



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 04:24 PM EST

PDB ID : 7JPX
EMDB ID : EMD-22426
Title : Rabbit Cav1.1 in the presence of 100 micromolar amlodipine in nanodiscs at 2.9 Angstrom resolution
Authors : Yan, N.; Gao, S.
Deposited on : 2020-08-10
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

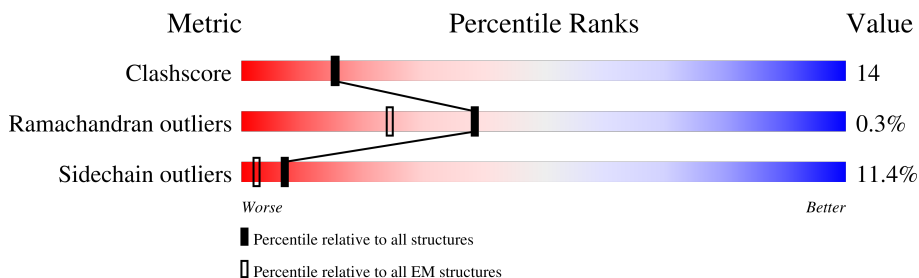
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	3PE	A	1903	-	-	X	-
5	3PE	A	1911	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18640 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	1116	Total	C	N	O	S	0	0
			9016	5977	1435	1544	60		

- 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		

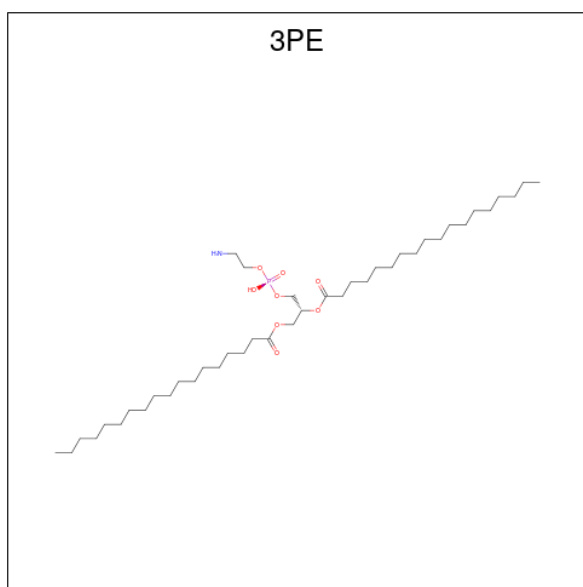
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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 (three-letter code: CA) (formula: Ca).

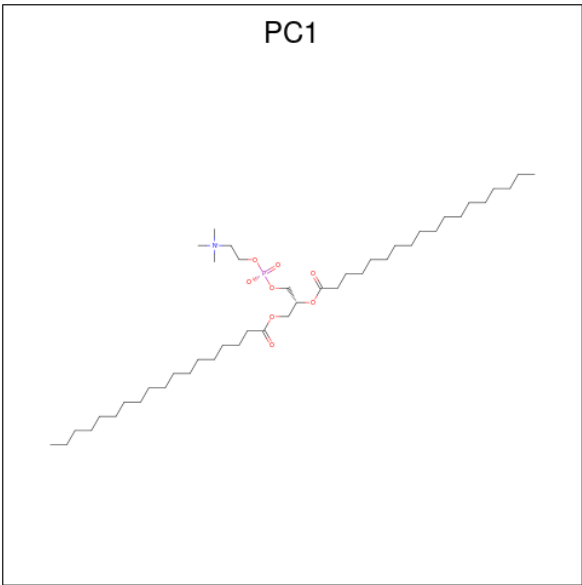
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



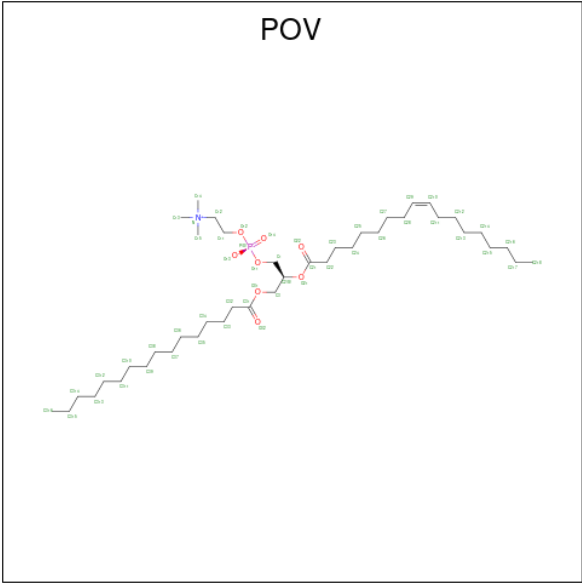
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
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 (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



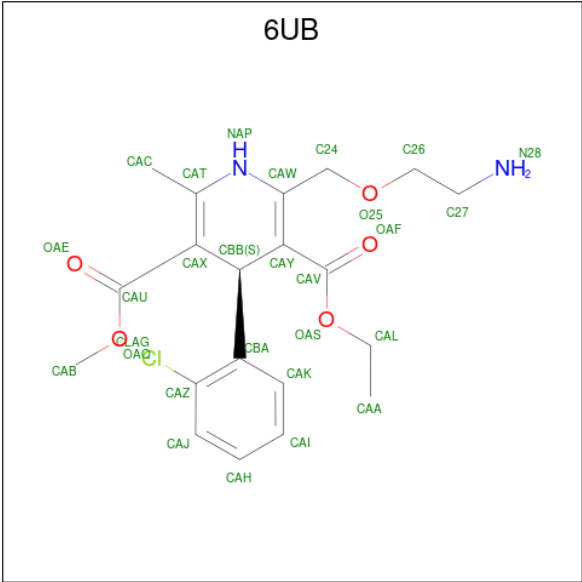
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



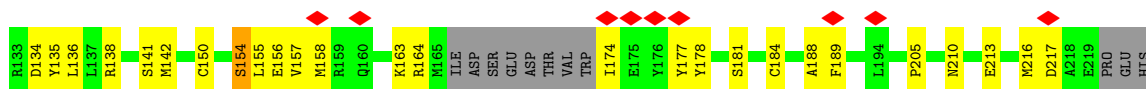
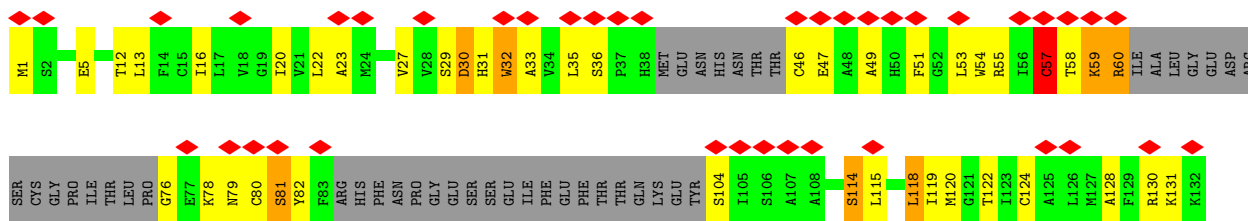
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 8 is amlodipine (three-letter code: 6UB) (formula: C₂₀H₂₅ClN₂O₅) (labeled as "Ligand of Interest" by depositor).



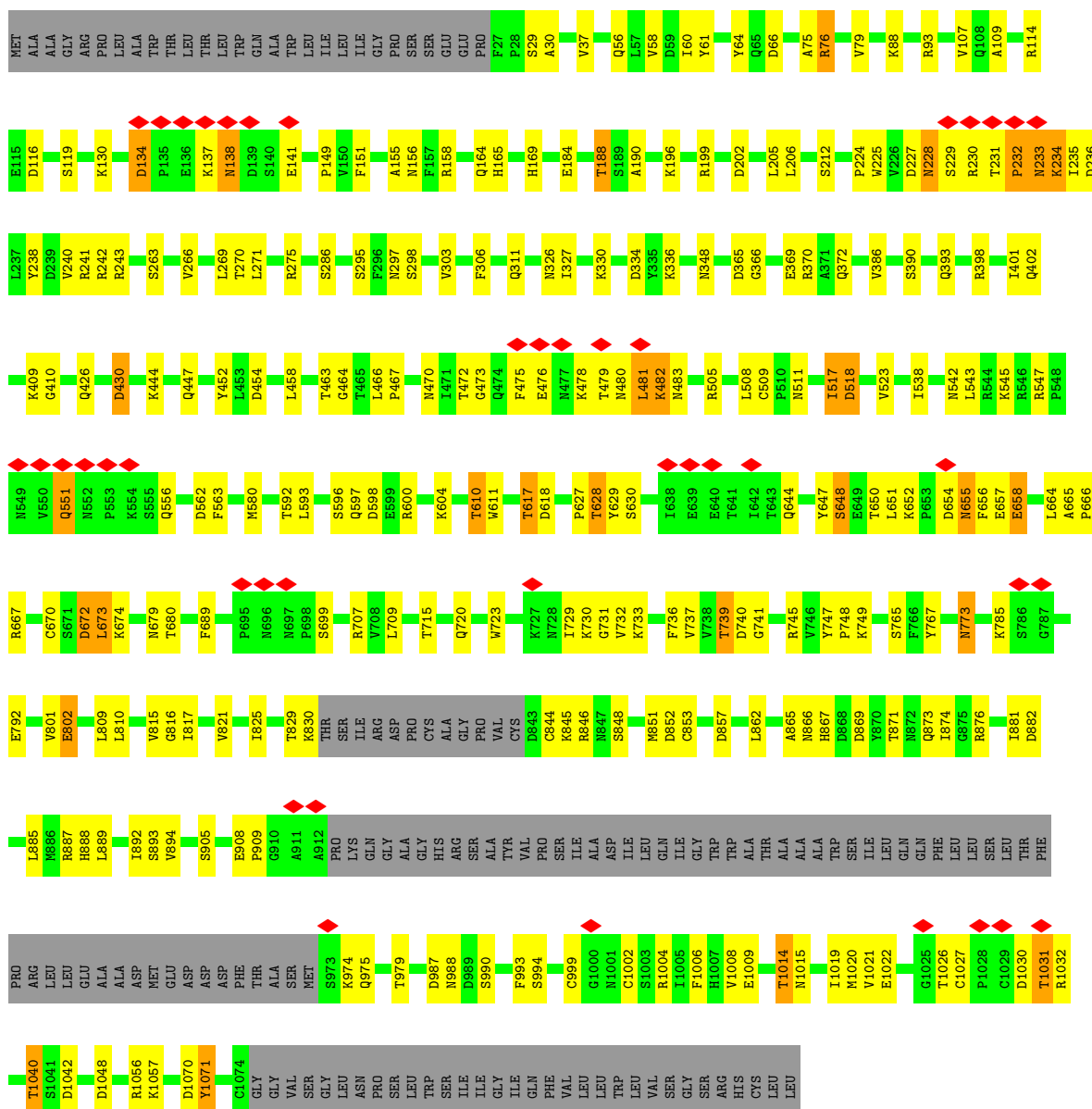
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
8	A	1	28	20	1	2	5	0





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

Chain F: 64% 21% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184373	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	0.186	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, 6UB, CA, 3PE, PC1

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	0.56	0/9240	0.55	1/12545 (0.0%)
2	E	0.39	0/1358	0.55	1/1832 (0.1%)
3	F	0.69	0/7974	0.57	0/10816
All	All	0.61	0/18572	0.56	2/25193 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	CYS	CA-CB-SG	6.87	126.37	114.00
1	A	520	THR	N-CA-C	5.33	125.38	111.00

