



## Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 09:56 PM EDT

PDB ID : 7JPV  
EMDB ID : EMD-22424  
Title : Rabbit Cav1.1 in the presence of 1 micromolar (S)-(-)-Bay K8644 in nanodiscs at 3.4 Angstrom resolution  
Authors : Yan, N.; Gao, S.  
Deposited on : 2020-08-10  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

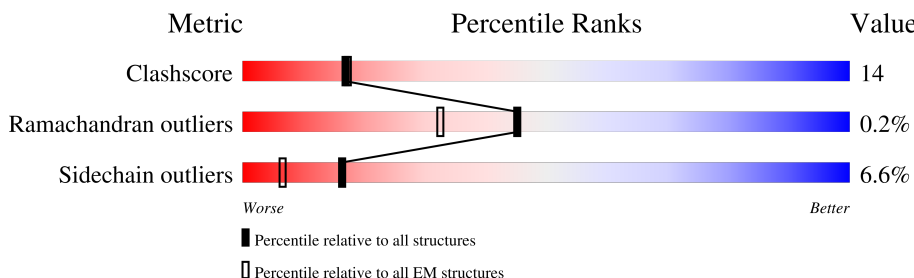
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 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	1905	-	-	X	-
5	3PE	A	1907	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PC1	E	301	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18288 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	1115	Total	C	N	O	S	0	0
			8987	5957	1439	1531	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	139	Total	C	N	O	S	0	0
			1080	713	171	181	15		

- 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).

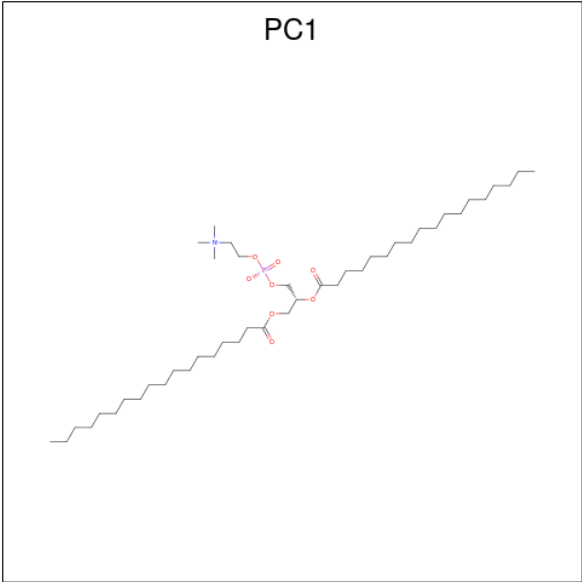
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



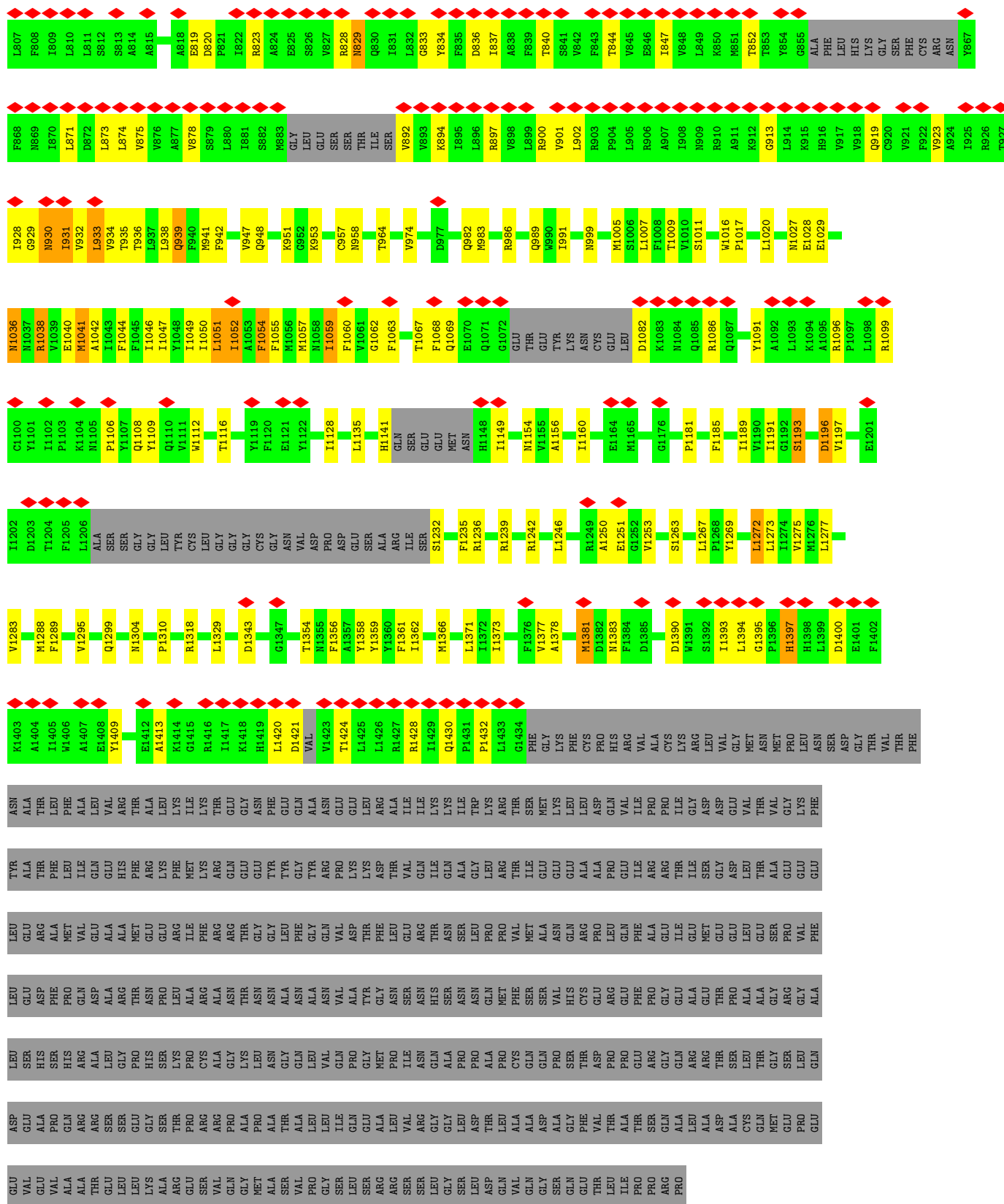
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
5	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).

