Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:55 PM EST

PDB ID	:	7JPK
EMDB ID	:	EMD-22414
Title	:	Rabbit Cav1.1 in the presence of 100 micromolar (S)-(-)-Bay K8644 in nanodiscs at 3.0 Angstrom resolution
Authors	:	Yan, N.; Gao, S.
Deposited on	:	2020-08-09
Resolution	:	3.00 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:

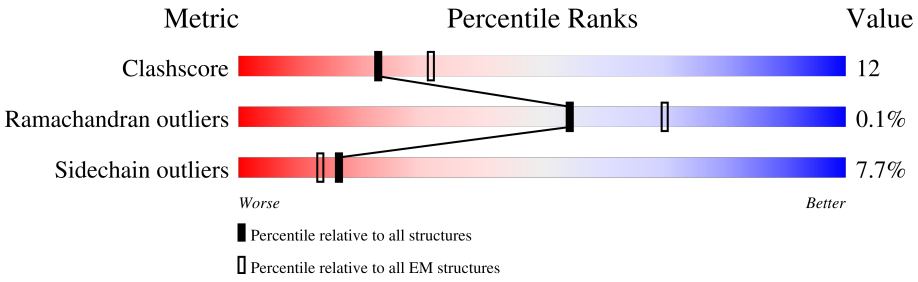
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	8% 40% 18% · 40%
2	E	222	20% 47% 27% · 24%
3	F	1105	· 66% 20% · 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18591 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
			Total	C	N	O	S		
1	A	1115	9009	5976	1437	1537	59	0	0

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

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

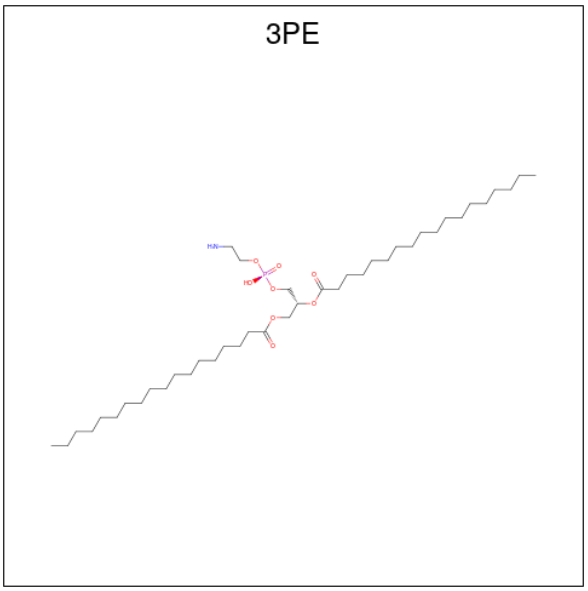
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

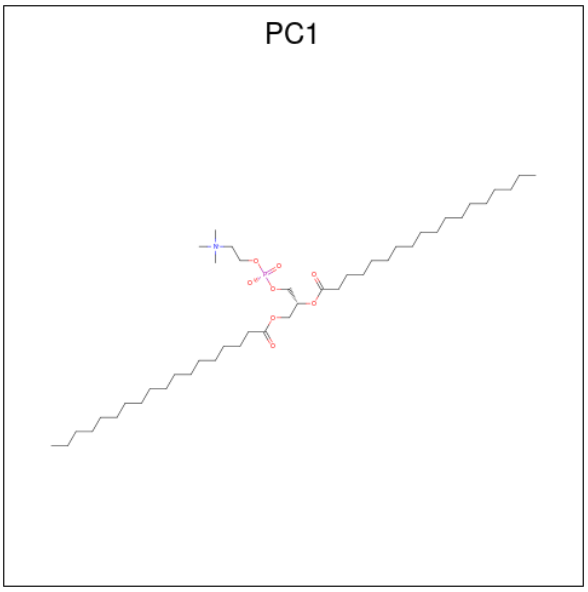
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	1	1	0

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



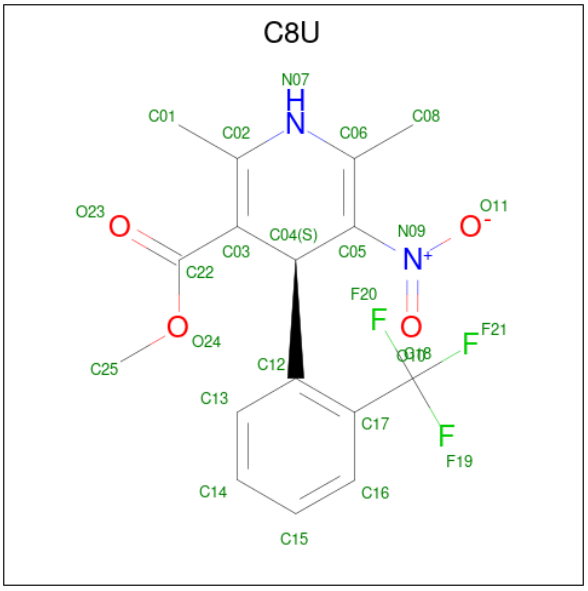
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	A	1	Total	C	N	O	P	0
			339	261	8	62	8	
5	E	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

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

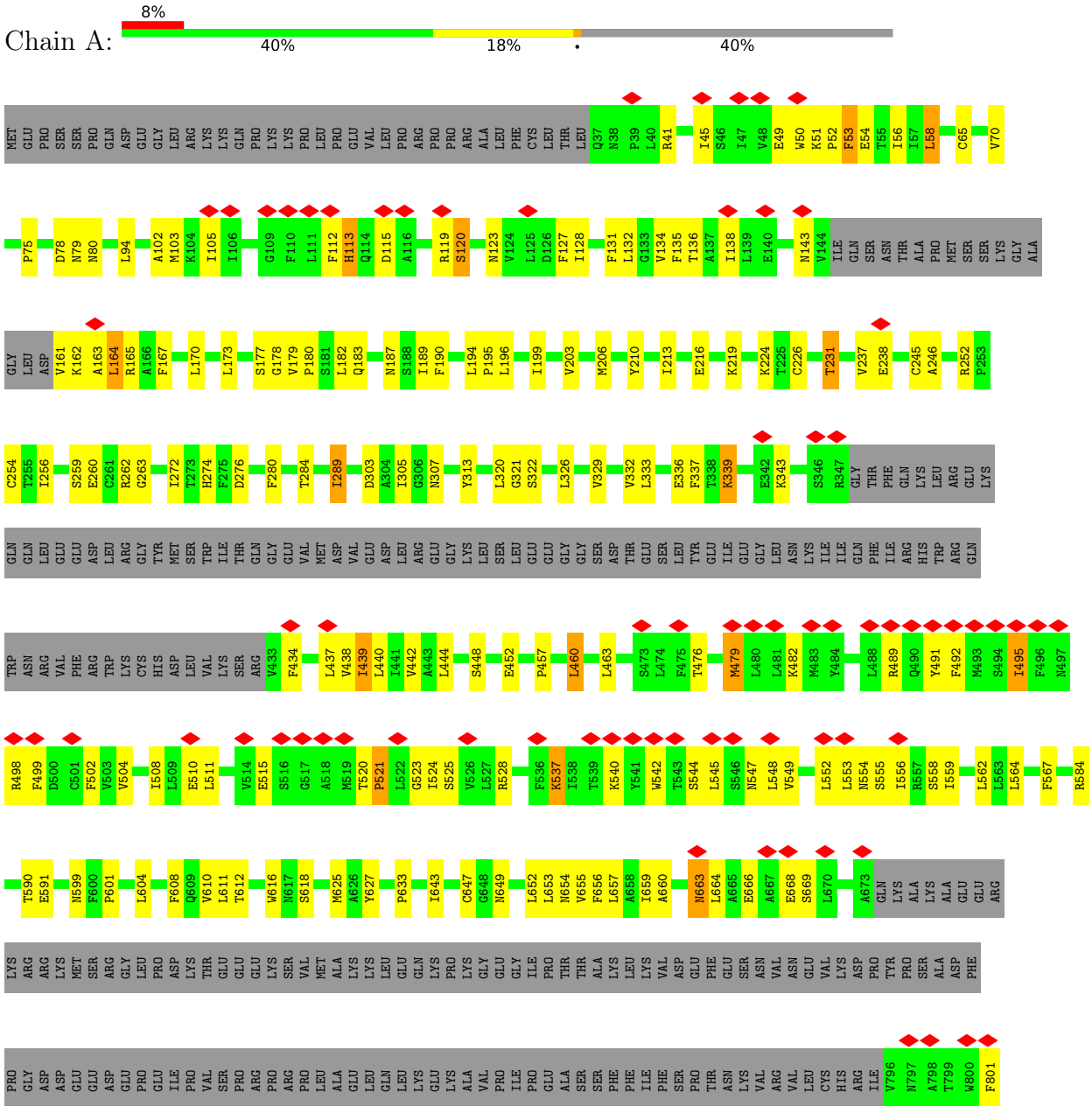


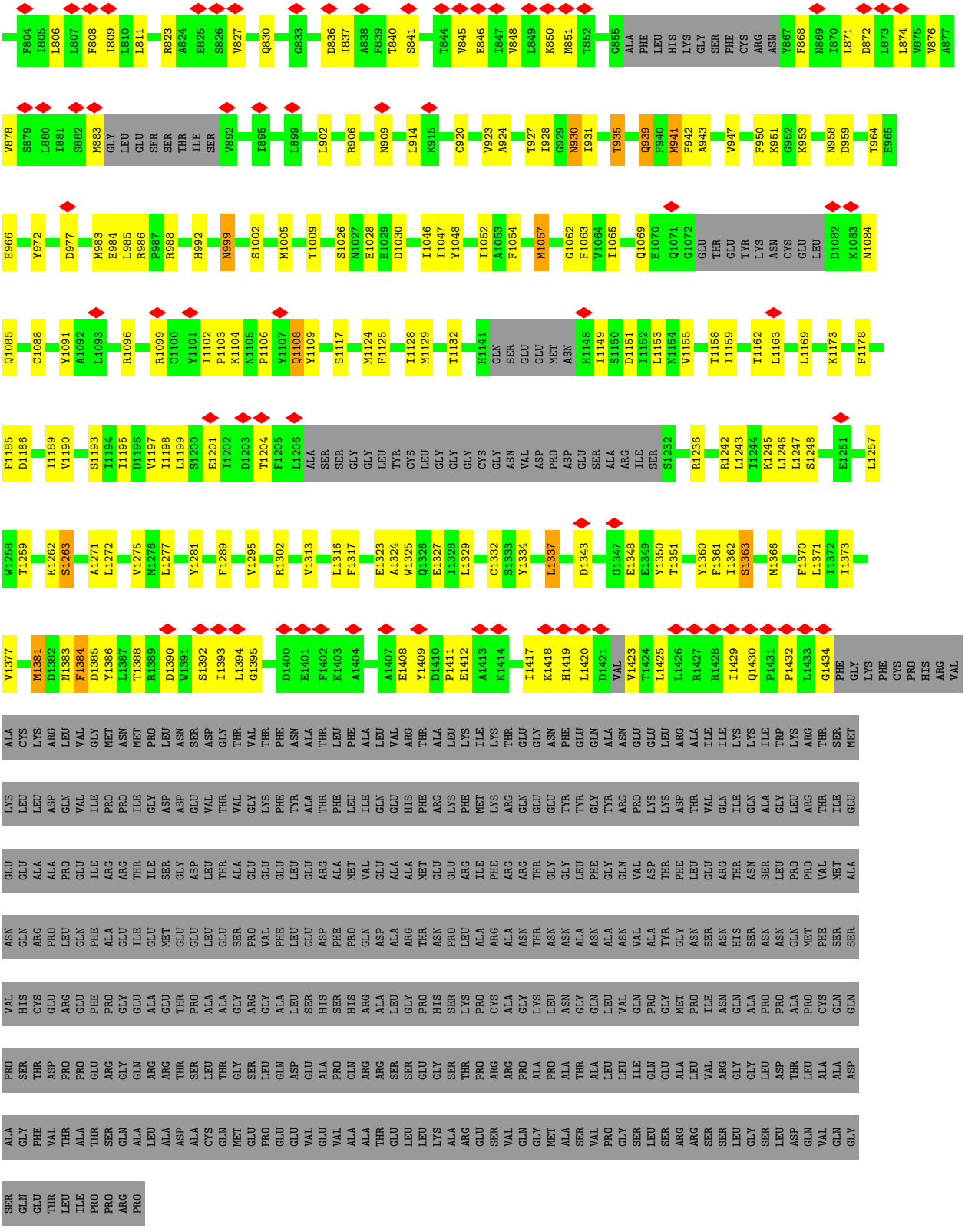
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
7	A	1	25	16	3	2	4	0

3 Residue-property plots (i)

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

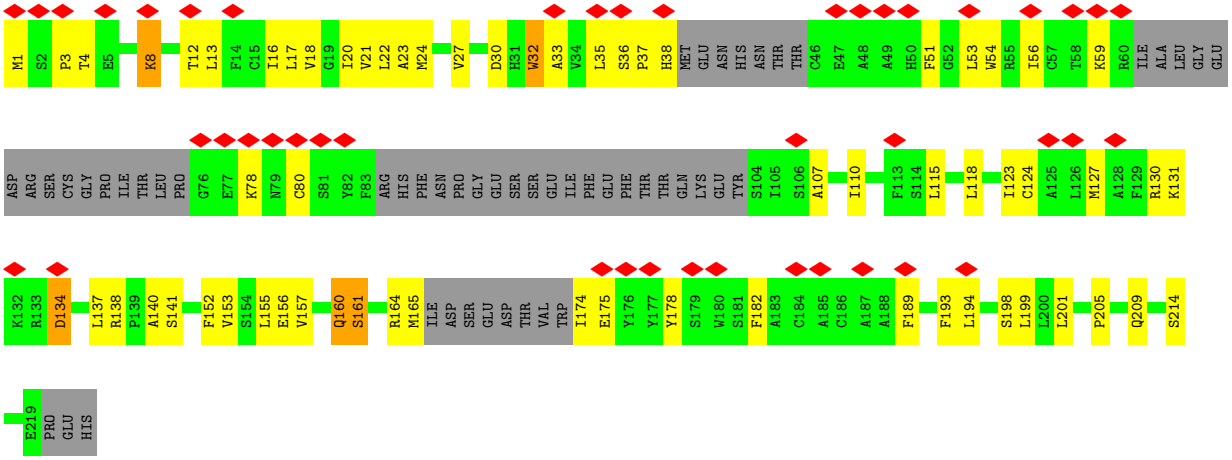
• Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S





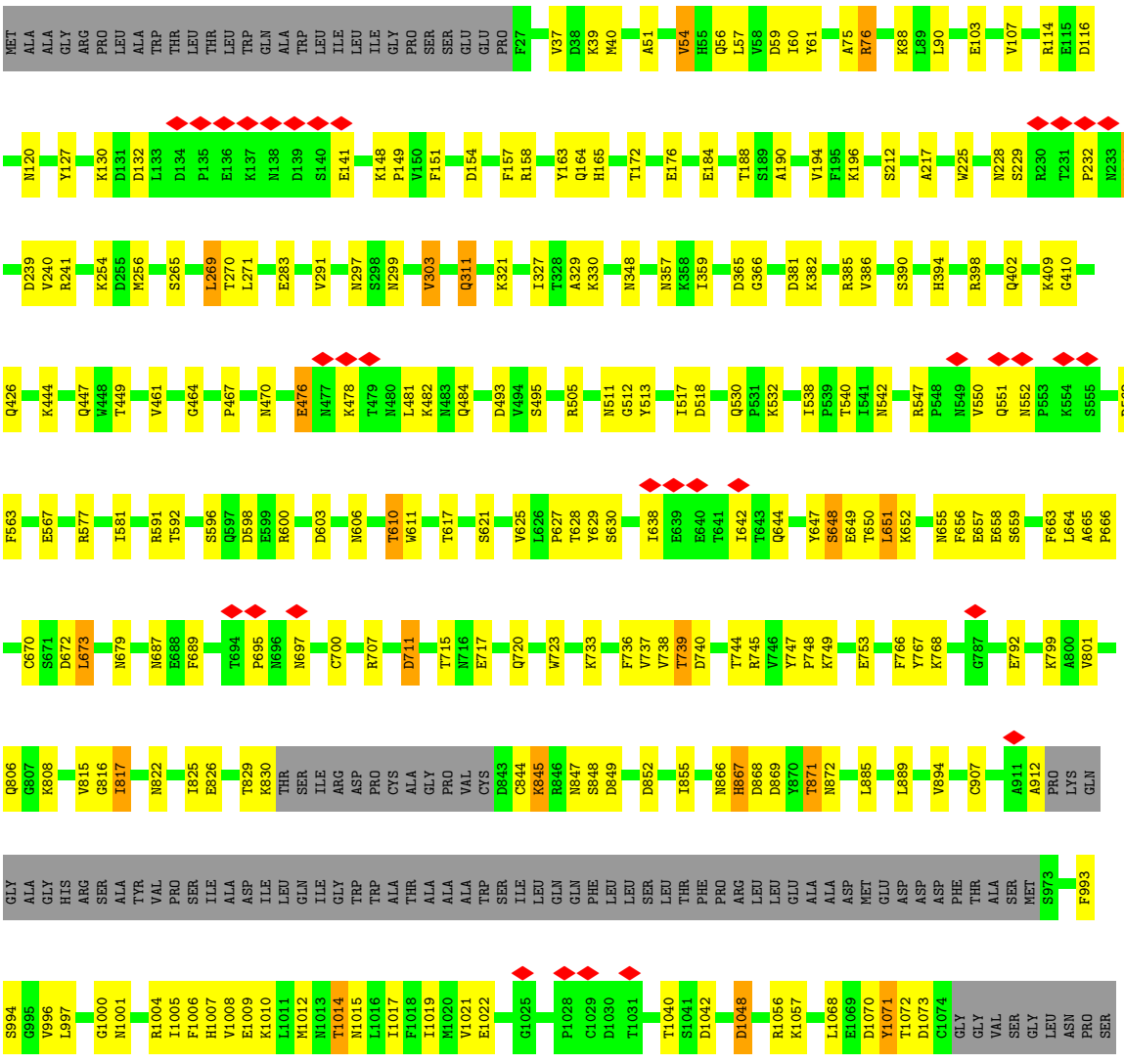
• Molecule 2: Voltage-dependent calcium channel gamma-1 subunit

Chain E:



• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain F:



LEU
TRP
SER
ILE
ILE
GLY
ILE
GLN
PHE
VAL
LEU
LEU
TRP
LEU
VAL
SER
GLY
SER
ARG
HIS
CYS
LEU
LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87516	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 ($e^-/Å^2$)	53	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	0.176	Depositor
Minimum map value	-0.096	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, PC1, CA, C8U

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	0/9233	0.45	0/12534
2	E	0.27	0/1358	0.44	0/1832
3	F	0.35	0/7974	0.48	0/10816
All	All	0.33	0/18565	0.46	0/25182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	9009	0	9146	258	0
2	E	1326	0	1345	42	0
3	F	7804	0	7617	128	0
4	A	1	0	0	0	0
5	A	339	0	504	79	0
5	E	33	0	40	1	0
6	A	54	0	88	16	0
7	A	25	0	0	6	0
All	All	18591	0	18740	462	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 12.

