1242:ARG:HG2	2.00	0.43
3:F:388:THR:OG1	3:F:405:ALA:HB2	2.19	0.43
3:F:1069:GLU:HB3	3:F:1071:TYR:CD2	2.54	0.43
1:A:973:TYR:HE1	3:F:235:ILE:HG21	1.84	0.42
2:E:154:SER:O	2:E:155:LEU:C	2.62	0.42
1:A:1257:LEU:HD23	1:A:1257:LEU:HA	1.78	0.42
3:F:470:ASN:HD21	3:F:482:LYS:HE3	1.84	0.42
3:F:664:LEU:H	3:F:679:ASN:HD21	1.67	0.42
3:F:688:GLU:O	3:F:692:ARG:CB	2.58	0.42
1:A:111:LEU:HG	1:A:112:PHE:CD1	2.54	0.42
1:A:483:MET:O	1:A:487:GLY:N	2.38	0.42
3:F:420:ALA:HB1	3:F:424:ASN:ND2	2.34	0.42
3:F:88:LYS:HB2	3:F:88:LYS:HE3	1.63	0.42
3:F:289:ASP:OD1	3:F:289:ASP:N	2.50	0.42
3:F:388:THR:HB	3:F:401:ILE:HG23	2.01	0.42
1:A:115:ASP:N	1:A:115:ASP:OD1	2.52	0.42
1:A:199:ILE:O	1:A:203:VAL:HG23	2.18	0.42
1:A:219:LYS:HB3	1:A:219:LYS:HE2	1.87	0.42
1:A:608:PHE:O	1:A:612:THR:HG23	2.20	0.42
2:E:106:SER:O	2:E:110:ILE:HG13	2.19	0.42
1:A:41:ARG:HD2	1:A:42:LYS:N	2.35	0.42
1:A:633:PRO:HB3	5:A:1906:3PE:H221	2.02	0.42
1:A:558:SER:O	1:A:559:ILE:HD13	2.20	0.42
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.78	0.42
1:A:933:LEU:HA	1:A:933:LEU:HD13	1.70	0.42
1:A:1234:PHE:HB3	6:A:1909:PC1:H232	2.01	0.42
6:A:1909:PC1:H232	6:A:1909:PC1:H262	1.89	0.42
5:A:1911:3PE:H291	5:A:1911:3PE:H262	1.42	0.42
3:F:126:TYR:CE2	3:F:128:ASN:HB2	2.55	0.42
1:A:468:ASN:OD1	1:A:531:ARG:NH2	2.45	0.42
1:A:576:LEU:HD21	5:A:1906:3PE:H2C1	2.02	0.42
1:A:599:ASN:OD1	1:A:599:ASN:N	2.52	0.42
1:A:600:PHE:HB3	1:A:601:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:242:ARG:NH2	3:F:284:THR:HG23	2.34	0.42
3:F:468:VAL:HG12	3:F:487:LEU:HD12	2.01	0.42
1:A:139:LEU:O	1:A:142:VAL:HG12	2.19	0.41
1:A:630:PRO:HA	1:A:635:VAL:HG13	2.02	0.41
1:A:931:ILE:HD12	1:A:931:ILE:HA	1.66	0.41
3:F:132:ASP:OD2	3:F:231:THR:HG21	2.20	0.41
1:A:45:ILE:HB	1:A:103:MET:HG3	2.02	0.41
1:A:1005:MET:O	1:A:1009:THR:HG23	2.21	0.41
1:A:1236:ARG:O	1:A:1239:ARG:HG2	2.21	0.41
1:A:1389:ARG:HD3	1:A:1397:HIS:HE1	1.85	0.41
3:F:185:LEU:HG	3:F:216:LEU:HD21	2.02	0.41
3:F:723:TRP:CE3	3:F:747:TYR:HB2	2.56	0.41
1:A:75:PRO:HB3	1:A:583:GLY:O	2.20	0.41
1:A:610:VAL:HG13	1:A:616:TRP:HB2	2.03	0.41
1:A:642:ILE:O	1:A:646:VAL:HB	2.20	0.41
2:E:135:TYR:CZ	2:E:136:LEU:HG	2.56	0.41
3:F:573:LYS:HE2	3:F:609:TYR:OH	2.19	0.41
3:F:628:THR:O	3:F:629:TYR:CD2	2.73	0.41
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.91	0.41
1:A:615:ASP:OD1	1:A:618:SER:OG	2.33	0.41
3:F:433:GLY:O	3:F:437:VAL:HG23	2.20	0.41
3:F:629:TYR:CD1	3:F:629:TYR:C	2.97	0.41
3:F:1065:ASN:O	3:F:1065:ASN:ND2	2.53	0.41
1:A:514:VAL:HG23	1:A:515:GLU:OE1	2.21	0.41
1:A:928:ILE:CD1	1:A:1064:VAL:CG2	2.99	0.41
1:A:1111:VAL:O	1:A:1114:VAL:HG12	2.21	0.41
2:E:32:TRP:HB3	2:E:181:SER:HB3	2.03	0.41
3:F:771:LEU:HD23	3:F:771:LEU:HA	1.90	0.41
1:A:584:ARG:NH1	5:A:1906:3PE:P	2.93	0.41
1:A:928:ILE:HD12	1:A:1064:VAL:HG22	2.03	0.41
5:A:1904:3PE:H3D2	5:A:1904:3PE:H3G2	1.79	0.41
2:E:30:ASP:HA	2:E:52:GLY:HA3	2.03	0.41
1:A:524:ILE:HD12	1:A:524:ILE:HA	1.82	0.41
3:F:97:LEU:HD11	3:F:464:GLY:O	2.20	0.41
1:A:1280:ILE:O	1:A:1284:ILE:HG13	2.20	0.41
1:A:1384:PHE:O	1:A:1388:THR:OG1	2.38	0.41
1:A:1418:LYS:HG2	1:A:1419:HIS:N	2.36	0.41
2:E:10:ARG:HA	2:E:13:LEU:HG	2.02	0.41
2:E:13:LEU:HA	2:E:16:ILE:HB	2.02	0.41
2:E:127:MET:HB3	2:E:127:MET:HE2	1.73	0.41
3:F:234:LYS:HD3	3:F:234:LYS:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:288:ASP:OD2	3:F:288:ASP:N	2.54	0.41
3:F:348:ASN:C	3:F:350:ASN:H	2.29	0.41
3:F:598:ASP:OD1	3:F:598:ASP:N	2.51	0.41
1:A:210:TYR:OH	6:A:1909:PC1:H3A1	2.20	0.41
1:A:497:ASN:OD1	1:A:497:ASN:N	2.54	0.41
1:A:553:LEU:HD23	1:A:553:LEU:O	2.21	0.41
3:F:470:ASN:HD21	3:F:482:LYS:NZ	2.19	0.41
3:F:664:LEU:HD23	3:F:682:PHE:HE2	1.86	0.41
1:A:268:PRO:HD2	1:A:273:THR:O	2.20	0.41
1:A:529:CYS:HA	1:A:532:LEU:HD21	2.03	0.41
3:F:851:MET:HE2	3:F:851:MET:HB3	1.84	0.41
3:F:987:ASP:OD1	3:F:987:ASP:N	2.54	0.41
1:A:1042:ALA:O	1:A:1046:ILE:HG13	2.21	0.40
2:E:127:MET:HG3	2:E:136:LEU:HD13	2.01	0.40
3:F:54:VAL:HG22	3:F:815:VAL:HG21	2.03	0.40
3:F:805:ILE:HD13	3:F:805:ILE:HA	1.88	0.40
1:A:1169:LEU:O	1:A:1173:LYS:N	2.50	0.40
1:A:1309:PHE:HB3	1:A:1310:PRO:HD3	2.03	0.40
5:A:1903:3PE:H352	5:A:1905:3PE:C34	2.38	0.40
5:A:1907:3PE:H112	5:A:1908:3PE:H111	2.02	0.40
5:A:1911:3PE:H2C1	5:A:1911:3PE:C2H	2.51	0.40
2:E:160:GLN:HE21	2:E:160:GLN:HB2	1.54	0.40
3:F:376:ALA:O	3:F:380:LYS:HB2	2.22	0.40
3:F:867:HIS:C	3:F:869:ASP:H	2.29	0.40
1:A:65:CYS:SG	5:A:1907:3PE:H282	2.61	0.40
1:A:441:ILE:HG23	1:A:471:LEU:HD23	2.04	0.40
3:F:44:LEU:HD23	3:F:44:LEU:HA	1.85	0.40
3:F:454:ASP:HB3	3:F:458:LEU:H	1.87	0.40
3:F:655:ASN:H	3:F:655:ASN:HD22	1.68	0.40
1:A:308:GLU:O	1:A:311:TRP:NE1	2.55	0.40
1:A:520:THR:O	1:A:521:PRO:C	2.64	0.40
1:A:633:PRO:HB2	5:A:1906:3PE:H222	2.00	0.40
1:A:943:ALA:O	1:A:947:VAL:HG23	2.21	0.40
5:A:1907:3PE:H371	5:A:1907:3PE:H341	1.79	0.40
6:A:1909:PC1:H322	6:A:1909:PC1:H32	1.83	0.40
3:F:41:GLN:HB2	3:F:1011:LEU:HD23	2.02	0.40
3:F:708:VAL:HG22	3:F:741:GLY:O	2.22	0.40
3:F:866:ASN:C	3:F:867:HIS:HD1	2.29	0.40
1:A:985:LEU:HD23	1:A:985:LEU:HA	1.80	0.40
1:A:1168:LYS:HB2	1:A:1168:LYS:HE3	1.78	0.40
6:A:1909:PC1:H112	6:A:1909:PC1:H152	1.79	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	1094/1873 (58%)	1017 (93%)	77 (7%)	0	100	100
2	E	159/222 (72%)	143 (90%)	15 (9%)	1 (1%)	21	50
3	F	968/1105 (88%)	876 (90%)	92 (10%)	0	100	100
All	All	2221/3200 (69%)	2036 (92%)	184 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	205	PRO

5.3.2 Protein sidechains [i](#)

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	980/1628 (60%)	853 (87%)	127 (13%)	4	16
2	E	143/192 (74%)	130 (91%)	13 (9%)	9	30
3	F	868/973 (89%)	798 (92%)	70 (8%)	11	36
All	All	1991/2793 (71%)	1781 (90%)	210 (10%)	9	23

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	58	LEU
1	A	61	ILE
1	A	65	CYS
1	A	74	MET
1	A	81	SER
1	A	94	LEU
1	A	95	THR
1	A	98	SER
1	A	100	GLU
1	A	106	ILE
1	A	113	HIS
1	A	115	ASP
1	A	123	ASN
1	A	125	LEU
1	A	144	VAL
1	A	161	VAL
1	A	176	VAL
1	A	184	VAL
1	A	193	MET
1	A	237	VAL
1	A	238	GLU
1	A	243	SER
1	A	245	CYS
1	A	248	THR
1	A	250	SER
1	A	252	ARG
1	A	256	ILE
1	A	270	HIS
1	A	282	MET
1	A	289	ILE
1	A	339	LYS
1	A	449	ILE
1	A	451	SER
1	A	460	LEU
1	A	468	ASN
1	A	473	SER
1	A	477	ILE
1	A	480	LEU
1	A	494	SER
1	A	495	ILE
1	A	511	LEU
1	A	519	MET