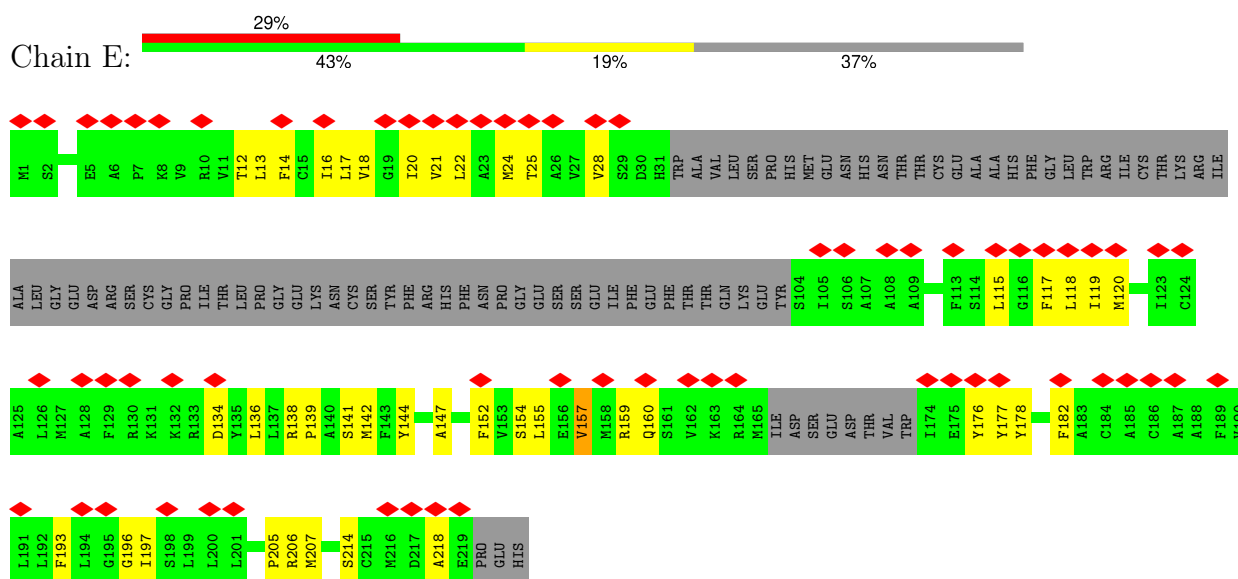


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	E	1	54	44	1	8	1	0

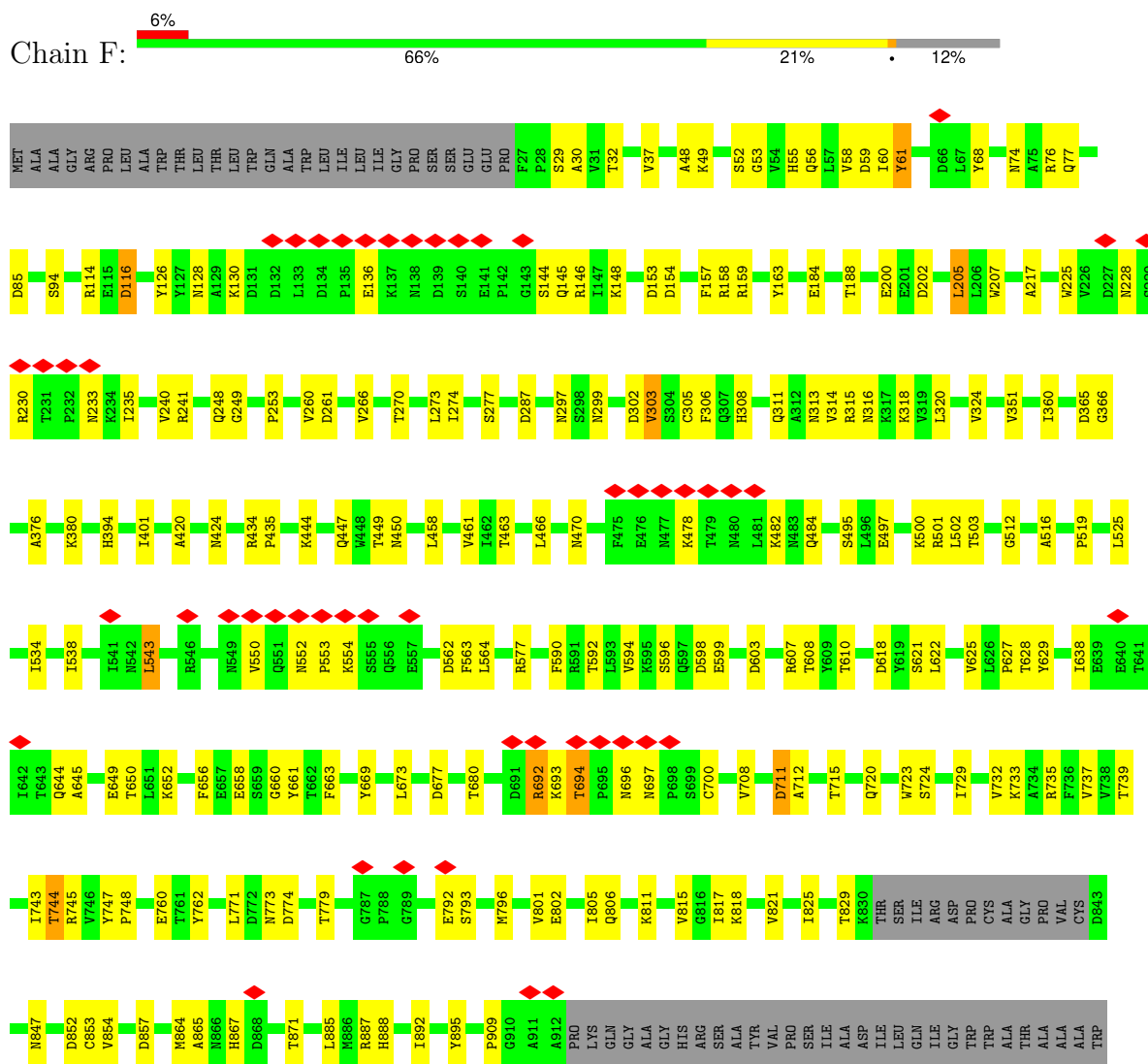


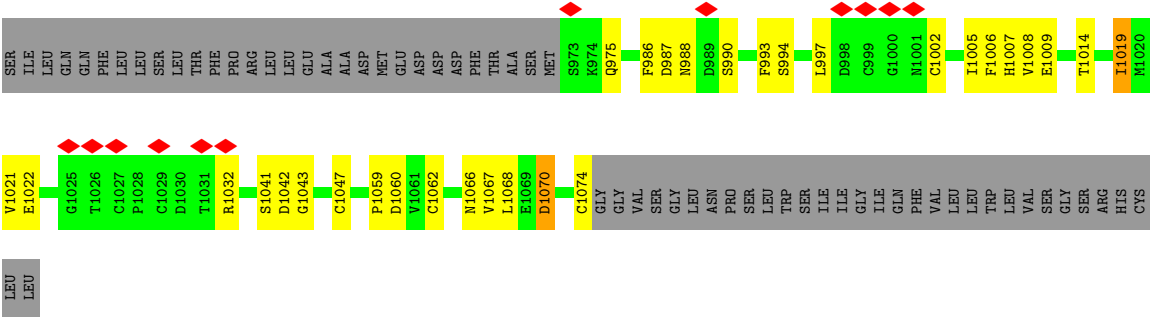






• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53341	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	0.140	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	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: PC1, CA, 3PE

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	0.30	1/9206 (0.0%)	0.41	0/12497
2	E	0.26	0/1104	0.40	0/1491
3	F	0.30	0/7974	0.46	0/10816
All	All	0.30	1/18284 (0.0%)	0.43	0/24804

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1036	ASN	C-N	-12.69	1.04	1.34

There are no bond angle outliers.