All (462) 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:1129:MET:CE	5:A:1902:3PE:H2C2	1.19	1.58
1:A:320:LEU:HD11	6:A:1908:PC1:C2I	1.24	1.57
1:A:320:LEU:CD1	6:A:1908:PC1:H2I1	1.19	1.55
1:A:1129:MET:HE1	5:A:1902:3PE:C2C	1.43	1.48
1:A:1366:MET:CE	5:A:1903:3PE:H2A1	1.55	1.34
1:A:1366:MET:CE	5:A:1903:3PE:C2A	2.24	1.16
1:A:1366:MET:HE3	5:A:1903:3PE:C2A	1.77	1.14
1:A:931:ILE:O	1:A:935:THR:HG23	1.45	1.14
1:A:559:ILE:HG21	1:A:659:ILE:HD11	1.28	1.11
1:A:1046:ILE:CD1	5:A:1907:3PE:H262	1.80	1.10
1:A:1129:MET:CE	5:A:1902:3PE:C2C	2.09	1.10
1:A:1046:ILE:HD13	5:A:1907:3PE:H262	1.30	1.09
5:A:1910:3PE:H2I1	5:A:1910:3PE:C3A	1.90	0.99
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.44	0.99
1:A:931:ILE:O	1:A:935:THR:CG2	2.11	0.98
5:A:1910:3PE:H3A1	5:A:1910:3PE:C2I	1.93	0.98
5:A:1910:3PE:H2I1	5:A:1910:3PE:H3A1	0.98	0.96
5:A:1903:3PE:H2I2	7:A:1911:C8U:F19	1.58	0.94
3:F:386:VAL:O	3:F:410:GLY:HA3	1.68	0.93
1:A:1366:MET:HE2	5:A:1903:3PE:C2A	2.00	0.92
1:A:1129:MET:HE3	5:A:1902:3PE:H2C2	1.49	0.89
1:A:1366:MET:HE3	5:A:1903:3PE:H2A1	0.89	0.88
1:A:337:PHE:HE2	1:A:657:LEU:HB3	1.39	0.87
5:A:1905:3PE:C3B	5:A:1905:3PE:H2G1	2.05	0.86
6:A:1908:PC1:O32	6:A:1908:PC1:H231	1.75	0.86
1:A:559:ILE:HD12	1:A:659:ILE:HG13	1.55	0.86
2:E:33:ALA:HB3	2:E:51:PHE:HB2	1.59	0.85
1:A:320:LEU:HD12	6:A:1908:PC1:H2I1	1.56	0.84
1:A:562:LEU:CG	1:A:655:VAL:HG22	2.07	0.84
1:A:1366:MET:CE	5:A:1903:3PE:H282	2.10	0.81
1:A:660:ALA:O	1:A:664:LEU:HD23	1.80	0.79
1:A:51:LYS:HG2	1:A:52:PRO:HD2	1.65	0.79
1:A:206:MET:HG2	6:A:1908:PC1:H3I2	1.64	0.78
3:F:297:ASN:ND2	3:F:330:LYS:O	2.18	0.77
1:A:1419:HIS:O	1:A:1423:VAL:N	2.18	0.77
1:A:559:ILE:HD12	1:A:659:ILE:CG1	2.15	0.77
1:A:1366:MET:HE2	5:A:1903:3PE:H2A2	1.67	0.76
1:A:305:ILE:HD12	6:A:1908:PC1:H12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:OD1	5:A:1910:3PE:H12	1.86	0.75
1:A:1313:VAL:HG12	5:A:1910:3PE:H362	1.69	0.74
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.69	0.74
1:A:567:PHE:HE1	5:A:1907:3PE:C29	2.01	0.74
1:A:320:LEU:HD11	6:A:1908:PC1:H2I2	1.64	0.73
3:F:37:VAL:HG21	3:F:1009:GLU:HG2	1.71	0.73
1:A:559:ILE:HD11	1:A:655:VAL:HG13	1.70	0.73
1:A:562:LEU:HG	1:A:655:VAL:CG2	2.19	0.73
3:F:738:VAL:HG22	3:F:744:THR:HG23	1.70	0.73
1:A:837:ILE:HD11	1:A:883:MET:HG2	1.69	0.72
3:F:658:GLU:O	3:F:720:GLN:NE2	2.23	0.72
1:A:559:ILE:CD1	1:A:659:ILE:HG13	2.20	0.72
1:A:1417:ILE:HG12	1:A:1418:LYS:H	1.54	0.72
5:A:1903:3PE:H11	5:A:1903:3PE:H112	1.72	0.71
1:A:656:PHE:CZ	1:A:1054:PHE:HB3	2.25	0.71
1:A:559:ILE:HG21	1:A:659:ILE:CD1	2.13	0.71
2:E:115:LEU:HA	2:E:118:LEU:HD12	1.72	0.71
1:A:1046:ILE:HD12	5:A:1907:3PE:H262	1.73	0.71
3:F:711:ASP:OD2	3:F:739:THR:OG1	2.05	0.71
1:A:231:THR:O	1:A:262:ARG:NH1	2.23	0.71
1:A:660:ALA:O	1:A:664:LEU:CD2	2.39	0.71
5:A:1903:3PE:H112	5:A:1903:3PE:C1	2.21	0.71
1:A:1046:ILE:CD1	5:A:1907:3PE:C26	2.67	0.70
1:A:1366:MET:HE1	5:A:1903:3PE:H282	1.72	0.70
3:F:994:SER:HB2	3:F:1007:HIS:HD2	1.57	0.69
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.75	0.69
1:A:599:ASN:HD22	1:A:601:PRO:HD2	1.57	0.69
1:A:237:VAL:HG12	1:A:238:GLU:H	1.58	0.68
5:A:1902:3PE:O14	5:A:1902:3PE:H121	1.93	0.68
1:A:559:ILE:HG12	1:A:562:LEU:HB3	1.76	0.68
1:A:850:LYS:NZ	1:A:851:MET:SD	2.66	0.68
1:A:549:VAL:HA	1:A:552:LEU:HB3	1.76	0.67
2:E:27:VAL:HA	2:E:53:LEU:HD12	1.77	0.67
1:A:1257:LEU:HB3	5:E:301:3PE:H231	1.77	0.66
5:A:1905:3PE:O14	5:A:1905:3PE:H122	1.93	0.66
5:A:1902:3PE:H322	5:A:1902:3PE:C22	2.25	0.66
3:F:642:ILE:HD12	3:F:642:ILE:H	1.60	0.66
1:A:559:ILE:HD13	1:A:659:ILE:HD11	1.76	0.66
1:A:542:TRP:HB3	1:A:545:LEU:HB2	1.77	0.65
3:F:647:TYR:O	3:F:650:THR:OG1	2.14	0.65
5:A:1902:3PE:O32	5:A:1904:3PE:H11	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:MET:HE2	5:A:1903:3PE:H282	1.79	0.65
1:A:320:LEU:CD1	6:A:1908:PC1:C2I	2.13	0.64
1:A:289:ILE:O	1:A:322:SER:OG	2.15	0.64
1:A:58:LEU:HD11	1:A:178:GLY:HA3	1.79	0.63
1:A:112:PHE:HB2	1:A:115:ASP:HA	1.80	0.63
5:A:1902:3PE:O32	5:A:1902:3PE:H341	1.97	0.63
1:A:1103:PRO:HG2	1:A:1108:GLN:HE22	1.63	0.63
3:F:1006:PHE:HB3	3:F:1021:VAL:HG23	1.80	0.63
1:A:1324:ALA:HB1	1:A:1327:GLU:HG3	1.81	0.63
3:F:54:VAL:HG11	3:F:799:LYS:HD3	1.79	0.63
1:A:643:ILE:HD13	5:A:1904:3PE:H3D2	1.79	0.63
1:A:1366:MET:CE	5:A:1903:3PE:C28	2.77	0.63
3:F:184:GLU:O	3:F:188:THR:OG1	2.15	0.63
6:A:1908:PC1:H3C2	6:A:1908:PC1:H2H1	1.81	0.62
1:A:1262:LYS:HG3	2:E:209:GLN:HA	1.80	0.62
1:A:206:MET:HE1	1:A:321:GLY:HA2	1.81	0.62
1:A:508:ILE:HA	1:A:511:LEU:HD12	1.82	0.62
1:A:643:ILE:HD13	5:A:1904:3PE:C3D	2.30	0.62
3:F:90:LEU:HD12	3:F:617:THR:HG21	1.81	0.62
2:E:152:PHE:O	2:E:155:LEU:HB2	2.01	0.61
1:A:964:THR:HG22	1:A:966:GLU:H	1.65	0.61
1:A:1384:PHE:O	1:A:1388:THR:OG1	2.19	0.61
1:A:337:PHE:CE2	1:A:657:LEU:HB3	2.29	0.61
1:A:939:GLN:NE2	7:A:1911:C8U:C01	2.63	0.61
3:F:638:ILE:O	3:F:644:GLN:NE2	2.34	0.60
1:A:1201:GLU:HA	1:A:1204:THR:HG22	1.84	0.60
3:F:481:LEU:HD23	3:F:482:LYS:H	1.66	0.60
3:F:444:LYS:NZ	3:F:467:PRO:O	2.35	0.60
3:F:283:GLU:OE1	3:F:321:LYS:NZ	2.34	0.60
1:A:45:ILE:HB	1:A:103:MET:HG3	1.83	0.60
1:A:102:ALA:HA	1:A:105:ILE:HG22	1.84	0.60
3:F:806:GLN:HG3	3:F:808:LYS:HE2	1.84	0.60
1:A:827:VAL:O	1:A:830:GLN:NE2	2.36	0.59
5:A:1903:3PE:H11	5:A:1903:3PE:C11	2.30	0.59
1:A:1132:THR:HG22	5:A:1902:3PE:H281	1.84	0.59
1:A:584:ARG:NH1	5:A:1905:3PE:O13	2.35	0.58
1:A:206:MET:CG	6:A:1908:PC1:H3I2	2.31	0.58
3:F:996:VAL:HB	3:F:1005:ILE:HD12	1.86	0.58
2:E:137:LEU:HD22	2:E:199:LEU:HD21	1.84	0.58
1:A:556:ILE:HA	1:A:559:ILE:HG22	1.85	0.58
3:F:868:ASP:HA	3:F:871:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:MET:HE1	5:A:1902:3PE:H2C2	0.59	0.58
1:A:1420:LEU:HA	1:A:1423:VAL:HG12	1.86	0.58
3:F:1014:THR:OG1	3:F:1015:ASN:N	2.36	0.57
3:F:1070:ASP:OD2	3:F:1072:THR:OG1	2.22	0.57
1:A:1129:MET:HE2	5:A:1902:3PE:C2C	2.28	0.57
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.18	0.57
1:A:559:ILE:CD1	1:A:659:ILE:CG1	2.80	0.57
1:A:1281:TYR:OH	1:A:1363:SER:OG	2.22	0.57
1:A:1129:MET:HE1	5:A:1902:3PE:C2D	2.29	0.56
1:A:1277:LEU:HD22	1:A:1371:LEU:HD12	1.87	0.56
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.86	0.56
1:A:567:PHE:CE1	5:A:1907:3PE:C29	2.87	0.56
1:A:70:VAL:HG12	5:A:1906:3PE:H11	1.86	0.56
1:A:1390:ASP:HB3	1:A:1393:ILE:HG12	1.88	0.56
3:F:172:THR:OG1	3:F:229:SER:OG	2.18	0.56
1:A:1178:PHE:O	2:E:138:ARG:NH1	2.38	0.55
1:A:163:ALA:HA	5:A:1905:3PE:H321	1.88	0.55
1:A:520:THR:O	1:A:523:GLY:N	2.39	0.55
3:F:56:GLN:O	3:F:60:ILE:HG23	2.05	0.55
3:F:164:GLN:O	3:F:196:LYS:NZ	2.32	0.55
1:A:1429:ILE:HB	1:A:1434:GLY:HA3	1.88	0.55
2:E:36:SER:HB3	2:E:38:HIS:CD2	2.42	0.55
3:F:1004:ARG:HB3	3:F:1022:GLU:HB2	1.88	0.55
5:A:1905:3PE:H12	5:A:1905:3PE:N	2.21	0.55
3:F:596:SER:OG	3:F:598:ASP:O	2.25	0.55
3:F:51:ALA:HB3	3:F:817:ILE:HD11	1.88	0.54
3:F:644:GLN:O	3:F:648:SER:OG	2.25	0.54
5:A:1903:3PE:C1	5:A:1903:3PE:C11	2.86	0.54
1:A:498:ARG:O	1:A:498:ARG:NH2	2.40	0.54
3:F:723:TRP:CH2	3:F:737:VAL:HG23	2.42	0.54
3:F:723:TRP:CE3	3:F:747:TYR:HB2	2.42	0.54
1:A:280:PHE:O	1:A:284:THR:HG22	2.07	0.54
1:A:1366:MET:HE1	5:A:1903:3PE:C28	2.38	0.54
1:A:521:PRO:HA	1:A:524:ILE:HD12	1.90	0.54
3:F:736:PHE:CZ	3:F:816:GLY:HA3	2.42	0.54
2:E:157:VAL:HA	2:E:160:GLN:HE21	1.73	0.54
1:A:94:LEU:HD21	1:A:134:VAL:HA	1.90	0.53
1:A:182:LEU:HD21	1:A:564:LEU:HD23	1.89	0.53
1:A:562:LEU:CD2	1:A:655:VAL:HG22	2.38	0.53
1:A:958:ASN:HD22	1:A:988:ARG:HA	1.72	0.53
1:A:1151:ASP:N	1:A:1151:ASP:OD2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:738:VAL:HG21	3:F:766:PHE:HZ	1.74	0.53
1:A:439:ILE:HA	1:A:442:VAL:HG12	1.90	0.53
1:A:1057:MET:CE	7:A:1911:C8U:C13	2.87	0.53
3:F:511:ASN:HD21	3:F:768:LYS:HB3	1.72	0.53
1:A:210:TYR:O	1:A:313:TYR:OH	2.26	0.53
2:E:59:LYS:HD3	2:E:78:LYS:HG2	1.91	0.53
3:F:154:ASP:OD2	3:F:163:TYR:OH	2.12	0.53
5:A:1902:3PE:H322	5:A:1902:3PE:H221	1.89	0.53
1:A:1057:MET:HE2	7:A:1911:C8U:C13	2.39	0.53
3:F:359:ILE:HG22	3:F:385:ARG:HB2	1.91	0.53
1:A:199:ILE:HD11	1:A:332:VAL:HG21	1.91	0.53
1:A:495:ILE:HA	1:A:498:ARG:HB2	1.90	0.53
5:A:1910:3PE:C2G	5:A:1910:3PE:C2C	2.85	0.53
3:F:235:ILE:H	3:F:551:GLN:HG2	1.74	0.52
3:F:993:PHE:HB2	3:F:1008:VAL:HG22	1.92	0.52
1:A:559:ILE:CD1	1:A:655:VAL:HG13	2.38	0.52
3:F:670:CYS:HB2	3:F:673:LEU:HD23	1.90	0.52
1:A:663:ASN:ND2	1:A:663:ASN:O	2.42	0.52
3:F:130:LYS:HB3	3:F:225:TRP:HB3	1.91	0.52
3:F:538:ILE:HG13	3:F:1042:ASP:HB3	1.91	0.52
1:A:1132:THR:CG2	5:A:1902:3PE:H281	2.39	0.52
1:A:1088:CYS:SG	1:A:1394:LEU:HD11	2.50	0.52
1:A:1048:TYR:CE1	1:A:1052:ILE:HG13	2.45	0.52
2:E:16:ILE:O	2:E:20:ILE:HG12	2.10	0.52
3:F:530:GLN:HB3	3:F:532:LYS:HE2	1.91	0.52
3:F:715:THR:HB	3:F:745:ARG:HH21	1.73	0.52
1:A:1099:ARG:NH2	1:A:1412:GLU:OE2	2.43	0.52
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.92	0.52
3:F:1042:ASP:OD1	3:F:1042:ASP:N	2.42	0.52
1:A:1394:LEU:HD13	1:A:1395:GLY:N	2.25	0.52
2:E:107:ALA:HB2	2:E:157:VAL:HB	1.92	0.52
3:F:470:ASN:HD21	3:F:482:LYS:NZ	2.08	0.51
1:A:213:ILE:HD13	6:A:1908:PC1:H381	1.92	0.51
1:A:476:THR:O	1:A:479:MET:HG3	2.10	0.51
1:A:1373:ILE:O	1:A:1377:VAL:HG23	2.10	0.51
1:A:112:PHE:CG	1:A:113:HIS:N	2.79	0.51
1:A:336:GLU:HA	1:A:339:LYS:HE3	1.92	0.51
3:F:695:PRO:HA	3:F:697:ASN:ND2	2.25	0.51
3:F:149:PRO:HG3	3:F:165:HIS:HE1	1.75	0.51
1:A:127:PHE:O	1:A:131:PHE:HB3	2.11	0.51
1:A:226:CYS:HA	1:A:260:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ILE:HD13	1:A:659:ILE:CD1	2.41	0.51
3:F:40:MET:SD	3:F:855:ILE:HD11	2.50	0.51
3:F:657:GLU:HG3	3:F:749:LYS:HD3	1.93	0.51
2:E:141:SER:HB3	2:E:199:LEU:HD22	1.93	0.51
5:A:1910:3PE:C2G	5:A:1910:3PE:H2C1	2.39	0.51
1:A:627:TYR:CE2	5:A:1905:3PE:H232	2.46	0.50
1:A:656:PHE:CE2	1:A:1054:PHE:HB3	2.46	0.50
2:E:17:LEU:O	2:E:21:VAL:HG22	2.12	0.50
2:E:198:SER:HA	2:E:201:LEU:HD12	1.93	0.50
1:A:1046:ILE:HD13	5:A:1907:3PE:C26	2.21	0.50
1:A:162:LYS:HE2	1:A:165:ARG:HG2	1.93	0.50
3:F:114:ARG:HH12	3:F:120:ASN:HB2	1.75	0.50
1:A:1046:ILE:HD12	5:A:1907:3PE:C24	2.41	0.50
1:A:489:ARG:NH1	1:A:492:PHE:HB2	2.27	0.50
6:A:1908:PC1:H132	6:A:1908:PC1:O14	2.11	0.50
2:E:20:ILE:HD13	2:E:118:LEU:HD22	1.94	0.50
1:A:1186:ASP:O	1:A:1190:VAL:HG23	2.11	0.50
3:F:825:ILE:O	3:F:829:THR:HG23	2.12	0.50
3:F:672:ASP:HB2	3:F:689:PHE:HE1	1.77	0.50
3:F:591:ARG:NH2	3:F:606:ASN:OD1	2.45	0.49
1:A:806:LEU:HA	1:A:809:ILE:HD12	1.93	0.49
1:A:868:PHE:HB3	1:A:909:ASN:OD1	2.12	0.49
1:A:1005:MET:O	1:A:1009:THR:HG23	2.12	0.49
1:A:1102:ILE:HB	1:A:1411:PRO:HB3	1.94	0.49
1:A:1323:GLU:O	1:A:1325:TRP:N	2.44	0.49
1:A:179:VAL:HG23	1:A:182:LEU:HB2	1.95	0.49
2:E:3:PRO:HG2	2:E:134:ASP:HB3	1.94	0.49
1:A:1057:MET:HE3	7:A:1911:C8U:C14	2.43	0.49
3:F:868:ASP:O	3:F:872:ASN:ND2	2.46	0.49
1:A:252:ARG:HG2	1:A:303:ASP:HB3	1.95	0.49
1:A:845:VAL:O	1:A:848:VAL:HG22	2.13	0.49
1:A:1005:MET:SD	1:A:1362:ILE:HD11	2.52	0.49