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Mol	Chain	Res	Type
1	A	524	ILE
1	A	526	VAL
1	A	529	CYS
1	A	532	LEU
1	A	555	SER
1	A	561	SER
1	A	619	VAL
1	A	646	VAL
1	A	647	CYS
1	A	659	ILE
1	A	668	GLU
1	A	672	SER
1	A	799	THR
1	A	807	LEU
1	A	812	SER
1	A	827	VAL
1	A	845	VAL
1	A	851	MET
1	A	852	THR
1	A	869	ASN
1	A	870	ILE
1	A	871	LEU
1	A	873	LEU
1	A	875	VAL
1	A	876	VAL
1	A	880	LEU
1	A	881	ILE
1	A	882	SER
1	A	892	VAL
1	A	899	LEU
1	A	903	ARG
1	A	908	ILE
1	A	910	ARG
1	A	921	VAL
1	A	927	THR
1	A	928	ILE
1	A	930	ASN
1	A	931	ILE
1	A	933	LEU
1	A	934	VAL
1	A	937	LEU
1	A	938	LEU

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Mol	Chain	Res	Type
1	A	939	GLN
1	A	961	SER
1	A	974	VAL
1	A	983	MET
1	A	985	LEU
1	A	991	ILE
1	A	994	ASP
1	A	999	ASN
1	A	1011	SER
1	A	1030	ASP
1	A	1093	LEU
1	A	1108	GLN
1	A	1115	VAL
1	A	1117	SER
1	A	1129	MET
1	A	1154	ASN
1	A	1164	GLU
1	A	1167	LEU
1	A	1189	ILE
1	A	1198	ILE
1	A	1202	ILE
1	A	1206	LEU
1	A	1235	PHE
1	A	1243	LEU
1	A	1247	LEU
1	A	1251	GLU
1	A	1263	SER
1	A	1265	GLN
1	A	1270	VAL
1	A	1287	GLN
1	A	1289	PHE
1	A	1296	ASP
1	A	1300	ILE
1	A	1302	ARG
1	A	1308	THR
1	A	1344	TYR
1	A	1352	CYS
1	A	1354	THR
1	A	1384	PHE
1	A	1397	HIS
1	A	1424	THR
1	A	1425	LEU

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Mol	Chain	Res	Type
2	E	4	THR
2	E	9	VAL
2	E	17	LEU
2	E	22	LEU
2	E	50	HIS
2	E	51	PHE
2	E	81	SER
2	E	115	LEU
2	E	160	GLN
2	E	161	SER
2	E	186	CYS
2	E	198	SER
2	E	203	SER
3	F	29	SER
3	F	61	TYR
3	F	66	ASP
3	F	69	THR
3	F	102	LEU
3	F	125	VAL
3	F	132	ASP
3	F	134	ASP
3	F	158	ARG
3	F	172	THR
3	F	205	LEU
3	F	209	VAL
3	F	237	LEU
3	F	263	SER
3	F	272	LYS
3	F	284	THR
3	F	289	ASP
3	F	303	VAL
3	F	304	SER
3	F	327	ILE
3	F	328	THR
3	F	332	ILE
3	F	348	ASN
3	F	355	ASN
3	F	381	ASP
3	F	417	SER
3	F	449	THR
3	F	475	PHE
3	F	476	GLU

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Mol	Chain	Res	Type
3	F	482	LYS
3	F	503	THR
3	F	508	LEU
3	F	517	ILE
3	F	523	VAL
3	F	524	LEU
3	F	543	LEU
3	F	581	ILE
3	F	592	THR
3	F	594	VAL
3	F	602	ILE
3	F	610	THR
3	F	612	THR
3	F	628	THR
3	F	639	GLU
3	F	648	SER
3	F	651	LEU
3	F	668	ASP
3	F	671	SER
3	F	680	THR
3	F	710	LEU
3	F	711	ASP
3	F	729	ILE
3	F	735	ARG
3	F	739	THR
3	F	774	ASP
3	F	775	ASN
3	F	793	SER
3	F	814	VAL
3	F	817	ILE
3	F	871	THR
3	F	881	ILE
3	F	906	VAL
3	F	976	SER
3	F	982	THR
3	F	997	LEU
3	F	1008	VAL
3	F	1014	THR
3	F	1033	LEU
3	F	1060	ASP
3	F	1068	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	277	ASN
1	A	302	ASN
1	A	445	ASN
1	A	453	HIS
1	A	464	GLN
1	A	663	ASN
1	A	797	ASN
1	A	803	ASN
1	A	939	GLN
1	A	992	HIS
1	A	999	ASN
1	A	1058	ASN
1	A	1087	GLN
1	A	1108	GLN
1	A	1110	GLN
1	A	1307	GLN
1	A	1311	GLN
1	A	1374	ASN
2	E	160	GLN
3	F	112	GLN
3	F	169	HIS
3	F	208	GLN
3	F	248	GLN
3	F	394	HIS
3	F	395	ASN
3	F	408	ASN
3	F	447	GLN
3	F	450	ASN
3	F	470	ASN
3	F	484	GLN
3	F	526	HIS
3	F	655	ASN
3	F	679	ASN
3	F	685	ASN
3	F	697	ASN
3	F	706	ASN
3	F	847	ASN
3	F	872	ASN
3	F	1052	GLN
3	F	1065	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	3PE	A	1911	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
5	3PE	A	1903	-	35,35,50	1.10	2 (5%)	38,40,55	1.16	3 (7%)
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.16	3 (7%)
6	PC1	A	1909	-	53,53,53	0.94	2 (3%)	59,61,61	1.00	3 (5%)
5	3PE	A	1906	-	43,43,50	0.99	2 (4%)	46,48,55	1.11	3 (6%)
5	3PE	A	1905	-	50,50,50	0.93	2 (4%)	53,55,55	1.08	3 (5%)
5	3PE	A	1908	-	20,20,50	1.03	1 (5%)	22,23,55	0.97	1 (4%)
5	3PE	A	1902	-	32,32,50	1.14	2 (6%)	35,37,55	1.22	3 (8%)
5	3PE	A	1904	-	50,50,50	0.93	2 (4%)	53,55,55	1.04	2 (3%)
5	3PE	A	1910	-	31,31,50	1.17	2 (6%)	34,36,55	1.23	3 (8%)
7	C8U	A	1912	-	24,26,26	4.13	8 (33%)	32,39,39	2.57	9 (28%)

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
5	3PE	A	1911	-	-	30/54/54/54	-
5	3PE	A	1903	-	-	23/39/39/54	-
5	3PE	A	1907	-	-	20/41/41/54	-
6	PC1	A	1909	-	-	31/57/57/57	-
5	3PE	A	1906	-	-	20/47/47/54	-
5	3PE	A	1905	-	-	32/54/54/54	-
5	3PE	A	1908	-	-	11/21/21/54	-
5	3PE	A	1902	-	-	19/36/36/54	-
5	3PE	A	1904	-	-	36/54/54/54	-
5	3PE	A	1910	-	-	14/35/35/54	-
7	C8U	A	1912	-	-	8/18/40/40	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	C8U	C02-C03	14.09	1.52	1.35
7	A	1912	C8U	O10-N09	10.27	1.40	1.22
7	A	1912	C8U	C06-N07	5.54	1.45	1.38
7	A	1912	C8U	C02-N07	4.69	1.44	1.38
5	A	1910	3PE	O31-C31	4.33	1.46	1.33
5	A	1905	3PE	O31-C31	4.32	1.45	1.33
5	A	1907	3PE	O31-C31	4.31	1.45	1.33
5	A	1906	3PE	O31-C31	4.29	1.45	1.33
5	A	1903	3PE	O31-C31	4.26	1.45	1.33
6	A	1909	PC1	O31-C31	4.24	1.45	1.33
5	A	1904	3PE	O31-C31	4.24	1.45	1.33
5	A	1902	3PE	O31-C31	4.19	1.45	1.33
5	A	1911	3PE	O31-C31	4.17	1.45	1.33
5	A	1904	3PE	O21-C21	4.14	1.46	1.34
5	A	1908	3PE	O21-C21	4.13	1.45	1.33
5	A	1902	3PE	O21-C21	4.11	1.45	1.34
5	A	1903	3PE	O21-C21	4.11	1.45	1.34
5	A	1907	3PE	O21-C21	4.10	1.45	1.34
5	A	1911	3PE	O21-C21	4.08	1.45	1.34
6	A	1909	PC1	O21-C21	4.08	1.45	1.34
5	A	1905	3PE	O21-C21	4.06	1.45	1.34
5	A	1910	3PE	O21-C21	4.04	1.45	1.34
5	A	1906	3PE	O21-C21	4.02	1.45	1.34
7	A	1912	C8U	C22-C03	3.32	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	C8U	O24-C22	3.30	1.40	1.33
7	A	1912	C8U	O11-N09	-2.58	1.18	1.35
7	A	1912	C8U	O24-C25	-2.13	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1912	C8U	C01-C02-C03	-7.77	119.88	127.61
7	A	1912	C8U	C01-C02-N07	5.63	119.96	113.42
7	A	1912	C8U	C08-C06-N07	5.37	119.67	113.42
5	A	1905	3PE	O21-C21-C22	4.60	121.43	111.48
5	A	1904	3PE	O21-C21-C22	4.28	120.73	111.48
5	A	1902	3PE	O21-C21-C22	4.22	120.62	111.48
5	A	1907	3PE	O21-C21-C22	4.22	120.61	111.48
7	A	1912	C8U	O24-C22-C03	4.19	120.02	112.31
5	A	1903	3PE	O21-C21-C22	4.12	120.39	111.48
5	A	1910	3PE	O21-C21-C22	4.11	120.38	111.48
5	A	1906	3PE	O21-C21-C22	3.99	120.11	111.48
5	A	1911	3PE	O21-C21-C22	3.94	120.00	111.48
6	A	1909	PC1	O21-C21-C22	3.84	119.79	111.48
7	A	1912	C8U	C05-C04-C03	3.79	113.33	108.62
7	A	1912	C8U	C06-N07-C02	-3.45	120.23	123.44
5	A	1911	3PE	O31-C31-C32	2.94	120.78	111.83
6	A	1909	PC1	O31-C31-C32	2.91	120.70	111.83
5	A	1903	3PE	O31-C31-C32	2.87	120.60	111.83
5	A	1907	3PE	O31-C31-C32	2.84	120.49	111.83
5	A	1902	3PE	O31-C31-C32	2.84	120.48	111.83
5	A	1905	3PE	O31-C31-C32	2.83	120.46	111.83
5	A	1910	3PE	O31-C31-C32	2.75	120.23	111.83
5	A	1906	3PE	O31-C31-C32	2.75	120.22	111.83
5	A	1904	3PE	O31-C31-C32	2.71	120.11	111.83
5	A	1906	3PE	C2-O21-C21	-2.65	111.44	117.80
5	A	1908	3PE	O21-C21-C22	2.65	119.92	111.83
5	A	1910	3PE	C2-O21-C21	-2.59	111.61	117.80
7	A	1912	C8U	C12-C04-C05	-2.56	108.70	112.52
7	A	1912	C8U	O23-C22-C03	-2.45	120.03	125.20
7	A	1912	C8U	C04-C05-N09	2.41	119.57	116.37
5	A	1907	3PE	C2-O21-C21	-2.33	112.22	117.80
5	A	1902	3PE	C2-O21-C21	-2.30	112.29	117.80
5	A	1905	3PE	O21-C21-O22	-2.19	118.58	123.70
5	A	1911	3PE	C2-O21-C21	-2.17	112.60	117.80
6	A	1909	PC1	C2-O21-C21	-2.15	112.65	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1903	3PE	C2-O21-C21	-2.13	112.70	117.80

There are no chirality outliers.