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	8987	0	9129	294	0
2	E	1080	0	1115	25	0
3	F	7804	0	7617	138	0
4	A	1	0	0	0	0
5	A	362	0	521	125	0
6	E	54	0	86	28	0
All	All	18288	0	18468	499	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 (499) 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:567:PHE:HE2	5:A:1907:3PE:C2C	1.18	1.53
1:A:567:PHE:CE2	5:A:1907:3PE:C2C	1.92	1.51
2:E:160:GLN:NE2	6:E:301:PC1:C14	1.70	1.51
1:A:643:ILE:CD1	5:A:1905:3PE:H3D1	1.60	1.30
1:A:1040:GLU:OE2	5:A:1909:3PE:H122	1.26	1.29
1:A:1359:TYR:CE2	5:A:1904:3PE:H232	1.66	1.29
1:A:567:PHE:HE2	5:A:1907:3PE:C2B	1.50	1.23
5:A:1904:3PE:H222	5:A:1904:3PE:H31	1.22	1.16
1:A:939:GLN:OE1	5:A:1904:3PE:H371	1.45	1.16
1:A:1275:VAL:HG22	5:A:1910:3PE:C2I	1.74	1.14
1:A:1068:PHE:CD2	1:A:1377:VAL:HG12	1.84	1.12
1:A:309:TRP:H	1:A:310:PRO:CD	1.64	1.09
1:A:635:VAL:HG11	5:A:1905:3PE:O22	1.50	1.09
1:A:938:LEU:HB3	1:A:1052:ILE:HD11	1.10	1.08
5:A:1903:3PE:O32	5:A:1905:3PE:H11	1.55	1.05
1:A:1275:VAL:HG22	5:A:1910:3PE:H2I3	1.38	1.05
1:A:1040:GLU:OE2	5:A:1909:3PE:C12	2.05	1.03
1:A:309:TRP:CD2	6:E:301:PC1:H242	1.93	1.03
1:A:643:ILE:HD11	5:A:1905:3PE:H3D1	1.06	1.03
1:A:931:ILE:HD12	1:A:1059:ILE:HD11	1.41	1.00
1:A:627:TYR:CD2	5:A:1906:3PE:H222	1.96	0.99
1:A:309:TRP:CE3	6:E:301:PC1:H242	1.98	0.98
1:A:647:CYS:HB3	5:A:1905:3PE:H3H2	1.44	0.98
1:A:939:GLN:OE1	5:A:1904:3PE:C37	2.12	0.98
1:A:209:ILE:HD12	6:E:301:PC1:H3H2	1.46	0.97
5:A:1902:3PE:H342	5:A:1902:3PE:H281	1.46	0.96
1:A:309:TRP:CE3	6:E:301:PC1:C24	2.51	0.93
1:A:567:PHE:CZ	5:A:1907:3PE:C2C	2.50	0.93
1:A:309:TRP:CD2	6:E:301:PC1:C24	2.51	0.93
1:A:1359:TYR:HE2	5:A:1904:3PE:H232	1.25	0.93
1:A:938:LEU:CB	1:A:1052:ILE:HD11	1.99	0.92
1:A:953:LYS:HE3	1:A:1028:GLU:O	1.68	0.92
1:A:931:ILE:CD1	1:A:1059:ILE:HD11	2.01	0.91
1:A:652:LEU:HD21	1:A:1054:PHE:CZ	2.06	0.91
1:A:210:TYR:OH	1:A:316:THR:HG22	1.70	0.90
1:A:627:TYR:HD2	5:A:1906:3PE:H222	1.31	0.90
1:A:567:PHE:CE2	5:A:1907:3PE:C2B	2.39	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:TYR:CD2	5:A:1904:3PE:H232	2.07	0.90
1:A:309:TRP:CE2	6:E:301:PC1:H241	2.08	0.88
2:E:160:GLN:CD	6:E:301:PC1:C14	2.42	0.87
5:A:1910:3PE:O14	5:A:1910:3PE:N	2.08	0.87
1:A:1038:ARG:HG3	1:A:1038:ARG:HH11	1.37	0.86
1:A:567:PHE:CE2	5:A:1907:3PE:H2B2	2.08	0.86
1:A:209:ILE:HD12	6:E:301:PC1:C3H	2.06	0.86
1:A:309:TRP:H	1:A:310:PRO:HD2	1.40	0.86
1:A:309:TRP:O	6:E:301:PC1:H321	1.76	0.85
5:A:1903:3PE:O14	5:A:1903:3PE:N	2.08	0.85
5:A:1905:3PE:O12	5:A:1905:3PE:H32	1.76	0.84
5:A:1905:3PE:H32	5:A:1905:3PE:P	2.18	0.83
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.57	0.83
1:A:1310:PRO:HB3	5:A:1910:3PE:H322	1.61	0.82
5:A:1904:3PE:H31	5:A:1904:3PE:C22	2.01	0.82
1:A:309:TRP:H	1:A:310:PRO:HD3	1.44	0.82
1:A:309:TRP:CZ2	6:E:301:PC1:H241	2.15	0.82
1:A:643:ILE:CD1	5:A:1905:3PE:C3D	2.51	0.82
5:A:1910:3PE:H2G1	5:A:1910:3PE:H2C1	1.62	0.82
1:A:309:TRP:N	1:A:310:PRO:CD	2.40	0.81
1:A:635:VAL:CG1	5:A:1905:3PE:O22	2.28	0.81
1:A:1275:VAL:HG22	5:A:1910:3PE:H2I2	1.60	0.81
1:A:65:CYS:SG	5:A:1907:3PE:H281	2.20	0.81
1:A:637:VAL:HG12	5:A:1906:3PE:H261	1.64	0.80
1:A:210:TYR:HD1	1:A:313:TYR:CE2	2.00	0.80
1:A:1359:TYR:CE2	5:A:1904:3PE:C23	2.59	0.80
1:A:601:PRO:HB3	5:A:1908:3PE:O22	1.82	0.79
1:A:522:LEU:HD23	5:A:1909:3PE:N	1.98	0.78
1:A:210:TYR:OH	1:A:316:THR:CG2	2.30	0.78
1:A:559:ILE:HG21	1:A:659:ILE:HG22	1.65	0.78
1:A:584:ARG:NH1	5:A:1906:3PE:O12	2.18	0.77
1:A:953:LYS:HG2	1:A:1028:GLU:O	1.85	0.77
1:A:209:ILE:CD1	6:E:301:PC1:H3H2	2.14	0.76
1:A:210:TYR:O	1:A:313:TYR:OH	2.04	0.76
1:A:643:ILE:HD11	5:A:1905:3PE:C3D	2.02	0.75
1:A:571:ILE:HD12	5:A:1907:3PE:H2A2	1.69	0.74
1:A:1068:PHE:HD2	1:A:1377:VAL:HG12	1.50	0.74
1:A:457:PRO:HD2	1:A:460:LEU:HD12	1.69	0.73
3:F:308:HIS:HD2	3:F:351:VAL:HG11	1.54	0.73
1:A:1196:ASP:OD2	1:A:1239:ARG:NH2	2.20	0.73
1:A:1068:PHE:CE2	1:A:1377:VAL:HG12	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:669:TYR:HE1	3:F:708:VAL:HG21	1.54	0.72
1:A:627:TYR:CE2	5:A:1906:3PE:C23	2.71	0.72
1:A:643:ILE:HD13	5:A:1905:3PE:H3D1	1.65	0.71
1:A:942:PHE:HD1	1:A:1044:PHE:HE1	1.39	0.71
1:A:1068:PHE:CD2	1:A:1377:VAL:CG1	2.69	0.71
1:A:309:TRP:CZ3	6:E:301:PC1:C25	2.74	0.71
2:E:17:LEU:HA	2:E:20:ILE:HD12	1.73	0.71
3:F:663:PHE:HB2	3:F:744:THR:HG23	1.73	0.71
1:A:65:CYS:SG	5:A:1907:3PE:C28	2.80	0.70
1:A:522:LEU:HD23	5:A:1909:3PE:HN3	1.56	0.70
3:F:154:ASP:OD2	3:F:163:TYR:OH	2.10	0.70
1:A:1275:VAL:CG2	5:A:1910:3PE:H2I3	2.21	0.69
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.73	0.68
1:A:1082:ASP:O	1:A:1086:ARG:NH1	2.27	0.68
1:A:636:LEU:CD2	5:A:1905:3PE:H322	2.24	0.67
1:A:309:TRP:CZ3	6:E:301:PC1:C24	2.78	0.67
1:A:1393:ILE:HG13	1:A:1394:LEU:H	1.60	0.67
1:A:489:ARG:HH12	1:A:493:MET:HB2	1.59	0.67
1:A:652:LEU:HD21	1:A:1054:PHE:CE2	2.30	0.67
1:A:1299:GLN:OE1	1:A:1318:ARG:NH2	2.28	0.67
1:A:660:ALA:HB1	1:A:1062:GLY:HA3	1.77	0.66
3:F:61:TYR:O	3:F:68:TYR:OH	2.13	0.66
1:A:928:ILE:HD13	1:A:928:ILE:N	2.09	0.66
3:F:658:GLU:O	3:F:720:GLN:NE2	2.28	0.66
1:A:1038:ARG:HG3	1:A:1038:ARG:NH1	2.10	0.66
6:E:301:PC1:H2H1	6:E:301:PC1:H3C1	1.77	0.66
3:F:512:GLY:HA2	3:F:625:VAL:O	1.95	0.66
1:A:599:ASN:HD22	1:A:601:PRO:HD2	1.60	0.66
5:A:1905:3PE:H321	5:A:1905:3PE:H221	1.77	0.66
3:F:217:ALA:HB2	3:F:240:VAL:HG21	1.76	0.66
3:F:248:GLN:NE2	3:F:447:GLN:O	2.29	0.66
1:A:309:TRP:CD2	6:E:301:PC1:H241	2.25	0.66
1:A:576:LEU:HD21	5:A:1906:3PE:H2D2	1.76	0.66
1:A:627:TYR:CE2	5:A:1906:3PE:H222	2.30	0.65
1:A:309:TRP:CH2	6:E:301:PC1:H241	2.32	0.65
1:A:307:ASN:O	1:A:307:ASN:ND2	2.30	0.65
1:A:647:CYS:CB	5:A:1905:3PE:H3H2	2.25	0.65
1:A:1409:TYR:OH	1:A:1428:ARG:NH1	2.29	0.65
1:A:627:TYR:CD2	5:A:1906:3PE:C22	2.77	0.65
1:A:1059:ILE:C	1:A:1059:ILE:HD12	2.17	0.64
5:A:1910:3PE:H2H2	5:A:1910:3PE:H3A2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:HB2	1:A:304:ALA:HB2	1.79	0.64
3:F:1006:PHE:HB3	3:F:1021:VAL:HG23	1.80	0.64
5:A:1910:3PE:H2H2	5:A:1910:3PE:C3A	2.27	0.63
1:A:65:CYS:SG	5:A:1907:3PE:H272	2.38	0.63
5:A:1902:3PE:H292	5:A:1902:3PE:H351	1.80	0.63
5:A:1903:3PE:HN1	5:A:1903:3PE:P	2.21	0.63
3:F:74:ASN:HD22	3:F:77:GLN:HG2	1.62	0.63
1:A:953:LYS:CE	1:A:1028:GLU:O	2.43	0.63
3:F:1005:ILE:H	3:F:1022:GLU:HG3	1.62	0.63
1:A:928:ILE:HD12	1:A:1063:PHE:CD1	2.33	0.63
3:F:638:ILE:O	3:F:644:GLN:NE2	2.30	0.63
1:A:1358:TYR:HB3	5:A:1904:3PE:O22	1.98	0.62
1:A:452:GLU:OE2	1:A:951:LYS:NZ	2.32	0.62
1:A:48:VAL:HG12	1:A:51:LYS:HD2	1.81	0.62
3:F:562:ASP:OD1	3:F:563:PHE:N	2.33	0.62
1:A:45:ILE:HD11	1:A:106:ILE:HG13	1.82	0.62
1:A:636:LEU:HD21	5:A:1905:3PE:H322	1.80	0.62
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.82	0.61
3:F:887:ARG:NH2	3:F:1032:ARG:O	2.33	0.61
5:A:1906:3PE:H12	5:A:1906:3PE:O22	1.98	0.61
3:F:697:ASN:HB3	3:F:700:CYS:HB3	1.82	0.61
1:A:210:TYR:CD1	1:A:313:TYR:CE2	2.87	0.61
1:A:1028:GLU:OE1	1:A:1028:GLU:HA	2.01	0.60
1:A:1041:MET:SD	5:A:1909:3PE:O12	2.60	0.60
1:A:942:PHE:HD1	1:A:1044:PHE:CE1	2.19	0.60
1:A:245:CYS:SG	1:A:246:ALA:N	2.75	0.60
1:A:215:LEU:O	1:A:219:LYS:HB2	2.02	0.59
1:A:1046:ILE:HD13	5:A:1908:3PE:H261	1.84	0.59
1:A:1359:TYR:CD2	5:A:1904:3PE:C23	2.83	0.59
3:F:114:ARG:NH2	3:F:116:ASP:O	2.35	0.59
1:A:453:HIS:CD2	1:A:456:GLN:HB3	2.38	0.59
1:A:604:LEU:CD1	5:A:1907:3PE:H331	2.32	0.59
3:F:987:ASP:OD1	3:F:988:ASN:N	2.35	0.59
1:A:524:ILE:HG22	1:A:528:ARG:HD2	1.85	0.59
3:F:854:VAL:HG23	3:F:1019:ILE:HG23	1.85	0.59
1:A:311:TRP:NE1	5:A:1910:3PE:H341	2.18	0.58
1:A:61:ILE:HG13	1:A:174:ARG:HB2	1.84	0.58
1:A:78:ASP:OD1	1:A:79:ASN:N	2.36	0.58
3:F:994:SER:HB3	3:F:1007:HIS:HD2	1.68	0.58
1:A:844:THR:HA	1:A:847:ILE:HG22	1.84	0.58
1:A:939:GLN:OE1	5:A:1904:3PE:H372	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:O	1:A:303:ASP:OD1	2.21	0.58