1:A:953:LYS:HB3	1:A:1026:SER:HB2	1.95	0.49
3:F:1048:ASP:OD1	3:F:1048:ASP:N	2.45	0.48
1:A:65:CYS:HB3	5:A:1906:3PE:H262	1.94	0.48
1:A:303:ASP:OD2	1:A:1302:ARG:NH2	2.35	0.48
2:E:110:ILE:HG21	2:E:153:VAL:HG13	1.95	0.48
3:F:737:VAL:HG12	3:F:739:THR:HG22	1.96	0.48
1:A:1366:MET:CE	5:A:1903:3PE:H2A2	2.22	0.48
5:A:1905:3PE:H12	5:A:1905:3PE:HN3	1.78	0.48
1:A:210:TYR:CZ	6:A:1908:PC1:H3A1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:ILE:O	2:E:80:CYS:HA	2.14	0.48
1:A:1197:VAL:O	1:A:1201:GLU:HG2	2.14	0.48
2:E:30:ASP:OD1	2:E:30:ASP:N	2.40	0.48
3:F:540:THR:HB	3:F:912:ALA:HB3	1.96	0.48
1:A:914:LEU:HD13	1:A:1272:LEU:HD23	1.96	0.47
1:A:196:LEU:HD11	1:A:333:LEU:HG	1.95	0.47
1:A:1062:GLY:HA2	1:A:1065:ILE:HG22	1.96	0.47
1:A:1242:ARG:O	1:A:1245:LYS:HG2	2.14	0.47
2:E:153:VAL:O	2:E:156:GLU:HB3	2.14	0.47
3:F:598:ASP:O	3:F:600:ARG:N	2.45	0.47
3:F:847:ASN:HD21	3:F:868:ASP:HB3	1.79	0.47
3:F:382:LYS:HB3	3:F:409:LYS:HD3	1.95	0.47
1:A:256:ILE:O	1:A:259:SER:OG	2.25	0.47
1:A:953:LYS:HG2	1:A:1028:GLU:O	2.13	0.47
3:F:132:ASP:OD2	3:F:132:ASP:N	2.41	0.47
1:A:657:LEU:HD12	1:A:657:LEU:HA	1.76	0.47
1:A:836:ASP:O	1:A:840:THR:OG1	2.22	0.47
1:A:1370:PHE:HB2	5:A:1903:3PE:H2H1	1.97	0.47
3:F:562:ASP:OD1	3:F:563:PHE:N	2.48	0.47
1:A:189:ILE:HG13	1:A:190:PHE:N	2.29	0.47
1:A:590:THR:HG22	3:F:269:LEU:HD21	1.95	0.47
1:A:841:SER:O	1:A:845:VAL:HG23	2.15	0.47
1:A:999:ASN:ND2	1:A:1002:SER:OG	2.48	0.47
1:A:1189:ILE:HG21	1:A:1242:ARG:HG2	1.97	0.47
2:E:193:PHE:HD2	2:E:194:LEU:HD12	1.80	0.47
1:A:920:CYS:HA	1:A:923:VAL:HG12	1.96	0.47
1:A:984:GLU:OE1	1:A:986:ARG:NH2	2.48	0.47
3:F:1010:LYS:HG3	3:F:1017:ILE:HG13	1.95	0.47
1:A:1158:THR:O	1:A:1162:THR:HG22	2.15	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.46
1:A:1381:MET:HA	1:A:1384:PHE:CD2	2.50	0.46
5:A:1906:3PE:H2A2	5:A:1906:3PE:H271	1.31	0.46
2:E:12:THR:O	2:E:16:ILE:HG12	2.15	0.46
1:A:434:PHE:O	1:A:438:VAL:HG23	2.15	0.46
1:A:928:ILE:HD12	1:A:928:ILE:O	2.15	0.46
3:F:303:VAL:HG21	3:F:327:ILE:HD11	1.98	0.46
1:A:1151:ASP:O	1:A:1155:VAL:HG23	2.16	0.46
3:F:447:GLN:O	3:F:464:GLY:HA2	2.16	0.46
3:F:513:TYR:OH	3:F:567:GLU:OE1	2.21	0.46
3:F:664:LEU:H	3:F:679:ASN:HD21	1.63	0.46
1:A:1247:LEU:HD21	1:A:1257:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:LEU:HD12	2:E:37:PRO:HD3	1.98	0.46
2:E:59:LYS:HD2	2:E:59:LYS:HA	1.67	0.46
1:A:1417:ILE:HG12	1:A:1418:LYS:N	2.28	0.46
5:A:1906:3PE:H12	5:A:1906:3PE:O22	2.16	0.46
1:A:50:TRP:CD1	1:A:50:TRP:N	2.84	0.46
3:F:57:LEU:HD23	3:F:801:VAL:HG21	1.96	0.46
3:F:311:GLN:HE21	3:F:1056:ARG:HD2	1.80	0.46
1:A:136:THR:HG21	1:A:164:LEU:HB2	1.97	0.46
1:A:177:SER:HA	1:A:183:GLN:NE2	2.31	0.46
1:A:272:ILE:HD11	1:A:625:MET:HE3	1.97	0.46
3:F:75:ALA:HB1	3:F:610:THR:HG21	1.98	0.46
1:A:219:LYS:HE2	1:A:219:LYS:HB3	1.73	0.46
1:A:1271:ALA:O	1:A:1275:VAL:HG13	2.16	0.45
5:A:1905:3PE:C3B	5:A:1905:3PE:C2G	2.88	0.45
1:A:115:ASP:HB3	1:A:119:ARG:HB2	1.98	0.45
3:F:663:PHE:HB2	3:F:744:THR:HB	1.99	0.45
1:A:180:PRO:HA	1:A:183:GLN:HB2	1.99	0.45
1:A:652:LEU:C	1:A:652:LEU:HD23	2.37	0.45
1:A:164:LEU:HA	1:A:167:PHE:HD1	1.82	0.45
1:A:555:SER:OG	1:A:663:ASN:HB2	2.17	0.45
5:A:1903:3PE:H221	5:A:1903:3PE:O31	2.16	0.45
5:A:1902:3PE:H262	5:A:1902:3PE:H291	1.54	0.45
5:A:1910:3PE:H2A1	5:A:1910:3PE:H2D2	1.74	0.45
2:E:23:ALA:O	2:E:27:VAL:HG23	2.17	0.45
3:F:867:HIS:C	3:F:869:ASP:H	2.19	0.45
1:A:112:PHE:HD2	1:A:115:ASP:H	1.65	0.45
1:A:1047:ILE:HG12	5:A:1906:3PE:C3B	2.47	0.45
2:E:37:PRO:HA	2:E:174:ILE:HG12	1.99	0.45
3:F:476:GLU:OE1	3:F:478:LYS:HB2	2.17	0.45
2:E:157:VAL:O	2:E:160:GLN:HG3	2.17	0.45
3:F:651:LEU:O	3:F:687:ASN:ND2	2.50	0.45
1:A:1337:LEU:HD12	1:A:1350:TYR:CZ	2.52	0.44
3:F:176:GLU:O	3:F:176:GLU:HG2	2.17	0.44
1:A:1329:LEU:HD12	1:A:1361:PHE:HB2	1.99	0.44
5:A:1909:3PE:H282	5:A:1909:3PE:H252	1.72	0.44
2:E:27:VAL:HG12	2:E:54:TRP:HE1	1.82	0.44
3:F:217:ALA:HB2	3:F:240:VAL:HG21	2.00	0.44
1:A:199:ILE:HG21	1:A:329:VAL:HG12	2.00	0.44
1:A:924:ALA:O	1:A:927:THR:OG1	2.34	0.44
5:A:1902:3PE:H322	5:A:1902:3PE:H222	1.99	0.44
1:A:504:VAL:O	1:A:508:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:SER:OG	1:A:1383:ASN:OD1	2.23	0.44
5:A:1909:3PE:H232	5:A:1909:3PE:H261	1.34	0.44
3:F:107:VAL:HG11	3:F:190:ALA:HB3	2.00	0.44
3:F:234:LYS:O	3:F:234:LYS:HG2	2.18	0.44
2:E:8:LYS:HD3	2:E:8:LYS:HA	1.73	0.44
2:E:124:CYS:HB3	2:E:140:ALA:HB2	2.00	0.44
1:A:660:ALA:C	1:A:664:LEU:HD23	2.38	0.44
1:A:939:GLN:HE22	7:A:1911:C8U:C01	2.30	0.44
1:A:1159:ILE:O	1:A:1163:LEU:HG	2.17	0.44
1:A:1193:SER:O	1:A:1197:VAL:HG13	2.17	0.44
5:A:1905:3PE:H12	5:A:1905:3PE:O22	2.18	0.44
2:E:161:SER:O	2:E:164:ARG:HG3	2.18	0.44
3:F:844:CYS:HB3	3:F:866:ASN:ND2	2.33	0.44
1:A:128:ILE:HG22	1:A:132:LEU:HD12	2.00	0.43
3:F:127:TYR:HH	3:F:151:PHE:HZ	1.65	0.43
3:F:239:ASP:OD2	3:F:426:GLN:NE2	2.42	0.43
1:A:51:LYS:O	1:A:53:PHE:N	2.51	0.43
1:A:608:PHE:O	1:A:612:THR:HG23	2.18	0.43
1:A:801:PHE:CE1	1:A:846:GLU:HB3	2.53	0.43
1:A:1104:LYS:HE2	1:A:1104:LYS:HB2	1.85	0.43
3:F:628:THR:O	3:F:629:TYR:CD2	2.71	0.43
3:F:511:ASN:ND2	3:F:768:LYS:HB3	2.33	0.43
1:A:664:LEU:HD13	1:A:664:LEU:HA	1.83	0.43
5:A:1910:3PE:C2C	5:A:1910:3PE:H2G1	2.48	0.43
3:F:517:ILE:HG22	3:F:621:SER:HB3	1.99	0.43
3:F:845:LYS:HG2	3:F:848:SER:HB2	2.01	0.43
1:A:439:ILE:HG13	1:A:440:LEU:N	2.33	0.43
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.79	0.43
1:A:633:PRO:O	5:A:1905:3PE:C22	2.66	0.43
1:A:977:ASP:OD2	3:F:547:ARG:NH2	2.47	0.43
1:A:1149:ILE:HG22	1:A:1153:LEU:HD12	2.01	0.43
1:A:224:LYS:HA	1:A:263:GLY:HA2	2.01	0.43
1:A:1317:PHE:CD1	5:A:1910:3PE:H391	2.53	0.43
1:A:601:PRO:HB3	5:A:1907:3PE:O22	2.19	0.43
1:A:1169:LEU:O	1:A:1173:LYS:N	2.52	0.43
1:A:245:CYS:SG	1:A:246:ALA:N	2.91	0.43
1:A:943:ALA:O	1:A:947:VAL:HG23	2.19	0.43
1:A:985:LEU:HD23	1:A:985:LEU:HA	1.79	0.43
2:E:32:TRP:HB2	2:E:182:PHE:HB2	2.00	0.43
3:F:656:PHE:HB3	3:F:749:LYS:HD2	2.01	0.43
1:A:132:LEU:O	1:A:136:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:HE3	1:A:165:ARG:NH1	2.34	0.43
1:A:542:TRP:HD1	1:A:545:LEU:H	1.65	0.43
1:A:1096:ARG:HE	1:A:1096:ARG:HB3	1.65	0.43
2:E:18:VAL:O	2:E:22:LEU:HG	2.19	0.43
3:F:88:LYS:HE3	3:F:88:LYS:HB2	1.61	0.43
3:F:733:LYS:HE3	3:F:733:LYS:HB2	1.90	0.43
1:A:452:GLU:OE2	1:A:528:ARG:NH2	2.52	0.43
1:A:941:MET:HG3	1:A:942:PHE:N	2.34	0.43
1:A:1259:THR:HG21	1:A:1386:TYR:CD2	2.54	0.43
3:F:1000:GLY:O	3:F:1001:ASN:HB3	2.19	0.43
1:A:78:ASP:OD1	1:A:79:ASN:N	2.52	0.42
3:F:39:LYS:HB3	3:F:39:LYS:HE3	1.75	0.42
3:F:792:GLU:OE1	3:F:792:GLU:N	2.34	0.42
3:F:885:LEU:HD21	3:F:1019:ILE:HG21	2.00	0.42
1:A:959:ASP:HB3	1:A:972:TYR:CD2	2.54	0.42
1:A:1084:ASN:OD1	1:A:1085:GLN:N	2.53	0.42
3:F:103:GLU:HG3	3:F:194:VAL:HG21	2.01	0.42
3:F:365:ASP:HB2	3:F:394:HIS:CD2	2.55	0.42
3:F:822:ASN:O	3:F:826:GLU:HG3	2.19	0.42
2:E:123:ILE:O	2:E:127:MET:HG3	2.19	0.42
3:F:148:LYS:HB2	3:F:148:LYS:HE2	1.65	0.42
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.91	0.42
3:F:697:ASN:HB3	3:F:700:CYS:HB2	2.01	0.42
1:A:457:PRO:HD2	1:A:460:LEU:HD12	2.00	0.42
1:A:643:ILE:HD11	5:A:1904:3PE:H3B1	2.00	0.42
2:E:137:LEU:HD23	2:E:137:LEU:HA	1.90	0.42
3:F:76:ARG:NH2	3:F:611:TRP:O	2.52	0.42
3:F:228:ASN:HB2	3:F:232:PRO:CD	2.50	0.42
1:A:54:GLU:O	1:A:58:LEU:HB2	2.19	0.42
1:A:194:LEU:N	1:A:195:PRO:HD2	2.35	0.42
1:A:216:GLU:OE1	1:A:1236:ARG:HB3	2.20	0.42
1:A:1185:PHE:O	1:A:1189:ILE:HG12	2.19	0.42
1:A:1195:ILE:HD13	1:A:1195:ILE:HA	1.90	0.42
3:F:655:ASN:HB2	3:F:658:GLU:OE1	2.19	0.42
1:A:1128:ILE:HG21	1:A:1246:LEU:HD13	2.01	0.42
1:A:135:PHE:O	1:A:138:ILE:HG13	2.20	0.42
1:A:274:HIS:CD2	1:A:276:ASP:HB2	2.55	0.42
5:A:1906:3PE:H322	5:A:1906:3PE:H31	1.78	0.42
5:A:1910:3PE:H291	5:A:1910:3PE:H262	1.42	0.42
3:F:394:HIS:CE1	3:F:398:ARG:HE	2.38	0.42
3:F:365:ASP:OD1	3:F:366:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:511:ASN:HB2	3:F:627:PRO:HG3	2.02	0.42
1:A:120:SER:HB3	1:A:123:ASN:HB2	2.01	0.41
1:A:537:LYS:HD3	1:A:537:LYS:HA	1.78	0.41
2:E:35:LEU:HA	2:E:175:GLU:O	2.20	0.41
3:F:381:ASP:OD1	3:F:381:ASP:N	2.49	0.41
1:A:610:VAL:HG13	1:A:616:TRP:HB2	2.02	0.41
1:A:537:LYS:O	1:A:540:LYS:HB3	2.21	0.41
1:A:1409:TYR:HE2	1:A:1425:LEU:HB3	1.85	0.41
3:F:271:LEU:HD22	3:F:329:ALA:HB2	2.02	0.41
1:A:53:PHE:HD1	1:A:53:PHE:HA	1.70	0.41
1:A:75:PRO:HG2	3:F:265:SER:HA	2.01	0.41
3:F:577:ARG:O	3:F:581:ILE:HG13	2.20	0.41
1:A:80:ASN:OD1	1:A:80:ASN:N	2.54	0.41
1:A:170:LEU:O	1:A:173:LEU:HB2	2.21	0.41
1:A:495:ILE:H	1:A:495:ILE:HD13	1.85	0.41
1:A:544:SER:OG	1:A:930:ASN:OD1	2.37	0.41
1:A:874:LEU:O	1:A:878:VAL:HG22	2.21	0.41
1:A:951:LYS:HB3	1:A:951:LYS:HE2	1.60	0.41
1:A:1348:GLU:HG2	1:A:1351:THR:HG21	2.03	0.41
3:F:130:LYS:HB3	3:F:225:TRP:CB	2.51	0.41
3:F:256:MET:O	3:F:291:VAL:HA	2.20	0.41
3:F:695:PRO:HA	3:F:697:ASN:HD21	1.84	0.41
3:F:652:LYS:HB2	3:F:655:ASN:HD22	1.86	0.41
1:A:950:PHE:HA	1:A:953:LYS:HD2	2.03	0.41
6:A:1908:PC1:H3G1	6:A:1908:PC1:H3D1	1.84	0.41
2:E:110:ILE:HD13	2:E:153:VAL:HG22	2.01	0.41
3:F:749:LYS:HB3	3:F:749:LYS:HE3	1.82	0.41
1:A:112:PHE:HB2	1:A:115:ASP:CA	2.50	0.41
1:A:643:ILE:HD13	5:A:1904:3PE:H3D1	2.01	0.41
1:A:663:ASN:ND2	1:A:663:ASN:C	2.73	0.41
6:A:1908:PC1:O12	6:A:1908:PC1:H122	2.21	0.41
2:E:4:THR:OG1	2:E:134:ASP:OD2	2.33	0.41
2:E:131:LYS:HB2	2:E:131:LYS:HE2	1.81	0.41
3:F:254:LYS:HA	3:F:357:ASN:HB2	2.03	0.41
3:F:665:ALA:HA	3:F:666:PRO:HD3	1.91	0.41
1:A:482:LYS:HD2	1:A:482:LYS:HA	1.87	0.41
2:E:51:PHE:HA	2:E:56:ILE:HG22	2.03	0.41
1:A:199:ILE:O	1:A:203:VAL:HG23	2.20	0.40
3:F:409:LYS:HG2	3:F:1071:TYR:CD2	2.56	0.40
3:F:461:VAL:HG12	3:F:495:SER:HA	2.02	0.40
3:F:552:ASN:OD1	3:F:552:ASN:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ALA:O	1:A:664:LEU:HD22	2.19	0.40
5:A:1910:3PE:H2C1	5:A:1910:3PE:C2H	2.51	0.40
3:F:398:ARG:O	3:F:402:GLN:HG3	2.21	0.40
3:F:484:GLN:HE22	3:F:1070:ASP:N	2.19	0.40
3:F:642:ILE:H	3:F:642:ILE:CD1	2.32	0.40
3:F:889:LEU:HD22	3:F:894:VAL:HG11	2.03	0.40
1:A:872:ASP:O	1:A:876:VAL:HG22	2.21	0.40
6:A:1908:PC1:H111	6:A:1908:PC1:H133	1.47	0.40
3:F:297:ASN:C	3:F:299:ASN:H	2.24	0.40
1:A:1129:MET:CE	5:A:1902:3PE:C2B	2.92	0.40
1:A:1248:SER:O	1:A:1248:SER:OG	2.40	0.40
3:F:627:PRO:O	3:F:630:SER:HB3	2.22	0.40
1:A:1195:ILE:HD13	1:A:1198:ILE:HD11	2.03	0.40
3:F:512:GLY:HA2	3:F:625:VAL:O	2.22	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	1095/1873 (58%)	1019 (93%)	74 (7%)	2 (0%)	47 82
2	E	159/222 (72%)	147 (92%)	11 (7%)	1 (1%)	25 64
3	F	968/1105 (88%)	901 (93%)	67 (7%)	0	100 100
All	All	2222/3200 (69%)	2067 (93%)	152 (7%)	3 (0%)	54 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1334	TYR
2	E	205	PRO
1	A	521	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	981/1628 (60%)	896 (91%)	85 (9%)	10 37
2	E	143/192 (74%)	130 (91%)	13 (9%)	9 34
3	F	868/973 (89%)	812 (94%)	56 (6%)	17 50
All	All	1992/2793 (71%)	1838 (92%)	154 (8%)	16 42