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1902	3PE	C11-O13-P-O11
5	A	1902	3PE	O13-C11-C12-N
5	A	1902	3PE	O22-C21-O21-C2
5	A	1902	3PE	C22-C21-O21-C2
5	A	1903	3PE	C1-O11-P-O12
5	A	1903	3PE	C1-O11-P-O13
5	A	1903	3PE	C1-O11-P-O14
5	A	1903	3PE	C11-O13-P-O11
5	A	1903	3PE	C11-O13-P-O12
5	A	1903	3PE	C11-O13-P-O14
5	A	1903	3PE	O32-C31-O31-C3
5	A	1903	3PE	C32-C31-O31-C3
5	A	1903	3PE	C22-C21-O21-C2
5	A	1904	3PE	C1-O11-P-O12
5	A	1904	3PE	C11-O13-P-O11
5	A	1904	3PE	O22-C21-O21-C2
5	A	1904	3PE	C22-C21-O21-C2
5	A	1905	3PE	C1-O11-P-O12
5	A	1905	3PE	C1-O11-P-O13
5	A	1905	3PE	C1-O11-P-O14
5	A	1905	3PE	C11-O13-P-O11
5	A	1905	3PE	O22-C21-O21-C2
5	A	1905	3PE	C22-C21-O21-C2
5	A	1906	3PE	C12-C11-O13-P
5	A	1907	3PE	C11-O13-P-O14
5	A	1907	3PE	C2-C1-O11-P
5	A	1908	3PE	C1-O11-P-O12
5	A	1908	3PE	C1-O11-P-O13
5	A	1908	3PE	C11-O13-P-O14
5	A	1908	3PE	C12-C11-O13-P
5	A	1908	3PE	O13-C11-C12-N
5	A	1908	3PE	O11-C1-C2-O21
5	A	1910	3PE	C1-O11-P-O13
5	A	1910	3PE	C12-C11-O13-P
5	A	1911	3PE	C11-O13-P-O11
5	A	1911	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
6	A	1909	PC1	C11-O13-P-O14
6	A	1909	PC1	C1-O11-P-O12
6	A	1909	PC1	C1-O11-P-O13
6	A	1909	PC1	O13-C11-C12-N
6	A	1909	PC1	O32-C31-O31-C3
6	A	1909	PC1	C32-C31-O31-C3
7	A	1912	C8U	C02-C03-C22-O24
5	A	1907	3PE	O32-C31-O31-C3
7	A	1912	C8U	C03-C22-O24-C25
5	A	1907	3PE	C32-C31-O31-C3
5	A	1906	3PE	O32-C31-O31-C3
7	A	1912	C8U	C02-C03-C22-O23
5	A	1903	3PE	O22-C21-O21-C2
5	A	1904	3PE	C32-C31-O31-C3
5	A	1905	3PE	C32-C31-O31-C3
5	A	1906	3PE	C32-C31-O31-C3
7	A	1912	C8U	O23-C22-O24-C25
5	A	1904	3PE	O32-C31-O31-C3
5	A	1905	3PE	O32-C31-O31-C3
5	A	1911	3PE	C26-C27-C28-C29
5	A	1907	3PE	C28-C29-C2A-C2B
6	A	1909	PC1	C23-C24-C25-C26
5	A	1911	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C2C-C2D-C2E-C2F
5	A	1904	3PE	C3D-C3E-C3F-C3G
5	A	1910	3PE	C25-C26-C27-C28
5	A	1905	3PE	C21-C22-C23-C24
6	A	1909	PC1	C31-C32-C33-C34
5	A	1907	3PE	C21-C22-C23-C24
7	A	1912	C8U	C04-C03-C22-O23
5	A	1910	3PE	C32-C31-O31-C3
5	A	1906	3PE	C22-C21-O21-C2
5	A	1907	3PE	C22-C21-O21-C2
5	A	1907	3PE	O22-C21-O21-C2
5	A	1904	3PE	C2A-C2B-C2C-C2D
7	A	1912	C8U	C04-C03-C22-O24
5	A	1905	3PE	C2-C1-O11-P
6	A	1909	PC1	C2E-C2F-C2G-C2H
5	A	1906	3PE	O22-C21-O21-C2
5	A	1907	3PE	C22-C23-C24-C25
5	A	1907	3PE	C25-C26-C27-C28
5	A	1905	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
5	A	1905	3PE	C29-C2A-C2B-C2C
5	A	1904	3PE	C2E-C2F-C2G-C2H
5	A	1905	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C25-C26-C27-C28
5	A	1905	3PE	C27-C28-C29-C2A
5	A	1906	3PE	C32-C33-C34-C35
5	A	1905	3PE	C31-C32-C33-C34
5	A	1902	3PE	C22-C23-C24-C25
5	A	1904	3PE	C39-C3A-C3B-C3C
5	A	1903	3PE	C25-C26-C27-C28
5	A	1905	3PE	C32-C33-C34-C35
5	A	1910	3PE	O32-C31-O31-C3
5	A	1906	3PE	C33-C34-C35-C36
6	A	1909	PC1	C3A-C3B-C3C-C3D
5	A	1902	3PE	C24-C25-C26-C27
5	A	1910	3PE	C26-C27-C28-C29
6	A	1909	PC1	C25-C26-C27-C28
6	A	1909	PC1	C38-C39-C3A-C3B
6	A	1909	PC1	C3C-C3D-C3E-C3F
5	A	1903	3PE	C37-C38-C39-C3A
5	A	1904	3PE	C34-C35-C36-C37
5	A	1904	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C3B-C3C-C3D-C3E
5	A	1911	3PE	C3C-C3D-C3E-C3F
6	A	1909	PC1	C35-C36-C37-C38
5	A	1910	3PE	C23-C24-C25-C26
5	A	1906	3PE	C35-C36-C37-C38
5	A	1910	3PE	C28-C29-C2A-C2B
5	A	1902	3PE	C34-C35-C36-C37
5	A	1906	3PE	C23-C24-C25-C26
5	A	1903	3PE	C36-C37-C38-C39
5	A	1905	3PE	C2A-C2B-C2C-C2D
5	A	1906	3PE	C34-C35-C36-C37
5	A	1911	3PE	C33-C34-C35-C36
6	A	1909	PC1	C32-C33-C34-C35
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1905	3PE	C3E-C3F-C3G-C3H
5	A	1911	3PE	C38-C39-C3A-C3B
5	A	1904	3PE	C32-C33-C34-C35
5	A	1903	3PE	C22-C23-C24-C25
5	A	1904	3PE	C25-C26-C27-C28
5	A	1906	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
5	A	1904	3PE	C23-C24-C25-C26
5	A	1910	3PE	C22-C21-O21-C2
5	A	1911	3PE	C22-C21-O21-C2
5	A	1908	3PE	C21-C22-C23-C24
5	A	1903	3PE	C33-C34-C35-C36
5	A	1906	3PE	C22-C23-C24-C25
5	A	1902	3PE	C26-C27-C28-C29
5	A	1906	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	C3D-C3E-C3F-C3G
5	A	1906	3PE	C36-C37-C38-C39
5	A	1907	3PE	C23-C24-C25-C26
5	A	1911	3PE	O22-C21-O21-C2
5	A	1904	3PE	C35-C36-C37-C38
5	A	1907	3PE	C32-C33-C34-C35
5	A	1902	3PE	C32-C33-C34-C35
6	A	1909	PC1	C36-C37-C38-C39
5	A	1911	3PE	C22-C23-C24-C25
5	A	1904	3PE	C22-C23-C24-C25
5	A	1910	3PE	O22-C21-O21-C2
5	A	1902	3PE	C31-C32-C33-C34
5	A	1910	3PE	C32-C33-C34-C35
5	A	1905	3PE	C1-C2-C3-O31
5	A	1905	3PE	C34-C35-C36-C37
5	A	1904	3PE	C3A-C3B-C3C-C3D
6	A	1909	PC1	C3D-C3E-C3F-C3G
6	A	1909	PC1	C29-C2A-C2B-C2C
5	A	1904	3PE	C2D-C2E-C2F-C2G
5	A	1911	3PE	C31-C32-C33-C34
5	A	1904	3PE	C3-C2-O21-C21
5	A	1905	3PE	C39-C3A-C3B-C3C
5	A	1903	3PE	O11-C1-C2-O21
6	A	1909	PC1	O11-C1-C2-O21
5	A	1904	3PE	C37-C38-C39-C3A
6	A	1909	PC1	C37-C38-C39-C3A
5	A	1908	3PE	C26-C27-C28-C29
5	A	1902	3PE	C32-C31-O31-C3
5	A	1906	3PE	C2E-C2F-C2G-C2H
5	A	1910	3PE	C33-C34-C35-C36
5	A	1904	3PE	C3F-C3G-C3H-C3I
5	A	1904	3PE	C2C-C2D-C2E-C2F
5	A	1911	3PE	C32-C31-O31-C3
5	A	1910	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
5	A	1904	3PE	O11-C1-C2-C3
5	A	1911	3PE	C23-C24-C25-C26
5	A	1904	3PE	C31-C32-C33-C34
5	A	1911	3PE	C3D-C3E-C3F-C3G
5	A	1911	3PE	C3E-C3F-C3G-C3H
5	A	1906	3PE	C24-C25-C26-C27
6	A	1909	PC1	C21-C22-C23-C24
6	A	1909	PC1	C33-C34-C35-C36
5	A	1902	3PE	C1-C2-C3-O31
5	A	1907	3PE	C1-C2-C3-O31
5	A	1905	3PE	C3B-C3C-C3D-C3E
5	A	1907	3PE	C24-C25-C26-C27
5	A	1911	3PE	C2E-C2F-C2G-C2H
5	A	1911	3PE	C3F-C3G-C3H-C3I
5	A	1902	3PE	C27-C28-C29-C2A
5	A	1904	3PE	C36-C37-C38-C39
6	A	1909	PC1	O21-C21-C22-C23
5	A	1903	3PE	O21-C2-C3-O31
5	A	1905	3PE	O21-C2-C3-O31
5	A	1907	3PE	C27-C28-C29-C2A
5	A	1903	3PE	C27-C28-C29-C2A
5	A	1908	3PE	C23-C24-C25-C26
5	A	1902	3PE	O32-C31-O31-C3
5	A	1905	3PE	C3A-C3B-C3C-C3D
5	A	1902	3PE	C33-C34-C35-C36
5	A	1911	3PE	O32-C31-O31-C3
5	A	1911	3PE	C2F-C2G-C2H-C2I
5	A	1907	3PE	C3-C2-O21-C21
5	A	1906	3PE	C2C-C2D-C2E-C2F
5	A	1904	3PE	O11-C1-C2-O21
5	A	1905	3PE	O11-C1-C2-O21
5	A	1911	3PE	O11-C1-C2-O21
5	A	1903	3PE	C1-C2-C3-O31
5	A	1907	3PE	O21-C2-C3-O31
5	A	1904	3PE	C2B-C2C-C2D-C2E
5	A	1902	3PE	C35-C36-C37-C38
5	A	1902	3PE	C25-C26-C27-C28
7	A	1912	C8U	C04-C05-N09-O10
6	A	1909	PC1	C39-C3A-C3B-C3C
5	A	1903	3PE	O11-C1-C2-C3
6	A	1909	PC1	O11-C1-C2-C3
5	A	1902	3PE	O21-C2-C3-O31