1:A:545:LEU:HD11	1:A:933:LEU:CD2	2.34	0.58
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.39	0.58
5:A:1902:3PE:H281	5:A:1902:3PE:C34	2.29	0.58
3:F:774:ASP:N	3:F:774:ASP:OD1	2.34	0.58
1:A:1082:ASP:OD1	1:A:1082:ASP:N	2.36	0.57
5:A:1909:3PE:H251	5:A:1909:3PE:H342	1.85	0.57
1:A:789:ARG:NH1	1:A:852:THR:O	2.32	0.57
1:A:1275:VAL:CG2	5:A:1910:3PE:C2I	2.67	0.57
5:A:1907:3PE:H381	5:A:1908:3PE:C25	2.34	0.57
1:A:643:ILE:HD12	5:A:1905:3PE:H3F1	1.85	0.57
1:A:1040:GLU:O	1:A:1040:GLU:HG2	2.00	0.57
3:F:793:SER:OG	3:F:818:LYS:NZ	2.33	0.57
1:A:91:TYR:OH	1:A:140:GLU:OE2	2.16	0.57
1:A:452:GLU:OE1	1:A:948:GLN:NE2	2.36	0.57
1:A:1046:ILE:HD13	5:A:1908:3PE:H242	1.86	0.56
1:A:226:CYS:HA	1:A:260:GLU:O	2.05	0.56
1:A:309:TRP:CZ3	6:E:301:PC1:H252	2.41	0.56
1:A:627:TYR:HE2	5:A:1906:3PE:H232	1.70	0.56
1:A:632:TYR:HA	5:A:1905:3PE:O12	2.05	0.56
1:A:522:LEU:CD2	5:A:1909:3PE:N	2.67	0.56
1:A:567:PHE:CD2	5:A:1907:3PE:H2B2	2.40	0.56
1:A:1275:VAL:HA	5:A:1910:3PE:H2I3	1.86	0.56
3:F:306:PHE:O	3:F:308:HIS:ND1	2.37	0.56
1:A:545:LEU:O	1:A:549:VAL:HG23	2.05	0.56
1:A:445:ASN:HB2	1:A:471:LEU:HD13	1.86	0.56
1:A:1046:ILE:HG21	5:A:1908:3PE:H261	1.87	0.56
3:F:48:ALA:HA	3:F:817:ILE:HD12	1.87	0.56
3:F:230:ARG:NH2	3:F:233:ASN:O	2.39	0.56
5:A:1907:3PE:H381	5:A:1908:3PE:H251	1.88	0.55
3:F:847:ASN:ND2	3:F:867:HIS:O	2.39	0.55
1:A:1059:ILE:HD12	1:A:1059:ILE:O	2.06	0.55
3:F:852:ASP:OD1	3:F:852:ASP:N	2.37	0.55
1:A:545:LEU:HD11	1:A:933:LEU:HD22	1.89	0.55
5:A:1907:3PE:H381	5:A:1908:3PE:H262	1.87	0.55
1:A:336:GLU:HA	1:A:339:LYS:HE3	1.89	0.54
1:A:1299:GLN:O	1:A:1304:ASN:ND2	2.39	0.54
3:F:308:HIS:CD2	3:F:351:VAL:HG11	2.40	0.54
1:A:1421:ASP:OD1	1:A:1424:THR:OG1	2.25	0.54
3:F:130:LYS:HB3	3:F:225:TRP:HB3	1.89	0.54
3:F:516:ALA:HB2	3:F:622:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:994:SER:HB3	3:F:1007:HIS:CD2	2.42	0.54
3:F:184:GLU:O	3:F:188:THR:OG1	2.16	0.54
1:A:1250:ALA:HB1	1:A:1253:VAL:HB	1.89	0.54
1:A:520:THR:O	1:A:523:GLY:N	2.34	0.54
1:A:947:VAL:O	1:A:951:LYS:HB2	2.08	0.54
1:A:244:PRO:HB2	1:A:304:ALA:CB	2.38	0.54
1:A:627:TYR:CE2	5:A:1906:3PE:H231	2.43	0.54
3:F:594:VAL:HG22	3:F:603:ASP:HB2	1.90	0.54
1:A:871:LEU:O	1:A:875:VAL:HG23	2.08	0.54
2:E:139:PRO:HA	2:E:142:MET:SD	2.49	0.53
1:A:627:TYR:HE2	5:A:1906:3PE:C23	2.17	0.53
1:A:833:GLY:O	1:A:837:ILE:HG13	2.09	0.53
1:A:627:TYR:CE2	5:A:1906:3PE:C22	2.91	0.53
3:F:503:THR:O	3:F:503:THR:OG1	2.25	0.53
1:A:983:MET:HG3	3:F:235:ILE:HD11	1.91	0.53
1:A:38:ASN:HB3	1:A:42:LYS:HG3	1.89	0.53
2:E:18:VAL:HA	2:E:21:VAL:HG12	1.91	0.53
3:F:993:PHE:HB2	3:F:1008:VAL:HG22	1.90	0.53
2:E:152:PHE:O	2:E:155:LEU:HB3	2.09	0.53
1:A:1068:PHE:CD2	1:A:1381:MET:HB3	2.44	0.53
5:A:1908:3PE:O14	5:A:1908:3PE:H122	2.10	0.52
3:F:52:SER:O	3:F:723:TRP:NE1	2.34	0.52
1:A:1099:ARG:HH22	1:A:1413:ALA:H	1.56	0.52
2:E:21:VAL:O	2:E:25:THR:HG23	2.08	0.52
3:F:852:ASP:HB3	3:F:867:HIS:CE1	2.44	0.52
1:A:1005:MET:O	1:A:1009:THR:HG23	2.10	0.52
2:E:18:VAL:O	2:E:22:LEU:HG	2.09	0.52
6:E:301:PC1:H3C1	6:E:301:PC1:C2H	2.39	0.52
3:F:56:GLN:O	3:F:60:ILE:HG23	2.09	0.52
2:E:138:ARG:HH21	2:E:205:PRO:HD3	1.74	0.52
1:A:1232:SER:O	1:A:1232:SER:OG	2.26	0.52
1:A:66:VAL:CG2	5:A:1907:3PE:H241	2.40	0.52
5:A:1902:3PE:O12	2:E:214:SER:HB2	2.09	0.52
1:A:957:CYS:SG	1:A:958:ASN:N	2.82	0.52
1:A:1354:THR:HG23	1:A:1356:PHE:HB3	1.92	0.52
6:E:301:PC1:H2E2	6:E:301:PC1:H391	1.92	0.52
3:F:500:LYS:HG2	3:F:525:LEU:HD11	1.92	0.52
3:F:596:SER:OG	3:F:598:ASP:O	2.28	0.52
3:F:865:ALA:HB3	3:F:871:THR:HB	1.92	0.52
3:F:37:VAL:HG11	3:F:1009:GLU:HG2	1.91	0.51
1:A:953:LYS:CG	1:A:1028:GLU:O	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:PHE:CE2	1:A:1377:VAL:CG1	2.93	0.51
3:F:366:GLY:HA2	3:F:401:ILE:HD13	1.92	0.51
3:F:825:ILE:O	3:F:829:THR:HG23	2.10	0.51
1:A:519:MET:SD	1:A:519:MET:N	2.83	0.51
1:A:309:TRP:CZ3	6:E:301:PC1:H241	2.46	0.51
1:A:989:GLN:HG3	1:A:991:ILE:HG23	1.93	0.51
3:F:49:LYS:HD2	3:F:55:HIS:CE1	2.45	0.51
1:A:309:TRP:CE2	6:E:301:PC1:C24	2.79	0.51
1:A:309:TRP:CD1	6:E:301:PC1:H222	2.46	0.51
3:F:656:PHE:O	3:F:660:GLY:N	2.39	0.51
1:A:323:PHE:HE2	5:A:1910:3PE:H3G1	1.76	0.51
3:F:297:ASN:O	3:F:297:ASN:ND2	2.44	0.51
1:A:61:ILE:HG12	1:A:97:PHE:CZ	2.46	0.51
1:A:652:LEU:HD11	1:A:1054:PHE:CE2	2.46	0.51
1:A:875:VAL:HG22	1:A:902:LEU:HB3	1.92	0.51
3:F:287:ASP:O	3:F:311:GLN:NE2	2.43	0.51
3:F:461:VAL:HG12	3:F:495:SER:HA	1.93	0.51
1:A:65:CYS:SG	5:A:1907:3PE:C27	2.99	0.50
3:F:711:ASP:OD1	3:F:712:ALA:N	2.43	0.50
1:A:820:ASP:OD1	1:A:828:ARG:NH2	2.38	0.50
1:A:1051:LEU:O	1:A:1055:PHE:N	2.44	0.50
1:A:545:LEU:CD1	1:A:930:ASN:HD21	2.25	0.50
1:A:931:ILE:CD1	1:A:1059:ILE:CD1	2.81	0.50
3:F:608:THR:O	3:F:608:THR:OG1	2.30	0.50
1:A:309:TRP:CE3	6:E:301:PC1:C25	2.94	0.50
1:A:1193:SER:O	1:A:1197:VAL:HG23	2.12	0.50
3:F:538:ILE:HG13	3:F:1042:ASP:HB3	1.93	0.50
1:A:643:ILE:CD1	5:A:1905:3PE:H3F1	2.42	0.50
1:A:1038:ARG:NH1	1:A:1038:ARG:CG	2.73	0.50
5:A:1907:3PE:H381	5:A:1908:3PE:C26	2.41	0.50
2:E:115:LEU:HA	2:E:118:LEU:HD12	1.94	0.49
3:F:628:THR:O	3:F:629:TYR:CG	2.65	0.49
1:A:794:ARG:HG3	1:A:795:ILE:HG13	1.93	0.49
1:A:1135:LEU:HD21	1:A:1239:ARG:HD3	1.94	0.49
3:F:895:TYR:HE1	3:F:986:PHE:CE1	2.30	0.49
1:A:57:ILE:HG13	1:A:100:GLU:HG3	1.93	0.49
1:A:627:TYR:CE2	5:A:1906:3PE:H232	2.46	0.49
1:A:1366:MET:HB2	5:A:1904:3PE:H2C1	1.95	0.49
5:A:1903:3PE:C31	5:A:1905:3PE:H11	2.38	0.49
3:F:130:LYS:HB2	3:F:228:ASN:HA	1.95	0.49
1:A:338:THR:O	1:A:342:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ALA:HA	1:A:664:LEU:HB3	1.93	0.49
1:A:901:VAL:HG21	1:A:1283:VAL:HG21	1.94	0.49
5:A:1905:3PE:P	5:A:1905:3PE:C3	2.94	0.49
5:A:1904:3PE:H341	5:A:1904:3PE:O32	2.12	0.49
5:A:1910:3PE:H2C1	5:A:1910:3PE:C2G	2.38	0.49
3:F:273:LEU:O	3:F:277:SER:OG	2.27	0.49
1:A:653:LEU:O	1:A:657:LEU:HB2	2.12	0.48
2:E:13:LEU:O	2:E:16:ILE:HG13	2.13	0.48
1:A:953:LYS:CD	1:A:1028:GLU:O	2.60	0.48
3:F:760:GLU:HG3	3:F:762:TYR:H	1.79	0.48
5:A:1906:3PE:C1	5:A:1906:3PE:H112	2.43	0.48
1:A:1395:GLY:HA3	1:A:1397:HIS:CE1	2.49	0.48
3:F:821:VAL:O	3:F:825:ILE:HG13	2.13	0.48
3:F:1066:ASN:OD1	3:F:1067:VAL:N	2.47	0.48
1:A:226:CYS:HB2	1:A:259:SER:HB2	1.93	0.48
3:F:313:ASN:OD1	3:F:316:ASN:ND2	2.47	0.48
3:F:645:ALA:O	3:F:649:GLU:HG2	2.13	0.48
3:F:692:ARG:HH11	3:F:693:LYS:HB2	1.79	0.48
3:F:792:GLU:N	3:F:792:GLU:OE1	2.46	0.48
1:A:309:TRP:N	1:A:310:PRO:HD3	2.17	0.48
1:A:938:LEU:HB3	1:A:1052:ILE:CD1	2.06	0.48
1:A:651:ILE:O	1:A:655:VAL:HG23	2.14	0.48
2:E:141:SER:OG	2:E:196:GLY:O	2.32	0.47
3:F:650:THR:O	3:F:745:ARG:NH1	2.47	0.47
1:A:309:TRP:CE3	1:A:309:TRP:HA	2.49	0.47
3:F:854:VAL:HG12	3:F:865:ALA:HA	1.97	0.47
1:A:522:LEU:CD2	5:A:1909:3PE:HN3	2.24	0.47
1:A:643:ILE:HD13	5:A:1905:3PE:C3D	2.32	0.47
3:F:885:LEU:HD21	3:F:1019:ILE:HD11	1.96	0.47
1:A:522:LEU:HD23	5:A:1909:3PE:HN2	1.74	0.47
3:F:484:GLN:HE22	3:F:1070:ASP:N	2.12	0.47
1:A:1020:LEU:HD11	1:A:1042:ALA:HA	1.96	0.47
3:F:802:GLU:HG2	3:F:811:LYS:HE2	1.96	0.47
3:F:909:PRO:HG3	3:F:975:GLN:HG3	1.97	0.47
2:E:154:SER:O	2:E:157:VAL:HG12	2.15	0.47
3:F:732:VAL:HG13	3:F:817:ILE:HG23	1.97	0.47
1:A:982:GLN:HG2	3:F:550:VAL:HG21	1.96	0.47
5:A:1903:3PE:H2A2	5:A:1903:3PE:H2D2	1.37	0.47
3:F:302:ASP:OD2	3:F:303:VAL:N	2.48	0.47
1:A:542:TRP:CD1	1:A:545:LEU:HD13	2.49	0.47
3:F:305:CYS:O	3:F:1047:CYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:206:ARG:NH1	2:E:207:MET:O	2.48	0.47
3:F:365:ASP:HB2	3:F:394:HIS:CD2	2.49	0.47
1:A:301:VAL:HG12	1:A:301:VAL:O	2.14	0.46
1:A:1185:PHE:HB2	5:A:1902:3PE:H372	1.96	0.46
3:F:58:VAL:HG22	3:F:801:VAL:HG13	1.97	0.46
1:A:874:LEU:O	1:A:878:VAL:HG13	2.15	0.46
3:F:434:ARG:HB2	3:F:435:PRO:HD3	1.96	0.46
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.97	0.46
1:A:328:LEU:O	1:A:332:VAL:HG22	2.15	0.46
1:A:333:LEU:HD13	1:A:333:LEU:HA	1.75	0.46