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	9016	0	9143	276	0
2	E	1326	0	1345	48	0
3	F	7804	0	7617	165	0
4	A	1	0	0	0	0
5	A	364	0	525	106	0
6	A	54	0	88	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	47	0	69	8	0
8	A	28	0	0	4	0
All	All	18640	0	18787	541	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 (541) 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:309:TRP:HB3	6:A:1909:PC1:O32	1.35	1.27
2:E:55:ARG:HG2	2:E:81:SER:O	1.39	1.20
1:A:307:ASN:ND2	5:A:1911:3PE:H12	1.59	1.17
5:A:1911:3PE:H2H2	5:A:1911:3PE:H3A1	1.32	1.12
5:A:1911:3PE:H2C1	5:A:1911:3PE:H2G2	1.36	1.06
3:F:231:THR:HB	3:F:232:PRO:HD3	1.37	1.06
1:A:286:TYR:CD2	1:A:286:TYR:CZ	2.36	1.04
1:A:935:THR:HG22	1:A:1056:MET:HG2	1.41	1.02
5:A:1911:3PE:C2I	5:A:1911:3PE:H3B2	1.89	1.00
2:E:55:ARG:CG	2:E:81:SER:O	2.09	1.00
5:A:1907:3PE:C2C	5:A:1907:3PE:H272	1.92	0.99
2:E:55:ARG:HG2	2:E:81:SER:C	1.83	0.99
1:A:309:TRP:CB	6:A:1909:PC1:O32	2.11	0.98
1:A:939:GLN:HE21	8:A:1913:6UB:CAC	1.77	0.97
5:A:1903:3PE:H222	5:A:1903:3PE:H322	1.45	0.95
1:A:1275:VAL:HG22	5:A:1911:3PE:H2I3	1.47	0.95
2:E:36:SER:O	2:E:174:ILE:HA	1.69	0.93
1:A:939:GLN:NE2	8:A:1913:6UB:CAC	2.32	0.92
1:A:1275:VAL:HG22	5:A:1911:3PE:C2I	2.02	0.90
1:A:935:THR:CG2	1:A:1056:MET:HG2	2.01	0.90
1:A:1046:ILE:CD1	5:A:1908:3PE:H262	2.03	0.89
7:A:1912:POV:H2	7:A:1912:POV:H24A	1.50	0.89
5:A:1911:3PE:H2H2	5:A:1911:3PE:C3A	2.03	0.89
1:A:1129:MET:HE3	5:A:1903:3PE:H2C1	1.52	0.89
6:A:1909:PC1:O14	6:A:1909:PC1:H133	1.74	0.88
1:A:200:ALA:HB1	5:A:1903:3PE:C3H	2.04	0.87
3:F:233:ASN:O	3:F:233:ASN:ND2	2.08	0.87
5:A:1908:3PE:O14	5:A:1908:3PE:N	2.08	0.86
5:A:1906:3PE:O11	5:A:1906:3PE:N	2.08	0.86
1:A:1046:ILE:HD12	5:A:1908:3PE:H262	1.58	0.85
1:A:200:ALA:HB1	5:A:1903:3PE:H3H1	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:386:VAL:O	3:F:410:GLY:HA3	1.76	0.84
1:A:529:CYS:HA	1:A:532:LEU:HD12	1.60	0.84
1:A:1125:PHE:HE2	1:A:1249:ARG:HB2	1.41	0.83
2:E:55:ARG:CB	2:E:81:SER:O	2.27	0.83
1:A:231:THR:O	1:A:262:ARG:NH1	2.15	0.80
6:A:1909:PC1:H133	6:A:1909:PC1:P	2.22	0.79
5:A:1904:3PE:C3	5:A:1904:3PE:H221	2.11	0.79
3:F:235:ILE:H	3:F:551:GLN:HG3	1.49	0.78
1:A:522:LEU:HD22	1:A:522:LEU:O	1.84	0.78
3:F:297:ASN:ND2	3:F:330:LYS:O	2.17	0.77
5:A:1911:3PE:H3B2	5:A:1911:3PE:H2I2	1.67	0.77
3:F:444:LYS:NZ	3:F:467:PRO:O	2.18	0.76
1:A:987:PRO:HD3	3:F:230:ARG:HH12	1.51	0.76
1:A:928:ILE:HD13	1:A:1060:PHE:CE1	2.20	0.76
1:A:905:LEU:HD22	1:A:908:ILE:HD11	1.68	0.75
1:A:307:ASN:ND2	5:A:1911:3PE:C1	2.45	0.75
2:E:32:TRP:HB3	2:E:181:SER:HB2	1.67	0.75
5:A:1911:3PE:H2C1	5:A:1911:3PE:C2G	2.16	0.75
3:F:231:THR:CB	3:F:232:PRO:HD3	2.12	0.75
3:F:235:ILE:O	3:F:551:GLN:NE2	2.20	0.75
1:A:559:ILE:HG21	1:A:659:ILE:HD11	1.68	0.74
1:A:307:ASN:HD21	5:A:1911:3PE:H12	1.49	0.74
7:A:1912:POV:H24A	7:A:1912:POV:C2	2.16	0.73
2:E:59:LYS:HD3	2:E:59:LYS:O	1.89	0.73
3:F:235:ILE:N	3:F:551:GLN:HG3	2.03	0.72
1:A:555:SER:HA	1:A:663:ASN:HD22	1.54	0.72
3:F:232:PRO:HG2	3:F:234:LYS:HD3	1.72	0.72
1:A:935:THR:HG22	1:A:1056:MET:CG	2.18	0.72
2:E:60:ARG:HB2	2:E:76:GLY:HA2	1.71	0.72
1:A:510:GLU:OE1	1:A:531:ARG:NH2	2.22	0.71
1:A:65:CYS:HB3	5:A:1907:3PE:H262	1.72	0.71
2:E:114:SER:HB2	2:E:150:CYS:HB2	1.73	0.71
6:A:1909:PC1:H122	6:A:1909:PC1:O12	1.89	0.71
5:A:1903:3PE:O14	5:A:1903:3PE:H121	1.89	0.71
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.73	0.71
5:A:1911:3PE:H3I3	5:A:1911:3PE:H3E1	1.73	0.70
1:A:277:ASN:HD22	5:A:1903:3PE:H32	1.56	0.70
1:A:878:VAL:HG11	1:A:899:LEU:HD11	1.74	0.70
3:F:452:TYR:HH	3:F:463:THR:HG1	1.26	0.70
1:A:1125:PHE:CE2	1:A:1249:ARG:HB2	2.26	0.69
1:A:70:VAL:HG12	5:A:1907:3PE:H11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:234:LYS:O	3:F:234:LYS:HG2	1.94	0.68
3:F:658:GLU:O	3:F:720:GLN:NE2	2.26	0.68
1:A:872:ASP:HB2	1:A:906:ARG:HD3	1.76	0.68
3:F:1006:PHE:HB3	3:F:1021:VAL:HG23	1.76	0.68
2:E:210:ASN:HB2	2:E:213:GLU:HG3	1.76	0.68
1:A:326:LEU:HD21	7:A:1912:POV:H22	1.76	0.68
2:E:55:ARG:HA	2:E:81:SER:O	1.94	0.68
2:E:128:ALA:HB2	2:E:136:LEU:HB3	1.76	0.67
3:F:733:LYS:NZ	3:F:792:GLU:O	2.28	0.67
1:A:928:ILE:HD13	1:A:1060:PHE:HE1	1.59	0.67
3:F:739:THR:OG1	3:F:740:ASP:O	2.13	0.67
1:A:936:THR:HG21	5:A:1904:3PE:H3E1	1.76	0.67
5:A:1911:3PE:H292	5:A:1911:3PE:H342	1.76	0.67
1:A:532:LEU:HD23	1:A:535:LEU:HD11	1.77	0.66
1:A:869:ASN:OD1	1:A:869:ASN:N	2.26	0.66
1:A:344:ALA:HA	1:A:347:ARG:HG2	1.77	0.66
5:A:1911:3PE:H3B2	5:A:1911:3PE:H2I1	1.77	0.66
3:F:470:ASN:HD21	3:F:482:LYS:NZ	1.92	0.66
1:A:295:THR:HG21	1:A:1318:ARG:HG3	1.77	0.66
5:A:1911:3PE:H2G2	5:A:1911:3PE:C2C	2.17	0.66
1:A:1366:MET:HG2	8:A:1913:6UB:OAF	1.97	0.65
3:F:657:GLU:OE2	3:F:749:LYS:NZ	2.29	0.65
5:A:1906:3PE:HN1	5:A:1906:3PE:C1	2.10	0.65
3:F:647:TYR:O	3:F:650:THR:OG1	2.14	0.65
1:A:542:TRP:HB3	1:A:545:LEU:HB3	1.77	0.64
5:A:1904:3PE:H221	5:A:1904:3PE:H31	1.78	0.64
3:F:656:PHE:HB3	3:F:749:LYS:HD2	1.78	0.64
1:A:928:ILE:HD12	1:A:928:ILE:O	1.97	0.64
1:A:205:PHE:CE1	5:A:1903:3PE:H2D1	2.32	0.64
1:A:928:ILE:CD1	1:A:1060:PHE:HE1	2.11	0.64
3:F:729:ILE:HG22	3:F:730:LYS:H	1.62	0.64
5:A:1911:3PE:H3B2	5:A:1911:3PE:C2H	2.28	0.64
1:A:445:ASN:HB2	1:A:471:LEU:HD13	1.80	0.63
1:A:1046:ILE:HD13	5:A:1908:3PE:H262	1.80	0.63
1:A:1129:MET:CE	5:A:1903:3PE:H2F1	2.28	0.63
1:A:205:PHE:CZ	5:A:1903:3PE:H2D1	2.34	0.63
1:A:522:LEU:HD22	1:A:522:LEU:C	2.17	0.63
2:E:35:LEU:HG	2:E:49:ALA:HB3	1.80	0.63
1:A:633:PRO:O	5:A:1906:3PE:H222	1.99	0.62
2:E:55:ARG:CA	2:E:81:SER:O	2.47	0.62
1:A:64:ASN:OD1	1:A:171:ARG:NH1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:LEU:O	1:A:875:VAL:HG23	1.99	0.62
1:A:917:VAL:HG21	1:A:1269:TYR:HB2	1.82	0.62
3:F:184:GLU:O	3:F:188:THR:OG1	2.17	0.62
1:A:217:LEU:HD13	6:A:1909:PC1:H322	1.82	0.62
1:A:947:VAL:O	1:A:951:LYS:HB2	2.01	0.61
1:A:1254:ARG:HG3	5:A:1902:3PE:H222	1.82	0.61
3:F:654:ASP:OD1	3:F:655:ASN:N	2.32	0.60
3:F:297:ASN:O	3:F:298:SER:OG	2.15	0.60
1:A:1046:ILE:CD1	5:A:1908:3PE:C26	2.79	0.60
3:F:993:PHE:HB2	3:F:1008:VAL:HG22	1.83	0.60
1:A:94:LEU:HD21	1:A:133:GLY:HA3	1.83	0.60
3:F:1004:ARG:HB3	3:F:1022:GLU:HB2	1.84	0.60
1:A:1241:MET:HE2	6:A:1909:PC1:H3A2	1.84	0.60
1:A:1349:GLU:HG2	1:A:1350:TYR:HD1	1.67	0.59
3:F:644:GLN:O	3:F:648:SER:OG	2.21	0.59
1:A:199:ILE:HD11	1:A:332:VAL:HG21	1.85	0.59
2:E:33:ALA:HB3	2:E:51:PHE:HB2	1.84	0.59
3:F:228:ASN:HB2	3:F:231:THR:HB	1.84	0.59
1:A:844:THR:O	1:A:848:VAL:HG23	2.02	0.59
2:E:33:ALA:HA	2:E:177:TYR:O	2.02	0.59
3:F:593:LEU:HD23	3:F:604:LYS:HG2	1.84	0.58
1:A:307:ASN:HD22	5:A:1911:3PE:H12	1.62	0.58
1:A:646:VAL:HG11	5:A:1905:3PE:H3G2	1.85	0.58
1:A:1298:THR:O	1:A:1301:ASN:ND2	2.36	0.58
1:A:984:GLU:OE1	1:A:986:ARG:NH2	2.37	0.58
3:F:311:GLN:HE21	3:F:1056:ARG:HD2	1.69	0.58
1:A:1046:ILE:HD12	5:A:1908:3PE:C26	2.31	0.58
5:A:1911:3PE:H2H2	5:A:1911:3PE:C3B	2.33	0.58
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.85	0.58
2:E:55:ARG:HD3	2:E:81:SER:HA	1.85	0.58
3:F:1031:THR:OG1	3:F:1032:ARG:NH1	2.36	0.58
5:A:1902:3PE:H241	5:A:1902:3PE:O22	2.03	0.58
1:A:434:PHE:HA	1:A:437:LEU:HD23	1.84	0.58
1:A:656:PHE:HB3	1:A:1058:ASN:OD1	2.04	0.58
1:A:1129:MET:CE	5:A:1903:3PE:C2F	2.81	0.58
5:A:1911:3PE:C1	5:A:1911:3PE:H111	2.33	0.58
1:A:80:ASN:OD1	1:A:80:ASN:N	2.36	0.57
2:E:55:ARG:HD3	2:E:80:CYS:O	2.02	0.57
1:A:200:ALA:HB1	5:A:1903:3PE:H3H2	1.83	0.57
5:A:1906:3PE:H242	5:A:1906:3PE:H322	1.86	0.57
3:F:672:ASP:HB2	3:F:689:PHE:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:O	1:A:284:THR:HG22	2.04	0.57
1:A:923:VAL:O	1:A:926:ARG:NH1	2.37	0.57
1:A:502:PHE:O	1:A:506:SER:OG	2.22	0.57
1:A:576:LEU:HD21	5:A:1906:3PE:H2C2	1.87	0.57
1:A:987:PRO:HD3	3:F:230:ARG:NH1	2.19	0.56
5:A:1907:3PE:H2	5:A:1907:3PE:O12	2.04	0.56
1:A:449:ILE:HD11	1:A:535:LEU:HD21	1.85	0.56
3:F:596:SER:OG	3:F:598:ASP:O	2.22	0.56
1:A:1385:ASP:OD1	1:A:1385:ASP:N	2.36	0.56
1:A:334:SER:O	1:A:338:THR:HG23	2.05	0.56
1:A:1129:MET:HE3	5:A:1903:3PE:H2F1	1.87	0.56
1:A:1247:LEU:CD2	5:A:1902:3PE:H231	2.36	0.56
3:F:481:LEU:HG	3:F:482:LYS:H	1.71	0.56
1:A:1129:MET:HE3	5:A:1903:3PE:C2F	2.36	0.56
3:F:999:CYS:SG	3:F:1002:CYS:HB3	2.46	0.56
1:A:892:VAL:HG12	1:A:893:VAL:H	1.70	0.55
5:A:1911:3PE:H2H2	5:A:1911:3PE:H3B2	1.88	0.55
1:A:1068:PHE:HB3	1:A:1381:MET:HG3	1.88	0.55
1:A:1112:TRP:O	1:A:1116:THR:HG22	2.05	0.55
3:F:134:ASP:HB2	3:F:137:LYS:HZ2	1.70	0.55
3:F:844:CYS:HB2	3:F:866:ASN:ND2	2.22	0.55
1:A:656:PHE:CE2	1:A:1054:PHE:HB3	2.41	0.55
1:A:1103:PRO:HG2	1:A:1109:TYR:HD1	1.70	0.55
1:A:1113:TYR:O	1:A:1117:SER:OG	2.23	0.55
1:A:532:LEU:HD23	1:A:535:LEU:CD1	2.37	0.55
5:A:1908:3PE:HN1	5:A:1908:3PE:P	2.29	0.55
2:E:1:MET:HB3	2:E:5:GLU:HG2	1.89	0.54
3:F:652:LYS:O	3:F:655:ASN:ND2	2.40	0.54
1:A:633:PRO:CB	5:A:1906:3PE:O22	2.55	0.54
1:A:636:LEU:HD21	5:A:1905:3PE:H342	1.88	0.54
2:E:32:TRP:HB3	2:E:181:SER:CB	2.36	0.54
3:F:75:ALA:HB1	3:F:610:THR:HG21	1.89	0.54
3:F:829:THR:HG21	3:F:846:ARG:HD3	1.89	0.54
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.89	0.54
3:F:75:ALA:O	3:F:79:VAL:HG23	2.07	0.54
3:F:76:ARG:NH2	3:F:611:TRP:O	2.32	0.54
3:F:987:ASP:OD1	3:F:987:ASP:N	2.39	0.54
2:E:57:CYS:HB2	2:E:80:CYS:HA	1.88	0.54
2:E:30:ASP:OD2	2:E:30:ASP:N	2.41	0.53
2:E:20:ILE:HG23	2:E:118:LEU:HD21	1.89	0.53
1:A:601:PRO:HB3	5:A:1908:3PE:O22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:644:GLN:HE21	3:F:709:LEU:HD12	1.72	0.53
1:A:173:LEU:O	1:A:176:VAL:HG13	2.08	0.53
1:A:277:ASN:HD22	5:A:1903:3PE:C3	2.22	0.53
1:A:1105:ASN:O	1:A:1108:GLN:N	2.41	0.53
3:F:470:ASN:HD21	3:F:482:LYS:HZ2	1.56	0.53
1:A:900:ARG:O	1:A:903:ARG:NH1	2.41	0.53
1:A:928:ILE:HD11	5:A:1904:3PE:H2I1	1.90	0.53
1:A:1103:PRO:HG3	1:A:1112:TRP:CG	2.44	0.53
1:A:973:TYR:HE1	3:F:235:ILE:HG21	1.73	0.53
1:A:1148:HIS:O	1:A:1152:ILE:HG12	2.09	0.53
3:F:538:ILE:HG13	3:F:1042:ASP:HB3	1.91	0.53
3:F:64:TYR:O	3:F:66:ASP:N	2.41	0.52
3:F:476:GLU:HG3	3:F:478:LYS:HB2	1.90	0.52
1:A:599:ASN:HD22	1:A:601:PRO:HD2	1.75	0.52
1:A:1413:ALA:O	1:A:1415:GLY:N	2.41	0.52
2:E:53:LEU:HD23	2:E:53:LEU:H	1.74	0.52
2:E:138:ARG:O	2:E:141:SER:OG	2.27	0.52
1:A:552:LEU:HD21	1:A:1059:ILE:HD13	1.92	0.52
1:A:667:ALA:HA	1:A:670:LEU:HB2	1.91	0.52
2:E:16:ILE:O	2:E:20:ILE:HG13	2.10	0.52
5:A:1908:3PE:N	5:A:1908:3PE:P	2.81	0.52
3:F:664:LEU:H	3:F:679:ASN:HD21	1.55	0.52
1:A:1111:VAL:O	1:A:1115:VAL:HG23	2.09	0.52
5:A:1911:3PE:H3I3	5:A:1911:3PE:C3E	2.39	0.52
3:F:164:GLN:O	3:F:196:LYS:NZ	2.38	0.52
3:F:235:ILE:HB	3:F:551:GLN:HE21	1.73	0.52
3:F:853:CYS:SG	3:F:1020:MET:HG3	2.50	0.52
1:A:307:ASN:HD21	5:A:1911:3PE:C1	2.19	0.52
3:F:114:ARG:HH11	3:F:114:ARG:HB2	1.75	0.52
3:F:657:GLU:HA	3:F:749:LYS:HD3	1.91	0.52
1:A:1005:MET:SD	1:A:1362:ILE:HD11	2.50	0.51
3:F:723:TRP:CE3	3:F:747:TYR:HB2	2.45	0.51
3:F:430:ASP:OD1	3:F:430:ASP:N	2.42	0.51
3:F:707:ARG:HH21	3:F:740:ASP:HB3	1.75	0.51
1:A:1349:GLU:HG2	1:A:1350:TYR:CD1	2.45	0.51
3:F:1014:THR:OG1	3:F:1015:ASN:N	2.44	0.51
1:A:1088:CYS:SG	1:A:1394:LEU:HD23	2.51	0.51
1:A:841:SER:O	1:A:845:VAL:HG23	2.10	0.51
7:A:1912:POV:C31	7:A:1912:POV:H25A	2.40	0.51
3:F:1026:THR:OG1	3:F:1027:CYS:N	2.43	0.51
1:A:92:PHE:O	1:A:96:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:LEU:O	1:A:918:VAL:HG23	2.11	0.51
1:A:1115:VAL:HG11	1:A:1168:LYS:HG2	1.94	0.50
3:F:736:PHE:CZ	3:F:816:GLY:HA3	2.46	0.50
3:F:888:HIS:O	3:F:892:ILE:HG13	2.11	0.50
1:A:180:PRO:HA	1:A:183:GLN:HG3	1.93	0.50
1:A:1367:LEU:HG	5:A:1904:3PE:H2C2	1.93	0.50
3:F:336:LYS:HE3	3:F:369:GLU:OE1	2.11	0.50
3:F:988:ASN:OD1	3:F:990:SER:N	2.42	0.50
1:A:237:VAL:HG12	1:A:238:GLU:H	1.76	0.50
5:A:1904:3PE:H221	5:A:1904:3PE:O31	2.12	0.50
3:F:447:GLN:O	3:F:464:GLY:HA2	2.10	0.50
1:A:820:ASP:HB2	1:A:828:ARG:NH2	2.27	0.50
1:A:938:LEU:HD21	1:A:1051:LEU:HD12	1.92	0.50
1:A:122:TRP:NE1	1:A:183:GLN:OE1	2.44	0.50
1:A:1129:MET:HE1	5:A:1903:3PE:C2F	2.42	0.50
1:A:112:PHE:CE2	1:A:115:ASP:HB2	2.47	0.50
1:A:633:PRO:HB2	5:A:1906:3PE:O22	2.12	0.50
1:A:950:PHE:HE1	1:A:1041:MET:HG2	1.76	0.50
3:F:670:CYS:HB2	3:F:673:LEU:HD23	1.93	0.50
1:A:182:LEU:HD21	1:A:564:LEU:HD23	1.93	0.49
5:A:1903:3PE:H322	5:A:1903:3PE:C22	2.32	0.49
3:F:1008:VAL:HG12	3:F:1019:ILE:HG23	1.93	0.49
1:A:56:ILE:O	1:A:60:THR:HG23	2.11	0.49
1:A:245:CYS:SG	1:A:246:ALA:N	2.85	0.49
1:A:483:MET:O	1:A:487:GLY:N	2.45	0.49
1:A:642:ILE:HD13	5:A:1905:3PE:H272	1.93	0.49
1:A:1299:GLN:HG3	1:A:1327:GLU:HB3	1.94	0.49
1:A:337:PHE:HE2	1:A:657:LEU:HB3	1.77	0.49
5:A:1903:3PE:H222	5:A:1903:3PE:C32	2.32	0.49
6:A:1909:PC1:P	6:A:1909:PC1:C13	2.98	0.49
1:A:631:SER:O	1:A:635:VAL:HG22	2.12	0.49
1:A:1409:TYR:HE2	1:A:1425:LEU:HB3	1.77	0.49
3:F:37:VAL:HG21	3:F:1009:GLU:HG2	1.95	0.49
3:F:56:GLN:O	3:F:60:ILE:HG23	2.13	0.49
3:F:882:ASP:OD1	3:F:885:LEU:HB3	2.13	0.49
2:E:35:LEU:HD23	2:E:51:PHE:HZ	1.78	0.49