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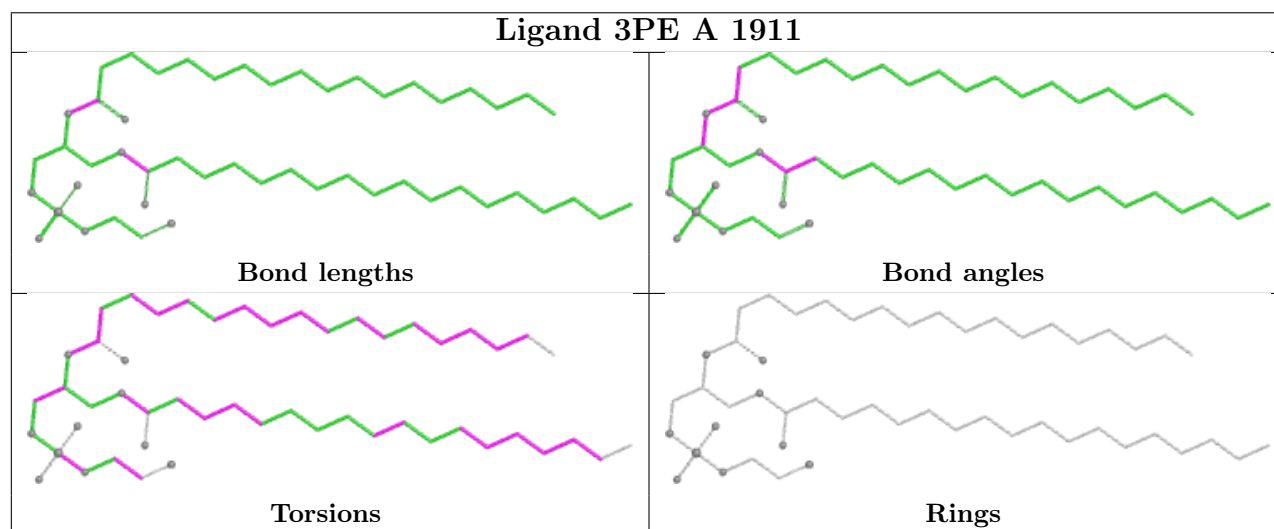
Mol	Chain	Res	Type	Atoms
5	A	1908	3PE	C22-C21-O21-C2
5	A	1902	3PE	C11-O13-P-O14
5	A	1904	3PE	C1-O11-P-O13
5	A	1904	3PE	C1-O11-P-O14
5	A	1904	3PE	C11-O13-P-O14
5	A	1904	3PE	O13-C11-C12-N
5	A	1905	3PE	C11-O13-P-O14
5	A	1907	3PE	C1-O11-P-O14
5	A	1910	3PE	C1-O11-P-O14
5	A	1911	3PE	O13-C11-C12-N
6	A	1909	PC1	C1-O11-P-O14
6	A	1909	PC1	C2-C1-O11-P
5	A	1905	3PE	C2E-C2F-C2G-C2H
5	A	1906	3PE	C27-C28-C29-C2A
5	A	1911	3PE	C27-C28-C29-C2A
5	A	1908	3PE	O22-C21-O21-C2
5	A	1904	3PE	C26-C27-C28-C29
5	A	1907	3PE	C37-C38-C39-C3A
5	A	1906	3PE	O11-C1-C2-O21
5	A	1906	3PE	C2F-C2G-C2H-C2I
5	A	1903	3PE	C34-C35-C36-C37
5	A	1903	3PE	C26-C27-C28-C29
6	A	1909	PC1	C28-C29-C2A-C2B
5	A	1905	3PE	O11-C1-C2-C3
5	A	1911	3PE	O11-C1-C2-C3
5	A	1904	3PE	C33-C34-C35-C36
5	A	1905	3PE	C2F-C2G-C2H-C2I
6	A	1909	PC1	C2A-C2B-C2C-C2D
5	A	1911	3PE	C32-C33-C34-C35
6	A	1909	PC1	O22-C21-C22-C23
5	A	1911	3PE	O21-C21-C22-C23
7	A	1912	C8U	C06-C05-N09-O10
6	A	1909	PC1	C3F-C3G-C3H-C3I
5	A	1911	3PE	C2D-C2E-C2F-C2G
5	A	1907	3PE	C29-C2A-C2B-C2C
5	A	1903	3PE	C23-C24-C25-C26
5	A	1911	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	O31-C31-C32-C33
5	A	1905	3PE	O32-C31-C32-C33
5	A	1904	3PE	C27-C28-C29-C2A

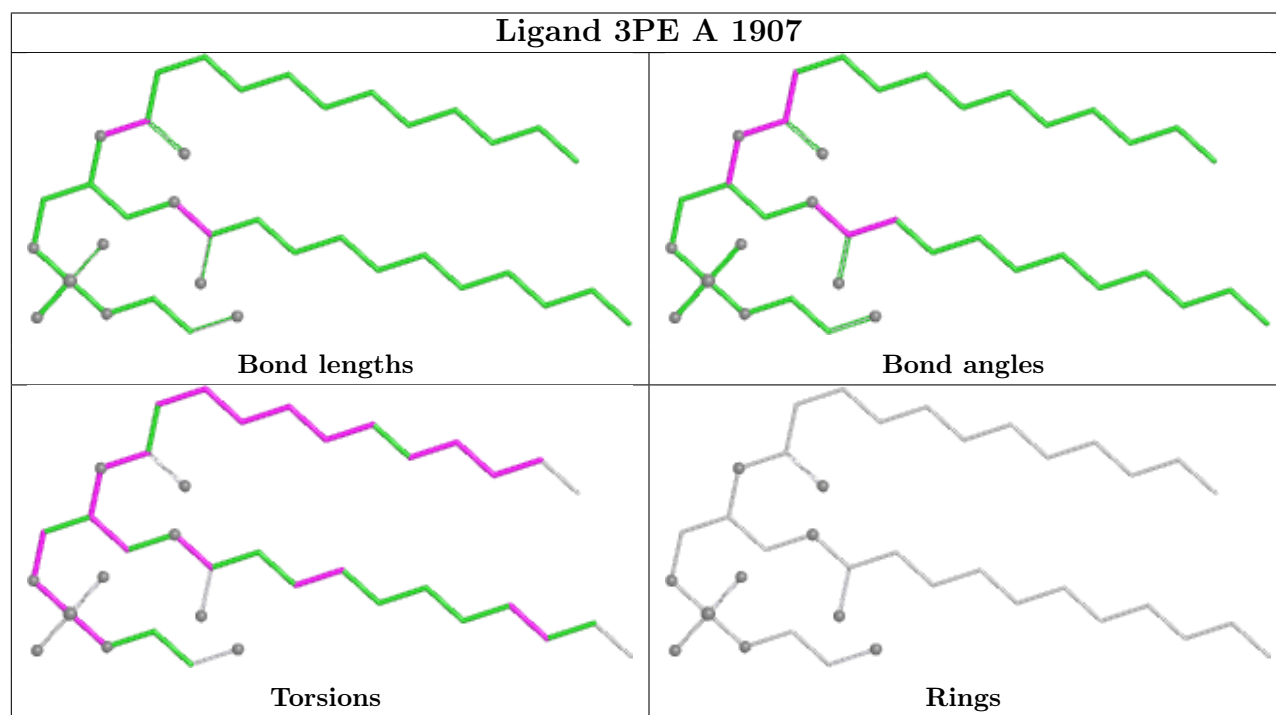
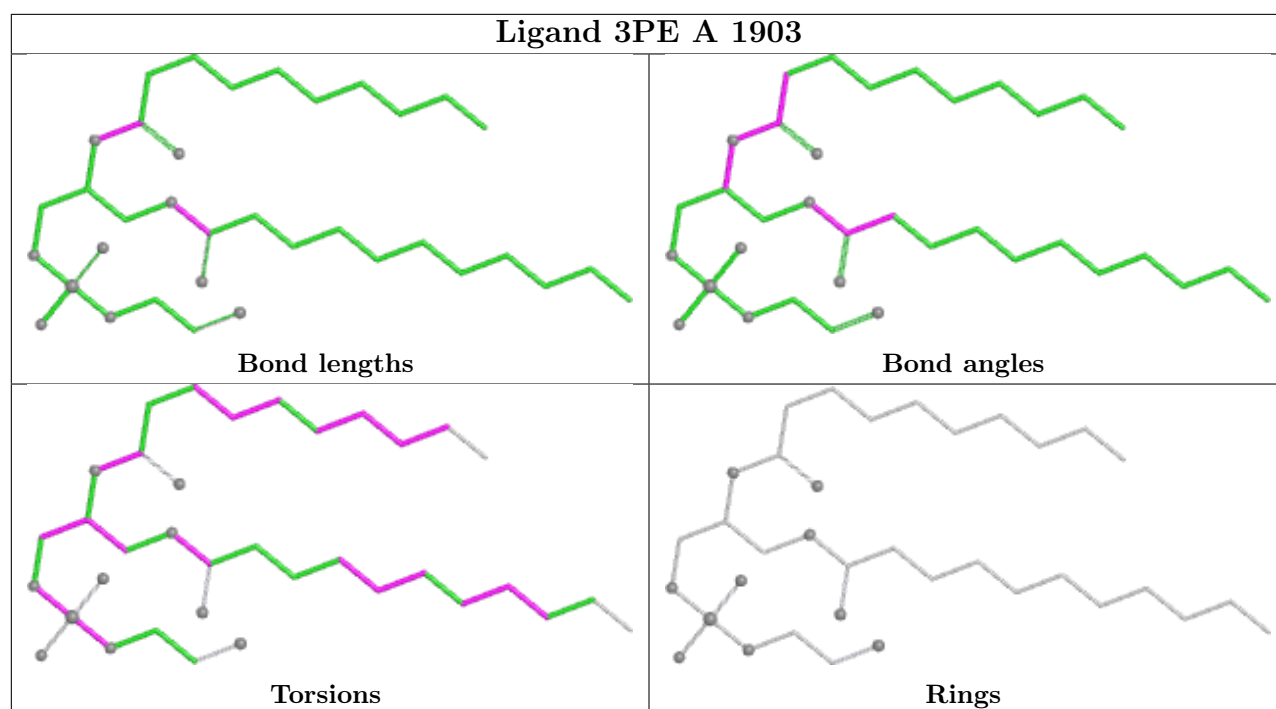
There are no ring outliers.