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	49	GLU
1	A	53	PHE
1	A	56	ILE
1	A	58	LEU
1	A	113	HIS
1	A	120	SER
1	A	143	ASN
1	A	161	VAL
1	A	164	LEU
1	A	187	ASN
1	A	231	THR
1	A	254	CYS
1	A	289	ILE
1	A	326	LEU
1	A	339	LYS
1	A	343	LYS
1	A	437	LEU
1	A	439	ILE
1	A	444	LEU
1	A	448	SER
1	A	460	LEU
1	A	463	LEU
1	A	479	MET
1	A	491	TYR
1	A	495	ILE

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Mol	Chain	Res	Type
1	A	499	PHE
1	A	502	PHE
1	A	510	GLU
1	A	515	GLU
1	A	525	SER
1	A	537	LYS
1	A	547	ASN
1	A	548	LEU
1	A	553	LEU
1	A	554	ASN
1	A	558	SER
1	A	591	GLU
1	A	604	LEU
1	A	618	SER
1	A	647	CYS
1	A	649	ASN
1	A	653	LEU
1	A	654	ASN
1	A	663	ASN
1	A	666	GLU
1	A	668	GLU
1	A	669	SER
1	A	808	PHE
1	A	811	LEU
1	A	823	ARG
1	A	871	LEU
1	A	902	LEU
1	A	906	ARG
1	A	930	ASN
1	A	935	THR
1	A	939	GLN
1	A	941	MET
1	A	983	MET
1	A	992	HIS
1	A	999	ASN
1	A	1030	ASP
1	A	1057	MET
1	A	1063	PHE
1	A	1069	GLN
1	A	1091	TYR
1	A	1108	GLN
1	A	1117	SER

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Mol	Chain	Res	Type
1	A	1124	MET
1	A	1125	PHE
1	A	1199	LEU
1	A	1243	LEU
1	A	1263	SER
1	A	1289	PHE
1	A	1295	VAL
1	A	1316	LEU
1	A	1332	CYS
1	A	1337	LEU
1	A	1343	ASP
1	A	1363	SER
1	A	1381	MET
1	A	1384	PHE
1	A	1385	ASP
1	A	1392	SER
1	A	1408	GLU
2	E	1	MET
2	E	8	LYS
2	E	13	LEU
2	E	24	MET
2	E	32	TRP
2	E	130	ARG
2	E	134	ASP
2	E	160	GLN
2	E	161	SER
2	E	165	MET
2	E	178	TYR
2	E	189	PHE
2	E	214	SER
3	F	54	VAL
3	F	59	ASP
3	F	61	TYR
3	F	76	ARG
3	F	116	ASP
3	F	141	GLU
3	F	157	PHE
3	F	158	ARG
3	F	212	SER
3	F	234	LYS
3	F	241	ARG
3	F	269	LEU

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Mol	Chain	Res	Type
3	F	270	THR
3	F	303	VAL
3	F	311	GLN
3	F	348	ASN
3	F	390	SER
3	F	449	THR
3	F	476	GLU
3	F	493	ASP
3	F	505	ARG
3	F	518	ASP
3	F	542	ASN
3	F	550	VAL
3	F	592	THR
3	F	603	ASP
3	F	610	THR
3	F	648	SER
3	F	649	GLU
3	F	651	LEU
3	F	659	SER
3	F	673	LEU
3	F	707	ARG
3	F	711	ASP
3	F	717	GLU
3	F	739	THR
3	F	740	ASP
3	F	753	GLU
3	F	767	TYR
3	F	817	ILE
3	F	830	LYS
3	F	845	LYS
3	F	849	ASP
3	F	852	ASP
3	F	867	HIS
3	F	871	THR
3	F	907	CYS
3	F	997	LEU
3	F	1012	MET
3	F	1014	THR
3	F	1040	THR
3	F	1048	ASP
3	F	1057	LYS
3	F	1068	LEU

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Mol	Chain	Res	Type
3	F	1071	TYR
3	F	1073	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	453	HIS
1	A	490	GLN
1	A	554	ASN
1	A	599	ASN
1	A	663	ASN
1	A	797	ASN
1	A	830	GLN
1	A	939	GLN
1	A	948	GLN
1	A	958	ASN
1	A	999	ASN
1	A	1071	GLN
1	A	1087	GLN
1	A	1108	GLN
1	A	1138	GLN
1	A	1307	GLN
2	E	31	HIS
2	E	38	HIS
2	E	209	GLN
3	F	55	HIS
3	F	56	GLN
3	F	145	GLN
3	F	156	ASN
3	F	164	GLN
3	F	165	HIS
3	F	169	HIS
3	F	186	ASN
3	F	233	ASN
3	F	308	HIS
3	F	394	HIS
3	F	450	ASN
3	F	470	ASN
3	F	484	GLN
3	F	511	ASN
3	F	542	ASN

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Mol	Chain	Res	Type
3	F	655	ASN
3	F	679	ASN
3	F	685	ASN
3	F	716	ASN
3	F	866	ASN
3	F	872	ASN
3	F	888	HIS
3	F	891	ASN
3	F	1007	HIS
3	F	1065	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1910	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	3 (5%)
5	3PE	E	301	-	32,32,50	1.14	2 (6%)	35,37,55	1.22	3 (8%)
5	3PE	A	1902	-	50,50,50	0.92	2 (4%)	53,55,55	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	3PE	A	1905	-	43,43,50	0.99	2 (4%)	46,48,55	1.03	2 (4%)
5	3PE	A	1903	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
5	3PE	A	1907	-	20,20,50	1.03	1 (5%)	22,23,55	0.95	1 (4%)
6	PC1	A	1908	-	53,53,53	0.94	2 (3%)	59,61,61	1.01	2 (3%)
5	3PE	A	1906	-	37,37,50	1.06	2 (5%)	40,42,55	1.13	3 (7%)
5	3PE	A	1909	-	31,31,50	1.17	2 (6%)	34,36,55	1.15	2 (5%)
5	3PE	A	1904	-	50,50,50	0.93	2 (4%)	53,55,55	1.07	3 (5%)
7	C8U	A	1911	-	22,26,26	4.11	7 (31%)	30,39,39	2.62	9 (30%)

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	1910	-	-	32/54/54/54	-
5	3PE	E	301	-	-	15/36/36/54	-
5	3PE	A	1902	-	-	34/54/54/54	-
5	3PE	A	1905	-	-	25/47/47/54	-
5	3PE	A	1903	-	-	25/54/54/54	-
5	3PE	A	1907	-	-	12/21/21/54	-
6	PC1	A	1908	-	-	36/57/57/57	-
5	3PE	A	1906	-	-	25/41/41/54	-
5	3PE	A	1909	-	-	20/35/35/54	-
5	3PE	A	1904	-	-	33/54/54/54	-
7	C8U	A	1911	-	-	3/18/40/40	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1911	C8U	C02-C03	13.30	1.51	1.35
7	A	1911	C8U	O10-N09	10.30	1.40	1.22
7	A	1911	C8U	C06-N07	5.21	1.45	1.38
7	A	1911	C8U	C02-N07	4.68	1.44	1.38
5	A	1904	3PE	O31-C31	4.31	1.45	1.33
5	A	1909	3PE	O31-C31	4.29	1.45	1.33
5	A	1902	3PE	O31-C31	4.28	1.45	1.33
6	A	1908	PC1	O31-C31	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1905	3PE	O31-C31	4.26	1.45	1.33
5	E	301	3PE	O31-C31	4.25	1.45	1.33
5	A	1906	3PE	O31-C31	4.24	1.45	1.33
5	A	1903	3PE	O31-C31	4.22	1.45	1.33
6	A	1908	PC1	O21-C21	4.18	1.46	1.34
5	A	1910	3PE	O31-C31	4.16	1.45	1.33
5	A	1907	3PE	O21-C21	4.12	1.45	1.33
5	A	1905	3PE	O21-C21	4.12	1.45	1.34
5	A	1906	3PE	O21-C21	4.10	1.45	1.34
5	E	301	3PE	O21-C21	4.09	1.45	1.34
5	A	1910	3PE	O21-C21	4.08	1.45	1.34
5	A	1903	3PE	O21-C21	4.08	1.45	1.34
5	A	1909	3PE	O21-C21	4.07	1.45	1.34
5	A	1904	3PE	O21-C21	4.05	1.45	1.34
5	A	1902	3PE	O21-C21	4.02	1.45	1.34
7	A	1911	C8U	C22-C03	3.20	1.53	1.47
7	A	1911	C8U	O24-C22	3.10	1.40	1.33
7	A	1911	C8U	O24-C25	-2.09	1.40	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1911	C8U	C01-C02-C03	-8.43	119.19	127.62
7	A	1911	C8U	C08-C06-N07	5.50	119.99	113.45
7	A	1911	C8U	C01-C02-N07	5.06	119.46	113.45
5	A	1904	3PE	O21-C21-C22	4.61	121.43	111.50
7	A	1911	C8U	O24-C22-C03	4.54	120.39	112.30
5	E	301	3PE	O21-C21-C22	4.29	120.74	111.50
5	A	1903	3PE	O21-C21-C22	4.22	120.59	111.50
5	A	1906	3PE	O21-C21-C22	4.16	120.47	111.50
5	A	1902	3PE	O21-C21-C22	4.13	120.40	111.50
5	A	1909	3PE	O21-C21-C22	3.98	120.08	111.50
5	A	1910	3PE	O21-C21-C22	3.94	120.00	111.50
6	A	1908	PC1	O21-C21-C22	3.91	119.94	111.50
5	A	1905	3PE	O21-C21-C22	3.67	119.40	111.50
7	A	1911	C8U	C04-C05-N09	3.07	120.51	116.37
5	A	1902	3PE	O31-C31-C32	2.95	121.16	111.91
6	A	1908	PC1	O31-C31-C32	2.94	121.12	111.91
7	A	1911	C8U	C06-N07-C02	-2.93	120.69	123.40
5	A	1910	3PE	O31-C31-C32	2.83	120.78	111.91
5	A	1904	3PE	O31-C31-C32	2.72	120.46	111.91
5	E	301	3PE	O31-C31-C32	2.71	120.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1905	3PE	O31-C31-C32	2.69	120.36	111.91
5	A	1909	3PE	O31-C31-C32	2.63	120.17	111.91
7	A	1911	C8U	C05-C04-C03	2.60	111.90	108.65
5	A	1903	3PE	O31-C31-C32	2.59	120.04	111.91
5	A	1907	3PE	O21-C21-C22	2.55	119.92	111.91
5	E	301	3PE	C2-O21-C21	-2.55	111.52	117.79
5	A	1906	3PE	O31-C31-C32	2.55	119.90	111.91
7	A	1911	C8U	O23-C22-C03	-2.47	120.09	125.20
5	A	1906	3PE	C2-O21-C21	-2.20	112.39	117.79
5	A	1904	3PE	O21-C21-O22	-2.12	118.58	123.70
5	A	1910	3PE	C2-O21-C21	-2.11	112.60	117.79
5	A	1902	3PE	C2-O21-C21	-2.11	112.60	117.79
7	A	1911	C8U	O24-C22-O23	-2.08	119.52	123.53

There are no chirality outliers.