1:A:1154:ASN:ND2	1:A:1242:ARG:HH12	2.14	0.46
5:A:1903:3PE:H392	5:A:1905:3PE:H371	1.98	0.46
1:A:247:ARG:HG2	1:A:248:THR:HG23	1.98	0.46
1:A:1193:SER:OG	1:A:1242:ARG:NH2	2.48	0.46
3:F:420:ALA:O	3:F:424:ASN:ND2	2.39	0.46
3:F:694:THR:HG23	3:F:696:ASN:H	1.80	0.46
3:F:1041:SER:OG	3:F:1042:ASP:N	2.48	0.46
1:A:799:THR:O	1:A:803:ASN:HB3	2.16	0.46
3:F:805:ILE:HG22	3:F:806:GLN:HG3	1.96	0.46
1:A:823:ARG:NH1	1:A:1343:ASP:OD1	2.48	0.46
5:A:1907:3PE:H3A1	5:A:1907:3PE:H371	1.73	0.46
3:F:543:LEU:H	3:F:543:LEU:HD12	1.80	0.46
2:E:193:PHE:O	2:E:197:ILE:HG13	2.15	0.46
3:F:29:SER:OG	3:F:30:ALA:N	2.48	0.46
1:A:309:TRP:N	1:A:310:PRO:HD2	2.15	0.46
1:A:801:PHE:O	1:A:805:ILE:HG12	2.15	0.46
1:A:1277:LEU:HD22	1:A:1371:LEU:HD12	1.98	0.45
1:A:1329:LEU:HD12	1:A:1361:PHE:HB2	1.98	0.45
1:A:836:ASP:O	1:A:840:THR:HG22	2.17	0.45
1:A:56:ILE:HD13	1:A:56:ILE:HA	1.84	0.45
1:A:265:TRP:CD1	1:A:266:PRO:HD2	2.51	0.45
1:A:1135:LEU:HD11	1:A:1239:ARG:HG3	1.97	0.45
3:F:598:ASP:N	3:F:598:ASP:OD1	2.49	0.45
3:F:153:ASP:OD1	3:F:154:ASP:N	2.47	0.45
3:F:253:PRO:HG2	3:F:1059:PRO:HG2	1.98	0.45
1:A:319:LEU:O	1:A:323:PHE:HB2	2.17	0.45
2:E:24:MET:O	2:E:28:VAL:HG22	2.16	0.45
3:F:895:TYR:HE1	3:F:986:PHE:HE1	1.65	0.45
1:A:1156:ALA:O	1:A:1160:ILE:HG13	2.17	0.45
1:A:66:VAL:HG23	5:A:1907:3PE:H241	1.97	0.45
1:A:309:TRP:O	6:E:301:PC1:C32	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TRP:CD1	1:A:311:TRP:O	2.70	0.45
1:A:555:SER:O	1:A:558:SER:OG	2.32	0.45
1:A:1362:ILE:HD13	5:A:1904:3PE:H322	1.98	0.45
2:E:115:LEU:O	2:E:119:ILE:HG13	2.16	0.45
2:E:159:ARG:HH21	2:E:182:PHE:HZ	1.65	0.45
2:E:178:TYR:HB3	2:E:182:PHE:HB3	1.98	0.45
3:F:315:ARG:HH22	3:F:318:LYS:HD2	1.82	0.45
3:F:519:PRO:HD3	3:F:618:ASP:O	2.17	0.45
5:A:1910:3PE:H281	5:A:1910:3PE:H2B2	1.80	0.44
3:F:599:GLU:OE2	3:F:599:GLU:N	2.39	0.44
3:F:202:ASP:HB3	3:F:205:LEU:HD12	1.99	0.44
1:A:659:ILE:HD12	1:A:1055:PHE:HE1	1.81	0.44
1:A:847:ILE:HG12	1:A:873:LEU:HD12	1.98	0.44
3:F:990:SER:HB2	3:F:993:PHE:CZ	2.51	0.44
1:A:173:LEU:O	1:A:176:VAL:HG13	2.16	0.44
1:A:913:GLY:HA3	1:A:1269:TYR:CZ	2.51	0.44
1:A:1267:LEU:HD22	1:A:1378:ALA:HB1	1.98	0.44
5:A:1903:3PE:H322	5:A:1903:3PE:H31	1.74	0.44
3:F:564:LEU:HG	3:F:577:ARG:HD2	1.99	0.44
5:A:1903:3PE:O12	5:A:1903:3PE:H121	2.17	0.44
5:A:1906:3PE:H2C2	5:A:1906:3PE:H2F2	1.71	0.44
1:A:1390:ASP:HB3	1:A:1393:ILE:HG12	2.00	0.44
3:F:720:GLN:O	3:F:724:SER:OG	2.23	0.44
1:A:66:VAL:HG23	5:A:1907:3PE:C24	2.47	0.44
3:F:552:ASN:N	3:F:552:ASN:OD1	2.49	0.44
1:A:958:ASN:HB2	1:A:989:GLN:H	1.82	0.44
1:A:309:TRP:CG	6:E:301:PC1:H222	2.53	0.44
1:A:298:LEU:O	1:A:302:ASN:CB	2.66	0.43
1:A:559:ILE:HD13	1:A:659:ILE:HG21	2.00	0.43
1:A:1373:ILE:O	1:A:1377:VAL:HG23	2.19	0.43
3:F:85:ASP:HB3	3:F:502:LEU:HD22	1.99	0.43
3:F:449:THR:HG22	3:F:463:THR:H	1.82	0.43
3:F:512:GLY:CA	3:F:625:VAL:O	2.65	0.43
5:A:1903:3PE:O32	5:A:1905:3PE:C1	2.46	0.43
6:E:301:PC1:H261	6:E:301:PC1:H231	1.35	0.43
3:F:314:VAL:HG21	3:F:534:ILE:HD11	1.99	0.43
3:F:825:ILE:HG12	3:F:864:MET:SD	2.59	0.43
3:F:871:THR:O	3:F:871:THR:OG1	2.35	0.43
1:A:163:ALA:HB2	5:A:1906:3PE:H321	2.01	0.43
1:A:897:ARG:O	1:A:900:ARG:HG2	2.18	0.43
1:A:1185:PHE:O	1:A:1189:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:733:LYS:HE2	3:F:733:LYS:HB2	1.83	0.43
1:A:1027:ASN:HB3	1:A:1028:GLU:H	1.60	0.43
3:F:779:THR:HB	3:F:796:MET:HB3	1.99	0.43
1:A:94:LEU:HD11	1:A:133:GLY:HA3	2.00	0.43
1:A:41:ARG:HG3	1:A:42:LYS:HG2	2.01	0.43
1:A:309:TRP:CE3	6:E:301:PC1:H252	2.54	0.43
1:A:829:ASN:OD1	1:A:829:ASN:N	2.52	0.43
3:F:248:GLN:HG3	3:F:249:GLY:N	2.34	0.43
3:F:554:LYS:HE2	3:F:554:LYS:HB3	1.93	0.43
1:A:1112:TRP:O	1:A:1116:THR:HG22	2.19	0.43
3:F:470:ASN:HD21	3:F:482:LYS:NZ	2.17	0.43
5:A:1907:3PE:C11	5:A:1908:3PE:H111	2.49	0.42
1:A:1128:ILE:HG21	1:A:1246:LEU:HG	2.01	0.42
1:A:1263:SER:HB3	1:A:1383:ASN:HD21	1.84	0.42
2:E:144:TYR:O	2:E:147:ALA:HB3	2.19	0.42
3:F:207:TRP:NE1	3:F:458:LEU:HD22	2.35	0.42
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.54	0.42
5:A:1903:3PE:N	5:A:1903:3PE:P	2.81	0.42
3:F:126:TYR:CE2	3:F:128:ASN:HB2	2.54	0.42
3:F:444:LYS:HE3	3:F:466:LEU:HD21	2.01	0.42
3:F:297:ASN:C	3:F:299:ASN:H	2.22	0.42
3:F:497:GLU:O	3:F:501:ARG:HG3	2.20	0.42
3:F:771:LEU:HD23	3:F:771:LEU:HA	1.87	0.42
1:A:299:TYR:O	1:A:303:ASP:CG	2.57	0.42
1:A:439:ILE:HD13	1:A:439:ILE:HA	1.83	0.42
3:F:773:ASN:OD1	3:F:773:ASN:N	2.53	0.42
1:A:452:GLU:CD	1:A:948:GLN:HE22	2.22	0.42
3:F:1060:ASP:OD1	3:F:1060:ASP:N	2.42	0.42
1:A:1191:ILE:HD13	1:A:1191:ILE:HA	1.93	0.42
3:F:1042:ASP:OD2	3:F:1043:GLY:N	2.53	0.42
1:A:1288:MET:HG3	1:A:1356:PHE:CE2	2.54	0.42
3:F:52:SER:OG	3:F:53:GLY:N	2.53	0.42
3:F:607:ARG:NE	3:F:627:PRO:HB3	2.34	0.42
3:F:712:ALA:HB2	3:F:743:ILE:HG13	2.02	0.42
3:F:715:THR:HG22	3:F:745:ARG:HD2	2.02	0.42
1:A:559:ILE:HD13	1:A:659:ILE:CG2	2.49	0.42
1:A:1049:ILE:O	1:A:1049:ILE:HG22	2.20	0.41
1:A:237:VAL:HG23	1:A:240:GLU:HB2	2.01	0.41
2:E:12:THR:O	2:E:16:ILE:HG23	2.20	0.41
3:F:228:ASN:N	3:F:228:ASN:OD1	2.54	0.41
3:F:484:GLN:HE22	3:F:1070:ASP:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:O	1:A:203:VAL:HG23	2.20	0.41
1:A:659:ILE:HD12	1:A:1055:PHE:CE1	2.56	0.41
5:A:1904:3PE:C22	5:A:1904:3PE:C3	2.85	0.41
1:A:307:ASN:ND2	1:A:307:ASN:C	2.73	0.41
1:A:894:LYS:HD2	1:A:894:LYS:HA	1.91	0.41
1:A:1430:GLN:HB3	1:A:1432:PRO:HD2	2.02	0.41
5:A:1909:3PE:H281	5:A:1909:3PE:H252	1.72	0.41
3:F:207:TRP:HE1	3:F:458:LEU:HD22	1.85	0.41
3:F:516:ALA:HA	3:F:621:SER:O	2.20	0.41
3:F:857:ASP:OD1	3:F:857:ASP:N	2.53	0.41
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.87	0.41
3:F:888:HIS:O	3:F:892:ILE:HG23	2.20	0.41
1:A:305:ILE:O	1:A:305:ILE:HG23	2.20	0.41
1:A:1393:ILE:HG13	1:A:1394:LEU:N	2.30	0.41
3:F:144:SER:OG	3:F:145:GLN:N	2.53	0.41
3:F:449:THR:OG1	3:F:450:ASN:N	2.53	0.41
3:F:669:TYR:CE1	3:F:708:VAL:HG21	2.44	0.41
1:A:246:ALA:HB3	1:A:251:GLY:HA3	2.02	0.41
1:A:269:ASN:HB2	1:A:273:THR:OG1	2.19	0.41
1:A:928:ILE:HG22	1:A:932:VAL:HG13	2.02	0.41
2:E:176:TYR:HE2	2:E:178:TYR:CZ	2.39	0.41
3:F:590:PHE:CE2	3:F:592:THR:HB	2.56	0.41
1:A:174:ARG:HH21	1:A:174:ARG:HB3	1.85	0.41
1:A:571:ILE:CD1	5:A:1907:3PE:H2A2	2.46	0.41
1:A:584:ARG:CZ	5:A:1906:3PE:O12	2.67	0.41
1:A:1420:LEU:HD23	1:A:1420:LEU:HA	1.97	0.41
3:F:693:LYS:HZ3	3:F:697:ASN:HA	1.86	0.41
1:A:340:GLU:HA	1:A:343:LYS:HG2	2.02	0.41
1:A:919:GLN:O	1:A:923:VAL:HG23	2.21	0.41
5:A:1907:3PE:C11	5:A:1908:3PE:C11	2.99	0.41
1:A:340:GLU:OE1	1:A:343:LYS:HD2	2.21	0.40
1:A:608:PHE:O	1:A:612:THR:HG23	2.21	0.40
1:A:643:ILE:HD13	5:A:1905:3PE:C3E	2.50	0.40
1:A:974:VAL:HG21	1:A:986:ARG:HG3	2.04	0.40
1:A:1068:PHE:HE2	1:A:1377:VAL:C	2.24	0.40
1:A:1269:TYR:HA	1:A:1272:LEU:HB2	2.02	0.40
3:F:126:TYR:O	3:F:146:ARG:HA	2.21	0.40
3:F:552:ASN:HA	3:F:553:PRO:HD3	1.91	0.40
3:F:320:LEU:O	3:F:324:VAL:HG23	2.20	0.40
1:A:66:VAL:CG2	5:A:1907:3PE:C24	2.99	0.40
1:A:544:SER:O	1:A:548:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:TYR:HA	1:A:837:ILE:HD12	2.04	0.40
1:A:1068:PHE:HD2	1:A:1381:MET:HB3	1.85	0.40
1:A:1096:ARG:CZ	2:E:218:ALA:HB3	2.52	0.40
1:A:1181:PRO:HB2	5:A:1902:3PE:H321	2.03	0.40
2:E:14:PHE:O	2:E:18:VAL:HG23	2.21	0.40
3:F:260:VAL:HG13	3:F:274:ILE:HG21	2.04	0.40
3:F:376:ALA:O	3:F:380:LYS:HB2	2.21	0.40
3:F:261:ASP:O	3:F:266:VAL:HG21	2.21	0.40
1:A:901:VAL:HG13	1:A:901:VAL:O	2.21	0.40
1:A:1236:ARG:O	1:A:1239:ARG:HG2	2.22	0.40
5:A:1909:3PE:H232	5:A:1909:3PE:H261	1.69	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	1093/1873 (58%)	1028 (94%)	61 (6%)	4 (0%)	30	60
2	E	133/222 (60%)	127 (96%)	6 (4%)	0	100	100
3	F	968/1105 (88%)	891 (92%)	77 (8%)	0	100	100
All	All	2194/3200 (69%)	2046 (93%)	144 (7%)	4 (0%)	45	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	TRP
1	A	305	ILE
1	A	929	GLY
1	A	307	ASN