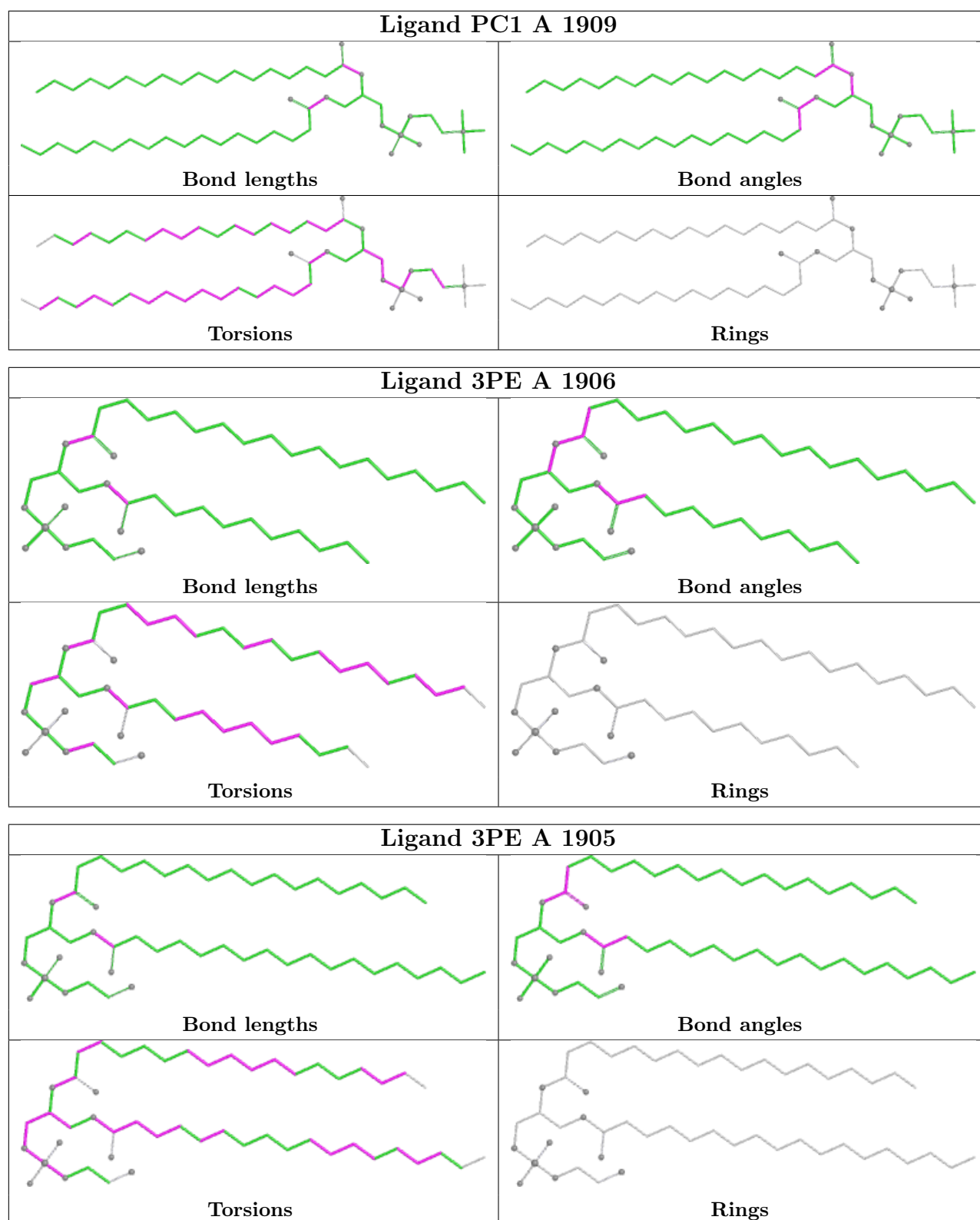
11 monomers are involved in 127 short contacts:

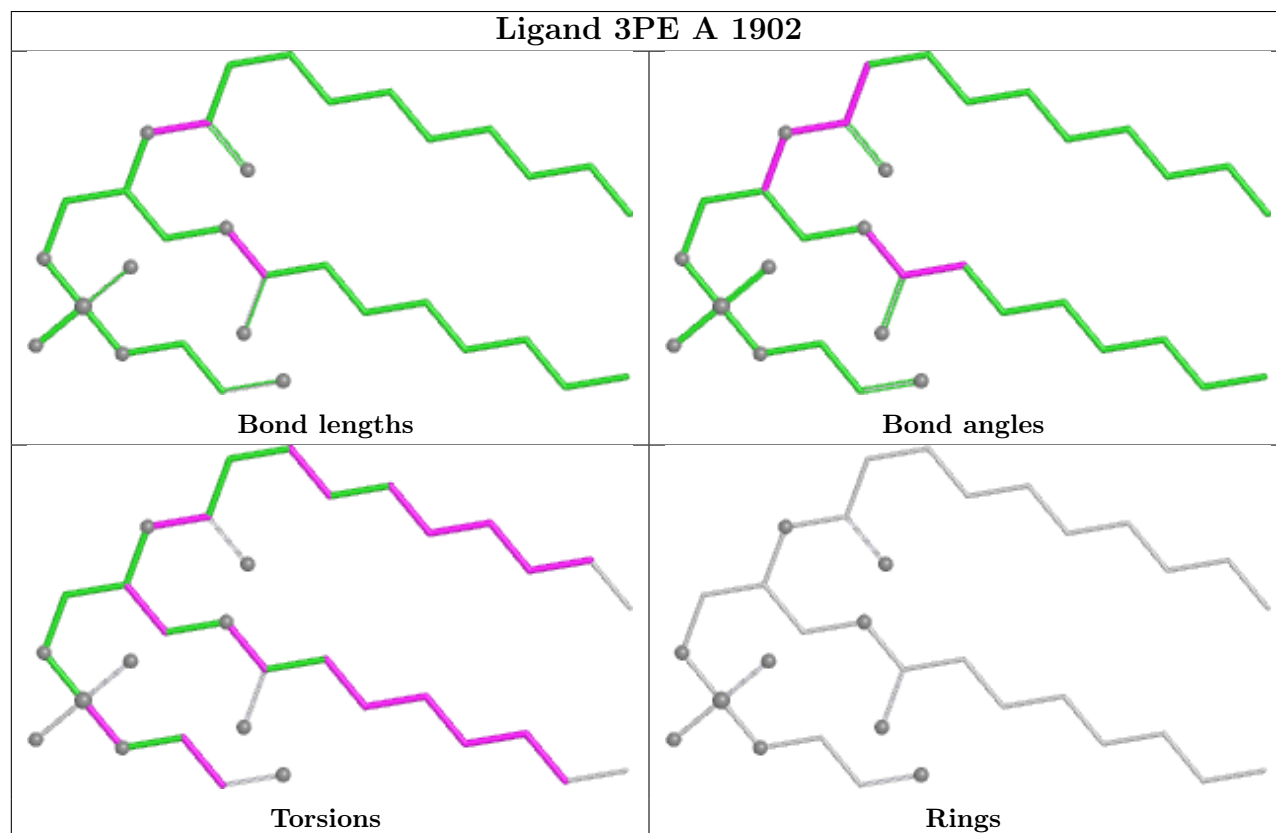
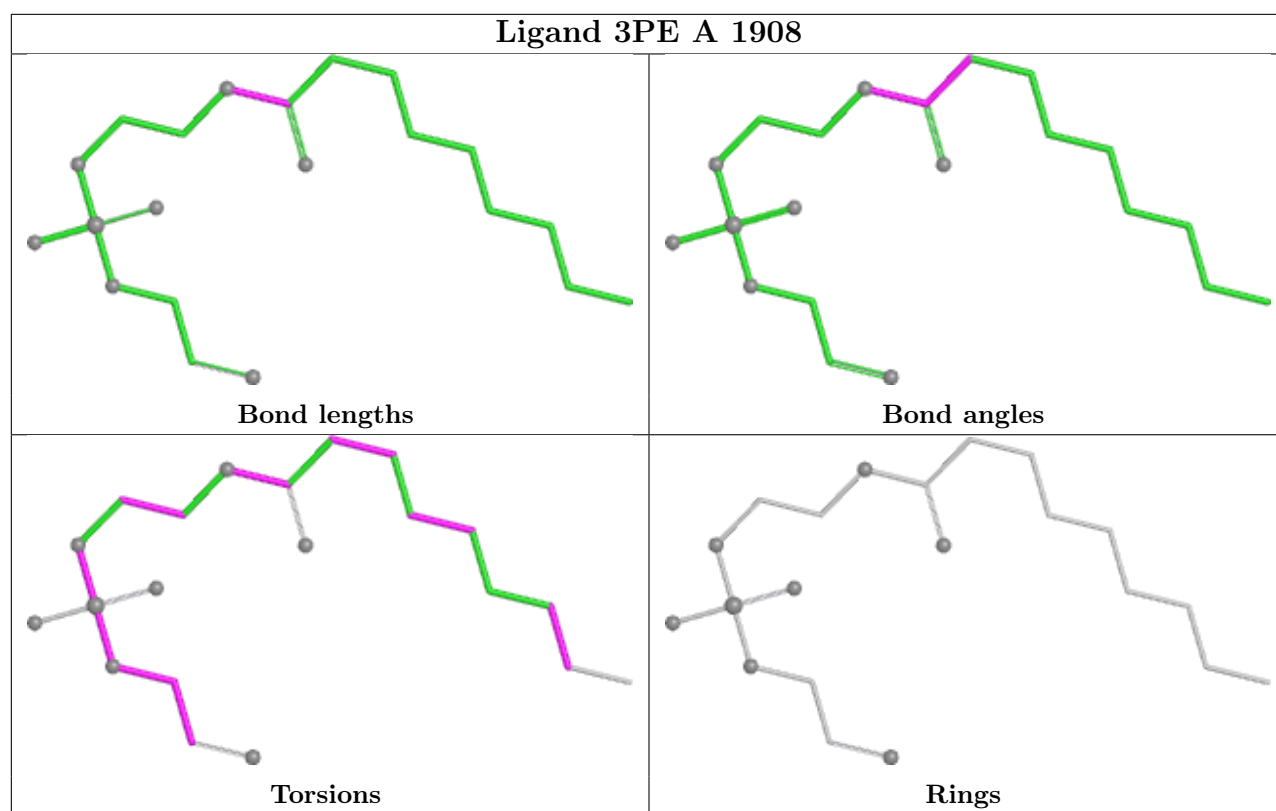
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1911	3PE	13	0
5	A	1903	3PE	17	0
5	A	1907	3PE	17	0
6	A	1909	PC1	12	0
5	A	1906	3PE	17	0
5	A	1905	3PE	17	0
5	A	1908	3PE	11	0
5	A	1902	3PE	2	0
5	A	1904	3PE	17	0
5	A	1910	3PE	9	0
7	A	1912	C8U	6	0