All (260) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C32-C31-O31-C3
5	A	1907	3PE	C1-O11-P-O12
5	A	1907	3PE	C11-O13-P-O14
5	A	1907	3PE	C12-C11-O13-P
5	A	1907	3PE	O13-C11-C12-N
5	A	1907	3PE	O11-C1-C2-O21
5	A	1909	3PE	C11-O13-P-O11
5	A	1909	3PE	O13-C11-C12-N
5	A	1910	3PE	C11-O13-P-O14
5	E	301	3PE	O13-C11-C12-N
5	E	301	3PE	C22-C21-O21-C2
6	A	1908	PC1	C11-O13-P-O11
6	A	1908	PC1	C12-C11-O13-P
6	A	1908	PC1	O13-C11-C12-N
7	A	1911	C8U	C03-C22-O24-C25
7	A	1911	C8U	O23-C22-O24-C25
5	A	1902	3PE	O22-C21-O21-C2
5	A	1906	3PE	O22-C21-O21-C2
5	E	301	3PE	O22-C21-O21-C2
5	A	1904	3PE	C32-C31-O31-C3
5	A	1903	3PE	C22-C21-O21-C2
5	A	1906	3PE	C22-C21-O21-C2
5	A	1909	3PE	C25-C26-C27-C28
6	A	1908	PC1	C32-C31-O31-C3
5	A	1904	3PE	O32-C31-O31-C3
6	A	1908	PC1	O32-C31-O31-C3
5	A	1902	3PE	C26-C27-C28-C29
5	A	1910	3PE	C28-C29-C2A-C2B
5	A	1906	3PE	C27-C28-C29-C2A
5	A	1909	3PE	C23-C24-C25-C26
5	A	1910	3PE	C26-C27-C28-C29
5	A	1910	3PE	C2C-C2D-C2E-C2F
6	A	1908	PC1	C3B-C3C-C3D-C3E
5	A	1906	3PE	C2-C1-O11-P
6	A	1908	PC1	C3D-C3E-C3F-C3G
5	A	1909	3PE	C32-C31-O31-C3
5	A	1904	3PE	C21-C22-C23-C24
5	E	301	3PE	C31-C32-C33-C34
5	A	1909	3PE	O32-C31-O31-C3
5	A	1909	3PE	C22-C21-O21-C2
5	A	1903	3PE	C1-O11-P-O13
5	A	1904	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
5	A	1904	3PE	C11-O13-P-O11
5	A	1905	3PE	C1-O11-P-O13
5	A	1907	3PE	C1-O11-P-O13
5	A	1910	3PE	C11-O13-P-O11
5	E	301	3PE	C11-O13-P-O11
6	A	1908	PC1	C1-O11-P-O13
5	A	1909	3PE	O22-C21-O21-C2
5	E	301	3PE	C33-C34-C35-C36
5	A	1903	3PE	C2C-C2D-C2E-C2F
5	E	301	3PE	C34-C35-C36-C37
5	A	1904	3PE	C26-C27-C28-C29
5	A	1904	3PE	C28-C29-C2A-C2B
5	A	1904	3PE	C29-C2A-C2B-C2C
6	A	1908	PC1	C33-C34-C35-C36
5	A	1902	3PE	C39-C3A-C3B-C3C
5	A	1904	3PE	C32-C33-C34-C35
6	A	1908	PC1	C25-C26-C27-C28
5	A	1904	3PE	C2-C1-O11-P
5	A	1902	3PE	C3D-C3E-C3F-C3G
5	A	1903	3PE	C33-C34-C35-C36
5	A	1910	3PE	C25-C26-C27-C28
6	A	1908	PC1	C24-C25-C26-C27
5	A	1904	3PE	C27-C28-C29-C2A
5	A	1903	3PE	C34-C35-C36-C37
6	A	1908	PC1	C37-C38-C39-C3A
5	A	1906	3PE	C33-C34-C35-C36
5	A	1910	3PE	C3B-C3C-C3D-C3E
5	A	1910	3PE	C3C-C3D-C3E-C3F
5	A	1904	3PE	C31-C32-C33-C34
5	A	1904	3PE	C2A-C2B-C2C-C2D
5	A	1910	3PE	C33-C34-C35-C36
5	A	1910	3PE	C38-C39-C3A-C3B
5	A	1903	3PE	C35-C36-C37-C38
5	A	1904	3PE	C3E-C3F-C3G-C3H
5	A	1902	3PE	C36-C37-C38-C39
5	A	1905	3PE	C25-C26-C27-C28
6	A	1908	PC1	C2A-C2B-C2C-C2D
6	A	1908	PC1	C36-C37-C38-C39
6	A	1908	PC1	C3A-C3B-C3C-C3D
5	A	1903	3PE	C37-C38-C39-C3A
5	A	1910	3PE	O13-C11-C12-N
5	A	1905	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
6	A	1908	PC1	C38-C39-C3A-C3B
5	E	301	3PE	C22-C23-C24-C25
5	A	1905	3PE	C23-C24-C25-C26
5	A	1905	3PE	C2B-C2C-C2D-C2E
6	A	1908	PC1	C2D-C2E-C2F-C2G
5	A	1904	3PE	C3D-C3E-C3F-C3G
5	A	1905	3PE	C35-C36-C37-C38
5	A	1906	3PE	C28-C29-C2A-C2B
5	A	1906	3PE	C21-C22-C23-C24
5	A	1906	3PE	C37-C38-C39-C3A
5	E	301	3PE	C25-C26-C27-C28
5	A	1903	3PE	C3E-C3F-C3G-C3H
5	A	1907	3PE	C21-C22-C23-C24
5	A	1902	3PE	C38-C39-C3A-C3B
6	A	1908	PC1	C22-C23-C24-C25
6	A	1908	PC1	C3F-C3G-C3H-C3I
5	A	1905	3PE	C27-C28-C29-C2A
5	A	1909	3PE	C28-C29-C2A-C2B
5	A	1905	3PE	C31-C32-C33-C34
5	A	1902	3PE	C2C-C2D-C2E-C2F
5	A	1903	3PE	C2B-C2C-C2D-C2E
5	A	1910	3PE	C22-C21-O21-C2
6	A	1908	PC1	C34-C35-C36-C37
5	A	1902	3PE	C2D-C2E-C2F-C2G
5	A	1904	3PE	C34-C35-C36-C37
5	A	1910	3PE	O22-C21-O21-C2
6	A	1908	PC1	O21-C2-C3-O31
5	A	1910	3PE	C22-C23-C24-C25
6	A	1908	PC1	C28-C29-C2A-C2B
5	A	1902	3PE	C3A-C3B-C3C-C3D
5	A	1904	3PE	C39-C3A-C3B-C3C
6	A	1908	PC1	O11-C1-C2-C3
5	A	1902	3PE	C2B-C2C-C2D-C2E
5	A	1904	3PE	C1-C2-C3-O31
5	A	1906	3PE	C1-C2-C3-O31
5	A	1907	3PE	C26-C27-C28-C29
5	A	1910	3PE	C31-C32-C33-C34
5	A	1905	3PE	C24-C25-C26-C27
6	A	1908	PC1	C2C-C2D-C2E-C2F
5	A	1902	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	C2E-C2F-C2G-C2H
5	A	1905	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C32-C33-C34-C35
5	A	1903	3PE	C22-C23-C24-C25
5	A	1910	3PE	C23-C24-C25-C26
5	A	1902	3PE	C29-C2A-C2B-C2C
5	A	1910	3PE	C3D-C3E-C3F-C3G
5	A	1910	3PE	C3E-C3F-C3G-C3H
5	A	1905	3PE	C38-C39-C3A-C3B
5	A	1909	3PE	C33-C34-C35-C36
5	A	1903	3PE	C2F-C2G-C2H-C2I
5	A	1902	3PE	C22-C23-C24-C25
5	A	1904	3PE	C3B-C3C-C3D-C3E
6	A	1908	PC1	C29-C2A-C2B-C2C
5	A	1910	3PE	C2E-C2F-C2G-C2H
5	A	1910	3PE	C32-C31-O31-C3
5	A	1902	3PE	C1-C2-C3-O31
6	A	1908	PC1	C1-C2-C3-O31
5	A	1902	3PE	C2E-C2F-C2G-C2H
5	A	1907	3PE	C11-O13-P-O11
6	A	1908	PC1	O11-C1-C2-O21
5	A	1905	3PE	C22-C23-C24-C25
5	A	1902	3PE	C37-C38-C39-C3A
5	A	1910	3PE	C3F-C3G-C3H-C3I
5	A	1904	3PE	O21-C2-C3-O31
5	A	1907	3PE	C23-C24-C25-C26
5	A	1909	3PE	C22-C23-C24-C25
5	A	1904	3PE	C3A-C3B-C3C-C3D
5	A	1910	3PE	C2F-C2G-C2H-C2I
6	A	1908	PC1	C23-C24-C25-C26
5	A	1905	3PE	C2C-C2D-C2E-C2F
5	E	301	3PE	C1-C2-C3-O31
5	A	1904	3PE	O11-C1-C2-O21
5	A	1910	3PE	O11-C1-C2-O21
5	E	301	3PE	O11-C1-C2-O21
5	A	1910	3PE	O32-C31-O31-C3
5	A	1902	3PE	O21-C2-C3-O31
5	A	1906	3PE	O21-C2-C3-O31
5	A	1909	3PE	O21-C2-C3-O31
5	E	301	3PE	O21-C2-C3-O31
5	A	1903	3PE	C3C-C3D-C3E-C3F
6	A	1908	PC1	C2E-C2F-C2G-C2H
5	E	301	3PE	C32-C33-C34-C35
5	A	1902	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
6	A	1908	PC1	C2B-C2C-C2D-C2E
5	A	1906	3PE	C11-O13-P-O11
7	A	1911	C8U	C04-C05-N09-O10
5	A	1902	3PE	C11-O13-P-O12
5	A	1904	3PE	C11-O13-P-O14
5	A	1905	3PE	C1-O11-P-O12
5	A	1906	3PE	C1-O11-P-O12
5	A	1909	3PE	C11-O13-P-O12
5	E	301	3PE	C11-O13-P-O14
6	A	1908	PC1	C11-O13-P-O12
6	A	1908	PC1	C1-O11-P-O12
6	A	1908	PC1	C1-O11-P-O14
5	A	1903	3PE	C32-C33-C34-C35
5	A	1902	3PE	O11-C1-C2-O21
5	A	1903	3PE	C3F-C3G-C3H-C3I
5	A	1904	3PE	C2E-C2F-C2G-C2H
5	A	1906	3PE	C29-C2A-C2B-C2C
5	A	1907	3PE	C22-C21-O21-C2
5	A	1905	3PE	O21-C21-C22-C23
5	A	1910	3PE	C27-C28-C29-C2A
5	A	1905	3PE	C36-C37-C38-C39
5	E	301	3PE	O11-C1-C2-C3
5	A	1907	3PE	O22-C21-O21-C2
5	A	1909	3PE	C1-O11-P-O13
5	A	1903	3PE	C1-C2-C3-O31
5	A	1903	3PE	C28-C29-C2A-C2B
5	A	1910	3PE	O11-C1-C2-C3
5	A	1902	3PE	C24-C25-C26-C27
5	A	1909	3PE	C1-C2-C3-O31
5	A	1903	3PE	C3A-C3B-C3C-C3D
5	A	1906	3PE	C3-C2-O21-C21
6	A	1908	PC1	C2F-C2G-C2H-C2I
5	A	1902	3PE	C3F-C3G-C3H-C3I
5	A	1903	3PE	C38-C39-C3A-C3B
5	A	1902	3PE	O11-C1-C2-C3
5	A	1904	3PE	O11-C1-C2-C3
5	A	1903	3PE	C2D-C2E-C2F-C2G
5	A	1902	3PE	C33-C34-C35-C36
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1910	3PE	C32-C33-C34-C35
5	A	1909	3PE	C2-C1-O11-P
5	A	1910	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
5	A	1905	3PE	O11-C1-C2-O21
5	A	1910	3PE	C2D-C2E-C2F-C2G
6	A	1908	PC1	C35-C36-C37-C38
5	A	1909	3PE	O31-C31-C32-C33
5	A	1909	3PE	C32-C33-C34-C35
5	A	1904	3PE	O31-C31-C32-C33
5	A	1906	3PE	C23-C24-C25-C26
5	A	1903	3PE	C3B-C3C-C3D-C3E
5	A	1910	3PE	C2A-C2B-C2C-C2D
5	A	1910	3PE	C11-O13-P-O12
6	A	1908	PC1	C11-C12-N-C13
5	A	1906	3PE	O13-C11-C12-N
5	A	1904	3PE	O32-C31-C32-C33
5	A	1906	3PE	C1-C2-O21-C21
5	A	1910	3PE	C12-C11-O13-P
5	A	1909	3PE	O32-C31-C32-C33
5	A	1905	3PE	O31-C31-C32-C33
5	A	1906	3PE	C35-C36-C37-C38
5	A	1903	3PE	C27-C28-C29-C2A
5	A	1902	3PE	O21-C21-C22-C23
5	A	1906	3PE	C34-C35-C36-C37
5	A	1906	3PE	C22-C23-C24-C25
5	A	1902	3PE	O22-C21-C22-C23
5	A	1909	3PE	C24-C25-C26-C27
5	A	1905	3PE	O32-C31-C32-C33
5	A	1904	3PE	C33-C34-C35-C36

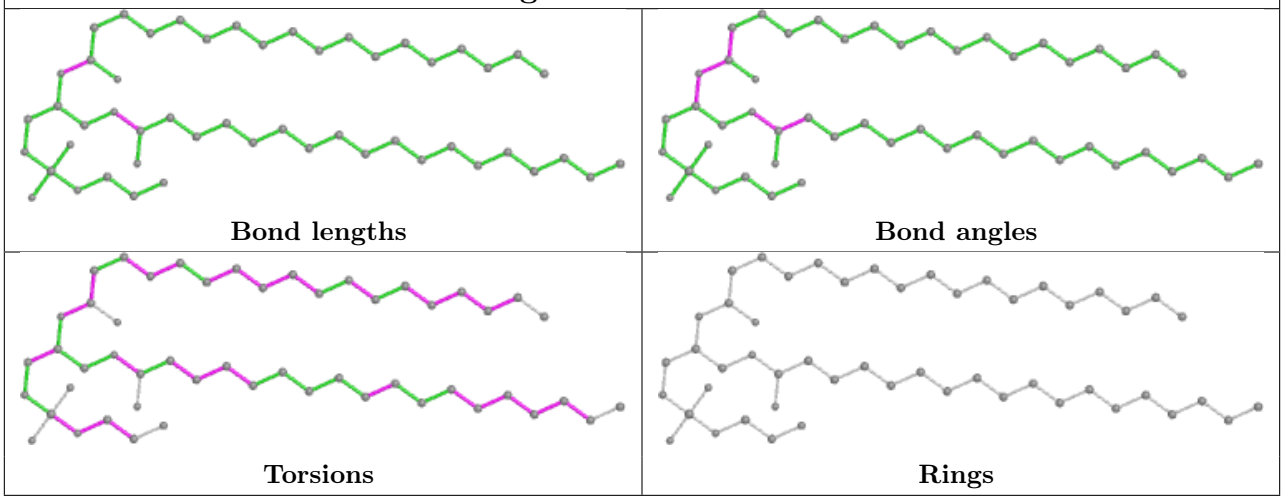
There are no ring outliers.

11 monomers are involved in 101 short contacts:

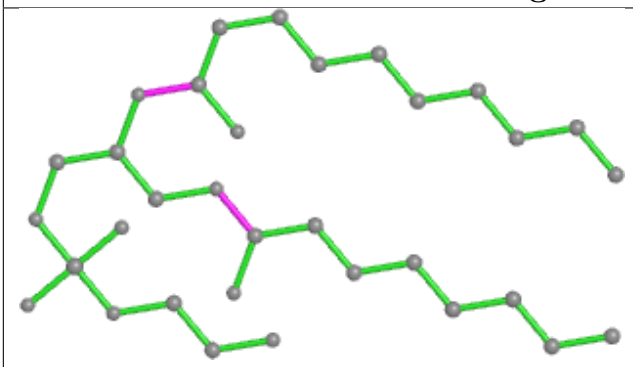
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1910	3PE	12	0
5	E	301	3PE	1	0
5	A	1902	3PE	17	0
5	A	1905	3PE	10	0
5	A	1903	3PE	19	0
5	A	1907	3PE	9	0
6	A	1908	PC1	16	0
5	A	1906	3PE	6	0
5	A	1909	3PE	2	0
5	A	1904	3PE	5	0
7	A	1911	C8U	6	0

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 then 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.