3:F:234:LYS:HA	3:F:551:GLN:HG3	1.94	0.49
3:F:729:ILE:HB	3:F:732:VAL:HB	1.95	0.49
3:F:627:PRO:O	3:F:630:SER:HB3	2.12	0.49
1:A:1105:ASN:O	1:A:1107:TYR:N	2.46	0.49
1:A:1188:LEU:HB2	2:E:142:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1906:3PE:HN1	5:A:1906:3PE:P	2.33	0.49
1:A:481:LEU:HD23	1:A:482:LYS:HD3	1.94	0.49
1:A:1359:TYR:O	1:A:1363:SER:OG	2.27	0.49
3:F:730:LYS:HG3	3:F:731:GLY:H	1.78	0.49
1:A:78:ASP:OD1	1:A:79:ASN:N	2.45	0.49
2:E:23:ALA:O	2:E:27:VAL:HG23	2.12	0.49
1:A:543:THR:HA	1:A:546:SER:HB3	1.95	0.48
1:A:1023:ALA:O	1:A:1026:SER:OG	2.26	0.48
2:E:29:SER:HG	2:E:31:HIS:CE1	2.32	0.48
2:E:135:TYR:CE2	2:E:136:LEU:HD13	2.49	0.48
3:F:597:GLN:HB3	3:F:765:SER:HB2	1.95	0.48
1:A:343:LYS:NZ	1:A:343:LYS:HB3	2.28	0.48
3:F:452:TYR:OH	3:F:463:THR:OG1	2.10	0.48
1:A:663:ASN:OD1	1:A:663:ASN:N	2.47	0.48
1:A:1005:MET:O	1:A:1009:THR:HG23	2.13	0.48
1:A:1298:THR:HG22	1:A:1299:GLN:H	1.77	0.48
2:E:27:VAL:O	2:E:54:TRP:NE1	2.46	0.48
1:A:928:ILE:CD1	5:A:1904:3PE:H2I1	2.44	0.48
1:A:1147:ASN:H	1:A:1147:ASN:ND2	2.12	0.48
1:A:1164:GLU:O	1:A:1168:LYS:HG3	2.13	0.48
1:A:974:VAL:HG22	1:A:984:GLU:HG2	1.96	0.48
1:A:446:THR:HG22	1:A:535:LEU:HD23	1.96	0.48
5:A:1903:3PE:H3I3	5:A:1903:3PE:H3F1	1.58	0.48
3:F:93:ARG:NH2	3:F:202:ASP:OD1	2.47	0.48
2:E:22:LEU:HB2	2:E:188:ALA:HB2	1.96	0.48
2:E:55:ARG:HD3	2:E:80:CYS:C	2.34	0.48
3:F:851:MET:HB2	3:F:1021:VAL:O	2.14	0.48
1:A:64:ASN:O	1:A:64:ASN:ND2	2.35	0.47
2:E:35:LEU:HB2	2:E:174:ILE:HD11	1.95	0.47
3:F:672:ASP:HB2	3:F:689:PHE:HE1	1.78	0.47
1:A:539:THR:HG22	1:A:545:LEU:HD21	1.96	0.47
3:F:88:LYS:HB2	3:F:88:LYS:HE3	1.49	0.47
1:A:181:SER:O	1:A:184:VAL:HG22	2.13	0.47
1:A:122:TRP:HB3	1:A:177:SER:HB2	1.97	0.47
1:A:161:VAL:HG22	1:A:162:LYS:HE2	1.94	0.47
1:A:559:ILE:HG12	1:A:559:ILE:O	2.15	0.47
1:A:1418:LYS:N	1:A:1418:LYS:HD2	2.29	0.47
3:F:130:LYS:HB3	3:F:225:TRP:HB3	1.96	0.47
3:F:398:ARG:O	3:F:402:GLN:HG3	2.14	0.47
3:F:889:LEU:HD22	3:F:894:VAL:HG11	1.95	0.47
1:A:162:LYS:HD2	1:A:165:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TRP:HE1	1:A:1321:THR:HG21	1.80	0.47
1:A:636:LEU:O	1:A:639:ILE:HG23	2.15	0.47
1:A:959:ASP:HB3	1:A:972:TYR:CE2	2.49	0.47
2:E:130:ARG:HB2	2:E:131:LYS:NZ	2.30	0.47
3:F:454:ASP:HB3	3:F:458:LEU:H	1.80	0.47
3:F:821:VAL:O	3:F:825:ILE:HG13	2.14	0.47
1:A:90:GLU:O	1:A:94:LEU:HB2	2.15	0.47
1:A:472:LEU:HD21	1:A:508:ILE:HG12	1.96	0.47
3:F:517:ILE:HG23	3:F:518:ASP:O	2.15	0.47
5:A:1904:3PE:H381	8:A:1913:6UB:CAB	2.45	0.47
1:A:1251:GLU:O	1:A:1255:THR:HG22	2.15	0.47
3:F:542:ASN:ND2	3:F:545:LYS:HG3	2.30	0.47
1:A:186:LEU:HD13	1:A:565:LEU:HD11	1.97	0.47
1:A:1175:ARG:HG3	2:E:135:TYR:CE1	2.50	0.47
1:A:1366:MET:HB3	5:A:1904:3PE:H2D2	1.96	0.47
3:F:580:MET:HB3	3:F:611:TRP:CD1	2.50	0.47
3:F:628:THR:O	3:F:629:TYR:CD2	2.68	0.47
3:F:1030:ASP:OD1	3:F:1031:THR:N	2.48	0.46
3:F:107:VAL:HG11	3:F:190:ALA:HB3	1.98	0.46
3:F:979:THR:HG22	3:F:1040:THR:HA	1.95	0.46
1:A:294:TRP:NE1	1:A:1321:THR:HG21	2.30	0.46
1:A:935:THR:HG21	1:A:1056:MET:HG2	1.91	0.46
3:F:470:ASN:HD21	3:F:482:LYS:HZ1	1.62	0.46
1:A:165:ARG:HH11	1:A:168:ARG:HH21	1.63	0.46
1:A:870:ILE:O	1:A:873:LEU:HB3	2.16	0.46
3:F:138:ASN:N	3:F:138:ASN:OD1	2.48	0.46
3:F:473:GLY:HA3	3:F:478:LYS:HB3	1.97	0.46
1:A:642:ILE:HG21	5:A:1905:3PE:H3C2	1.98	0.46
1:A:928:ILE:HD11	5:A:1904:3PE:C2I	2.46	0.46
5:A:1910:3PE:H232	5:A:1910:3PE:H261	1.60	0.46
3:F:231:THR:CB	3:F:232:PRO:CD	2.88	0.46
1:A:476:THR:OG1	1:A:504:VAL:HG13	2.15	0.46
1:A:1115:VAL:CG1	1:A:1168:LYS:HG2	2.45	0.46
1:A:506:SER:HB2	1:A:530:ILE:HD13	1.97	0.46
2:E:130:ARG:HB2	2:E:131:LYS:HZ2	1.81	0.46
1:A:906:ARG:HD2	1:A:906:ARG:HA	1.71	0.46
1:A:1310:PRO:HB3	5:A:1911:3PE:H322	1.97	0.46
1:A:1406:TRP:HZ2	1:A:1415:GLY:O	1.99	0.46
2:E:156:GLU:HA	2:E:156:GLU:OE1	2.15	0.46
1:A:45:ILE:HG13	1:A:107:ALA:HB2	1.96	0.46
6:A:1909:PC1:H3F2	6:A:1909:PC1:H3I3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:802:GLU:OE1	3:F:809:LEU:HD11	2.16	0.46
3:F:134:ASP:O	3:F:137:LYS:HG2	2.16	0.46
1:A:226:CYS:HA	1:A:260:GLU:O	2.16	0.45
1:A:308:GLU:O	1:A:311:TRP:NE1	2.49	0.45
1:A:1040:GLU:HG3	5:A:1910:3PE:O12	2.16	0.45
1:A:1311:GLN:OE1	5:A:1911:3PE:H11	2.16	0.45
3:F:598:ASP:O	3:F:600:ARG:N	2.47	0.45
3:F:617:THR:HG22	3:F:618:ASP:H	1.81	0.45
1:A:1129:MET:HE1	5:A:1903:3PE:H2F1	1.96	0.45
3:F:134:ASP:HB2	3:F:137:LYS:NZ	2.30	0.45
3:F:466:LEU:HD12	3:F:467:PRO:HD2	1.97	0.45
3:F:509:CYS:SG	3:F:511:ASN:HB2	2.57	0.45
2:E:115:LEU:O	2:E:119:ILE:HG12	2.16	0.45
3:F:630:SER:O	3:F:630:SER:OG	2.26	0.45
3:F:243:ARG:HH21	3:F:556:GLN:HE21	1.64	0.45
1:A:489:ARG:CZ	1:A:489:ARG:HA	2.46	0.45
2:E:181:SER:HA	2:E:184:CYS:SG	2.56	0.45
3:F:908:GLU:HG2	3:F:974:LYS:HD3	1.97	0.45
1:A:70:VAL:CG1	5:A:1907:3PE:H11	2.44	0.45
1:A:140:GLU:OE2	1:A:161:VAL:HG21	2.17	0.45
1:A:931:ILE:HD12	1:A:934:VAL:HG13	1.99	0.45
1:A:1142:GLN:NE2	1:A:1147:ASN:OD1	2.45	0.45
3:F:275:ARG:NH2	3:F:327:ILE:O	2.48	0.45
3:F:370:ARG:HG3	3:F:372:GLN:HG3	1.98	0.45
1:A:538:ILE:HD12	1:A:538:ILE:H	1.81	0.45
1:A:1275:VAL:HG22	5:A:1911:3PE:H2I1	1.94	0.45
1:A:499:PHE:O	1:A:502:PHE:HB3	2.17	0.45
1:A:939:GLN:NE2	1:A:1048:TYR:OH	2.50	0.45
5:A:1903:3PE:H3C2	5:A:1905:3PE:H3C1	1.98	0.45
6:A:1909:PC1:H152	6:A:1909:PC1:H111	1.59	0.45
1:A:44:CYS:O	1:A:47:ILE:HG12	2.17	0.45
1:A:959:ASP:HB3	1:A:972:TYR:CD2	2.52	0.45
3:F:479:THR:O	3:F:481:LEU:HD23	2.17	0.45
3:F:672:ASP:OD1	3:F:672:ASP:N	2.50	0.45
5:A:1903:3PE:O32	5:A:1903:3PE:H341	2.17	0.45
3:F:715:THR:HB	3:F:745:ARG:HH21	1.81	0.45
1:A:199:ILE:O	1:A:203:VAL:HG23	2.17	0.44
1:A:923:VAL:HG13	1:A:926:ARG:HH12	1.83	0.44
3:F:409:LYS:HB3	3:F:409:LYS:HE2	1.78	0.44
3:F:867:HIS:HB3	3:F:869:ASP:OD1	2.17	0.44
1:A:204:LEU:HD13	5:A:1903:3PE:H3F2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ILE:O	1:A:898:VAL:HG12	2.17	0.44
1:A:520:THR:HA	1:A:521:PRO:HD3	1.70	0.44
2:E:55:ARG:HD3	2:E:81:SER:CA	2.47	0.44
1:A:633:PRO:HB3	5:A:1906:3PE:O22	2.17	0.44
1:A:66:VAL:O	1:A:70:VAL:HG22	2.17	0.44
1:A:519:MET:HG2	1:A:520:THR:H	1.82	0.44
3:F:76:ARG:O	3:F:76:ARG:HG3	2.18	0.44
1:A:176:VAL:HA	1:A:182:LEU:HD12	1.99	0.44
1:A:210:TYR:O	1:A:313:TYR:OH	2.33	0.44
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.68	0.44
1:A:1129:MET:CE	5:A:1903:3PE:H2F2	2.47	0.44
5:A:1907:3PE:O22	5:A:1907:3PE:H12	2.18	0.44
5:A:1911:3PE:H3E2	5:A:1911:3PE:H3H1	1.65	0.44
7:A:1912:POV:H14B	7:A:1912:POV:H11A	1.54	0.44
1:A:291:MET:HE3	1:A:1321:THR:HG23	2.00	0.44
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.88	0.44
1:A:914:LEU:HD23	1:A:914:LEU:HA	1.83	0.44
3:F:234:LYS:HA	3:F:551:GLN:CG	2.48	0.44
5:A:1911:3PE:H3A1	5:A:1911:3PE:C2H	2.23	0.44
1:A:252:ARG:HG2	1:A:303:ASP:HB3	2.00	0.43
1:A:529:CYS:HA	1:A:532:LEU:CD1	2.38	0.43
5:A:1904:3PE:H2F1	5:A:1904:3PE:H2I2	1.80	0.43
5:A:1911:3PE:H12	5:A:1911:3PE:H111	2.00	0.43
3:F:298:SER:HA	3:F:334:ASP:HB2	2.00	0.43
1:A:45:ILE:H	1:A:45:ILE:HG12	1.64	0.43
3:F:830:LYS:HE3	3:F:830:LYS:HB3	1.66	0.43
3:F:867:HIS:C	3:F:869:ASP:H	2.21	0.43
1:A:193:MET:HG3	1:A:650:TYR:CZ	2.53	0.43
1:A:847:ILE:HA	1:A:850:LYS:HB2	2.00	0.43
3:F:773:ASN:OD1	3:F:773:ASN:N	2.51	0.43
3:F:857:ASP:OD1	3:F:857:ASP:N	2.51	0.43
3:F:130:LYS:HE3	3:F:169:HIS:CD2	2.54	0.43
3:F:225:TRP:HD1	3:F:227:ASP:O	2.02	0.43
3:F:862:LEU:HD22	3:F:881:ILE:HD12	2.01	0.43
1:A:94:LEU:HA	1:A:94:LEU:HD22	1.70	0.43
1:A:224:LYS:HD3	1:A:247:ARG:HH21	1.84	0.43
1:A:442:VAL:O	1:A:446:THR:HG23	2.18	0.43
1:A:548:LEU:O	1:A:552:LEU:HG	2.19	0.43
3:F:243:ARG:NH2	3:F:556:GLN:HG3	2.33	0.43
1:A:435:TYR:CE1	1:A:541:TYR:HE1	2.36	0.43
5:A:1911:3PE:H2D1	5:A:1911:3PE:H2A2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:543:LEU:HD23	3:F:543:LEU:HA	1.80	0.43
1:A:193:MET:HG3	1:A:650:TYR:OH	2.19	0.43
1:A:433:VAL:HG23	1:A:434:PHE:H	1.83	0.43
2:E:20:ILE:HG12	2:E:118:LEU:HD11	2.00	0.43
1:A:61:ILE:HD11	1:A:174:ARG:HD3	2.00	0.43
1:A:1291:LYS:HD3	1:A:1342:SER:HB2	2.01	0.43
1:A:295:THR:OG1	1:A:1323:GLU:HG2	2.18	0.43
1:A:802:THR:O	1:A:805:ILE:HG22	2.19	0.43
2:E:29:SER:OG	2:E:31:HIS:ND1	2.50	0.43
1:A:65:CYS:SG	5:A:1907:3PE:H282	2.59	0.43
3:F:64:TYR:C	3:F:66:ASP:H	2.22	0.43
3:F:232:PRO:HB2	3:F:233:ASN:H	1.52	0.43
3:F:243:ARG:HD2	3:F:243:ARG:HA	1.82	0.43
1:A:277:ASN:ND2	5:A:1903:3PE:H32	2.28	0.42
3:F:242:ARG:NH1	3:F:426:GLN:HB3	2.33	0.42
3:F:263:SER:O	3:F:266:VAL:HG22	2.18	0.42
3:F:365:ASP:OD1	3:F:366:GLY:N	2.48	0.42
3:F:409:LYS:HG2	3:F:1071:TYR:CD2	2.54	0.42
3:F:472:THR:H	3:F:483:ASN:HD21	1.67	0.42
1:A:1365:TYR:OH	7:A:1912:POV:C14	2.67	0.42
3:F:206:LEU:HD13	3:F:458:LEU:HD21	2.00	0.42
1:A:112:PHE:CZ	1:A:115:ASP:HB2	2.54	0.42
5:A:1905:3PE:C2A	7:A:1912:POV:C311	2.98	0.42
1:A:1131:ASN:O	1:A:1131:ASN:ND2	2.53	0.42
3:F:887:ARG:NH2	3:F:1032:ARG:HG3	2.35	0.42
1:A:1091:TYR:CG	1:A:1399:LEU:HD12	2.54	0.42
3:F:845:LYS:O	3:F:848:SER:OG	2.25	0.42
1:A:1161:PHE:O	1:A:1164:GLU:HG3	2.19	0.42
3:F:480:ASN:HA	3:F:483:ASN:HB2	2.02	0.42
1:A:53:PHE:O	1:A:53:PHE:CG	2.72	0.42
1:A:632:TYR:CE1	5:A:1905:3PE:H322	2.55	0.42
1:A:1416:ARG:NH1	1:A:1417:ILE:O	2.52	0.42
2:E:154:SER:O	2:E:155:LEU:C	2.57	0.42
1:A:237:VAL:HG22	1:A:256:ILE:HD11	2.01	0.42
1:A:1406:TRP:CZ3	1:A:1417:ILE:HD11	2.55	0.42
3:F:655:ASN:H	3:F:655:ASN:HD22	1.67	0.42
3:F:665:ALA:HA	3:F:666:PRO:HD3	1.85	0.42
1:A:127:PHE:HA	1:A:130:VAL:HG22	2.01	0.42
1:A:647:CYS:SG	5:A:1905:3PE:H3H1	2.60	0.42
1:A:893:VAL:HG23	1:A:894:LYS:H	1.84	0.42
1:A:900:ARG:HB2	1:A:903:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:ALA:O	1:A:1327:GLU:N	2.45	0.42
1:A:1370:PHE:HB2	5:A:1904:3PE:H2H2	2.01	0.42
3:F:723:TRP:CH2	3:F:737:VAL:HG23	2.55	0.42
3:F:862:LEU:HD22	3:F:881:ILE:CD1	2.50	0.42
1:A:174:ARG:HE	1:A:174:ARG:HB3	1.66	0.42
3:F:390:SER:HB2	3:F:401:ILE:HD11	2.02	0.42
1:A:1105:ASN:HB3	1:A:1108:GLN:HB3	2.02	0.41
1:A:520:THR:O	1:A:520:THR:HG23	2.19	0.41
1:A:1100:CYS:HB3	1:A:1411:PRO:HB3	2.01	0.41
3:F:58:VAL:HG22	3:F:801:VAL:HG13	2.02	0.41
1:A:172:PRO:O	1:A:175:LEU:HB2	2.20	0.41
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.86	0.41
1:A:636:LEU:CD2	5:A:1905:3PE:H342	2.50	0.41
3:F:29:SER:OG	3:F:30:ALA:N	2.53	0.41
3:F:169:HIS:CE1	3:F:238:TYR:HD1	2.37	0.41
2:E:12:THR:O	2:E:16:ILE:HG23	2.21	0.41
3:F:109:ALA:HA	3:F:472:THR:HG22	2.02	0.41
3:F:865:ALA:HB3	3:F:871:THR:OG1	2.20	0.41
1:A:1412:GLU:HG3	1:A:1414:LYS:NZ	2.36	0.41
3:F:228:ASN:N	3:F:228:ASN:OD1	2.52	0.41
1:A:212:ILE:O	1:A:216:GLU:HG3	2.21	0.41
1:A:224:LYS:HZ3	1:A:224:LYS:HG3	1.78	0.41
1:A:653:LEU:O	1:A:657:LEU:HB2	2.20	0.41
5:A:1911:3PE:C1	5:A:1911:3PE:C11	2.99	0.41
1:A:1410:ASP:HB2	1:A:1417:ILE:CG2	2.51	0.41
2:E:32:TRP:CH2	2:E:53:LEU:HD22	2.56	0.41
3:F:871:THR:HG23	3:F:874:ILE:HD11	2.03	0.41
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.77	0.41
1:A:1397:HIS:O	1:A:1401:GLU:HG2	2.21	0.41
3:F:562:ASP:OD1	3:F:563:PHE:N	2.53	0.41
3:F:873:GLN:H	3:F:873:GLN:HG2	1.64	0.41
3:F:909:PRO:HG3	3:F:975:GLN:HE21	1.85	0.41
1:A:532:LEU:HD21	1:A:944:CYS:HB2	2.03	0.41
1:A:1103:PRO:HB2	1:A:1108:GLN:HG2	2.03	0.41
1:A:1276:MET:HE2	1:A:1276:MET:HB3	1.83	0.41
3:F:151:PHE:CZ	3:F:224:PRO:HD3	2.56	0.41
1:A:642:ILE:CD1	5:A:1905:3PE:H272	2.51	0.41
1:A:931:ILE:HD12	1:A:934:VAL:CG1	2.50	0.41
1:A:1146:MET:O	1:A:1149:ILE:HG13	2.21	0.41
3:F:271:LEU:HD11	3:F:327:ILE:HG22	2.03	0.41
3:F:852:ASP:OD1	3:F:852:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:HD2	1:A:482:LYS:HA	1.80	0.40
1:A:539:THR:HA	1:A:545:LEU:HG	2.04	0.40
1:A:552:LEU:O	1:A:555:SER:OG	2.35	0.40
7:A:1912:POV:H23	7:A:1912:POV:H26	1.56	0.40
1:A:1170:LEU:HD23	1:A:1170:LEU:HA	1.76	0.40
5:A:1906:3PE:N	5:A:1906:3PE:P	2.91	0.40
2:E:60:ARG:HA	2:E:60:ARG:HD3	1.43	0.40
3:F:149:PRO:HB3	3:F:165:HIS:CE1	2.56	0.40
3:F:785:LYS:HD3	3:F:785:LYS:HA	1.80	0.40
3:F:1048:ASP:N	3:F:1048:ASP:OD1	2.52	0.40
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	2.04	0.40
3:F:155:ALA:O	3:F:156:ASN:HB2	2.21	0.40
1:A:499:PHE:HE2	1:A:537:LYS:HD3	1.86	0.40
1:A:943:ALA:O	1:A:947:VAL:HG23	2.22	0.40
1:A:1120:PHE:HA	1:A:1123:LEU:HD23	2.04	0.40
1:A:1329:LEU:HD12	1:A:1329:LEU:O	2.21	0.40
3:F:466:LEU:HD12	3:F:466:LEU:HA	1.85	0.40
3:F:667:ARG:NH1	3:F:741:GLY:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1100/1873 (59%)	1010 (92%)	86 (8%)	4 (0%)	30	60
2	E	159/222 (72%)	142 (89%)	16 (10%)	1 (1%)	22	52
3	F	968/1105 (88%)	886 (92%)	81 (8%)	1 (0%)	48	77
All	All	2227/3200 (70%)	2038 (92%)	183 (8%)	6 (0%)	38	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	232	PRO
1	A	520	THR
1	A	521	PRO
2	E	205	PRO
1	A	1106	PRO
1	A	1414	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	983/1628 (60%)	852 (87%)	131 (13%)	3	10
2	E	143/192 (74%)	114 (80%)	29 (20%)	1	3
3	F	868/973 (89%)	800 (92%)	68 (8%)	10	31
All	All	1994/2793 (71%)	1766 (89%)	228 (11%)	7	15