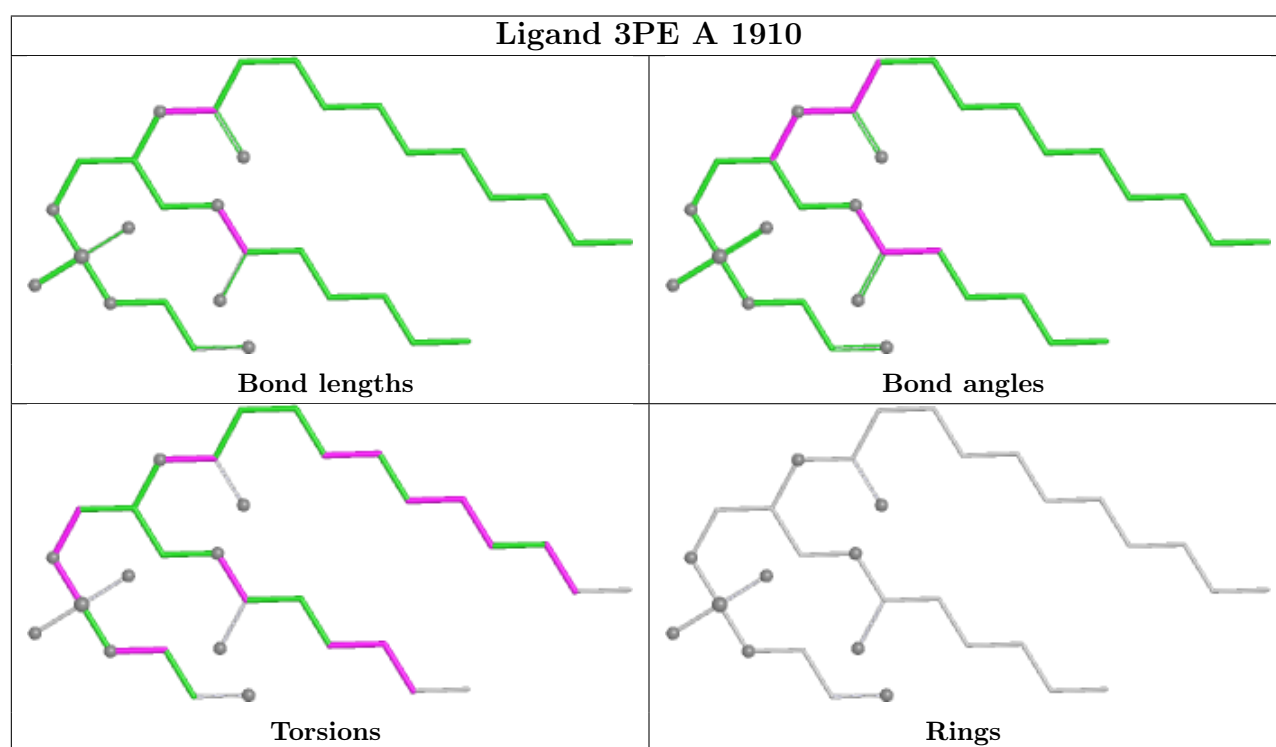
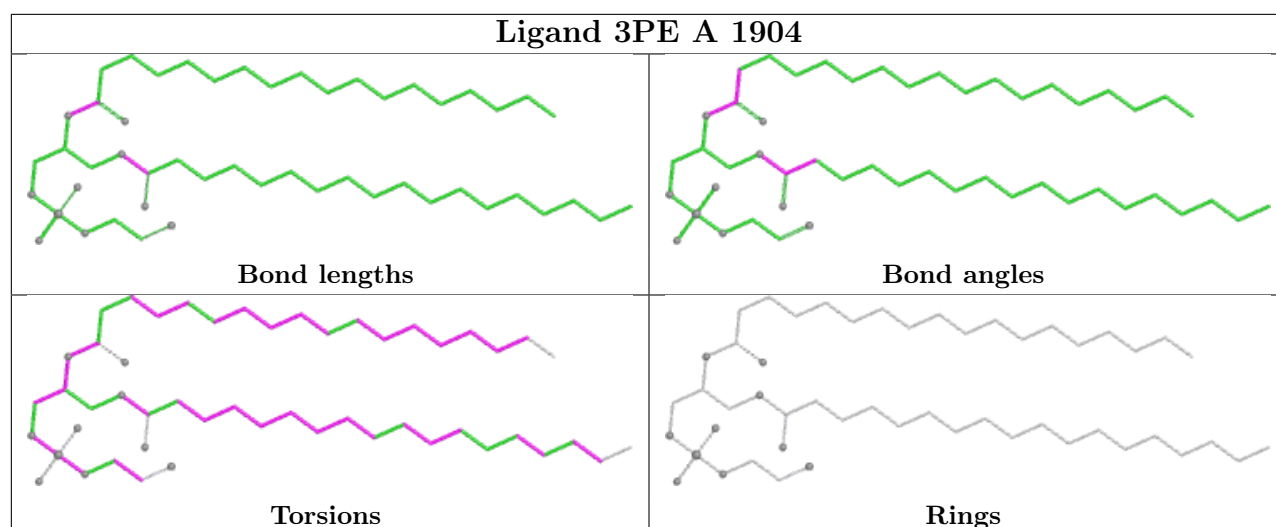
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

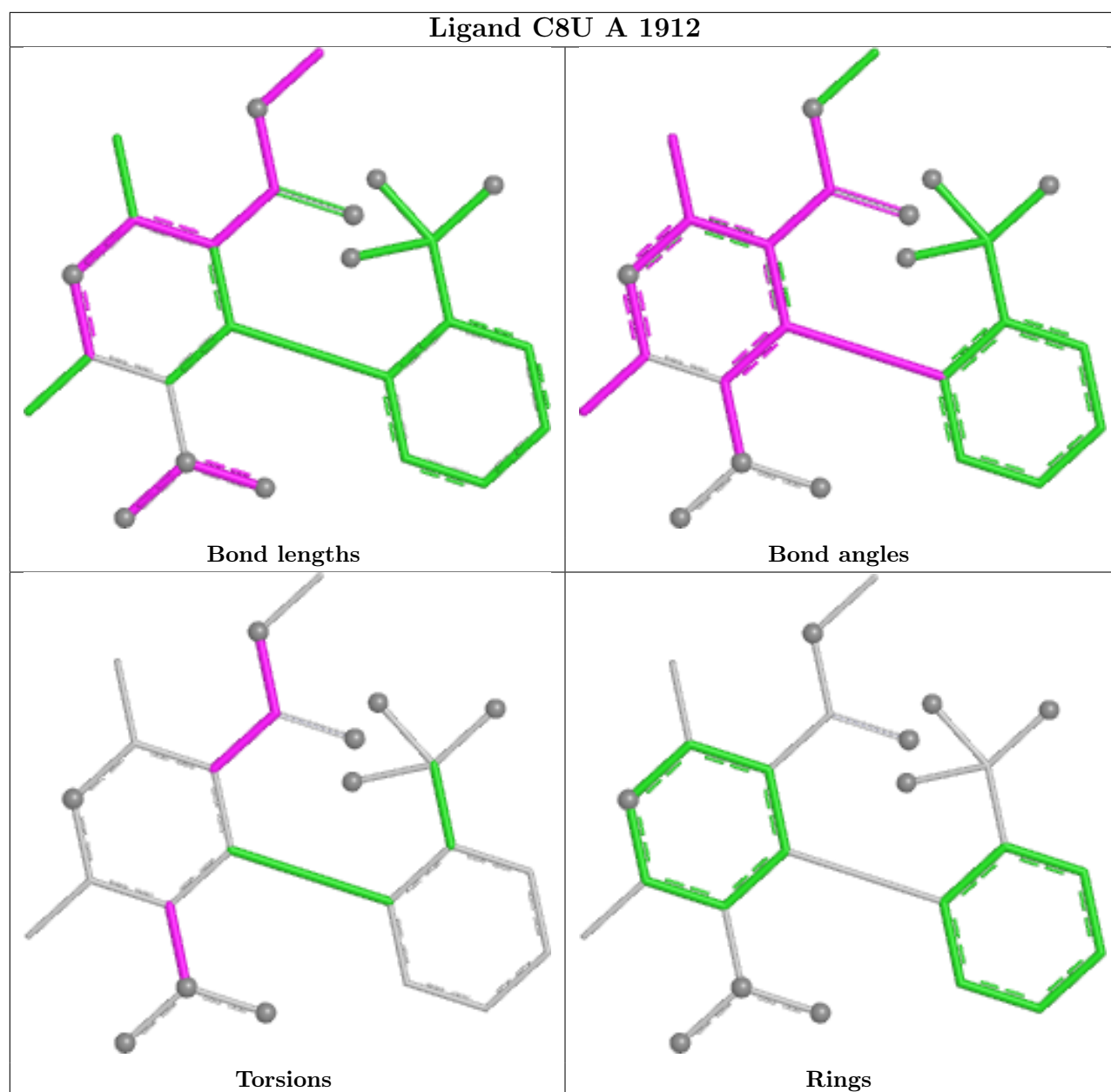












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

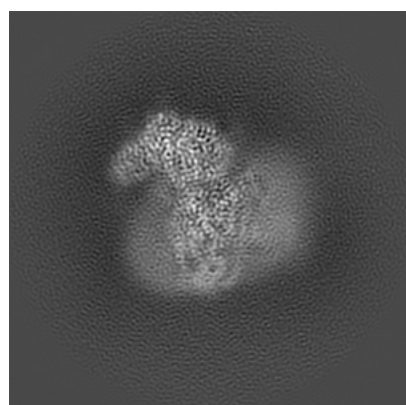
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22415. These allow visual inspection of the internal detail of the map and identification of artifacts.

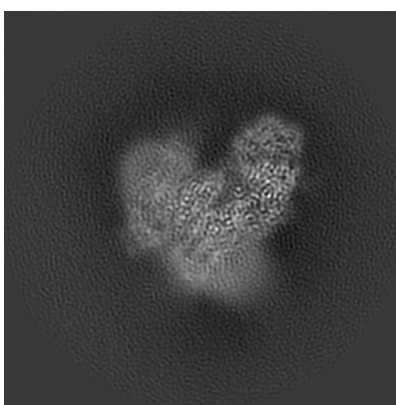
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

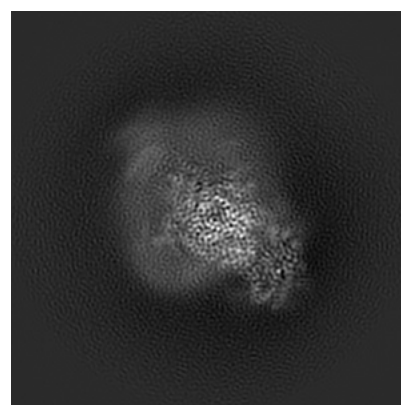
6.1.1 Primary map



X



Y

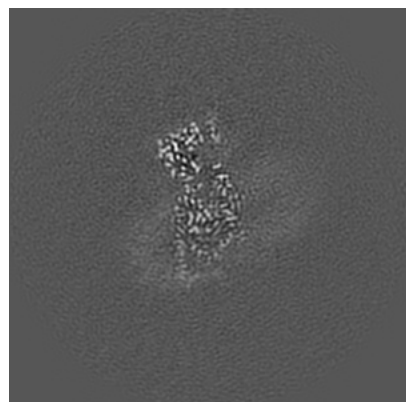


Z

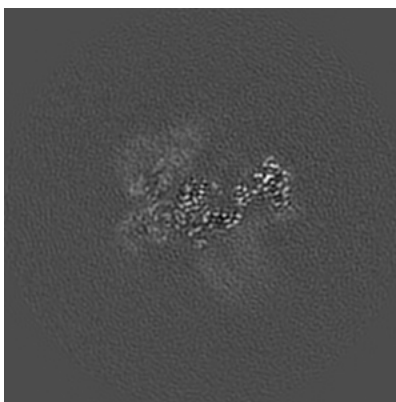
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