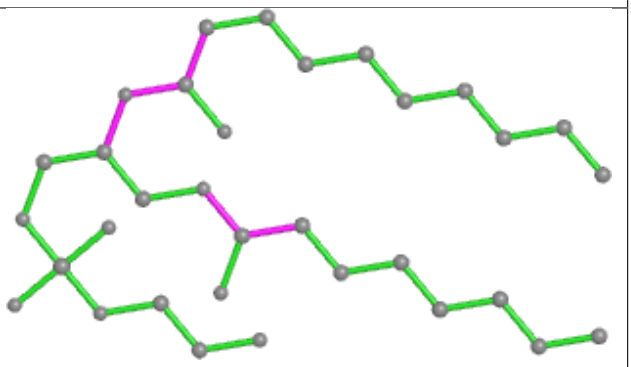
Ligand 3PE A 1910



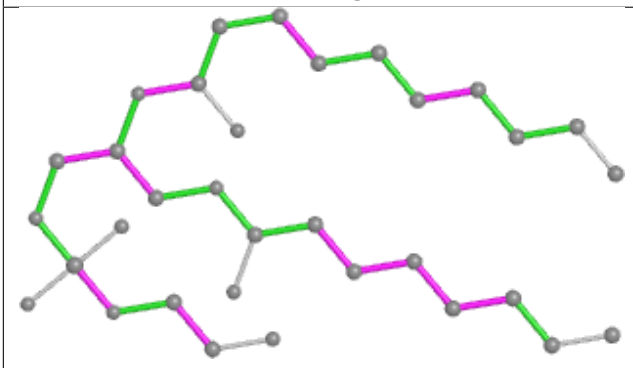
Ligand 3PE E 301



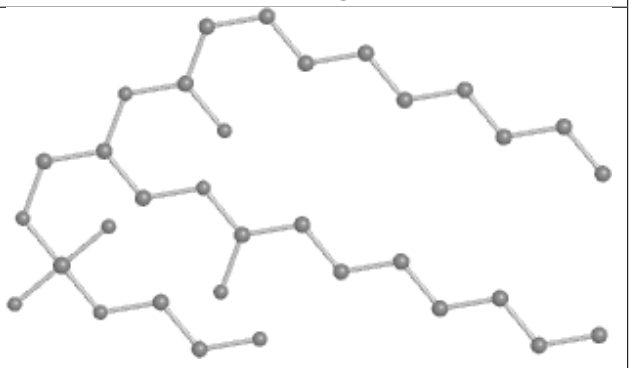
Bond lengths



Bond angles

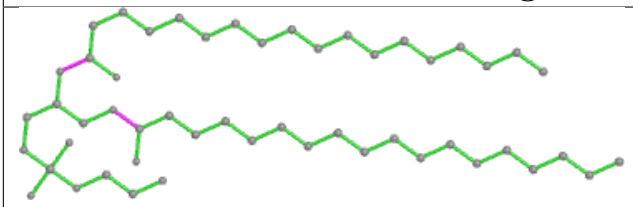


Torsions

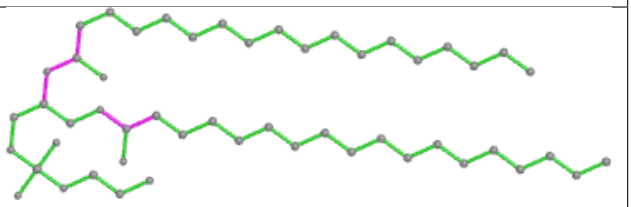


Rings

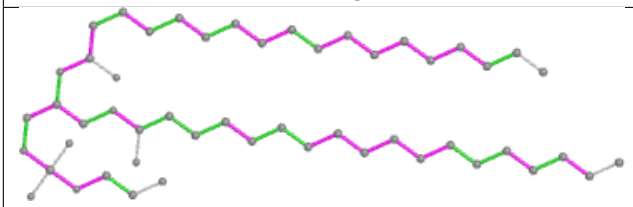
Ligand 3PE A 1902



Bond lengths



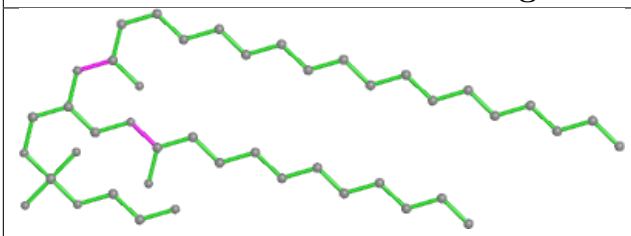
Bond angles



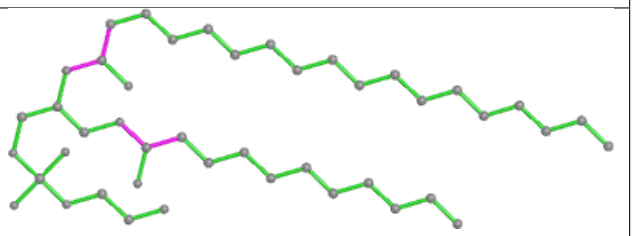
Torsions

Rings

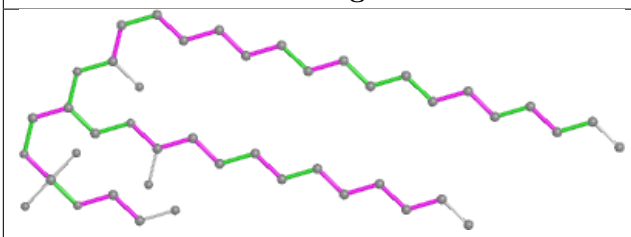
Ligand 3PE A 1905



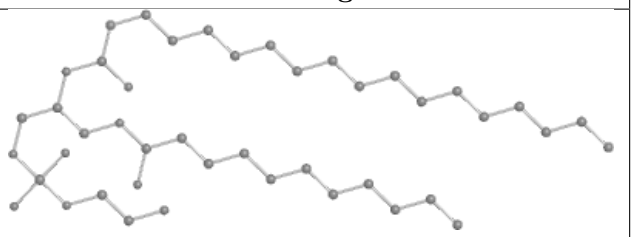
Bond lengths



Bond angles

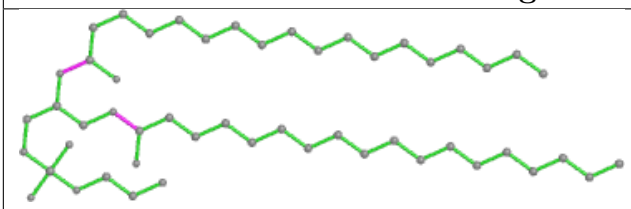


Torsions

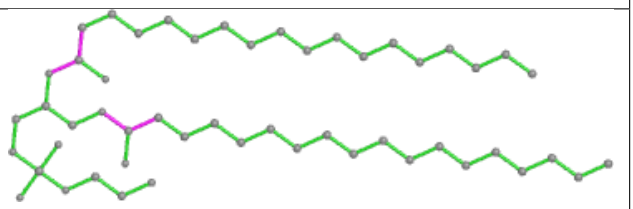


Rings

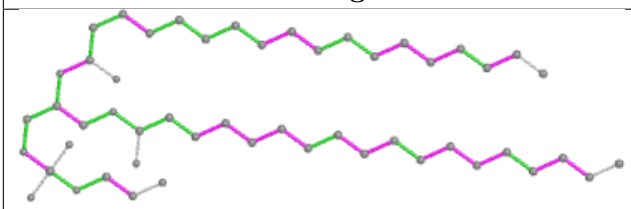
Ligand 3PE A 1903



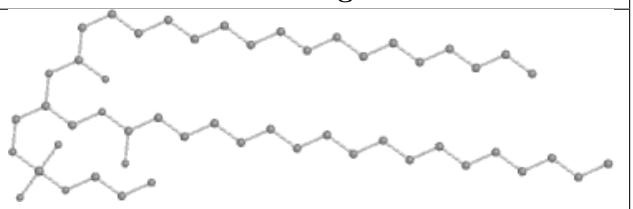
Bond lengths



Bond angles

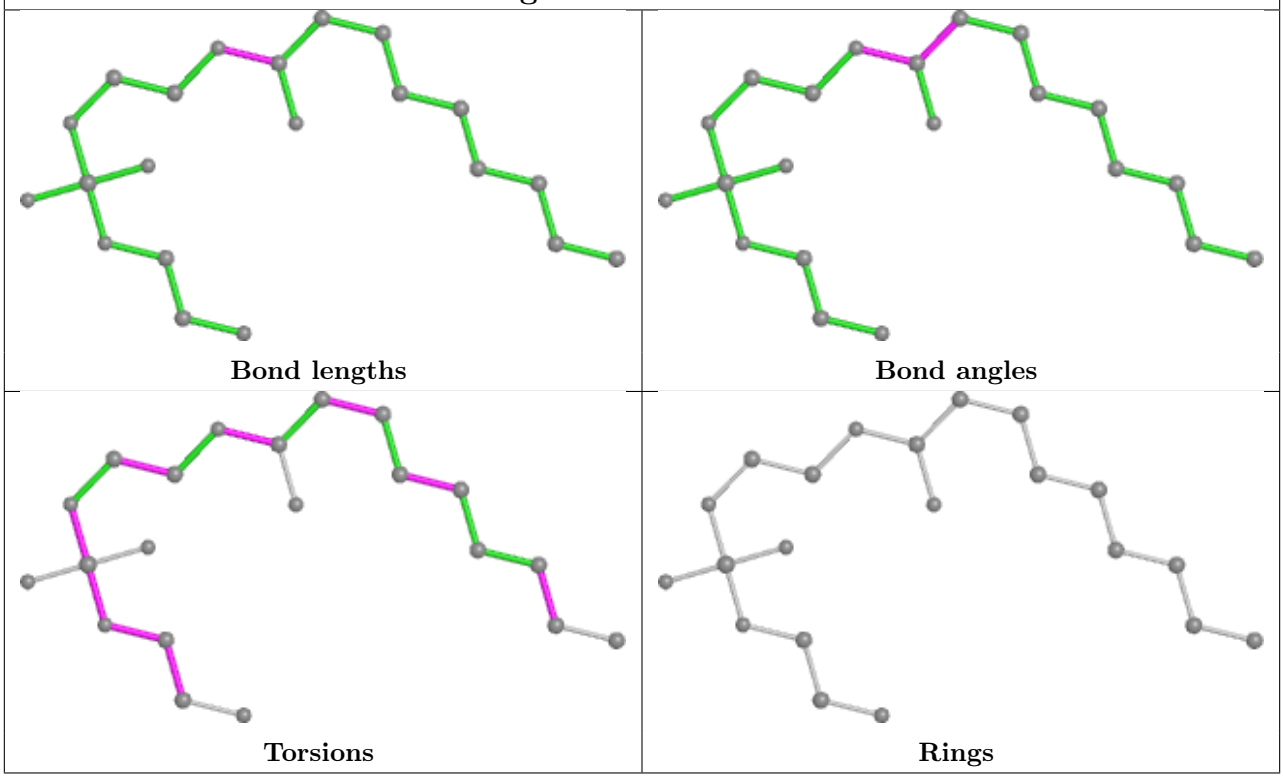


Torsions

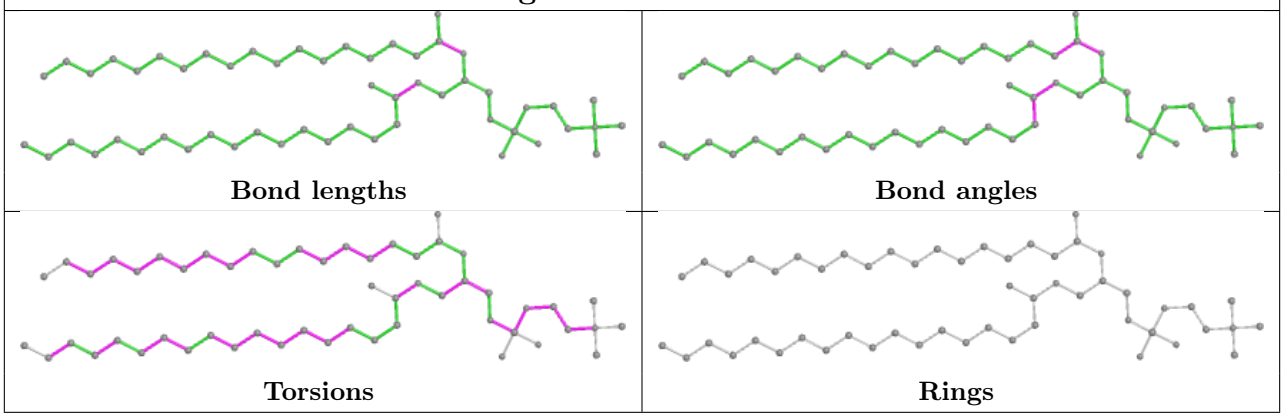


Rings

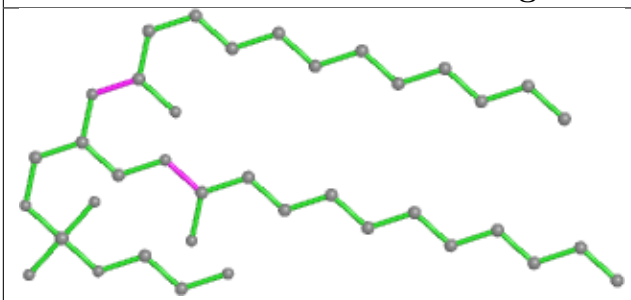
Ligand 3PE A 1907



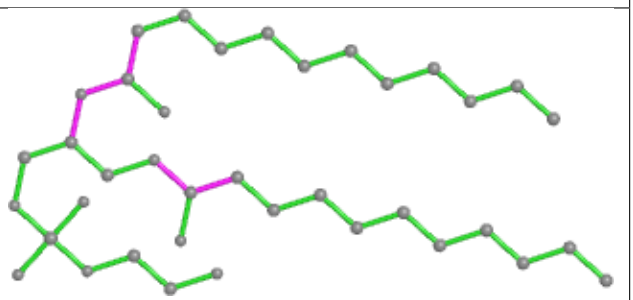
Ligand PC1 A 1908



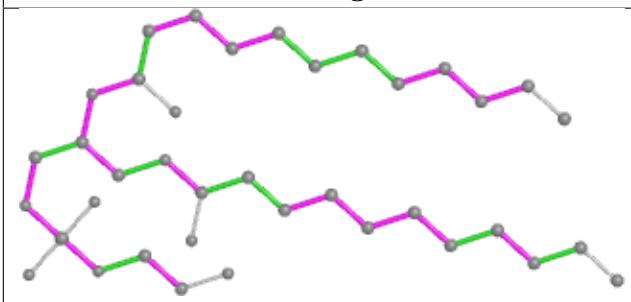
Ligand 3PE A 1906



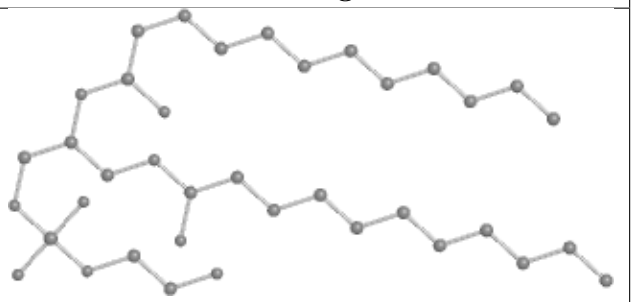
Bond lengths



Bond angles

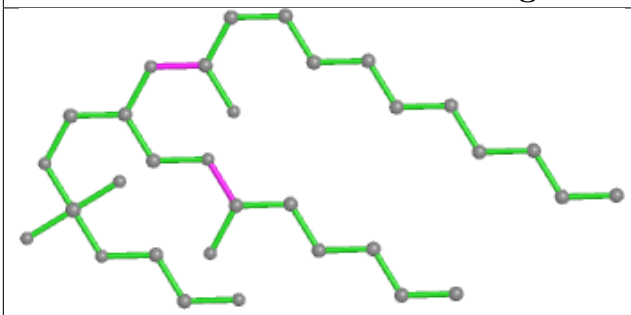


Torsions

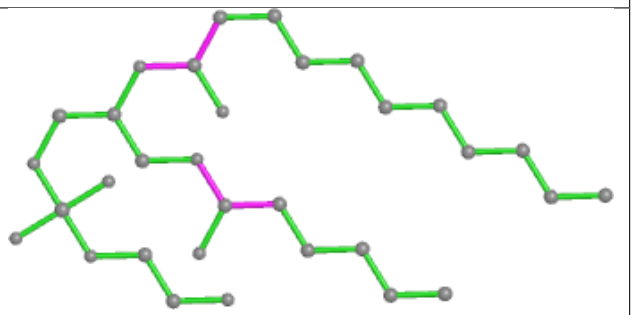


Rings

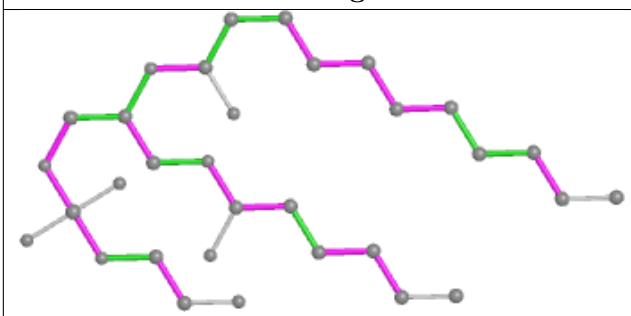
Ligand 3PE A 1909



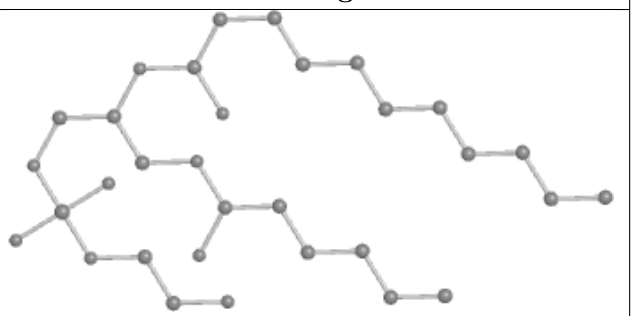
Bond lengths



Bond angles

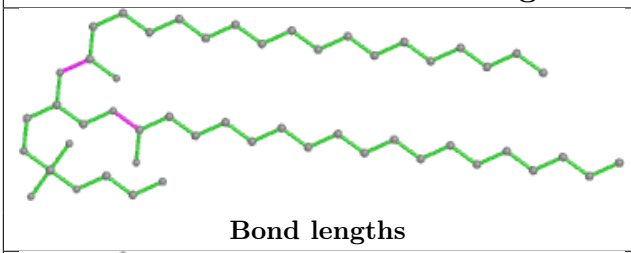