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	64	ASN
1	A	80	ASN
1	A	94	LEU
1	A	100	GLU
1	A	110	PHE
1	A	117	TYR
1	A	124	VAL
1	A	134	VAL
1	A	164	LEU
1	A	175	LEU
1	A	176	VAL
1	A	226	CYS
1	A	247	ARG
1	A	250	SER
1	A	281	SER
1	A	289	ILE

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Mol	Chain	Res	Type
1	A	307	ASN
1	A	319	LEU
1	A	320	LEU
1	A	325	ILE
1	A	333	LEU
1	A	347	ARG
1	A	433	VAL
1	A	435	TYR
1	A	437	LEU
1	A	441	ILE
1	A	442	VAL
1	A	444	LEU
1	A	451	SER
1	A	458	LEU
1	A	460	LEU
1	A	477	ILE
1	A	481	LEU
1	A	483	MET
1	A	489	ARG
1	A	490	GLN
1	A	494	SER
1	A	495	ILE
1	A	497	ASN
1	A	499	PHE
1	A	512	LEU
1	A	522	LEU
1	A	524	ILE
1	A	527	LEU
1	A	528	ARG
1	A	532	LEU
1	A	536	PHE
1	A	540	LYS
1	A	541	TYR
1	A	546	SER
1	A	547	ASN
1	A	554	ASN
1	A	555	SER
1	A	589	ASP
1	A	599	ASN
1	A	604	LEU
1	A	639	ILE
1	A	654	ASN

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Mol	Chain	Res	Type
1	A	663	ASN
1	A	666	GLU
1	A	669	SER
1	A	670	LEU
1	A	800	TRP
1	A	808	PHE
1	A	816	LEU
1	A	822	ILE
1	A	826	SER
1	A	830	GLN
1	A	835	PHE
1	A	869	ASN
1	A	871	LEU
1	A	880	LEU
1	A	898	VAL
1	A	912	LYS
1	A	914	LEU
1	A	920	CYS
1	A	926	ARG
1	A	927	THR
1	A	928	ILE
1	A	934	VAL
1	A	936	THR
1	A	937	LEU
1	A	938	LEU
1	A	939	GLN
1	A	956	SER
1	A	961	SER
1	A	962	LYS
1	A	983	MET
1	A	985	LEU
1	A	992	HIS
1	A	999	ASN
1	A	1022	ARG
1	A	1041	MET
1	A	1051	LEU
1	A	1056	MET
1	A	1063	PHE
1	A	1067	THR
1	A	1071	GLN
1	A	1091	TYR
1	A	1104	LYS

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Mol	Chain	Res	Type
1	A	1105	ASN
1	A	1117	SER
1	A	1123	LEU
1	A	1130	LEU
1	A	1141	HIS
1	A	1145	GLU
1	A	1147	ASN
1	A	1148	HIS
1	A	1153	LEU
1	A	1163	LEU
1	A	1164	GLU
1	A	1165	MET
1	A	1188	LEU
1	A	1196	ASP
1	A	1200	SER
1	A	1204	THR
1	A	1234	PHE
1	A	1246	LEU
1	A	1249	ARG
1	A	1262	LYS
1	A	1267	LEU
1	A	1308	THR
1	A	1339	ASP
1	A	1354	THR
1	A	1363	SER
1	A	1384	PHE
1	A	1392	SER
1	A	1408	GLU
1	A	1418	LYS
1	A	1426	LEU
2	E	13	LEU
2	E	30	ASP
2	E	32	TRP
2	E	46	CYS
2	E	47	GLU
2	E	57	CYS
2	E	58	THR
2	E	59	LYS
2	E	60	ARG
2	E	78	LYS
2	E	79	ASN
2	E	81	SER

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Mol	Chain	Res	Type
2	E	82	TYR
2	E	104	SER
2	E	114	SER
2	E	118	LEU
2	E	120	MET
2	E	122	THR
2	E	124	CYS
2	E	134	ASP
2	E	154	SER
2	E	157	VAL
2	E	158	MET
2	E	163	LYS
2	E	164	ARG
2	E	178	TYR
2	E	189	PHE
2	E	216	MET
2	E	217	ASP
3	F	61	TYR
3	F	76	ARG
3	F	116	ASP
3	F	119	SER
3	F	134	ASP
3	F	138	ASN
3	F	141	GLU
3	F	158	ARG
3	F	188	THR
3	F	199	ARG
3	F	205	LEU
3	F	212	SER
3	F	228	ASN
3	F	229	SER
3	F	233	ASN
3	F	234	LYS
3	F	236	ASP
3	F	240	VAL
3	F	241	ARG
3	F	269	LEU
3	F	270	THR
3	F	286	SER
3	F	295	SER
3	F	303	VAL
3	F	306	PHE

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Mol	Chain	Res	Type
3	F	326	ASN
3	F	348	ASN
3	F	393	GLN
3	F	430	ASP
3	F	475	PHE
3	F	481	LEU
3	F	482	LYS
3	F	505	ARG
3	F	508	LEU
3	F	517	ILE
3	F	518	ASP
3	F	523	VAL
3	F	547	ARG
3	F	551	GLN
3	F	592	THR
3	F	610	THR
3	F	617	THR
3	F	628	THR
3	F	648	SER
3	F	651	LEU
3	F	655	ASN
3	F	658	GLU
3	F	672	ASP
3	F	673	LEU
3	F	674	LYS
3	F	680	THR
3	F	699	SER
3	F	739	THR
3	F	767	TYR
3	F	773	ASN
3	F	802	GLU
3	F	810	LEU
3	F	817	ILE
3	F	876	ARG
3	F	893	SER
3	F	905	SER
3	F	994	SER
3	F	1014	THR
3	F	1031	THR
3	F	1040	THR
3	F	1057	LYS
3	F	1070	ASP

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Mol	Chain	Res	Type
3	F	1071	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	183	GLN
1	A	239	ASN
1	A	277	ASN
1	A	307	ASN
1	A	455	ASN
1	A	599	ASN
1	A	803	ASN
1	A	939	GLN
1	A	999	ASN
1	A	1037	ASN
1	A	1105	ASN
1	A	1131	ASN
1	A	1138	GLN
1	A	1383	ASN
1	A	1419	HIS
2	E	38	HIS
3	F	145	GLN
3	F	165	HIS
3	F	169	HIS
3	F	450	ASN
3	F	470	ASN
3	F	511	ASN
3	F	551	GLN
3	F	552	ASN
3	F	556	GLN
3	F	644	GLN
3	F	655	ASN
3	F	679	ASN
3	F	685	ASN
3	F	696	ASN
3	F	806	GLN
3	F	847	ASN
3	F	866	ASN
3	F	975	GLN
3	F	1007	HIS
3	F	1039	GLN

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	1908	-	20,20,50	1.04	1 (5%)	22,23,55	0.98	1 (4%)
5	3PE	A	1910	-	31,31,50	1.16	2 (6%)	34,36,55	1.18	3 (8%)
8	6UB	A	1913	-	28,29,29	4.28	11 (39%)	38,39,39	2.28	12 (31%)
5	3PE	A	1904	-	50,50,50	0.92	2 (4%)	53,55,55	1.08	3 (5%)
5	3PE	A	1906	-	43,43,50	0.99	2 (4%)	46,48,55	1.08	3 (6%)
5	3PE	A	1903	-	50,50,50	0.93	2 (4%)	53,55,55	1.05	3 (5%)
5	3PE	A	1905	-	42,42,50	1.00	2 (4%)	45,47,55	1.11	4 (8%)
5	3PE	A	1911	-	50,50,50	0.90	2 (4%)	53,55,55	1.06	3 (5%)
7	POV	A	1912	-	46,46,51	1.00	2 (4%)	52,54,59	1.10	4 (7%)
5	3PE	A	1907	-	37,37,50	1.06	2 (5%)	40,42,55	1.14	3 (7%)
5	3PE	A	1902	-	32,32,50	1.15	2 (6%)	35,37,55	1.25	3 (8%)
6	PC1	A	1909	-	53,53,53	0.92	2 (3%)	59,61,61	1.02	4 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PE	A	1908	-	-	10/21/21/54	-
5	3PE	A	1910	-	-	20/35/35/54	-
8	6UB	A	1913	-	-	11/22/42/42	0/2/2/2
5	3PE	A	1904	-	-	23/54/54/54	-
5	3PE	A	1906	-	-	26/47/47/54	-
5	3PE	A	1903	-	-	32/54/54/54	-
5	3PE	A	1905	-	-	27/46/46/54	-
5	3PE	A	1911	-	-	31/54/54/54	-
7	POV	A	1912	-	-	24/50/50/55	-
5	3PE	A	1907	-	-	20/41/41/54	-
5	3PE	A	1902	-	-	18/36/36/54	-
6	PC1	A	1909	-	-	35/57/57/57	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1913	6UB	CAT-CAX	14.69	1.52	1.35
8	A	1913	6UB	CAW-CAY	13.31	1.53	1.36
8	A	1913	6UB	CAT-NAP	5.38	1.45	1.38
8	A	1913	6UB	CAW-NAP	5.02	1.45	1.37
5	A	1906	3PE	O31-C31	4.36	1.46	1.33
5	A	1905	3PE	O31-C31	4.30	1.45	1.33
5	A	1903	3PE	O31-C31	4.29	1.45	1.33
7	A	1912	POV	O31-C31	4.23	1.45	1.33
5	A	1910	3PE	O31-C31	4.23	1.45	1.33
5	A	1902	3PE	O31-C31	4.22	1.45	1.33
5	A	1904	3PE	O31-C31	4.22	1.45	1.33
5	A	1907	3PE	O31-C31	4.22	1.45	1.33
6	A	1909	PC1	O31-C31	4.19	1.45	1.33
5	A	1908	3PE	O21-C21	4.14	1.45	1.33
5	A	1911	3PE	O31-C31	4.10	1.45	1.33
5	A	1902	3PE	O21-C21	4.08	1.45	1.34
5	A	1904	3PE	O21-C21	4.08	1.45	1.34
5	A	1903	3PE	O21-C21	4.06	1.45	1.34
7	A	1912	POV	O21-C21	4.06	1.45	1.34
5	A	1907	3PE	O21-C21	4.06	1.45	1.34
5	A	1910	3PE	O21-C21	4.05	1.45	1.34
5	A	1905	3PE	O21-C21	4.03	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1909	PC1	O21-C21	4.02	1.45	1.34
5	A	1906	3PE	O21-C21	4.02	1.45	1.34
5	A	1911	3PE	O21-C21	3.99	1.45	1.34
8	A	1913	6UB	OAS-CAV	3.29	1.40	1.33
8	A	1913	6UB	CAV-CAY	2.98	1.52	1.47
8	A	1913	6UB	CAU-CAX	2.93	1.52	1.47
8	A	1913	6UB	OAQ-CAU	2.90	1.39	1.33
8	A	1913	6UB	OAQ-CAB	-2.28	1.40	1.45
8	A	1913	6UB	OAS-CAL	-2.14	1.40	1.46
8	A	1913	6UB	CAZ-CLAG	2.08	1.78	1.73

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1913	6UB	CAC-CAT-CAX	-7.86	119.80	127.61
8	A	1913	6UB	CAC-CAT-NAP	4.95	119.17	113.42
8	A	1913	6UB	OAS-CAV-CAY	4.62	120.60	112.28
5	A	1904	3PE	O21-C21-C22	4.51	121.24	111.48
5	A	1902	3PE	O21-C21-C22	4.25	120.67	111.48
5	A	1905	3PE	O21-C21-C22	4.23	120.64	111.48
5	A	1903	3PE	O21-C21-C22	4.13	120.42	111.48
7	A	1912	POV	O21-C21-C22	4.10	120.36	111.48
8	A	1913	6UB	OAQ-CAU-CAX	4.03	119.72	112.31
6	A	1909	PC1	O21-C21-C22	4.01	120.16	111.48
5	A	1907	3PE	O21-C21-C22	3.98	120.08	111.48
5	A	1911	3PE	O21-C21-C22	3.97	120.08	111.48
5	A	1910	3PE	O21-C21-C22	3.86	119.84	111.48
5	A	1906	3PE	O21-C21-C22	3.77	119.64	111.48
8	A	1913	6UB	CAK-CBA-CAZ	3.27	120.10	116.82
7	A	1912	POV	O31-C31-C32	3.05	121.12	111.83
5	A	1905	3PE	O31-C31-C32	2.91	120.70	111.83
5	A	1903	3PE	O31-C31-C32	2.87	120.58	111.83
5	A	1904	3PE	O31-C31-C32	2.86	120.54	111.83
5	A	1906	3PE	O31-C31-C32	2.83	120.46	111.83
5	A	1902	3PE	O31-C31-C32	2.82	120.43	111.83
5	A	1911	3PE	O31-C31-C32	2.81	120.39	111.83
8	A	1913	6UB	CAZ-CBA-CBB	-2.79	120.27	123.97
6	A	1909	PC1	O31-C31-C32	2.75	120.22	111.83
5	A	1908	3PE	O21-C21-C22	2.75	120.22	111.83
8	A	1913	6UB	CAT-NAP-CAW	-2.75	120.04	122.35
5	A	1910	3PE	O31-C31-C32	2.67	119.99	111.83
6	A	1909	PC1	C2-O21-C21	-2.66	111.42	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1902	3PE	C2-O21-C21	-2.65	111.45	117.80
5	A	1907	3PE	C2-O21-C21	-2.61	111.55	117.80
7	A	1912	POV	C2-O21-C21	-2.60	111.57	117.80
5	A	1907	3PE	O31-C31-C32	2.60	119.75	111.83
5	A	1911	3PE	C2-O21-C21	-2.58	111.62	117.80
8	A	1913	6UB	OAF-CAV-CAY	-2.55	119.82	125.20
5	A	1906	3PE	C2-O21-C21	-2.48	111.86	117.80
8	A	1913	6UB	OAE-CAU-CAX	-2.33	120.28	125.20
5	A	1910	3PE	C2-O21-C21	-2.32	112.24	117.80
5	A	1903	3PE	C2-O21-C21	-2.32	112.25	117.80
8	A	1913	6UB	CAJ-CAZ-CBA	-2.23	119.87	121.98
5	A	1904	3PE	O21-C21-O22	-2.19	118.57	123.70
5	A	1905	3PE	C2-O21-C21	-2.13	112.70	117.80
8	A	1913	6UB	OAS-CAV-OAF	-2.11	119.58	123.37
8	A	1913	6UB	C24-CAW-NAP	2.06	118.75	115.53
6	A	1909	PC1	O21-C21-O22	-2.06	118.90	123.70
5	A	1905	3PE	O21-C21-O22	-2.02	118.97	123.70
7	A	1912	POV	C11-C12-N	-2.02	109.33	115.82

There are no chirality outliers.