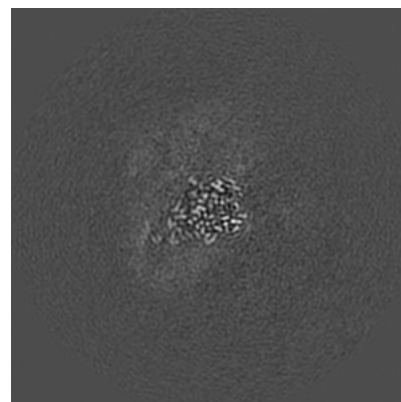
6.2.1 Primary map



X Index: 140



Y Index: 140

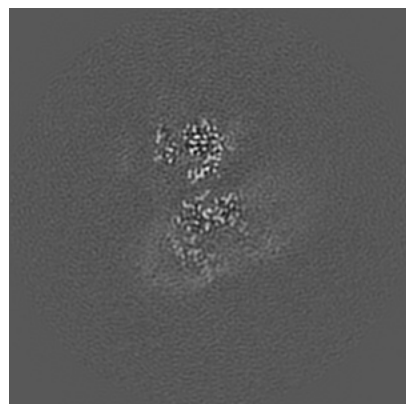


Z Index: 140

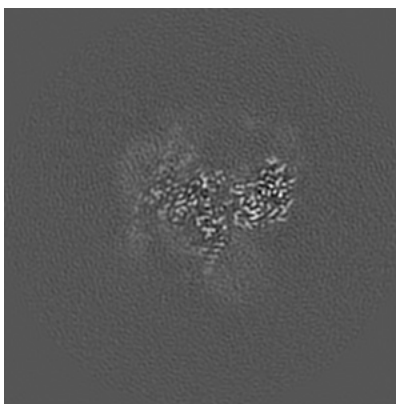
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

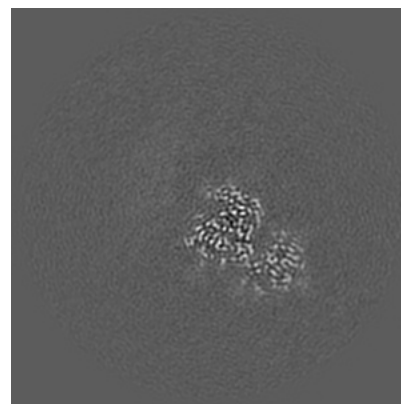
6.3.1 Primary map



X Index: 151



Y Index: 130

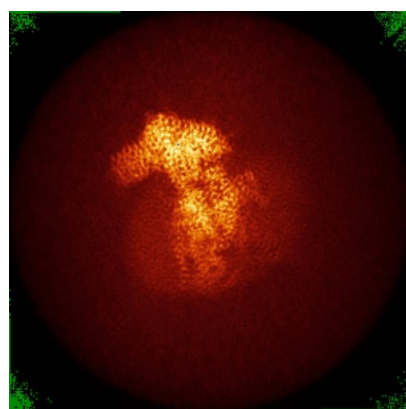


Z Index: 184

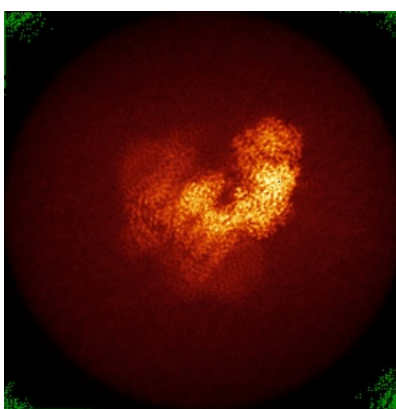
The images above show the largest variance slices of the map in three orthogonal directions.

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

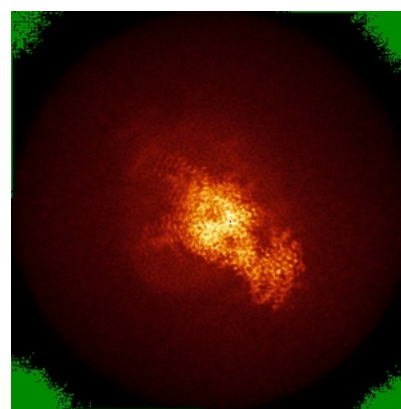
6.4.1 Primary map



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

This section was not generated.

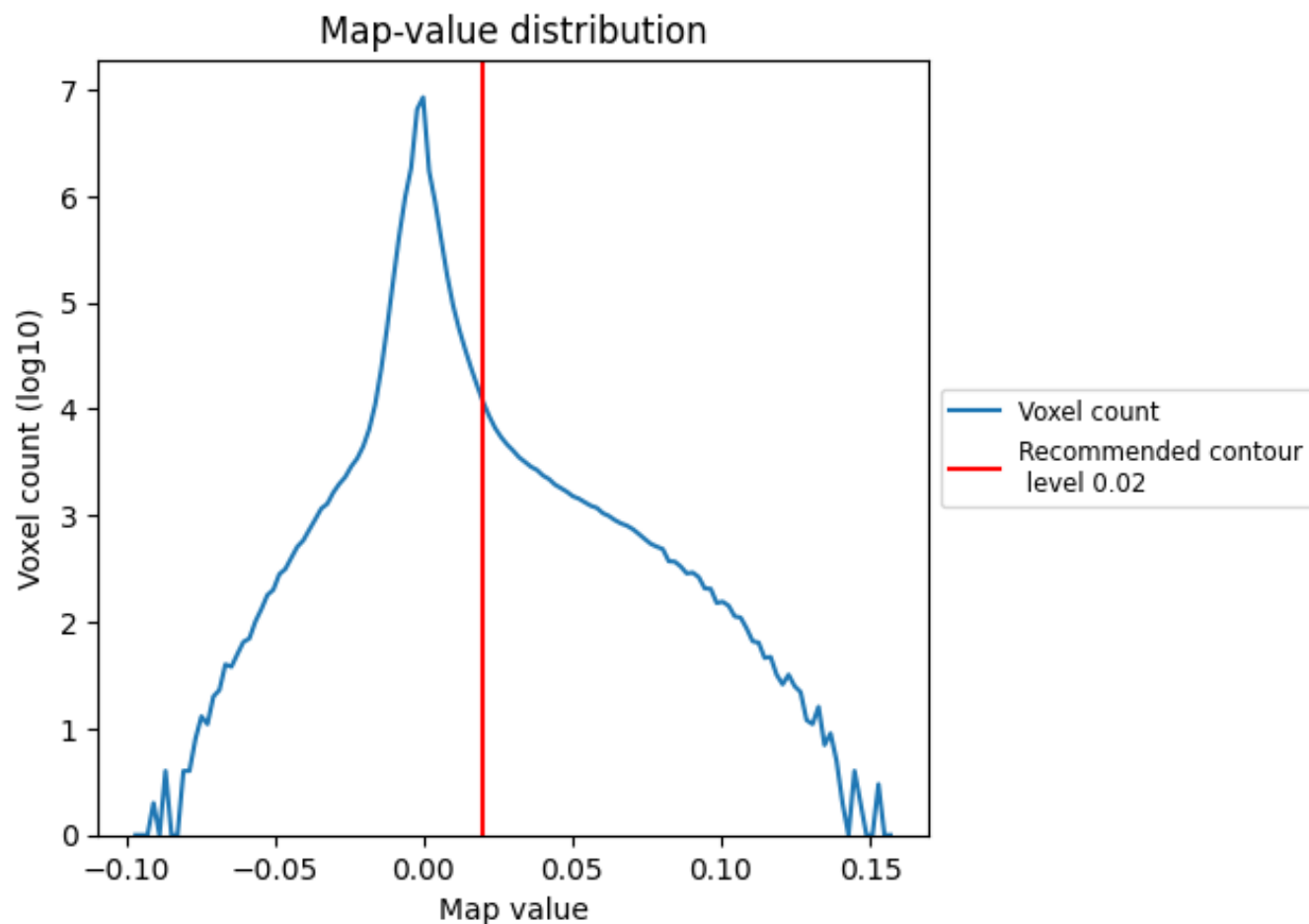
6.6 Mask visualisation

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

7 Map analysis [i](#)

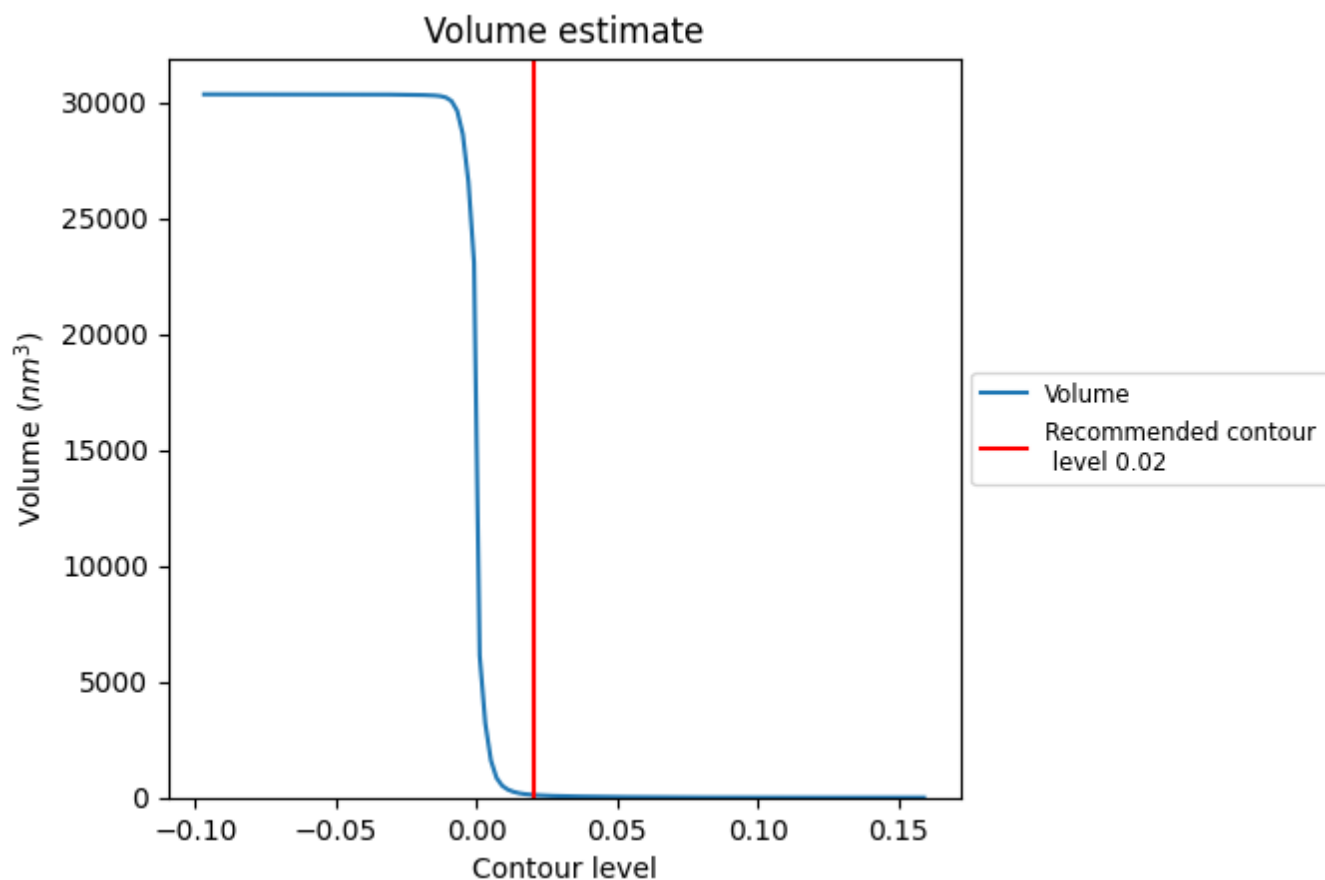
This section contains the results of statistical analysis of the map.