### 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	978/1628 (60%)	895 (92%)	83 (8%)	8	29
2	E	118/192 (62%)	112 (95%)	6 (5%)	20	46
3	F	868/973 (89%)	827 (95%)	41 (5%)	22	49
All	All	1964/2793 (70%)	1834 (93%)	130 (7%)	16	39

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	61	ILE
1	A	65	CYS
1	A	135	PHE
1	A	139	LEU
1	A	171	ARG
1	A	176	VAL
1	A	226	CYS
1	A	245	CYS
1	A	247	ARG
1	A	255	THR
1	A	274	HIS
1	A	289	ILE
1	A	305	ILE
1	A	307	ASN
1	A	308	GLU
1	A	311	TRP
1	A	312	ILE
1	A	324	PHE
1	A	333	LEU
1	A	433	VAL
1	A	436	TRP
1	A	437	LEU
1	A	453	HIS
1	A	468	ASN
1	A	491	TYR

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Mol	Chain	Res	Type
1	A	510	GLU
1	A	528	ARG
1	A	533	LEU
1	A	541	TYR
1	A	547	ASN
1	A	589	ASP
1	A	647	CYS
1	A	653	LEU
1	A	670	LEU
1	A	791	LEU
1	A	792	CYS
1	A	803	ASN
1	A	804	PHE
1	A	819	GLU
1	A	829	ASN
1	A	892	VAL
1	A	930	ASN
1	A	931	ILE
1	A	933	LEU
1	A	934	VAL
1	A	935	THR
1	A	936	THR
1	A	939	GLN
1	A	941	MET
1	A	964	THR
1	A	999	ASN
1	A	1007	LEU
1	A	1011	SER
1	A	1029	GLU
1	A	1036	ASN
1	A	1038	ARG
1	A	1041	MET
1	A	1047	ILE
1	A	1050	ILE
1	A	1051	LEU
1	A	1052	ILE
1	A	1054	PHE
1	A	1057	MET
1	A	1059	ILE
1	A	1060	PHE
1	A	1067	THR
1	A	1069	GLN

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Mol	Chain	Res	Type
1	A	1091	TYR
1	A	1108	GLN
1	A	1141	HIS
1	A	1149	ILE
1	A	1193	SER
1	A	1196	ASP
1	A	1235	PHE
1	A	1251	GLU
1	A	1272	LEU
1	A	1273	LEU
1	A	1289	PHE
1	A	1295	VAL
1	A	1381	MET
1	A	1397	HIS
1	A	1400	ASP
2	E	117	PHE
2	E	120	MET
2	E	134	ASP
2	E	136	LEU
2	E	157	VAL
2	E	177	TYR
3	F	32	THR
3	F	59	ASP
3	F	61	TYR
3	F	76	ARG
3	F	94	SER
3	F	116	ASP
3	F	136	GLU
3	F	148	LYS
3	F	157	PHE
3	F	158	ARG
3	F	159	ARG
3	F	200	GLU
3	F	205	LEU
3	F	241	ARG
3	F	270	THR
3	F	303	VAL
3	F	360	ILE
3	F	478	LYS
3	F	543	LEU
3	F	610	THR
3	F	652	LYS

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Mol	Chain	Res	Type
3	F	661	TYR
3	F	673	LEU
3	F	677	ASP
3	F	680	THR
3	F	692	ARG
3	F	694	THR
3	F	711	ASP
3	F	729	ILE
3	F	735	ARG
3	F	739	THR
3	F	744	THR
3	F	853	CYS
3	F	997	LEU
3	F	1002	CYS
3	F	1014	THR
3	F	1019	ILE
3	F	1062	CYS
3	F	1068	LEU
3	F	1070	ASP
3	F	1074	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	302	ASN
1	A	307	ASN
1	A	453	HIS
1	A	547	ASN
1	A	599	ASN
1	A	797	ASN
1	A	930	ASN
1	A	999	ASN
1	A	1085	GLN
1	A	1108	GLN
1	A	1138	GLN
1	A	1154	ASN
3	F	55	HIS
3	F	65	GLN
3	F	74	ASN
3	F	120	ASN
3	F	299	ASN

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Mol	Chain	Res	Type
3	F	307	GLN
3	F	316	ASN
3	F	470	ASN
3	F	484	GLN
3	F	511	ASN
3	F	679	ASN
3	F	685	ASN
3	F	728	ASN
3	F	847	ASN
3	F	872	ASN
3	F	983	GLN
3	F	1007	HIS
3	F	1039	GLN
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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	1902	-	32,32,50	1.15	2 (6%)	35,37,55	1.19	3 (8%)
5	3PE	A	1903	-	50,50,50	0.92	2 (4%)	53,55,55	1.11	4 (7%)
5	3PE	A	1910	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
5	3PE	A	1904	-	40,40,50	1.02	2 (5%)	43,45,55	1.12	4 (9%)
5	3PE	A	1908	-	20,20,50	1.06	1 (5%)	22,23,55	0.94	1 (4%)
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.15	3 (7%)
5	3PE	A	1905	-	50,50,50	0.93	2 (4%)	53,55,55	1.06	4 (7%)
6	PC1	E	301	-	53,53,53	0.94	2 (3%)	59,61,61	1.02	3 (5%)
5	3PE	A	1906	-	43,43,50	0.99	2 (4%)	46,48,55	1.04	2 (4%)
5	3PE	A	1909	-	31,31,50	1.17	2 (6%)	34,36,55	1.22	4 (11%)

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	1902	-	-	15/36/36/54	-
5	3PE	A	1903	-	-	27/54/54/54	-
5	3PE	A	1910	-	-	28/54/54/54	-
5	3PE	A	1904	-	-	25/44/44/54	-
5	3PE	A	1908	-	-	13/21/21/54	-
5	3PE	A	1907	-	-	22/41/41/54	-
5	3PE	A	1905	-	-	24/54/54/54	-
6	PC1	E	301	-	-	34/57/57/57	-
5	3PE	A	1906	-	-	24/47/47/54	-
5	3PE	A	1909	-	-	17/35/35/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1907	3PE	O31-C31	4.31	1.45	1.33
5	A	1908	3PE	O21-C21	4.31	1.45	1.33
5	A	1909	3PE	O31-C31	4.30	1.45	1.33
5	A	1910	3PE	O31-C31	4.29	1.45	1.33
5	A	1903	3PE	O31-C31	4.29	1.45	1.33
5	A	1905	3PE	O31-C31	4.28	1.45	1.33
5	A	1906	3PE	O31-C31	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1902	3PE	O31-C31	4.25	1.45	1.33
6	E	301	PC1	O31-C31	4.24	1.45	1.33
5	A	1904	3PE	O31-C31	4.22	1.45	1.33
6	E	301	PC1	O21-C21	4.14	1.46	1.34
5	A	1902	3PE	O21-C21	4.10	1.45	1.34
5	A	1905	3PE	O21-C21	4.08	1.45	1.34
5	A	1906	3PE	O21-C21	4.06	1.45	1.34
5	A	1907	3PE	O21-C21	4.05	1.45	1.34
5	A	1904	3PE	O21-C21	4.04	1.45	1.34
5	A	1909	3PE	O21-C21	4.04	1.45	1.34
5	A	1910	3PE	O21-C21	4.03	1.45	1.34
5	A	1903	3PE	O21-C21	4.02	1.45	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1903	3PE	O21-C21-C22	4.32	120.82	111.48
5	A	1905	3PE	O21-C21-C22	4.26	120.70	111.48
5	A	1902	3PE	O21-C21-C22	4.14	120.43	111.48
5	A	1904	3PE	O21-C21-C22	4.12	120.40	111.48
5	A	1907	3PE	O21-C21-C22	4.10	120.36	111.48
5	A	1909	3PE	O21-C21-C22	4.07	120.29	111.48
6	E	301	PC1	O21-C21-C22	3.97	120.08	111.48
5	A	1910	3PE	O21-C21-C22	3.92	119.97	111.48
5	A	1906	3PE	O21-C21-C22	3.69	119.47	111.48
5	A	1903	3PE	C2-O21-C21	-2.93	110.77	117.80
5	A	1903	3PE	O31-C31-C32	2.91	120.70	111.83
5	A	1907	3PE	O31-C31-C32	2.88	120.61	111.83
5	A	1910	3PE	O31-C31-C32	2.87	120.59	111.83
5	A	1906	3PE	O31-C31-C32	2.85	120.53	111.83
5	A	1905	3PE	O31-C31-C32	2.82	120.44	111.83
6	E	301	PC1	O31-C31-C32	2.81	120.39	111.83
5	A	1908	3PE	O21-C21-C22	2.78	120.32	111.83
5	A	1904	3PE	O31-C31-C32	2.73	120.16	111.83
5	A	1902	3PE	O31-C31-C32	2.71	120.11	111.83
5	A	1909	3PE	O31-C31-C32	2.71	120.11	111.83
5	A	1909	3PE	C2-O21-C21	-2.68	111.39	117.80
5	A	1902	3PE	C2-O21-C21	-2.57	111.65	117.80
5	A	1910	3PE	C2-O21-C21	-2.43	111.97	117.80
5	A	1907	3PE	C2-O21-C21	-2.34	112.18	117.80
5	A	1904	3PE	C2-O21-C21	-2.31	112.27	117.80
5	A	1905	3PE	C2-O21-C21	-2.31	112.28	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	PC1	C2-O21-C21	-2.24	112.44	117.80
5	A	1903	3PE	O21-C21-O22	-2.16	118.66	123.70
5	A	1905	3PE	O21-C21-O22	-2.08	118.85	123.70
5	A	1904	3PE	O21-C21-O22	-2.03	118.97	123.70
5	A	1909	3PE	O21-C21-O22	-2.01	119.01	123.70