All (277) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C11-O13-P-O14
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	C12-C11-O13-P
5	A	1903	3PE	O13-C11-C12-N
5	A	1903	3PE	C22-C21-O21-C2
5	A	1904	3PE	C11-O13-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-O12
5	A	1905	3PE	C1-O11-P-O13
5	A	1905	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
5	A	1905	3PE	C11-O13-P-O14
5	A	1905	3PE	C22-C21-O21-C2
5	A	1906	3PE	C1-O11-P-O12
5	A	1906	3PE	C1-O11-P-O13
5	A	1906	3PE	C11-O13-P-O11
5	A	1906	3PE	O32-C31-O31-C3
5	A	1906	3PE	C32-C31-O31-C3
5	A	1906	3PE	C22-C21-O21-C2
5	A	1907	3PE	C11-O13-P-O11
5	A	1907	3PE	C2-C1-O11-P
5	A	1907	3PE	O32-C31-O31-C3
5	A	1907	3PE	C32-C31-O31-C3
5	A	1908	3PE	C12-C11-O13-P
5	A	1910	3PE	C1-O11-P-O12
5	A	1910	3PE	C1-O11-P-O13
5	A	1910	3PE	C11-O13-P-O11
5	A	1910	3PE	C11-O13-P-O14
5	A	1910	3PE	O13-C11-C12-N
5	A	1911	3PE	C11-O13-P-O11
5	A	1911	3PE	C11-O13-P-O12
6	A	1909	PC1	C1-O11-P-O12
6	A	1909	PC1	C1-O11-P-O13
6	A	1909	PC1	C12-C11-O13-P
7	A	1912	POV	C1-O11-P-O12
7	A	1912	POV	C1-O11-P-O13
7	A	1912	POV	C1-O11-P-O14
7	A	1912	POV	O12-C11-C12-N
7	A	1912	POV	C22-C21-O21-C2
8	A	1913	6UB	OAS-CAV-CAY-CAW
8	A	1913	6UB	OAF-CAV-CAY-CAW
8	A	1913	6UB	O25-C26-C27-N28
5	A	1903	3PE	O32-C31-O31-C3
6	A	1909	PC1	O32-C31-O31-C3
7	A	1912	POV	O32-C31-O31-C3
8	A	1913	6UB	OAF-CAV-OAS-CAL
8	A	1913	6UB	CAY-CAV-OAS-CAL
6	A	1909	PC1	C32-C31-O31-C3
7	A	1912	POV	C32-C31-O31-C3
5	A	1905	3PE	O22-C21-O21-C2
5	A	1906	3PE	O22-C21-O21-C2
8	A	1913	6UB	CAX-CAU-OAQ-CAB
5	A	1903	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
5	A	1903	3PE	O22-C21-O21-C2
7	A	1912	POV	O22-C21-O21-C2
5	A	1911	3PE	C3C-C3D-C3E-C3F
5	A	1910	3PE	C25-C26-C27-C28
6	A	1909	PC1	C2E-C2F-C2G-C2H
7	A	1912	POV	C214-C215-C216-C217
7	A	1912	POV	C23-C24-C25-C26
5	A	1902	3PE	C33-C34-C35-C36
5	A	1911	3PE	C3E-C3F-C3G-C3H
8	A	1913	6UB	OAE-CAU-OAQ-CAB
5	A	1907	3PE	C27-C28-C29-C2A
7	A	1912	POV	C21-C22-C23-C24
5	A	1903	3PE	C2A-C2B-C2C-C2D
5	A	1911	3PE	C31-C32-C33-C34
6	A	1909	PC1	C11-C12-N-C15
5	A	1905	3PE	C21-C22-C23-C24
5	A	1905	3PE	C32-C31-O31-C3
5	A	1907	3PE	C22-C21-O21-C2
5	A	1910	3PE	C22-C21-O21-C2
5	A	1911	3PE	C21-C22-C23-C24
5	A	1907	3PE	O22-C21-O21-C2
5	A	1910	3PE	O22-C21-O21-C2
6	A	1909	PC1	C23-C24-C25-C26
5	A	1910	3PE	C32-C31-O31-C3
5	A	1911	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	O32-C31-O31-C3
5	A	1911	3PE	C32-C31-O31-C3
6	A	1909	PC1	C11-C12-N-C13
5	A	1911	3PE	C39-C3A-C3B-C3C
5	A	1911	3PE	C28-C29-C2A-C2B
5	A	1904	3PE	C2B-C2C-C2D-C2E
6	A	1909	PC1	C3E-C3F-C3G-C3H
5	A	1906	3PE	C36-C37-C38-C39
5	A	1906	3PE	C2C-C2D-C2E-C2F
6	A	1909	PC1	C36-C37-C38-C39
5	A	1911	3PE	C36-C37-C38-C39
5	A	1911	3PE	C22-C21-O21-C2
6	A	1909	PC1	C3C-C3D-C3E-C3F
5	A	1902	3PE	C21-C22-C23-C24
5	A	1907	3PE	C24-C25-C26-C27
5	A	1906	3PE	C35-C36-C37-C38
6	A	1909	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	A	1903	3PE	C3E-C3F-C3G-C3H
5	A	1902	3PE	C31-C32-C33-C34
5	A	1904	3PE	C38-C39-C3A-C3B
5	A	1907	3PE	C34-C35-C36-C37
5	A	1911	3PE	C35-C36-C37-C38
5	A	1911	3PE	C24-C25-C26-C27
5	A	1911	3PE	C29-C2A-C2B-C2C
5	A	1910	3PE	O32-C31-O31-C3
5	A	1903	3PE	C22-C23-C24-C25
5	A	1903	3PE	C28-C29-C2A-C2B
5	A	1910	3PE	C23-C24-C25-C26
6	A	1909	PC1	C3D-C3E-C3F-C3G
5	A	1903	3PE	C3F-C3G-C3H-C3I
5	A	1905	3PE	C31-C32-C33-C34
5	A	1902	3PE	C35-C36-C37-C38
5	A	1903	3PE	C2B-C2C-C2D-C2E
5	A	1904	3PE	C34-C35-C36-C37
5	A	1911	3PE	O32-C31-O31-C3
5	A	1902	3PE	C25-C26-C27-C28
5	A	1904	3PE	C3E-C3F-C3G-C3H
5	A	1906	3PE	C2B-C2C-C2D-C2E
5	A	1904	3PE	C32-C33-C34-C35
5	A	1904	3PE	C37-C38-C39-C3A
5	A	1905	3PE	C34-C35-C36-C37
5	A	1906	3PE	C34-C35-C36-C37
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1910	3PE	C28-C29-C2A-C2B
6	A	1909	PC1	C11-C12-N-C14
5	A	1903	3PE	C39-C3A-C3B-C3C
5	A	1907	3PE	C37-C38-C39-C3A
6	A	1909	PC1	C26-C27-C28-C29
5	A	1911	3PE	O22-C21-O21-C2
5	A	1903	3PE	C38-C39-C3A-C3B
5	A	1904	3PE	C33-C34-C35-C36
6	A	1909	PC1	C31-C32-C33-C34
5	A	1903	3PE	C2D-C2E-C2F-C2G
5	A	1908	3PE	C25-C26-C27-C28
5	A	1902	3PE	C24-C25-C26-C27
8	A	1913	6UB	OAF-CAV-CAY-CBB
5	A	1905	3PE	C26-C27-C28-C29
8	A	1913	6UB	OAS-CAV-CAY-CBB
5	A	1904	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	A	1912	POV	C2-C1-O11-P
5	A	1903	3PE	C3C-C3D-C3E-C3F
5	A	1905	3PE	C3D-C3E-C3F-C3G
6	A	1909	PC1	C25-C26-C27-C28
5	A	1906	3PE	C22-C23-C24-C25
6	A	1909	PC1	O11-C1-C2-C3
5	A	1903	3PE	C3A-C3B-C3C-C3D
6	A	1909	PC1	C3F-C3G-C3H-C3I
5	A	1911	3PE	C27-C28-C29-C2A
5	A	1903	3PE	C1-C2-C3-O31
5	A	1904	3PE	C1-C2-C3-O31
5	A	1908	3PE	C24-C25-C26-C27
7	A	1912	POV	C22-C23-C24-C25
5	A	1911	3PE	C2D-C2E-C2F-C2G
5	A	1906	3PE	C29-C2A-C2B-C2C
5	A	1905	3PE	C39-C3A-C3B-C3C
6	A	1909	PC1	C32-C33-C34-C35
6	A	1909	PC1	C2F-C2G-C2H-C2I
5	A	1910	3PE	C33-C34-C35-C36
5	A	1906	3PE	C32-C33-C34-C35
5	A	1904	3PE	C22-C23-C24-C25
5	A	1911	3PE	C32-C33-C34-C35
7	A	1912	POV	C35-C36-C37-C38
5	A	1907	3PE	C29-C2A-C2B-C2C
5	A	1911	3PE	C3B-C3C-C3D-C3E
6	A	1909	PC1	C22-C21-O21-C2
5	A	1906	3PE	C38-C39-C3A-C3B
6	A	1909	PC1	C34-C35-C36-C37
5	A	1911	3PE	C2F-C2G-C2H-C2I
7	A	1912	POV	C34-C35-C36-C37
6	A	1909	PC1	C33-C34-C35-C36
5	A	1903	3PE	C24-C25-C26-C27
5	A	1902	3PE	C1-C2-C3-O31
5	A	1907	3PE	C1-C2-C3-O31
5	A	1911	3PE	O11-C1-C2-O21
6	A	1909	PC1	O11-C1-C2-O21
7	A	1912	POV	O11-C1-C2-O21
5	A	1902	3PE	O21-C2-C3-O31
5	A	1903	3PE	O21-C2-C3-O31
5	A	1906	3PE	O21-C2-C3-O31
5	A	1908	3PE	C21-C22-C23-C24
5	A	1904	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C37-C38-C39-C3A
5	A	1902	3PE	O11-C1-C2-C3
5	A	1908	3PE	C26-C27-C28-C29
5	A	1904	3PE	C39-C3A-C3B-C3C
5	A	1903	3PE	C32-C33-C34-C35
6	A	1909	PC1	C2D-C2E-C2F-C2G
6	A	1909	PC1	C2A-C2B-C2C-C2D
5	A	1911	3PE	C25-C26-C27-C28
5	A	1910	3PE	C27-C28-C29-C2A
6	A	1909	PC1	O22-C21-O21-C2
5	A	1906	3PE	O11-C1-C2-O21
5	A	1910	3PE	C12-C11-O13-P
7	A	1912	POV	C12-C11-O12-P
5	A	1906	3PE	C2E-C2F-C2G-C2H
5	A	1905	3PE	O21-C2-C3-O31
5	A	1905	3PE	C36-C37-C38-C39
5	A	1911	3PE	C23-C24-C25-C26
5	A	1911	3PE	C2E-C2F-C2G-C2H
5	A	1903	3PE	C26-C27-C28-C29
5	A	1908	3PE	C22-C21-O21-C2
5	A	1904	3PE	C21-C22-C23-C24
5	A	1904	3PE	O11-C1-C2-C3
5	A	1905	3PE	O11-C1-C2-C3
5	A	1903	3PE	C2E-C2F-C2G-C2H
6	A	1909	PC1	C37-C38-C39-C3A
5	A	1902	3PE	O11-C1-C2-O21
5	A	1904	3PE	O11-C1-C2-O21
5	A	1905	3PE	O11-C1-C2-O21
5	A	1905	3PE	C3E-C3F-C3G-C3H
5	A	1908	3PE	O22-C21-O21-C2
5	A	1904	3PE	O21-C2-C3-O31
5	A	1907	3PE	O21-C2-C3-O31
7	A	1912	POV	C215-C216-C217-C218
5	A	1902	3PE	C1-O11-P-O12
5	A	1905	3PE	C11-O13-P-O12
5	A	1907	3PE	C1-O11-P-O14
5	A	1907	3PE	C11-O13-P-O14
5	A	1911	3PE	C11-O13-P-O14
6	A	1909	PC1	C11-O13-P-O14
6	A	1909	PC1	C1-O11-P-O14
5	A	1905	3PE	C38-C39-C3A-C3B
5	A	1905	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
8	A	1913	6UB	C27-C26-O25-C24
5	A	1907	3PE	C3-C2-O21-C21
5	A	1911	3PE	C22-C23-C24-C25
7	A	1912	POV	C311-C310-C39-C38
5	A	1911	3PE	O11-C1-C2-C3
7	A	1912	POV	O11-C1-C2-C3
7	A	1912	POV	C33-C34-C35-C36
5	A	1910	3PE	O21-C2-C3-O31
5	A	1907	3PE	C32-C33-C34-C35
5	A	1903	3PE	C36-C37-C38-C39
6	A	1909	PC1	C3B-C3C-C3D-C3E
5	A	1907	3PE	C22-C23-C24-C25
5	A	1903	3PE	O11-C1-C2-O21
7	A	1912	POV	C27-C28-C29-C210
8	A	1913	6UB	O25-C24-CAW-NAP
5	A	1907	3PE	C21-C22-C23-C24
5	A	1911	3PE	C3F-C3G-C3H-C3I
5	A	1906	3PE	C24-C25-C26-C27
5	A	1905	3PE	C3F-C3G-C3H-C3I
6	A	1909	PC1	O21-C2-C3-O31
5	A	1911	3PE	C2C-C2D-C2E-C2F
5	A	1906	3PE	C27-C28-C29-C2A
5	A	1910	3PE	C26-C27-C28-C29
5	A	1905	3PE	C2-C1-O11-P
5	A	1903	3PE	C37-C38-C39-C3A
5	A	1905	3PE	C33-C34-C35-C36
5	A	1906	3PE	C33-C34-C35-C36
5	A	1907	3PE	C36-C37-C38-C39
5	A	1906	3PE	C2-C1-O11-P
5	A	1903	3PE	C33-C34-C35-C36
5	A	1908	3PE	C22-C23-C24-C25
5	A	1910	3PE	C22-C23-C24-C25
5	A	1910	3PE	C1-C2-C3-O31
5	A	1904	3PE	C2E-C2F-C2G-C2H
7	A	1912	POV	C32-C33-C34-C35
5	A	1906	3PE	O11-C1-C2-C3
5	A	1906	3PE	C1-C2-C3-O31
5	A	1904	3PE	C2D-C2E-C2F-C2G
7	A	1912	POV	C29-C210-C211-C212
5	A	1903	3PE	O11-C1-C2-C3
5	A	1903	3PE	C23-C24-C25-C26
6	A	1909	PC1	O13-C11-C12-N