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.

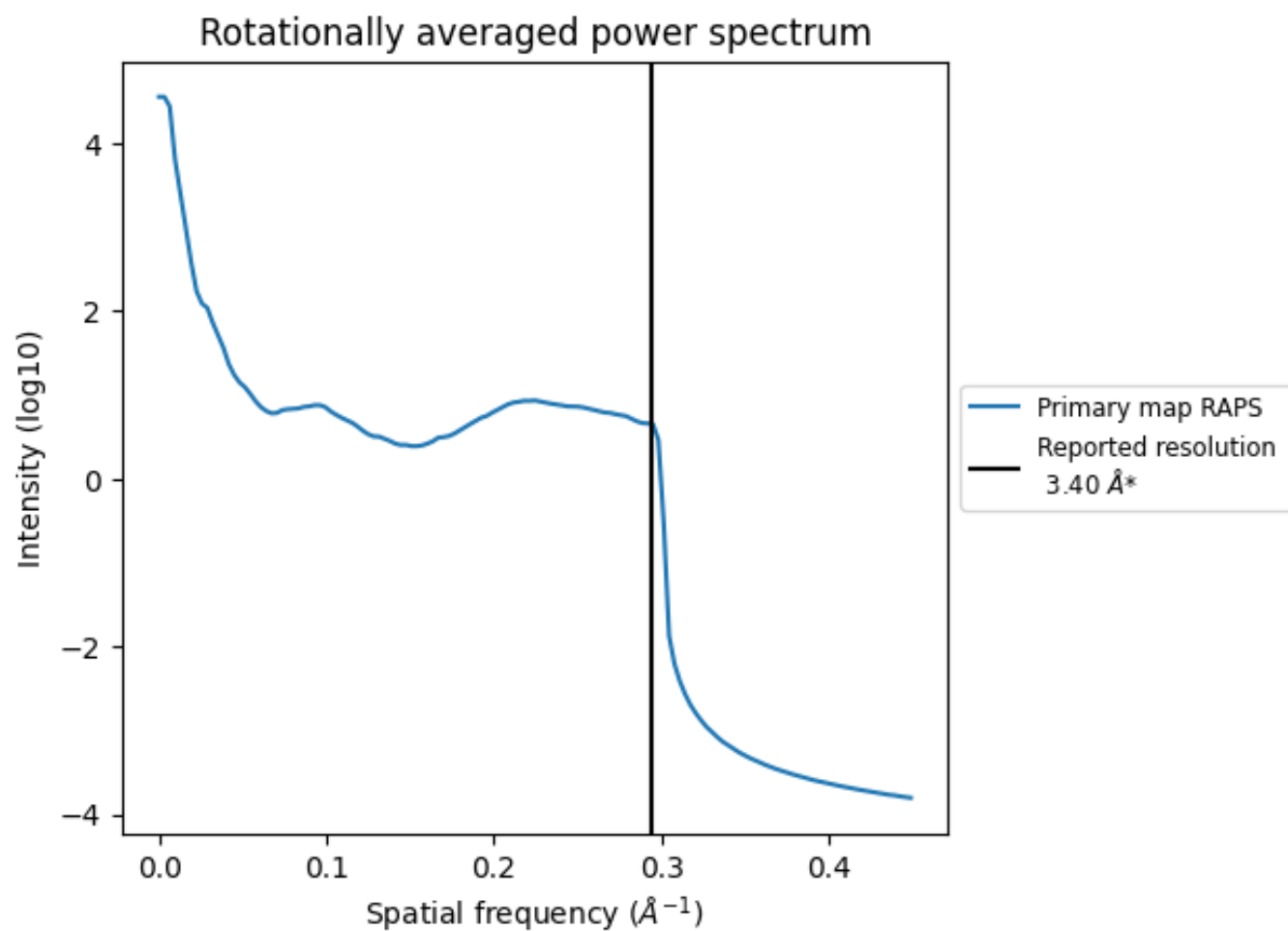
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 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 0.294 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

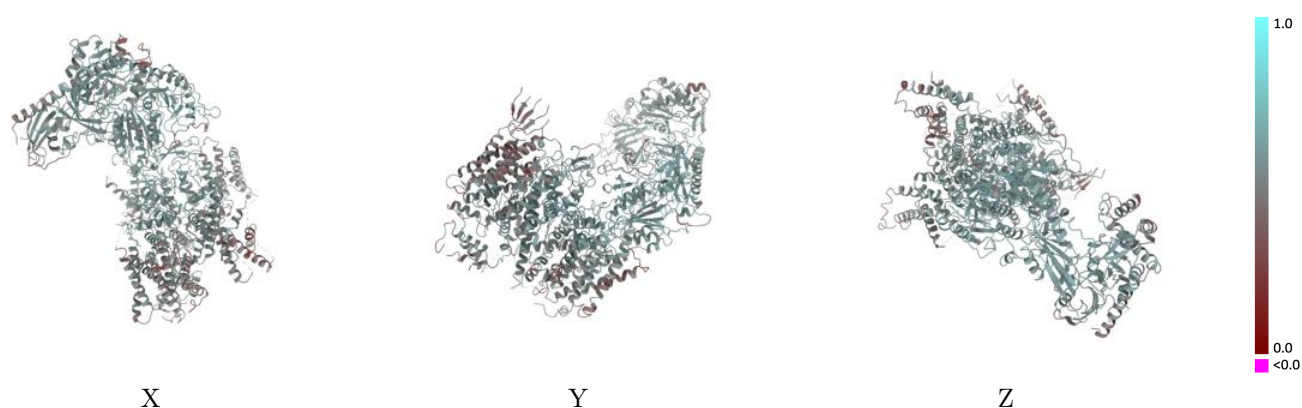
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-22415 and PDB model 7JPL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

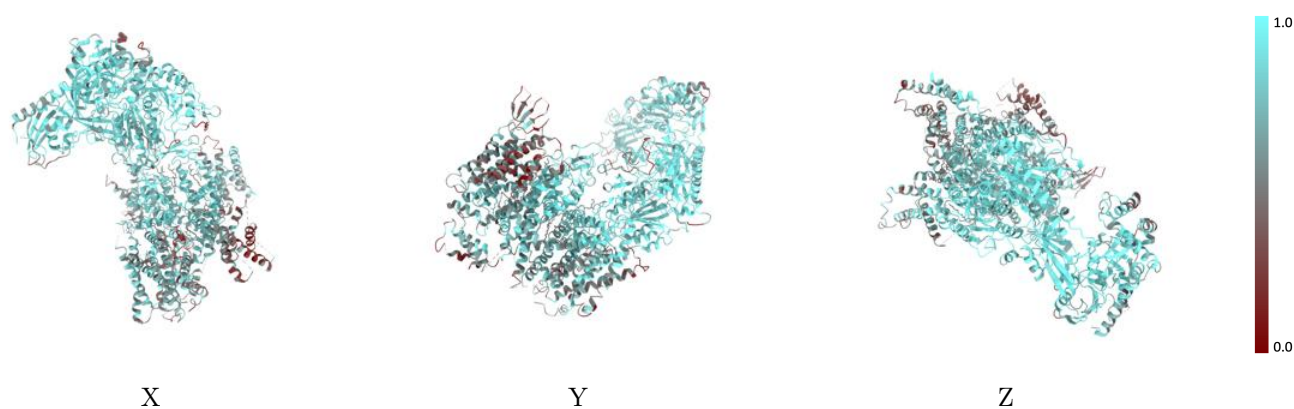
This section was not generated.

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



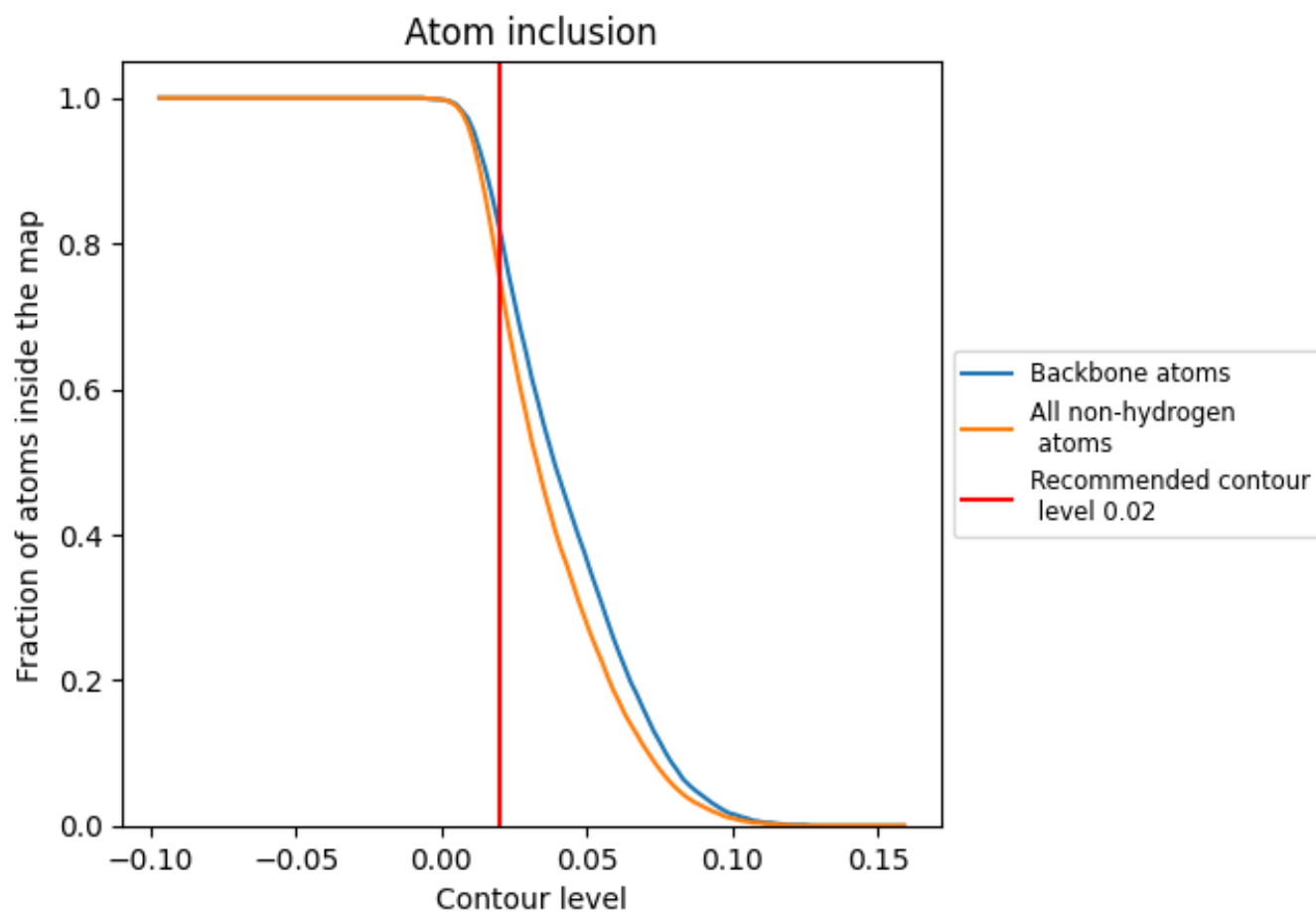
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.5300
A	0.7080	0.5230
E	0.5670	0.4570
F	0.8350	0.5510