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1902	3PE	C11-O13-P-O14
5	A	1903	3PE	C1-O11-P-O12
5	A	1903	3PE	C12-C11-O13-P
5	A	1903	3PE	O32-C31-O31-C3
5	A	1903	3PE	C32-C31-O31-C3
5	A	1904	3PE	C1-O11-P-O12
5	A	1904	3PE	O22-C21-O21-C2
5	A	1904	3PE	C22-C21-O21-C2
5	A	1905	3PE	C1-O11-P-O12
5	A	1905	3PE	C1-O11-P-O13
5	A	1905	3PE	C1-O11-P-O14
5	A	1905	3PE	C11-O13-P-O11
5	A	1905	3PE	C11-O13-P-O12
5	A	1905	3PE	C2-C1-O11-P
5	A	1905	3PE	O32-C31-O31-C3
5	A	1905	3PE	C32-C31-O31-C3
5	A	1905	3PE	O22-C21-O21-C2
5	A	1905	3PE	C22-C21-O21-C2
5	A	1906	3PE	O13-C11-C12-N
5	A	1907	3PE	C1-O11-P-O12
5	A	1907	3PE	C1-O11-P-O13
5	A	1907	3PE	C11-O13-P-O12
5	A	1908	3PE	C1-O11-P-O13
5	A	1908	3PE	C12-C11-O13-P
5	A	1908	3PE	O13-C11-C12-N
5	A	1909	3PE	C1-O11-P-O13
5	A	1909	3PE	C11-O13-P-O11
5	A	1909	3PE	C11-O13-P-O12
5	A	1909	3PE	O13-C11-C12-N
5	A	1910	3PE	C11-O13-P-O11
5	A	1910	3PE	C11-O13-P-O12
5	A	1910	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
5	A	1910	3PE	C12-C11-O13-P
6	E	301	PC1	C11-O13-P-O14
6	E	301	PC1	C12-C11-O13-P
5	A	1906	3PE	O32-C31-O31-C3
5	A	1907	3PE	O32-C31-O31-C3
5	A	1906	3PE	C32-C31-O31-C3
5	A	1907	3PE	C32-C31-O31-C3
6	E	301	PC1	C2-C3-O31-C31
5	A	1904	3PE	C32-C31-O31-C3
5	A	1909	3PE	C22-C21-O21-C2
5	A	1904	3PE	O32-C31-O31-C3
5	A	1907	3PE	C37-C38-C39-C3A
6	E	301	PC1	C23-C24-C25-C26
5	A	1909	3PE	O22-C21-O21-C2
5	A	1909	3PE	C32-C31-O31-C3
5	A	1910	3PE	C32-C31-O31-C3
5	A	1903	3PE	C2A-C2B-C2C-C2D
5	A	1910	3PE	O32-C31-O31-C3
5	A	1903	3PE	C21-C22-C23-C24
5	A	1906	3PE	C31-C32-C33-C34
5	A	1905	3PE	C21-C22-C23-C24
5	A	1902	3PE	C31-C32-C33-C34
5	A	1904	3PE	C21-C22-C23-C24
5	A	1909	3PE	O32-C31-O31-C3
6	E	301	PC1	C31-C32-C33-C34
5	A	1909	3PE	C25-C26-C27-C28
5	A	1906	3PE	C2C-C2D-C2E-C2F
5	A	1907	3PE	C22-C21-O21-C2
5	A	1906	3PE	C1-C2-O21-C21
5	A	1907	3PE	O22-C21-O21-C2
5	A	1906	3PE	C22-C21-O21-C2
5	A	1909	3PE	C23-C24-C25-C26
5	A	1904	3PE	C33-C34-C35-C36
6	E	301	PC1	C2C-C2D-C2E-C2F
6	E	301	PC1	C38-C39-C3A-C3B
5	A	1909	3PE	C22-C23-C24-C25
5	A	1903	3PE	C2D-C2E-C2F-C2G
5	A	1904	3PE	C25-C26-C27-C28
6	E	301	PC1	C2B-C2C-C2D-C2E
5	A	1910	3PE	C23-C24-C25-C26
6	E	301	PC1	C36-C37-C38-C39
5	A	1907	3PE	C27-C28-C29-C2A

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

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Mol	Chain	Res	Type	Atoms
5	A	1908	3PE	C24-C25-C26-C27
6	E	301	PC1	C28-C29-C2A-C2B
5	A	1907	3PE	C35-C36-C37-C38
5	A	1904	3PE	C2D-C2E-C2F-C2G
5	A	1903	3PE	C31-C32-C33-C34
5	A	1907	3PE	C26-C27-C28-C29
5	A	1910	3PE	C33-C34-C35-C36
6	E	301	PC1	C35-C36-C37-C38
5	A	1908	3PE	C23-C24-C25-C26
5	A	1904	3PE	C28-C29-C2A-C2B
5	A	1905	3PE	C2A-C2B-C2C-C2D
5	A	1910	3PE	C35-C36-C37-C38
5	A	1905	3PE	C39-C3A-C3B-C3C
5	A	1906	3PE	C27-C28-C29-C2A
6	E	301	PC1	C24-C25-C26-C27
5	A	1903	3PE	C2F-C2G-C2H-C2I
5	A	1906	3PE	O21-C21-C22-C23
5	A	1910	3PE	C2F-C2G-C2H-C2I
5	A	1910	3PE	C38-C39-C3A-C3B
5	A	1903	3PE	C38-C39-C3A-C3B
5	A	1902	3PE	O11-C1-C2-C3
5	A	1910	3PE	O11-C1-C2-C3
5	A	1906	3PE	C38-C39-C3A-C3B
5	A	1910	3PE	C24-C25-C26-C27
5	A	1902	3PE	C1-C2-C3-O31
5	A	1906	3PE	C29-C2A-C2B-C2C
5	A	1910	3PE	O11-C1-C2-O21
6	E	301	PC1	O21-C2-C3-O31
5	A	1903	3PE	C36-C37-C38-C39
5	A	1902	3PE	C32-C33-C34-C35
5	A	1904	3PE	C27-C28-C29-C2A
5	A	1905	3PE	C2C-C2D-C2E-C2F
5	A	1903	3PE	C34-C35-C36-C37
5	A	1910	3PE	C39-C3A-C3B-C3C
5	A	1905	3PE	O11-C1-C2-C3
6	E	301	PC1	C2A-C2B-C2C-C2D
5	A	1910	3PE	C26-C27-C28-C29
5	A	1907	3PE	C3-C2-O21-C21
5	A	1903	3PE	C3C-C3D-C3E-C3F
6	E	301	PC1	C1-C2-C3-O31
5	A	1905	3PE	C2F-C2G-C2H-C2I
6	E	301	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
5	A	1909	3PE	C2-C1-O11-P
6	E	301	PC1	O13-C11-C12-N
5	A	1905	3PE	C2B-C2C-C2D-C2E
5	A	1910	3PE	C2A-C2B-C2C-C2D
5	A	1907	3PE	C36-C37-C38-C39
5	A	1902	3PE	O11-C1-C2-O21
5	A	1905	3PE	O11-C1-C2-O21
5	A	1902	3PE	O21-C2-C3-O31
5	A	1902	3PE	C1-O11-P-O14
5	A	1902	3PE	C11-O13-P-O11
5	A	1902	3PE	C11-O13-P-O12
5	A	1903	3PE	C1-O11-P-O13
5	A	1903	3PE	C1-O11-P-O14
5	A	1904	3PE	C1-O11-P-O13
5	A	1904	3PE	O13-C11-C12-N
5	A	1905	3PE	O13-C11-C12-N
5	A	1907	3PE	O13-C11-C12-N
5	A	1908	3PE	C1-O11-P-O14
5	A	1909	3PE	C1-O11-P-O14
5	A	1907	3PE	C2-C1-O11-P
5	A	1903	3PE	C3-C2-O21-C21
5	A	1910	3PE	C2C-C2D-C2E-C2F
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1903	3PE	O21-C2-C3-O31
5	A	1908	3PE	C26-C27-C28-C29
5	A	1910	3PE	C25-C26-C27-C28
5	A	1910	3PE	C37-C38-C39-C3A
5	A	1910	3PE	C32-C33-C34-C35
5	A	1907	3PE	C25-C26-C27-C28
6	E	301	PC1	C32-C31-O31-C3
5	A	1906	3PE	O22-C21-C22-C23
6	E	301	PC1	O32-C31-O31-C3
6	E	301	PC1	C2F-C2G-C2H-C2I
5	A	1910	3PE	O21-C2-C3-O31
5	A	1906	3PE	C23-C24-C25-C26
5	A	1903	3PE	C25-C26-C27-C28
5	A	1907	3PE	C33-C34-C35-C36
5	A	1908	3PE	O11-C1-C2-O21
5	A	1908	3PE	C21-C22-C23-C24
5	A	1906	3PE	C26-C27-C28-C29
6	E	301	PC1	C11-C12-N-C15
5	A	1909	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
5	A	1910	3PE	C3D-C3E-C3F-C3G
5	A	1908	3PE	C1-C2-O21-C21
5	A	1906	3PE	C36-C37-C38-C39
5	A	1904	3PE	C1-C2-C3-O31
5	A	1910	3PE	C3A-C3B-C3C-C3D
5	A	1907	3PE	C29-C2A-C2B-C2C
6	E	301	PC1	C3B-C3C-C3D-C3E
5	A	1904	3PE	O21-C2-C3-O31
5	A	1904	3PE	O11-C1-C2-C3
5	A	1907	3PE	O11-C1-C2-C3
5	A	1902	3PE	O22-C21-O21-C2
5	A	1906	3PE	C34-C35-C36-C37
5	A	1906	3PE	C37-C38-C39-C3A
5	A	1909	3PE	C27-C28-C29-C2A
5	A	1904	3PE	C26-C27-C28-C29
5	A	1903	3PE	C1-C2-C3-O31
5	A	1903	3PE	C26-C27-C28-C29
5	A	1902	3PE	C22-C21-O21-C2
6	E	301	PC1	C22-C23-C24-C25
5	A	1905	3PE	C25-C26-C27-C28
5	A	1908	3PE	O21-C21-C22-C23
5	A	1904	3PE	C1-C2-O21-C21
5	A	1904	3PE	C3-C2-O21-C21
5	A	1903	3PE	C2-C1-O11-P
5	A	1907	3PE	O11-C1-C2-O21
6	E	301	PC1	C11-C12-N-C14
6	E	301	PC1	O22-C21-O21-C2
5	A	1910	3PE	C27-C28-C29-C2A
5	A	1908	3PE	O22-C21-C22-C23

There are no ring outliers.

10 monomers are involved in 153 short contacts:

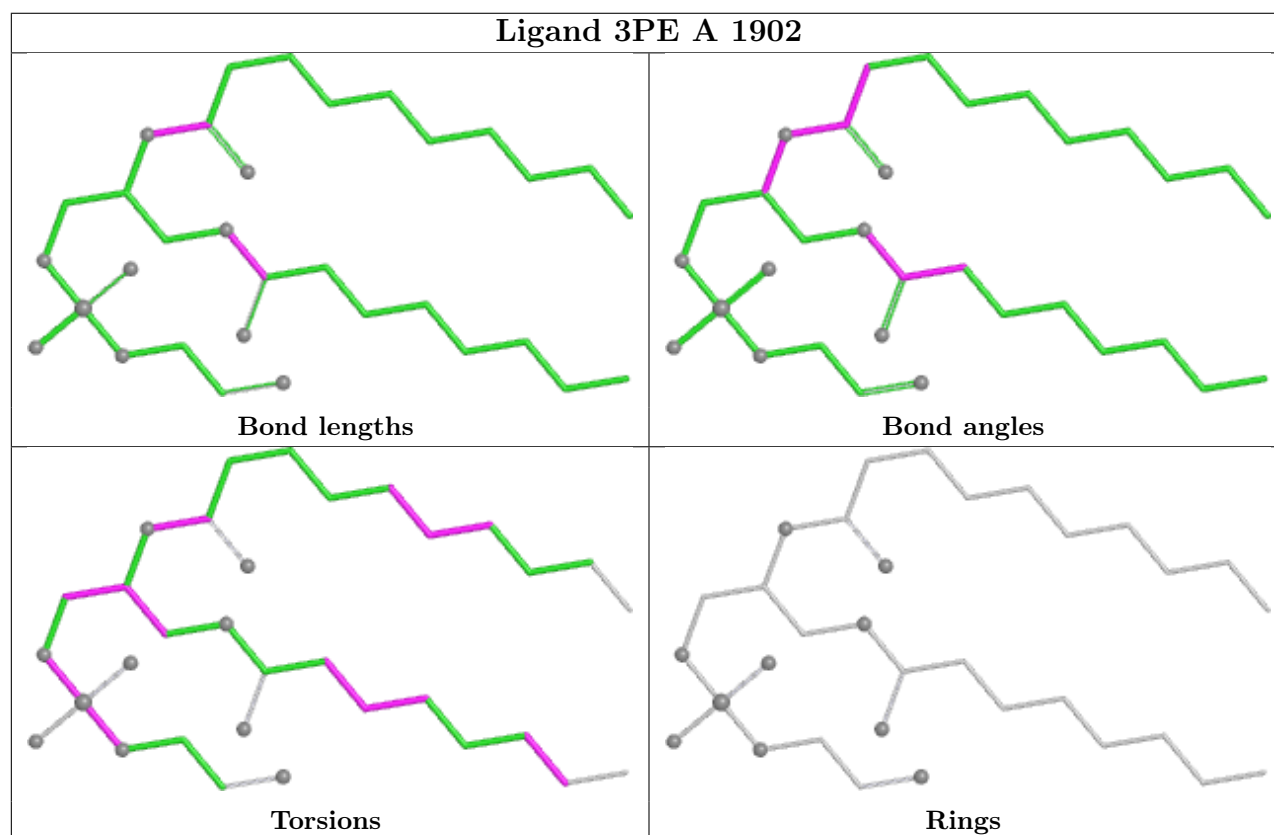
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1902	3PE	6	0
5	A	1903	3PE	10	0
5	A	1910	3PE	15	0
5	A	1904	3PE	15	0
5	A	1908	3PE	11	0
5	A	1907	3PE	25	0
5	A	1905	3PE	24	0
6	E	301	PC1	28	0