Torsions

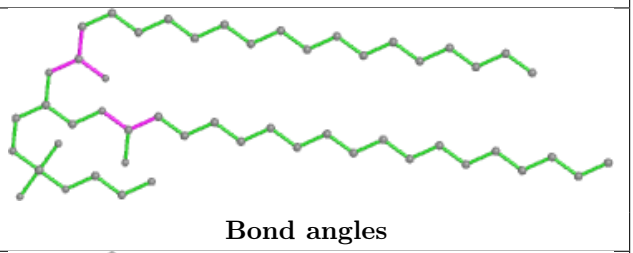


Rings

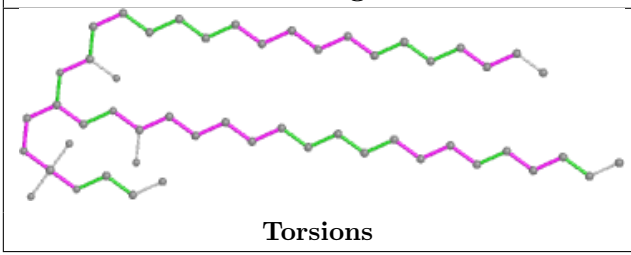
Ligand 3PE A 1904



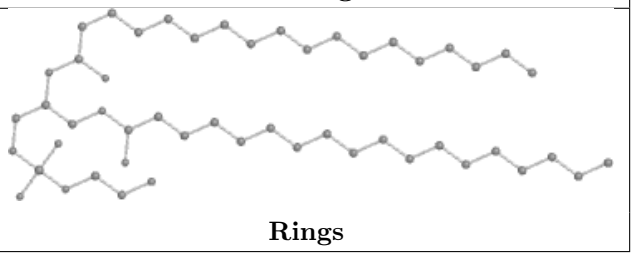
Bond lengths



Bond angles

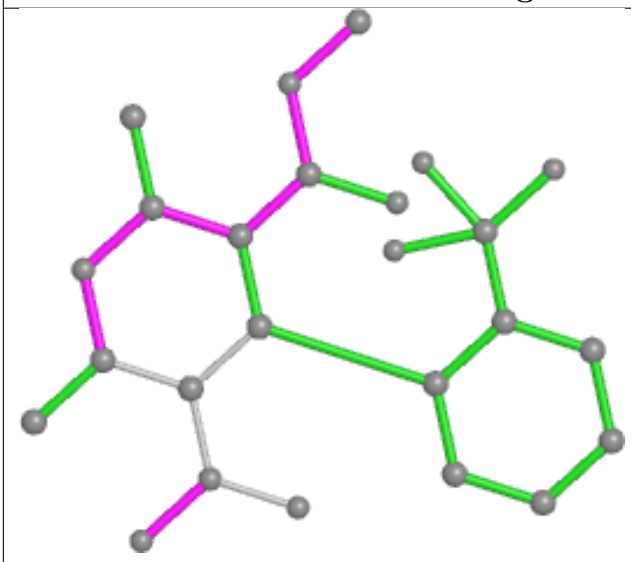


Torsions

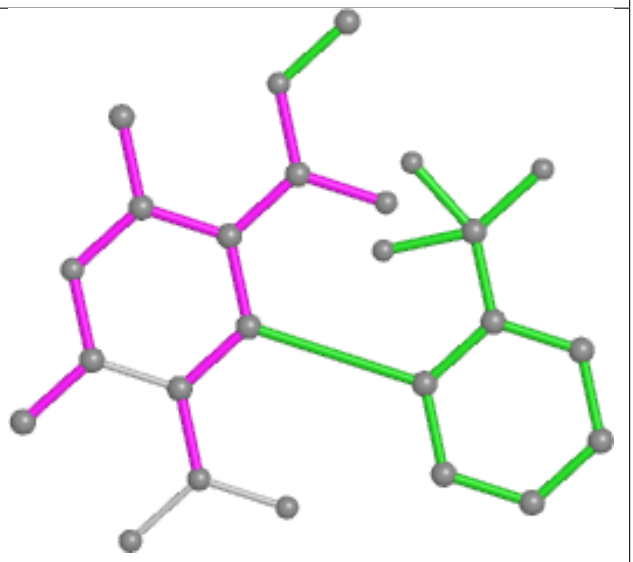


Rings

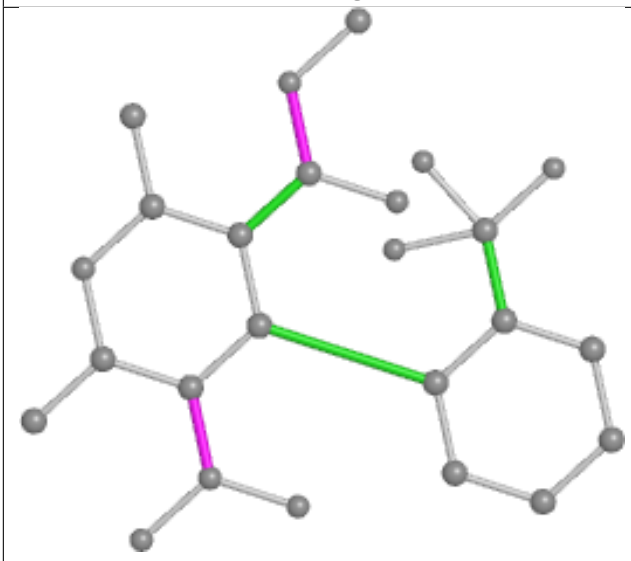
Ligand C8U A 1911



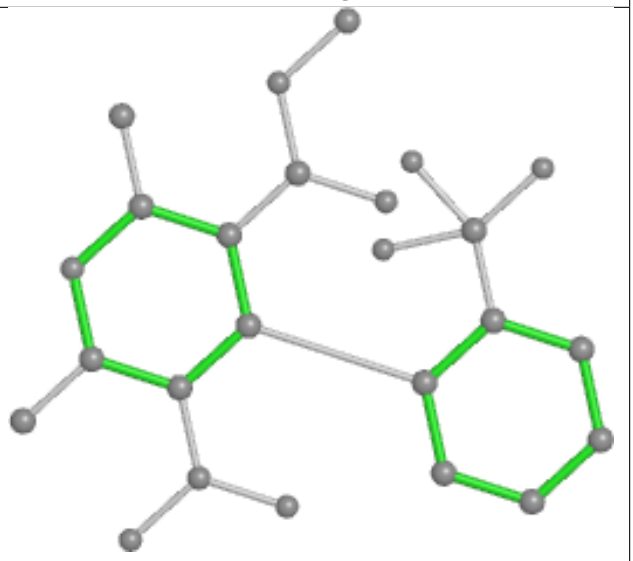
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

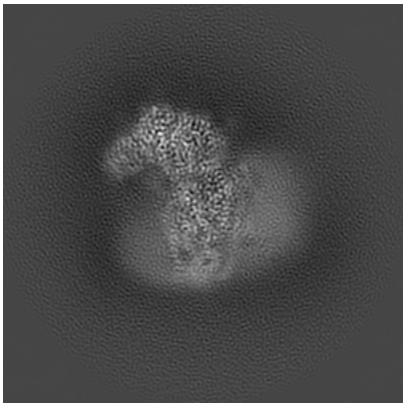
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22414. These allow visual inspection of the internal detail of the map and identification of artifacts.

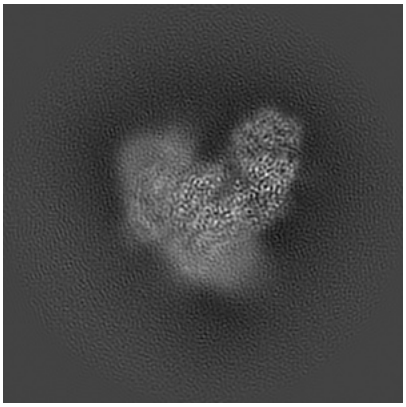
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

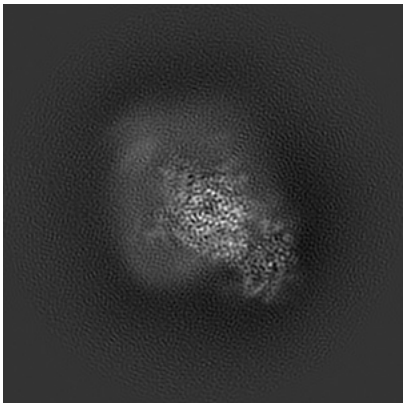
6.1.1 Primary map



X



Y

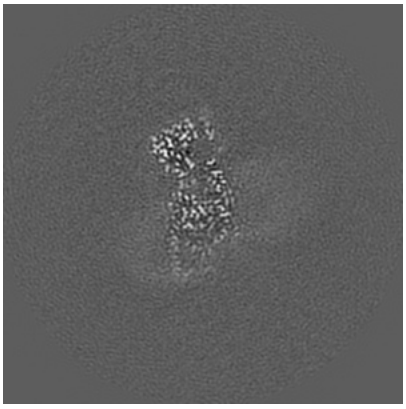


Z

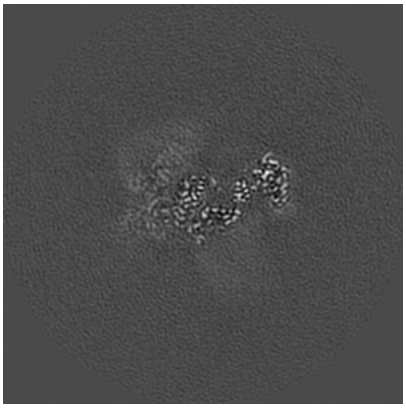
The images above show the map projected in three orthogonal directions.

6.2 Central slices

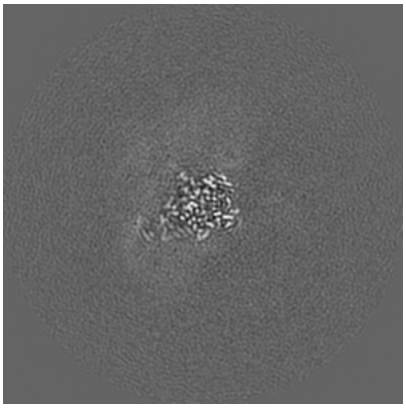
6.2.1 Primary map



X Index: 140



Y Index: 140

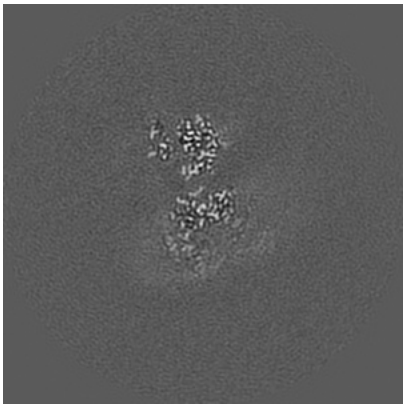


Z Index: 140

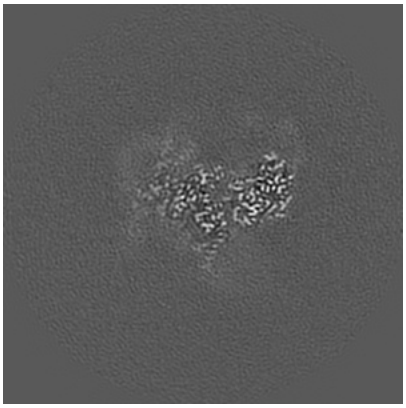
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

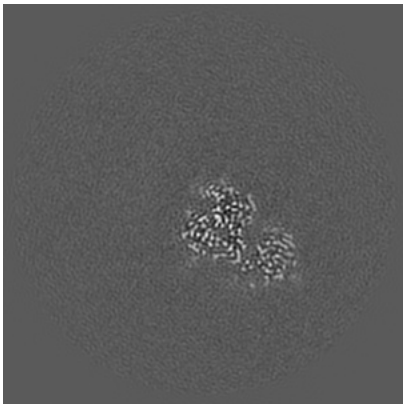
6.3.1 Primary map



X Index: 151



Y Index: 130



Z Index: 185

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

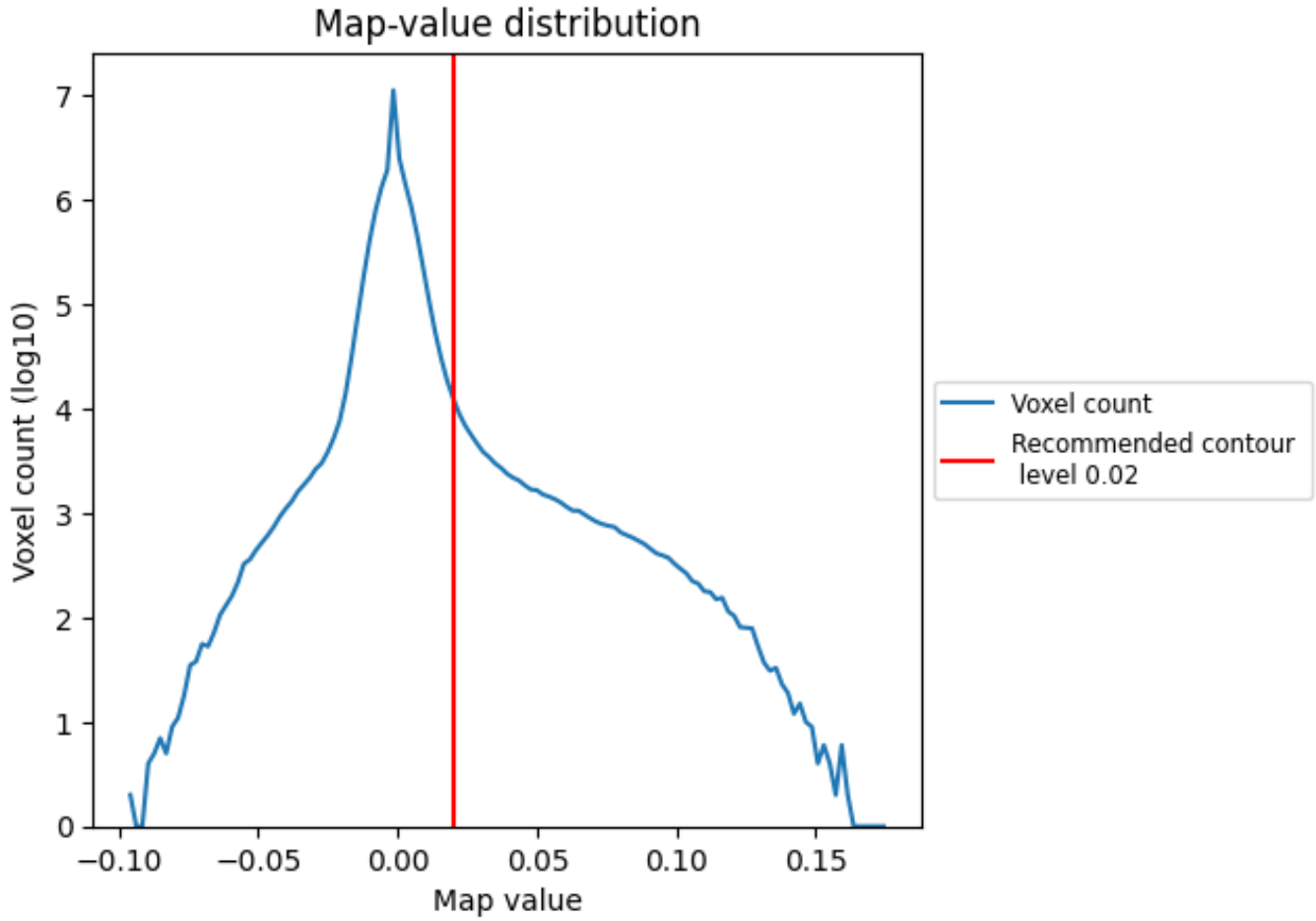
6.5 Mask visualisation (i)