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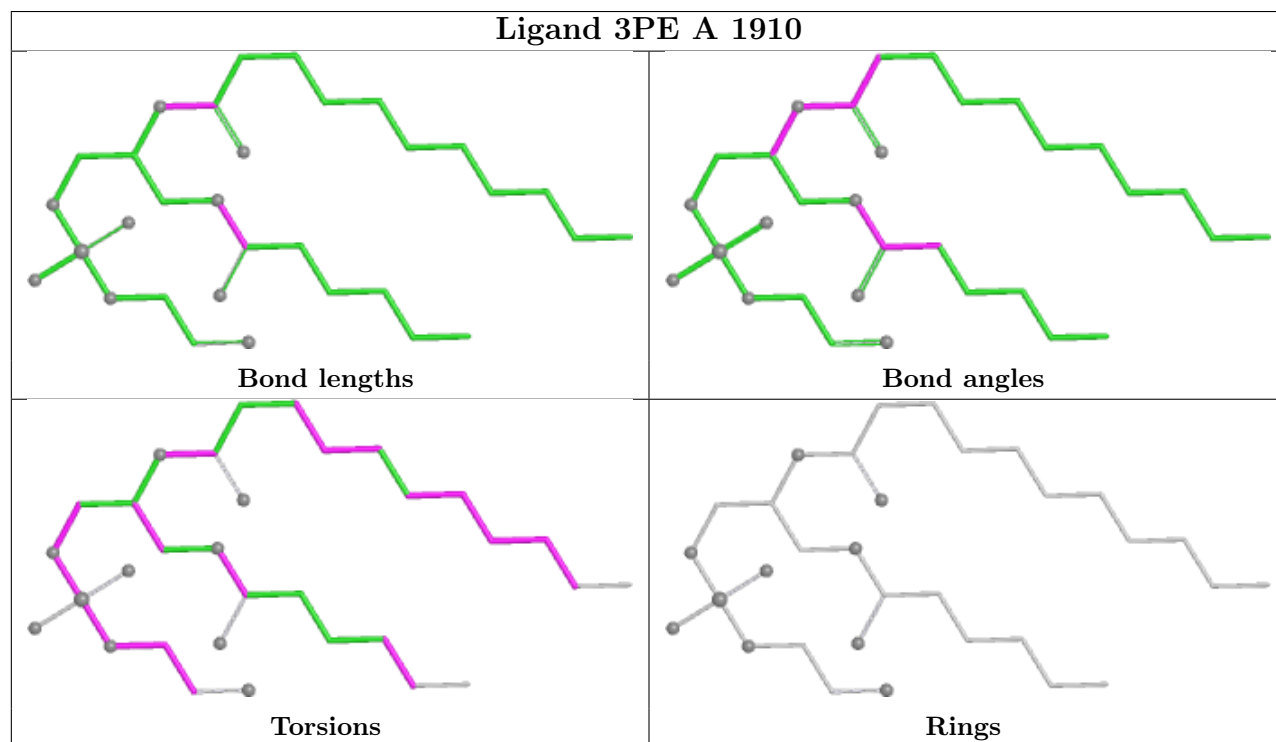
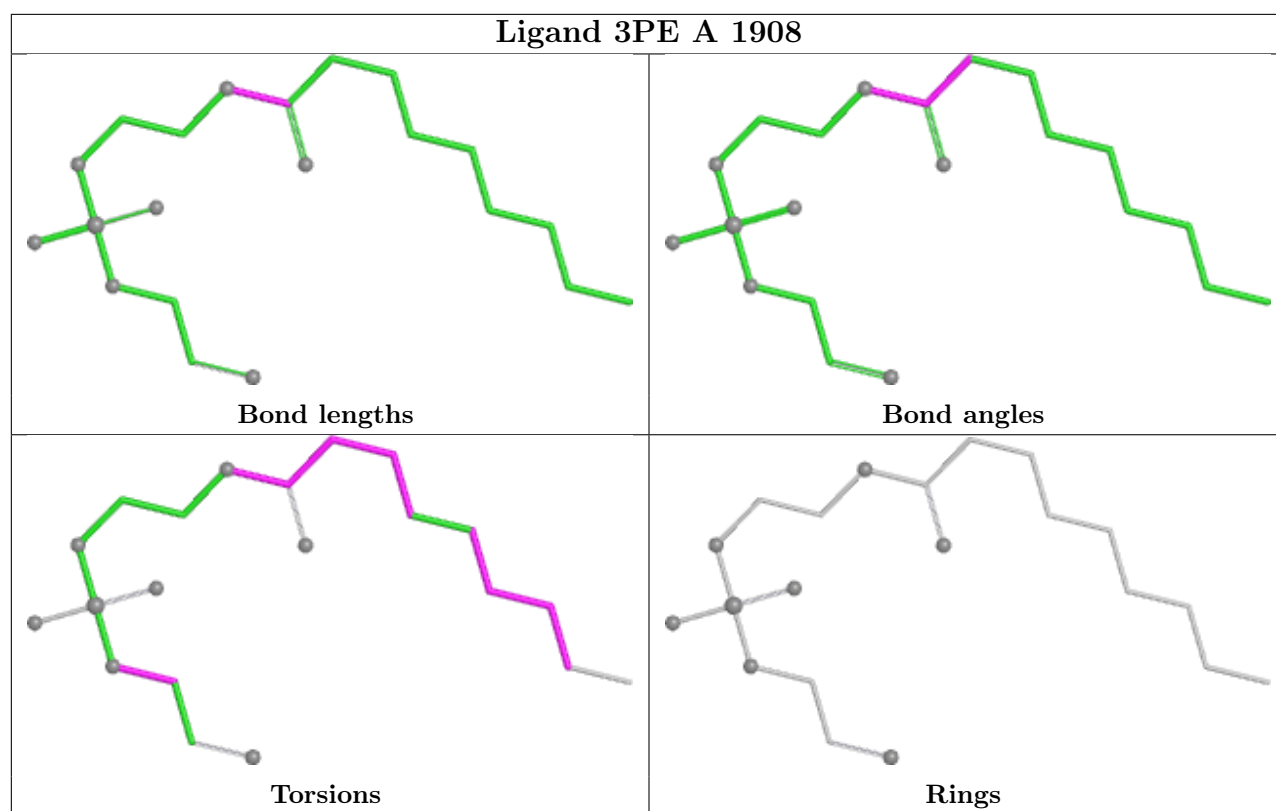
Mol	Chain	Res	Type	Atoms
5	A	1905	3PE	C35-C36-C37-C38
5	A	1904	3PE	C3B-C3C-C3D-C3E
5	A	1905	3PE	C1-C2-C3-O31
5	A	1908	3PE	O21-C21-C22-C23
5	A	1910	3PE	C2-C1-O11-P
5	A	1908	3PE	O22-C21-C22-C23

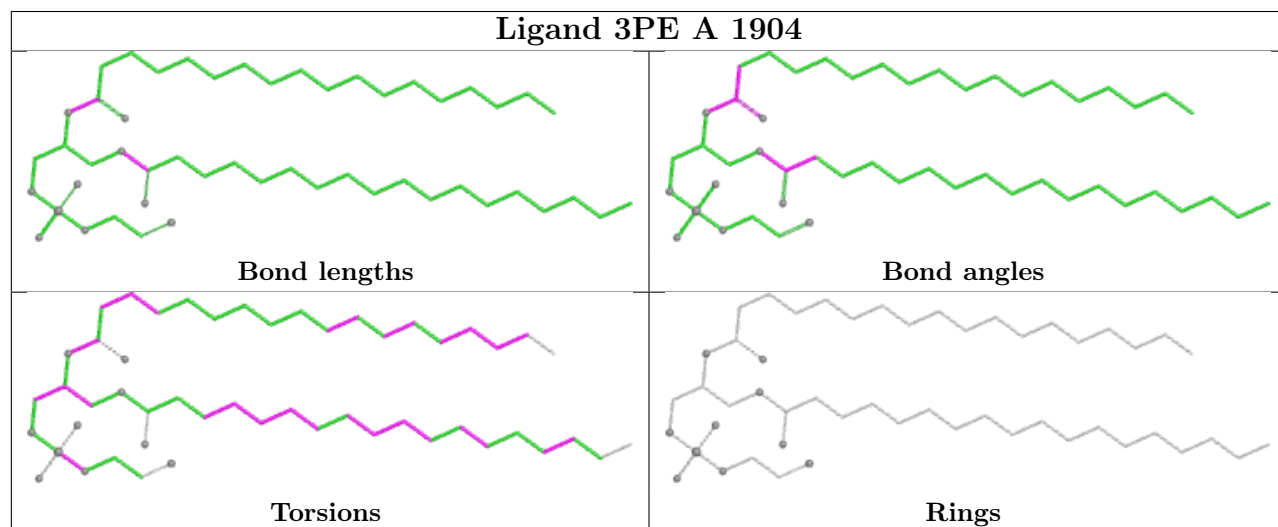
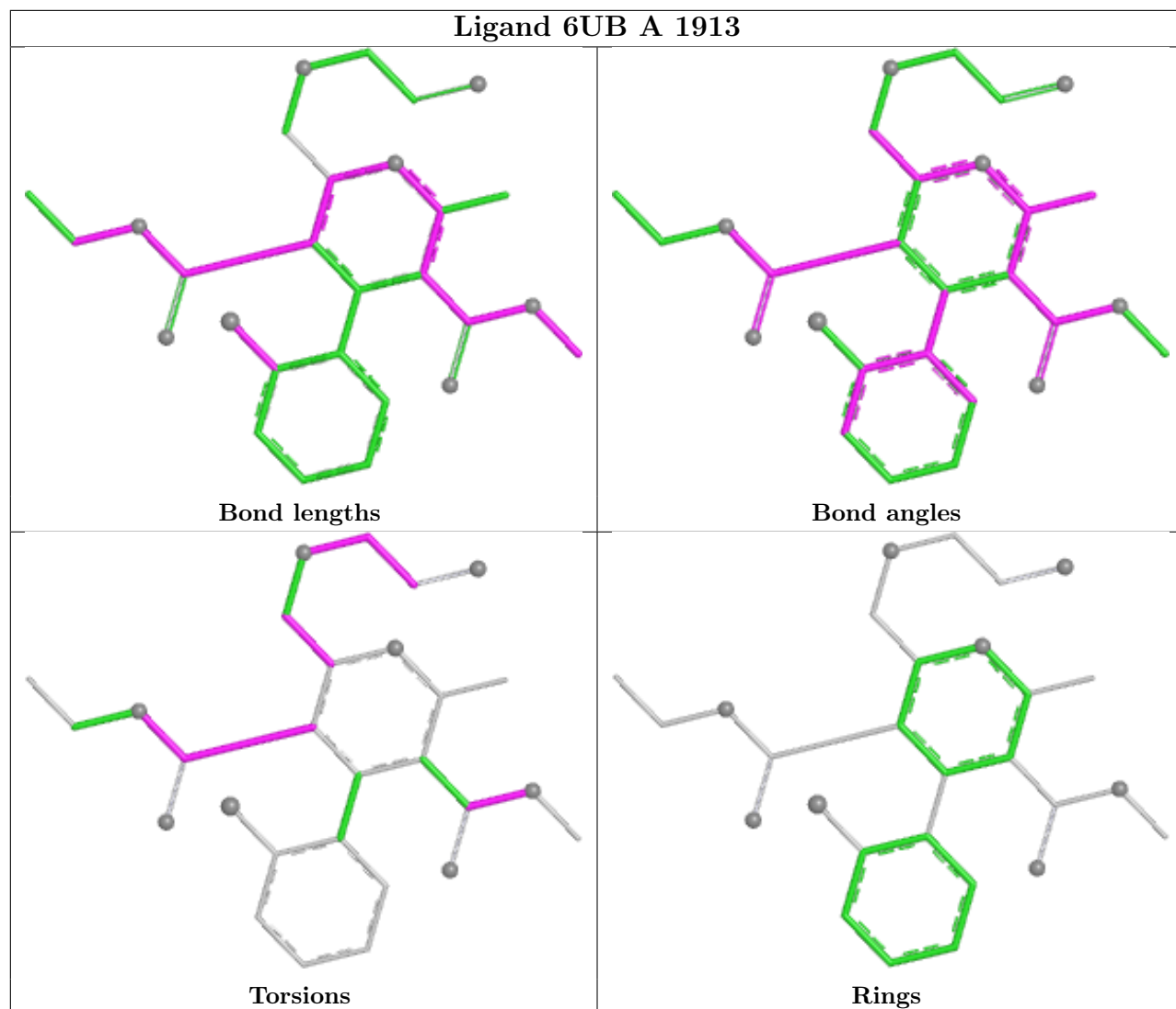
There are no ring outliers.

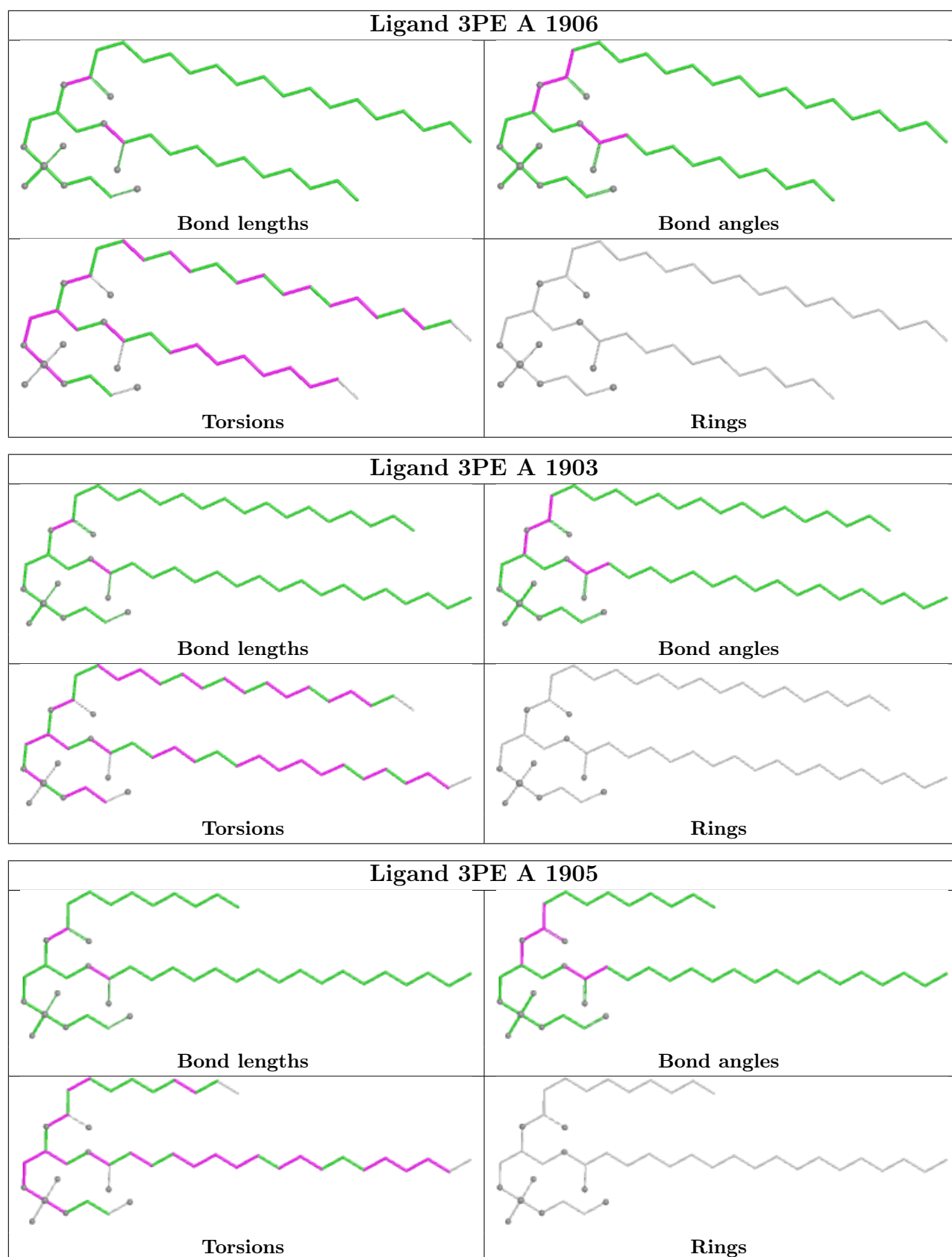
12 monomers are involved in 126 short contacts:

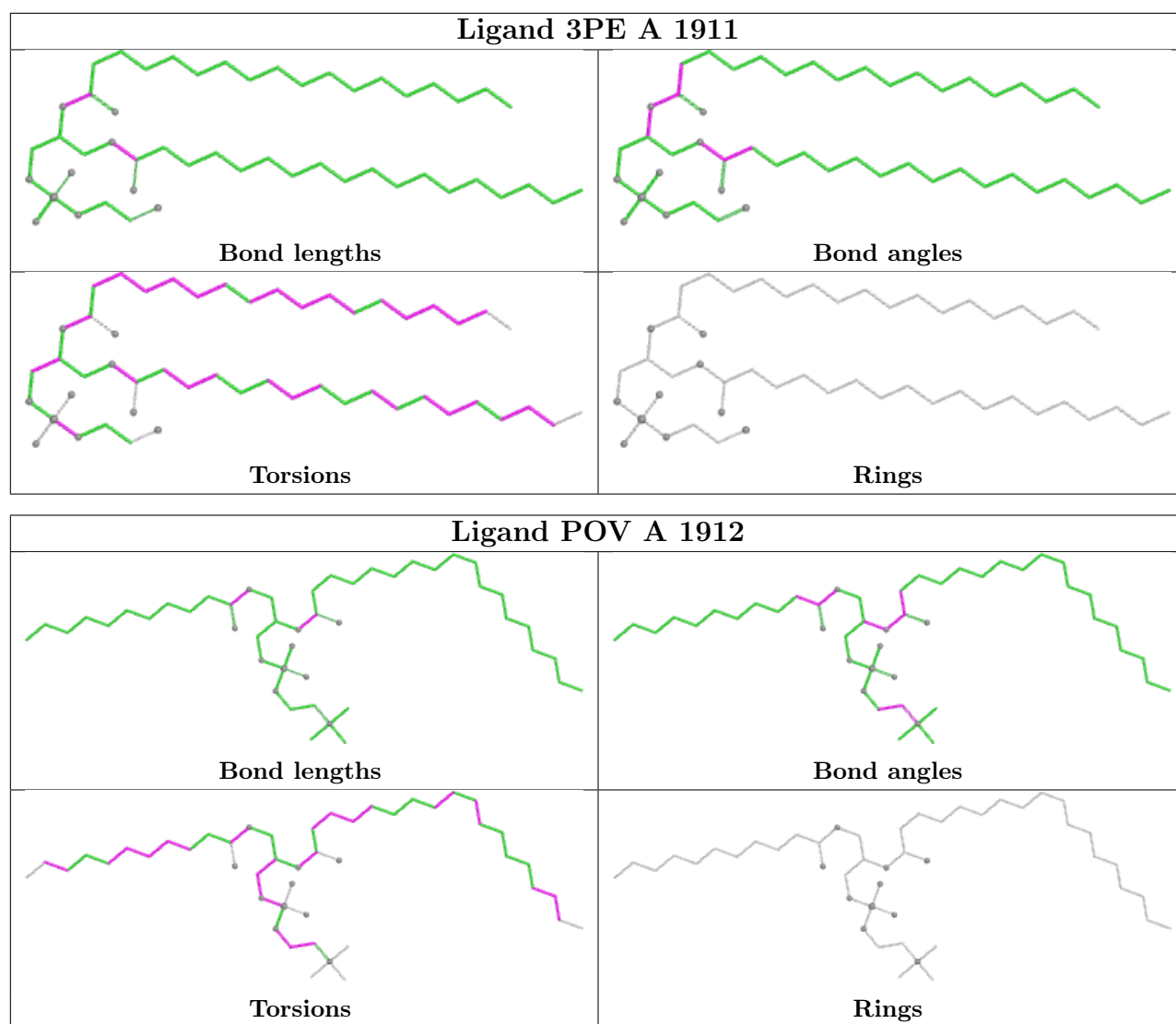
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1908	3PE	9	0
5	A	1910	3PE	2	0
8	A	1913	6UB	4	0
5	A	1904	3PE	12	0
5	A	1906	3PE	10	0
5	A	1903	3PE	24	0
5	A	1905	3PE	10	0
5	A	1911	3PE	30	0
7	A	1912	POV	8	0
5	A	1907	3PE	7	0
5	A	1902	3PE	3	0
6	A	1909	PC1	10	0