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

7 Map analysis

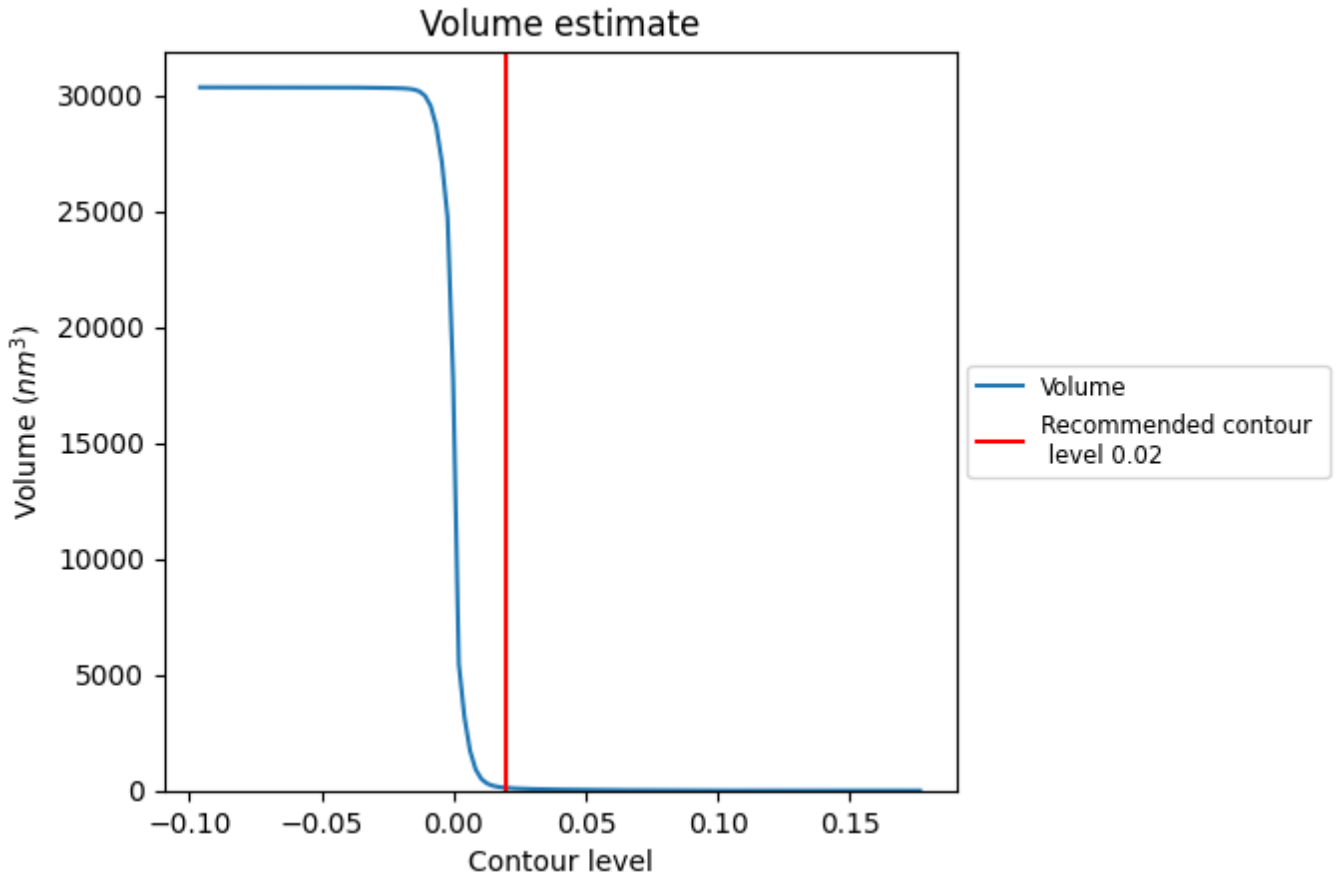
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

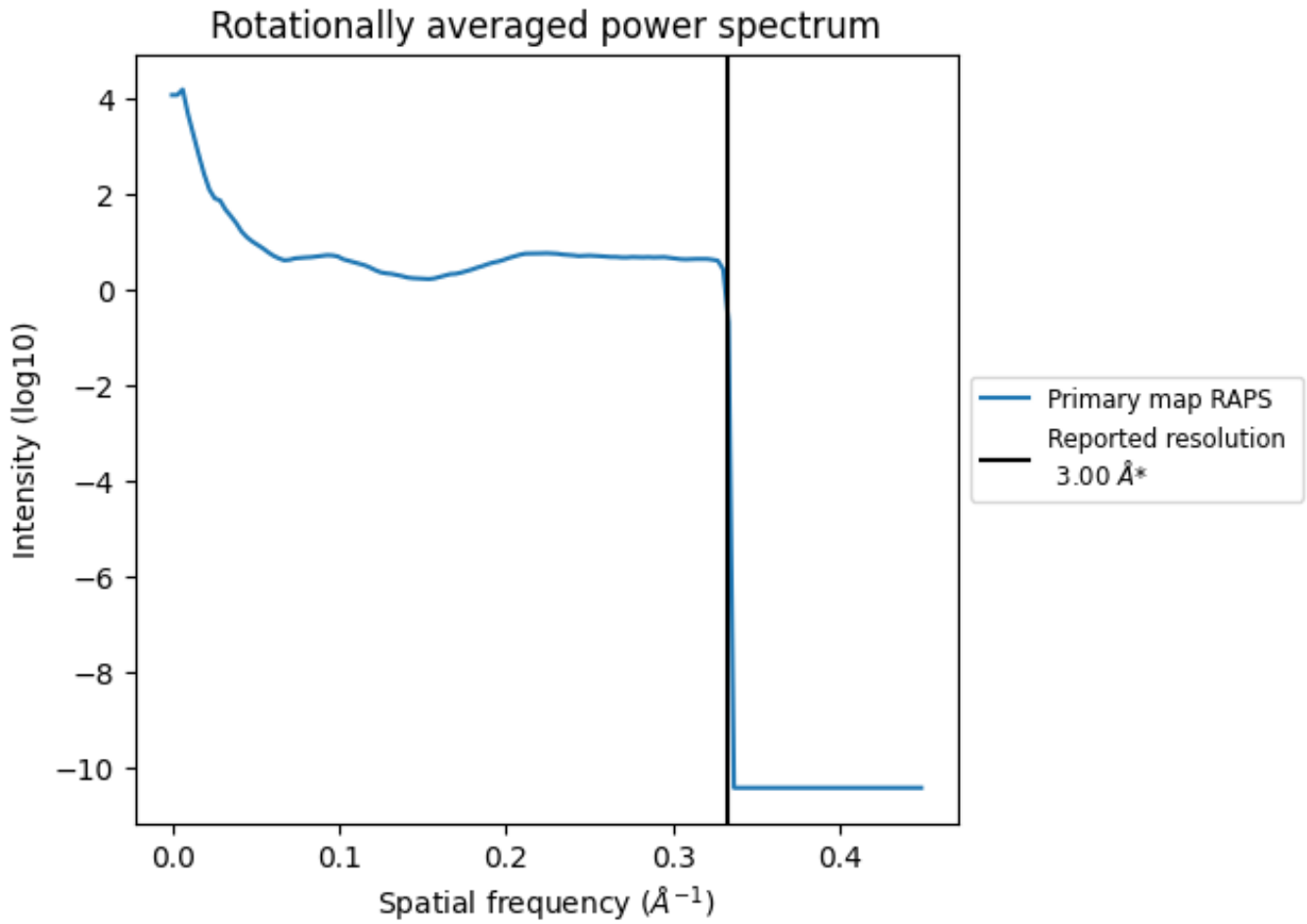
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 106 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 (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

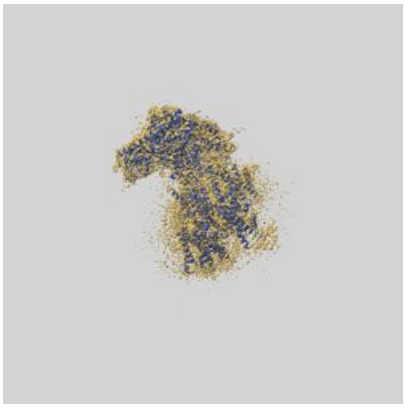
8 Fourier-Shell correlation (i)

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

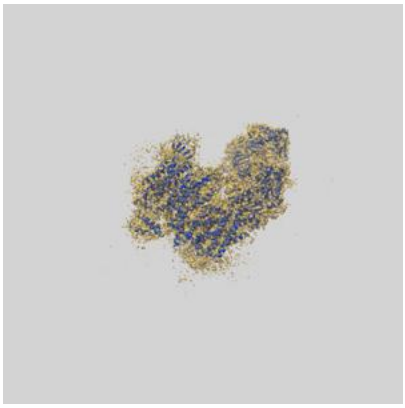
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22414 and PDB model 7JPK. Per-residue inclusion information can be found in section 3 on page 6.

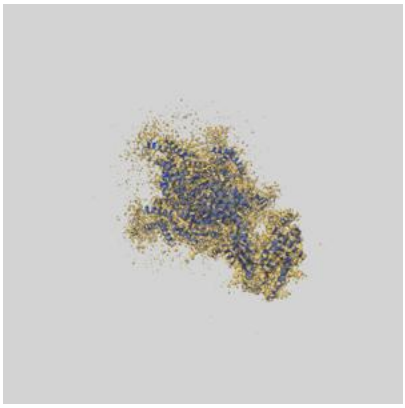
9.1 Map-model overlay



X



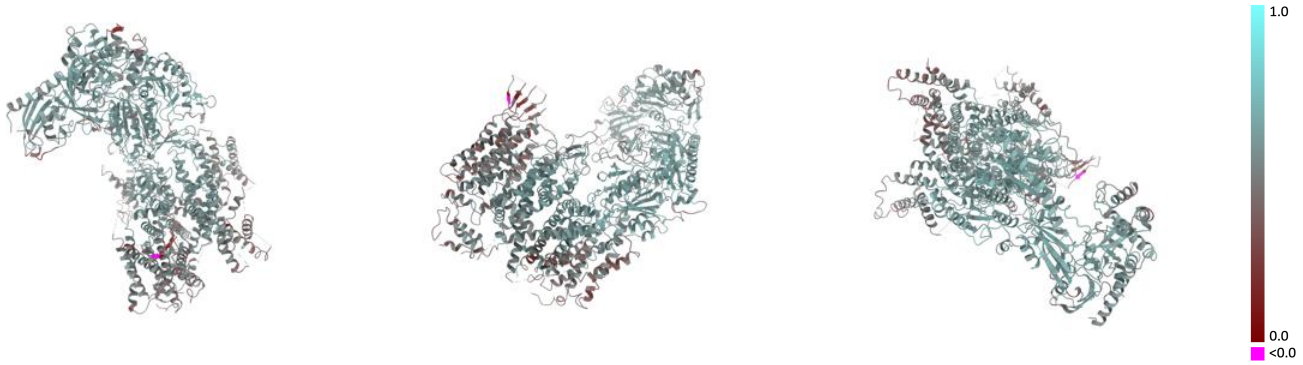
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

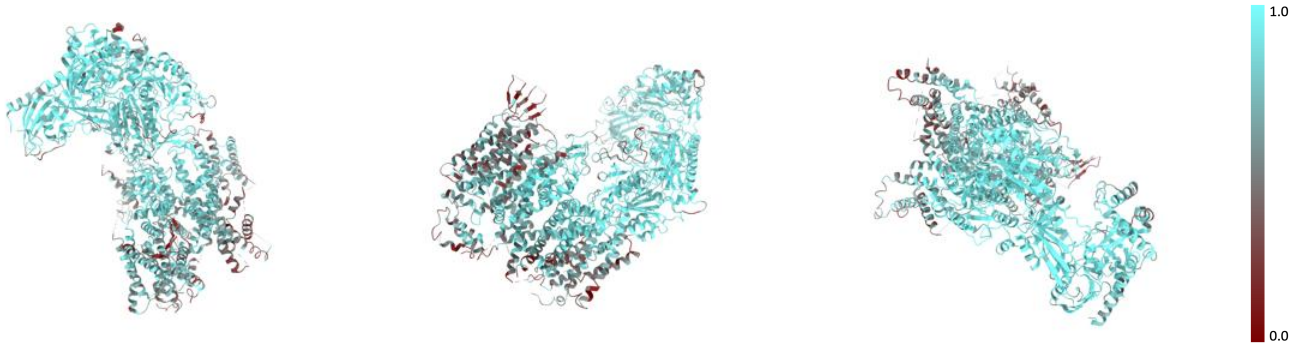
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

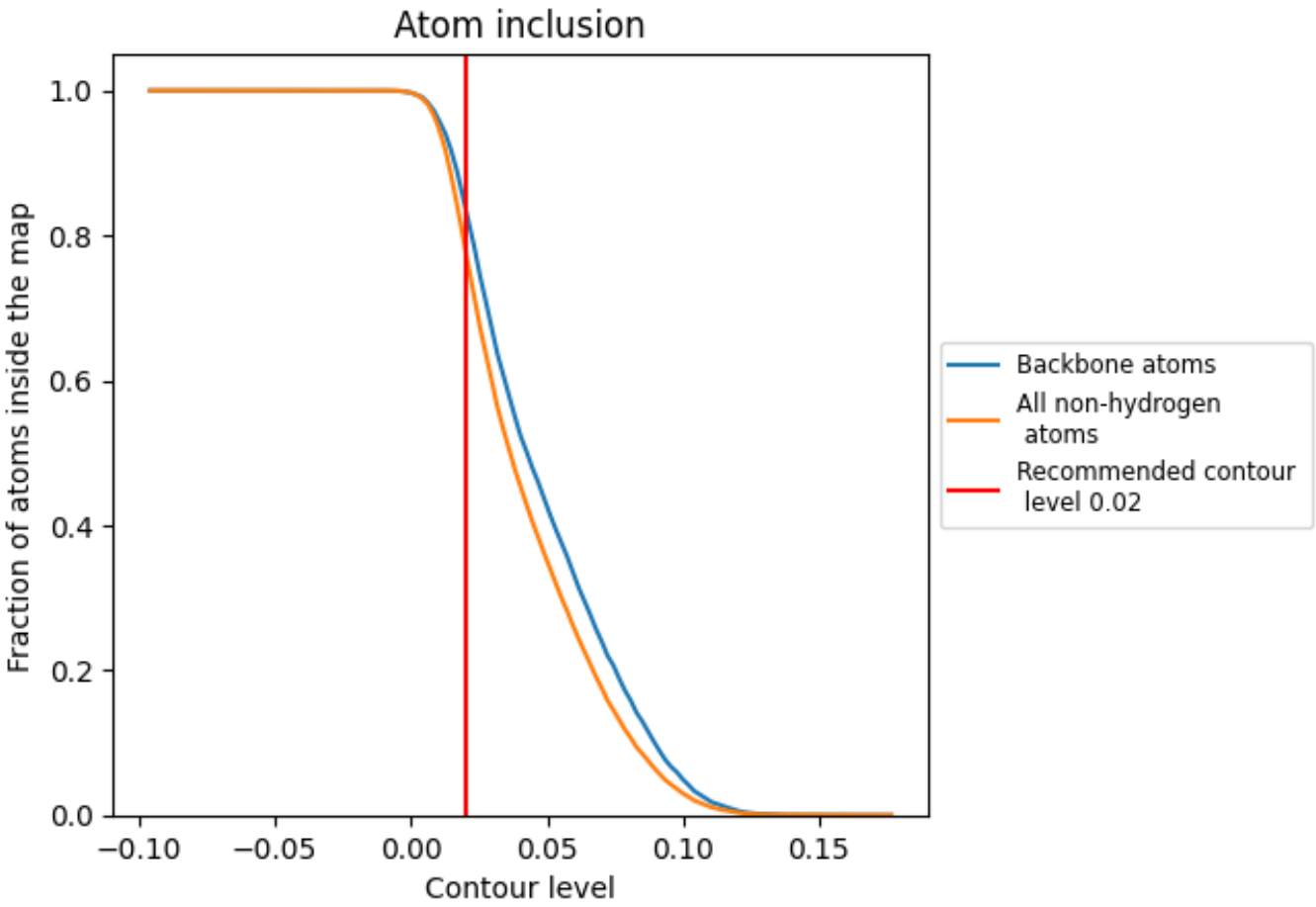
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 84% of all backbone atoms, 78% 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	0.7789	0.5500
A	0.7305	0.5380
E	0.5733	0.4520
F	0.8733	0.5820