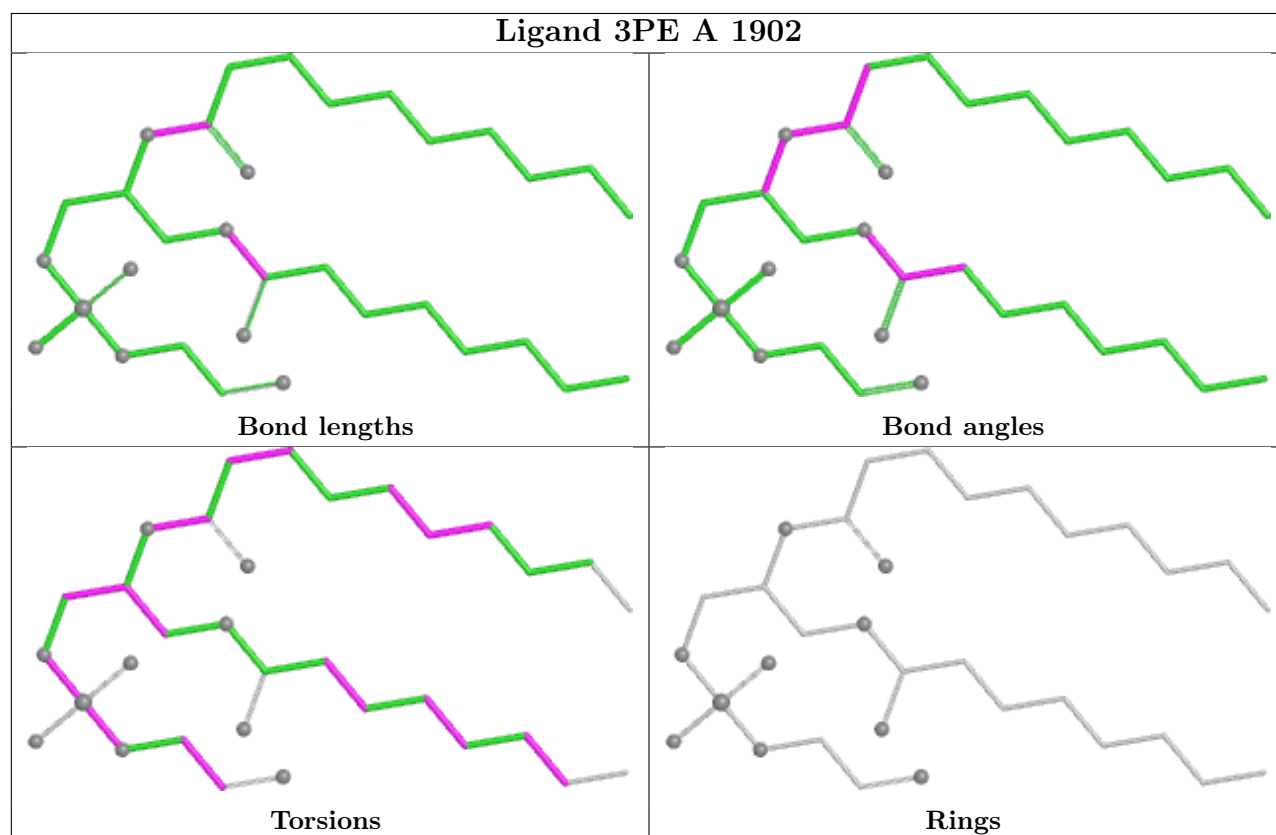
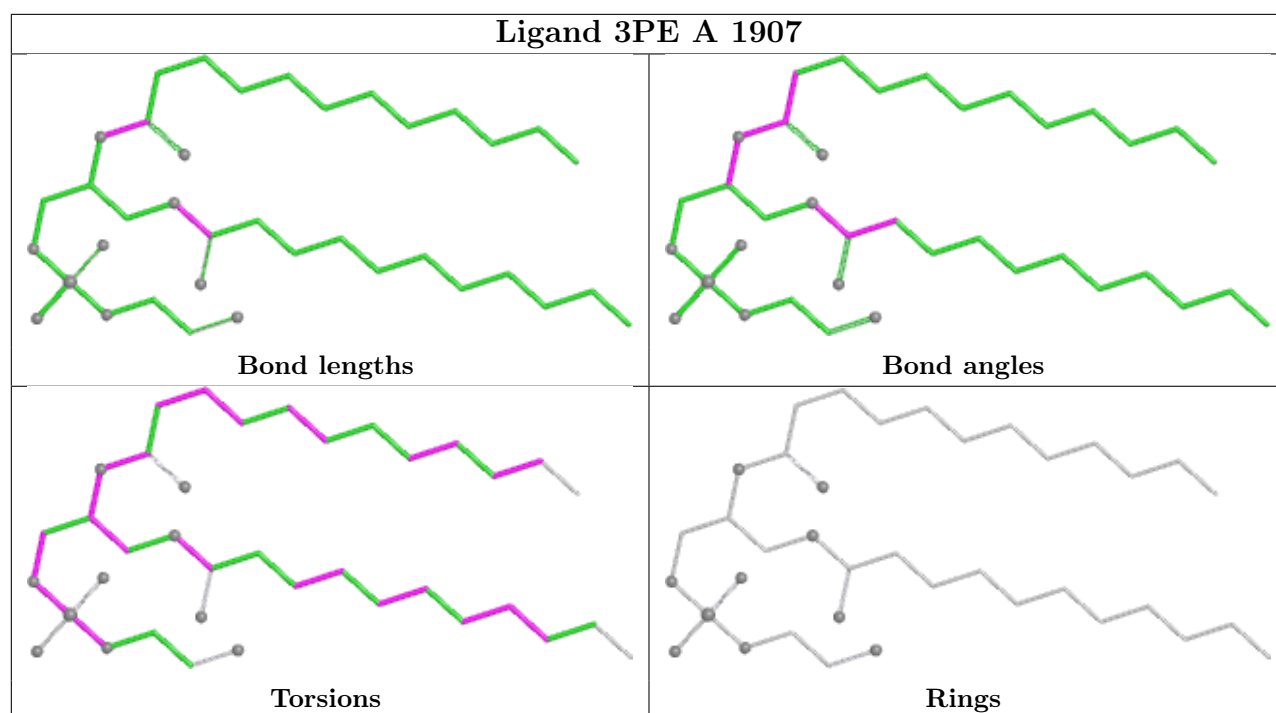
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

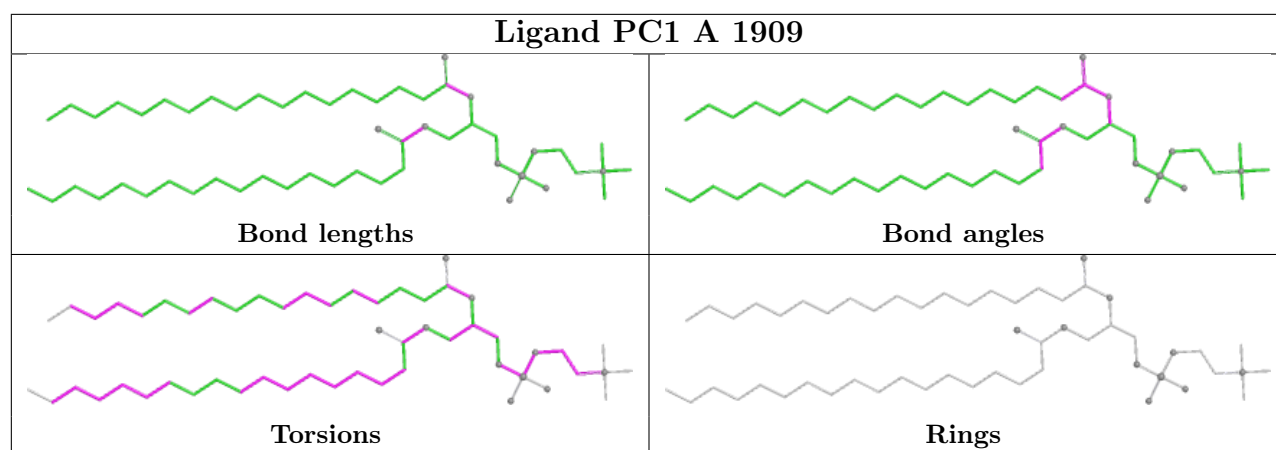












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

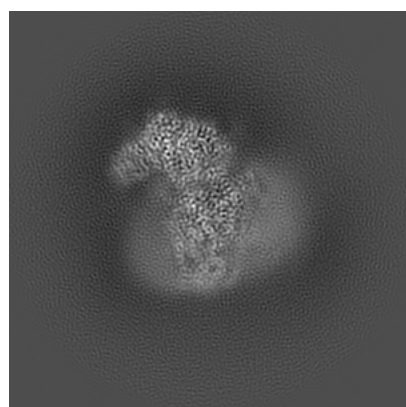
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22426. These allow visual inspection of the internal detail of the map and identification of artifacts.

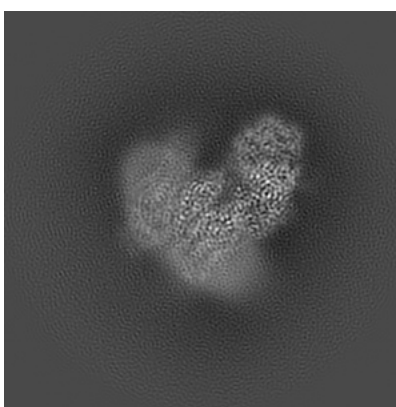
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

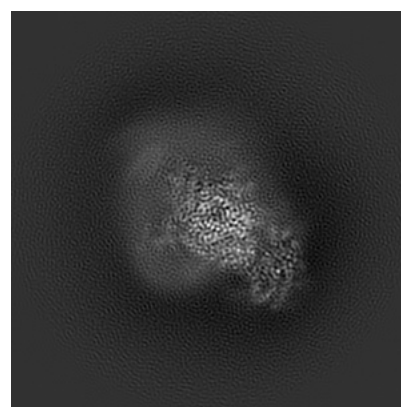
6.1.1 Primary map



X



Y

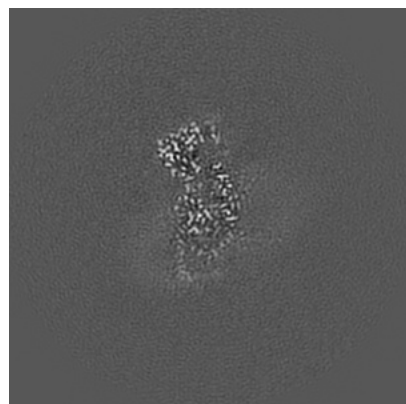


Z

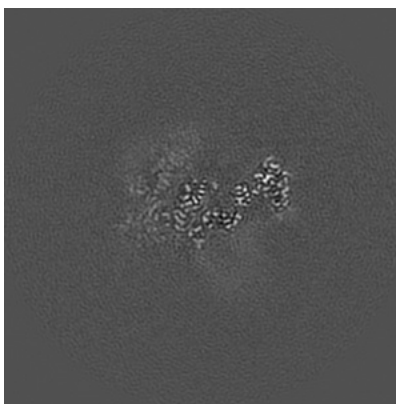
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

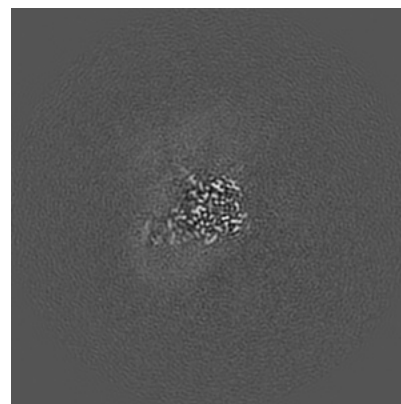
6.2.1 Primary map



X Index: 140



Y Index: 140

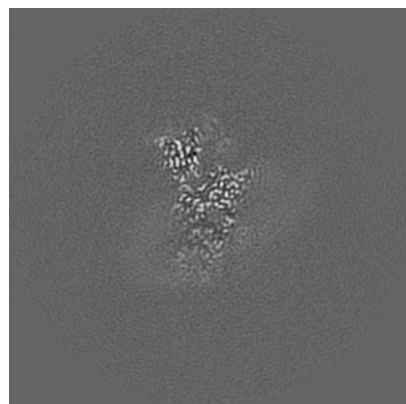


Z Index: 140

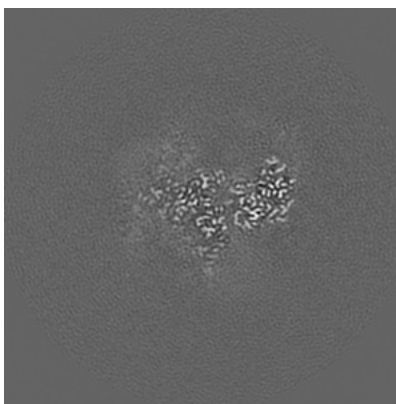
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

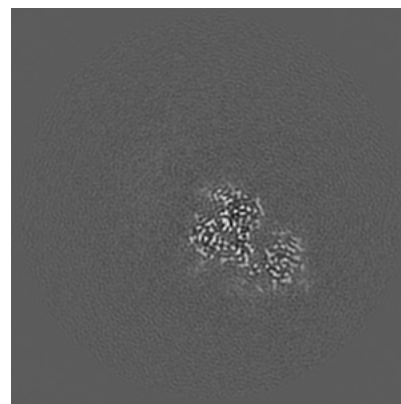
6.3.1 Primary map



X Index: 136



Y Index: 130

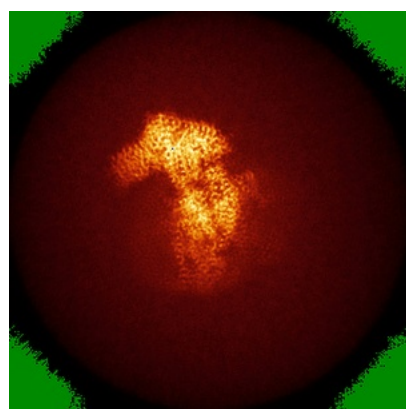


Z Index: 185

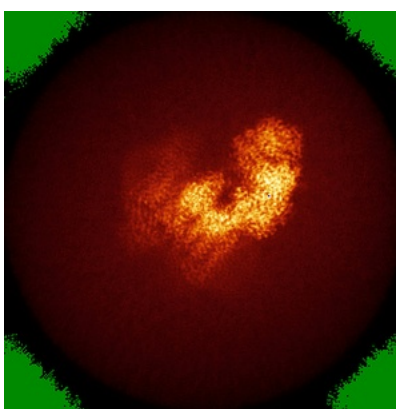
The images above show the largest variance slices of the map in three orthogonal directions.

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

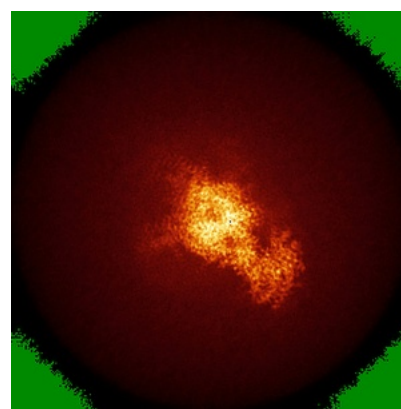
6.4.1 Primary map



X



Y



Z

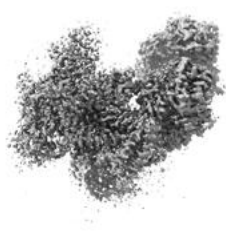
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

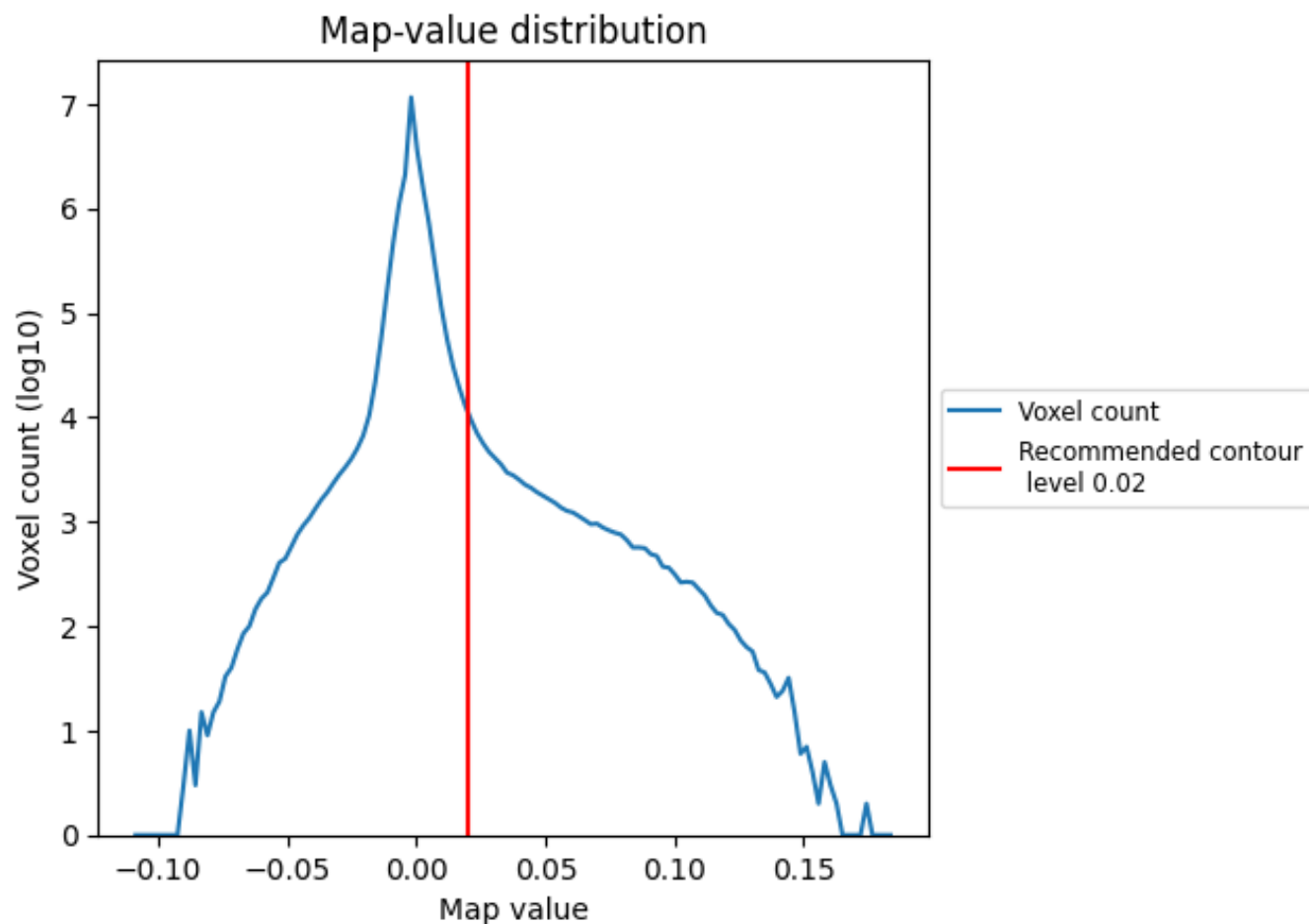
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

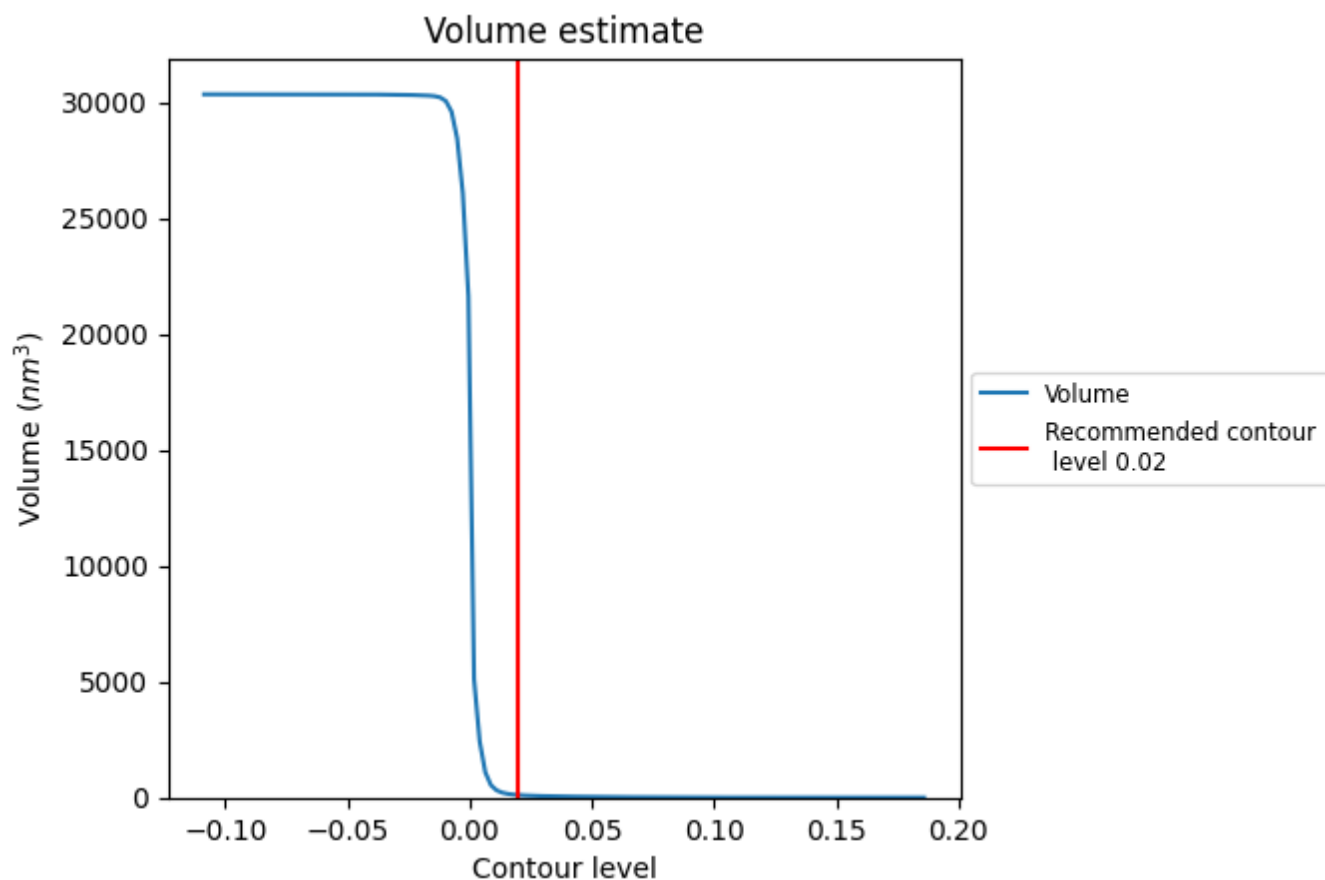
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

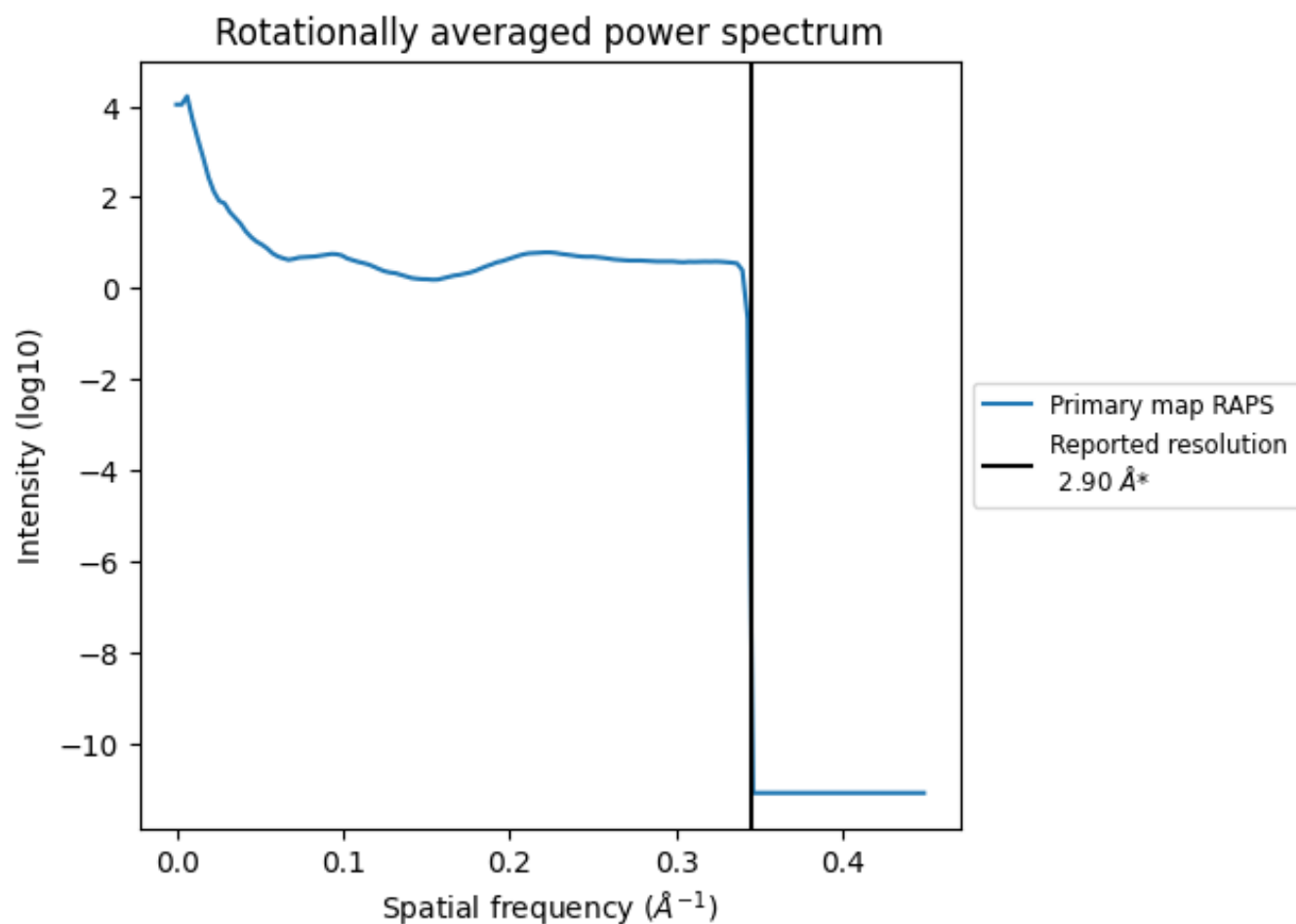
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 97 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 0.345 Å⁻¹

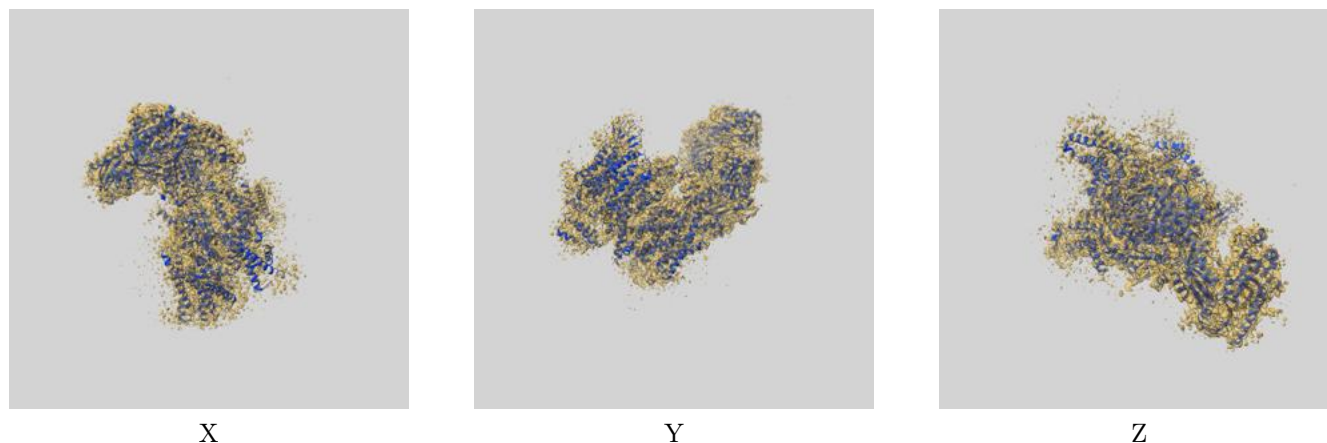
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

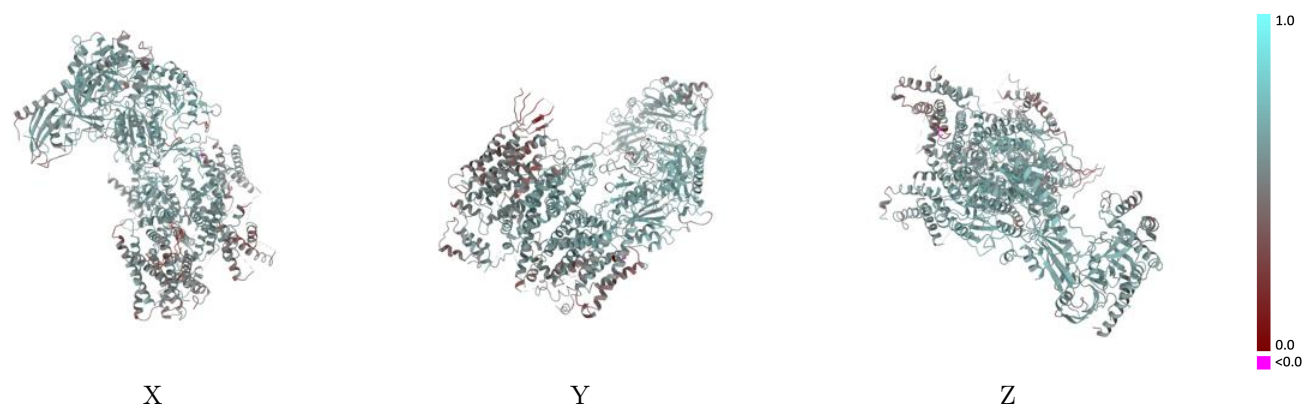
This section contains information regarding the fit between EMDB map EMD-22426 and PDB model 7JPX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



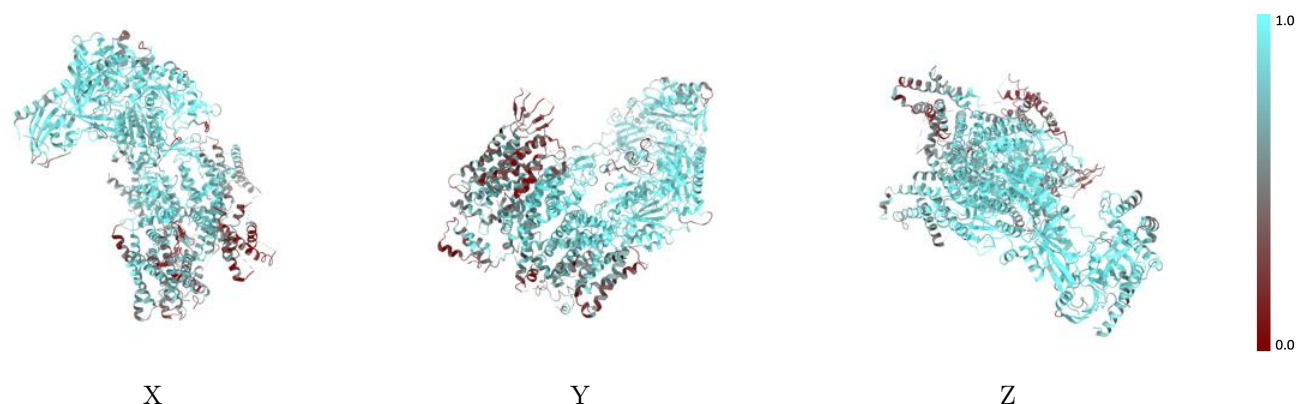
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



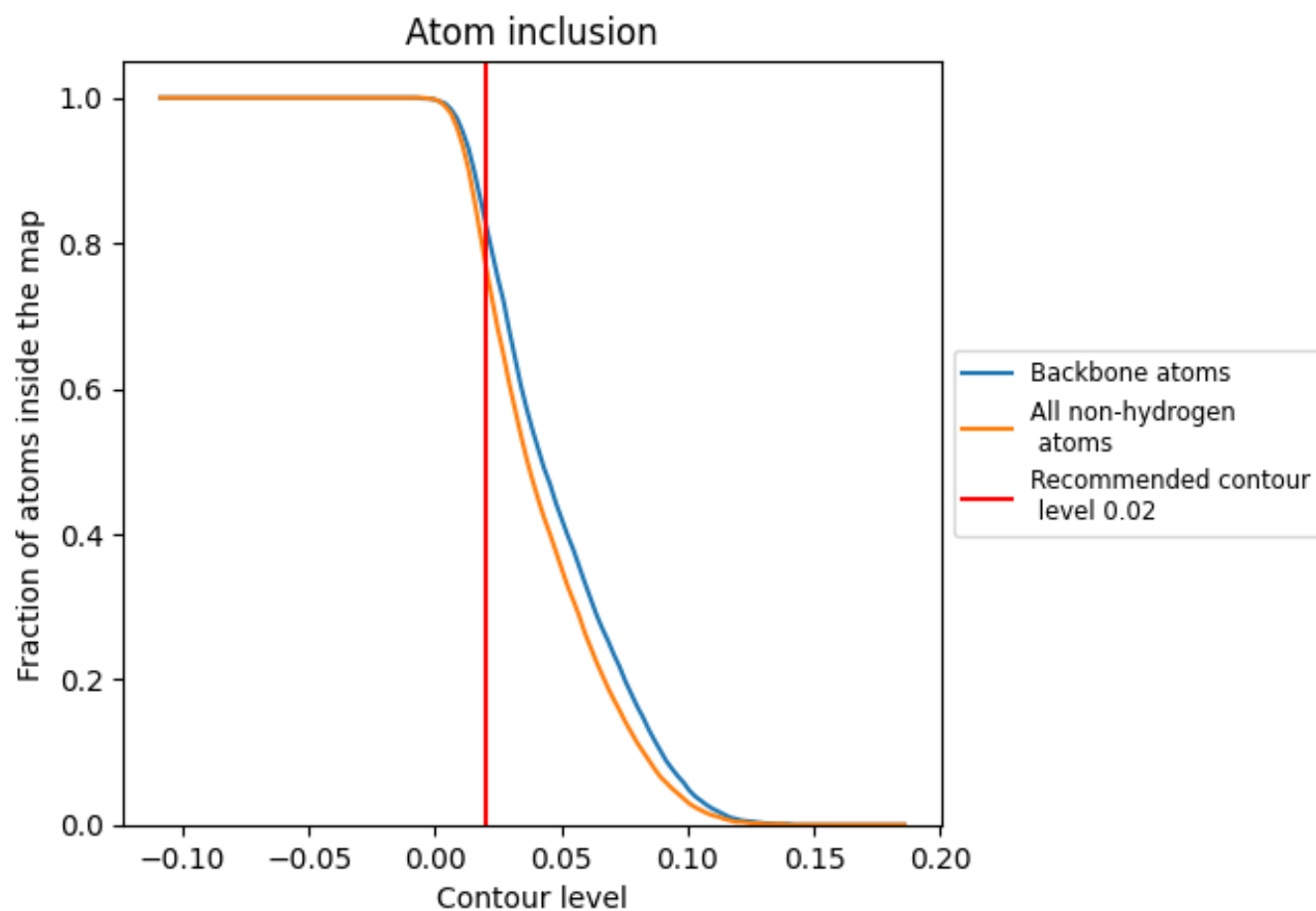
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 77% 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	<div></div> 0.7710	<div></div> 0.5630
A	<div></div> 0.7220	<div></div> 0.5540
E	<div></div> 0.5280	<div></div> 0.4530
F	<div></div> 0.8720	<div></div> 0.5930