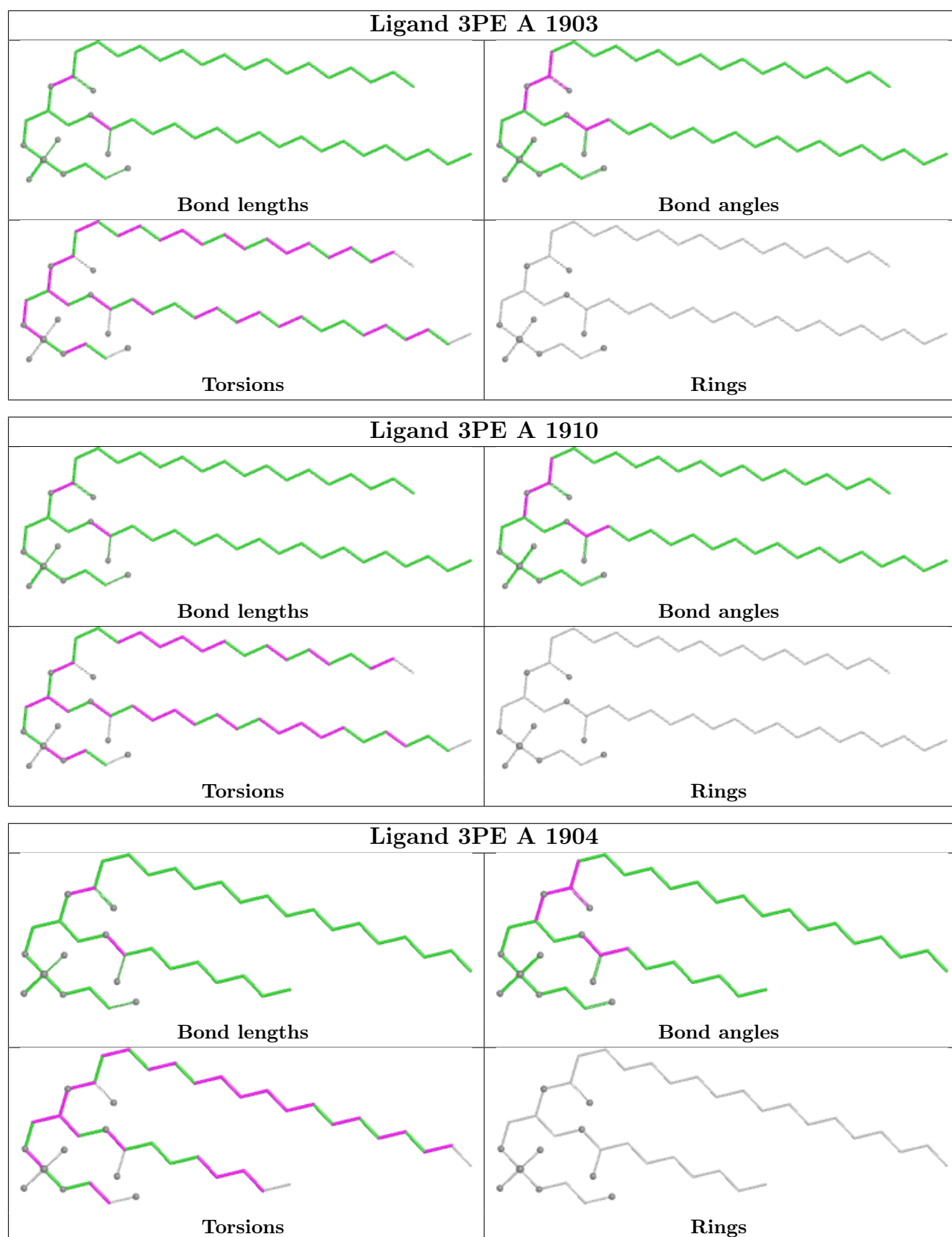
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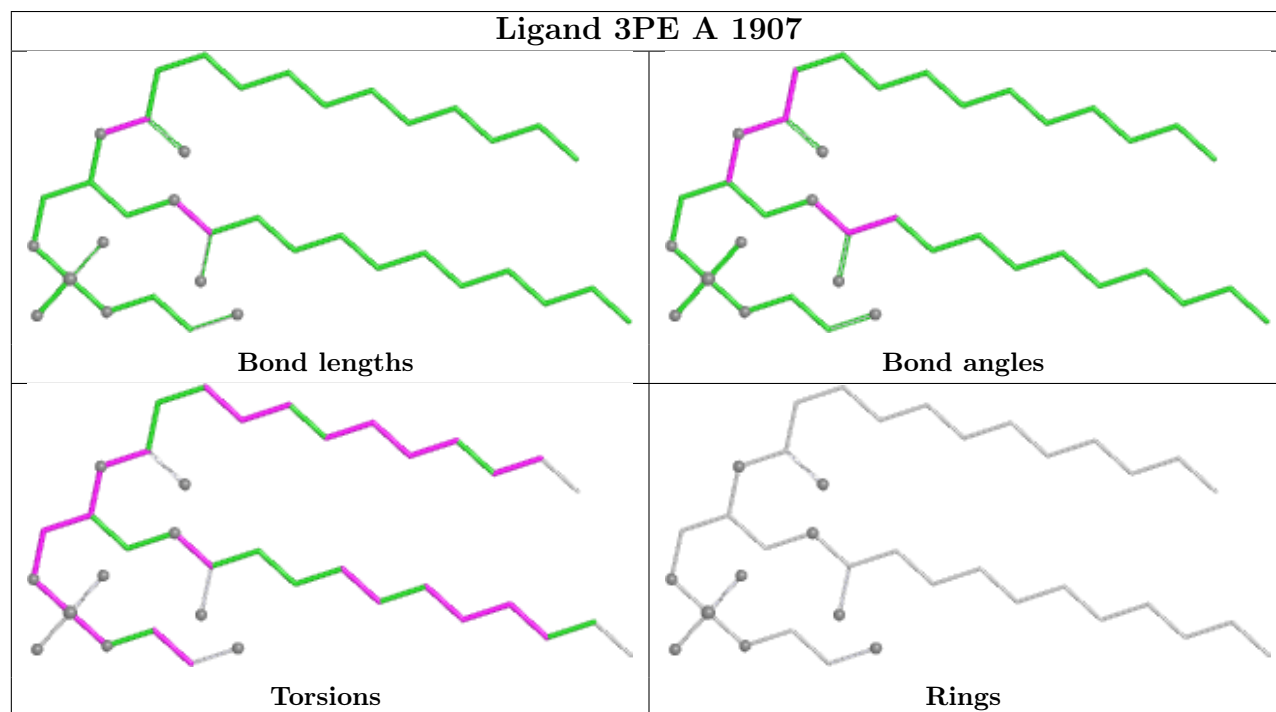
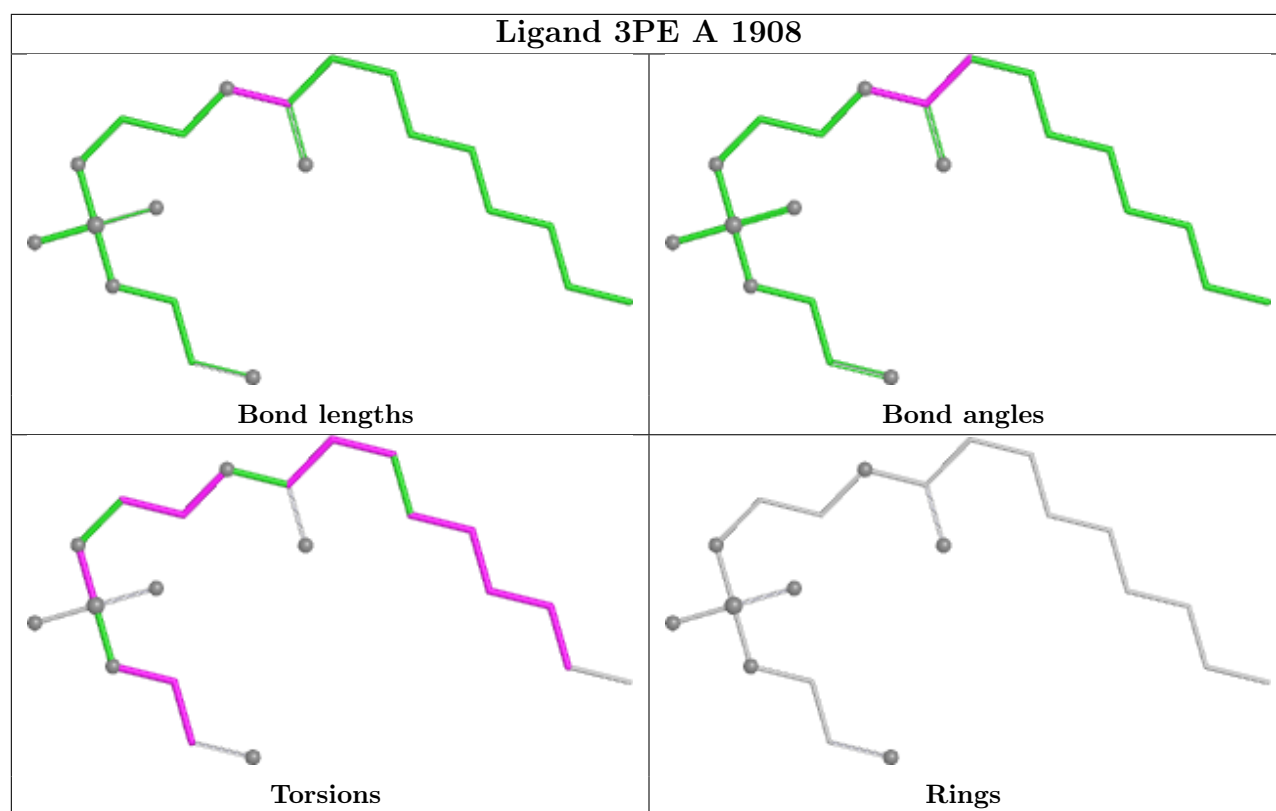
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1906	3PE	18	0
5	A	1909	3PE	11	0

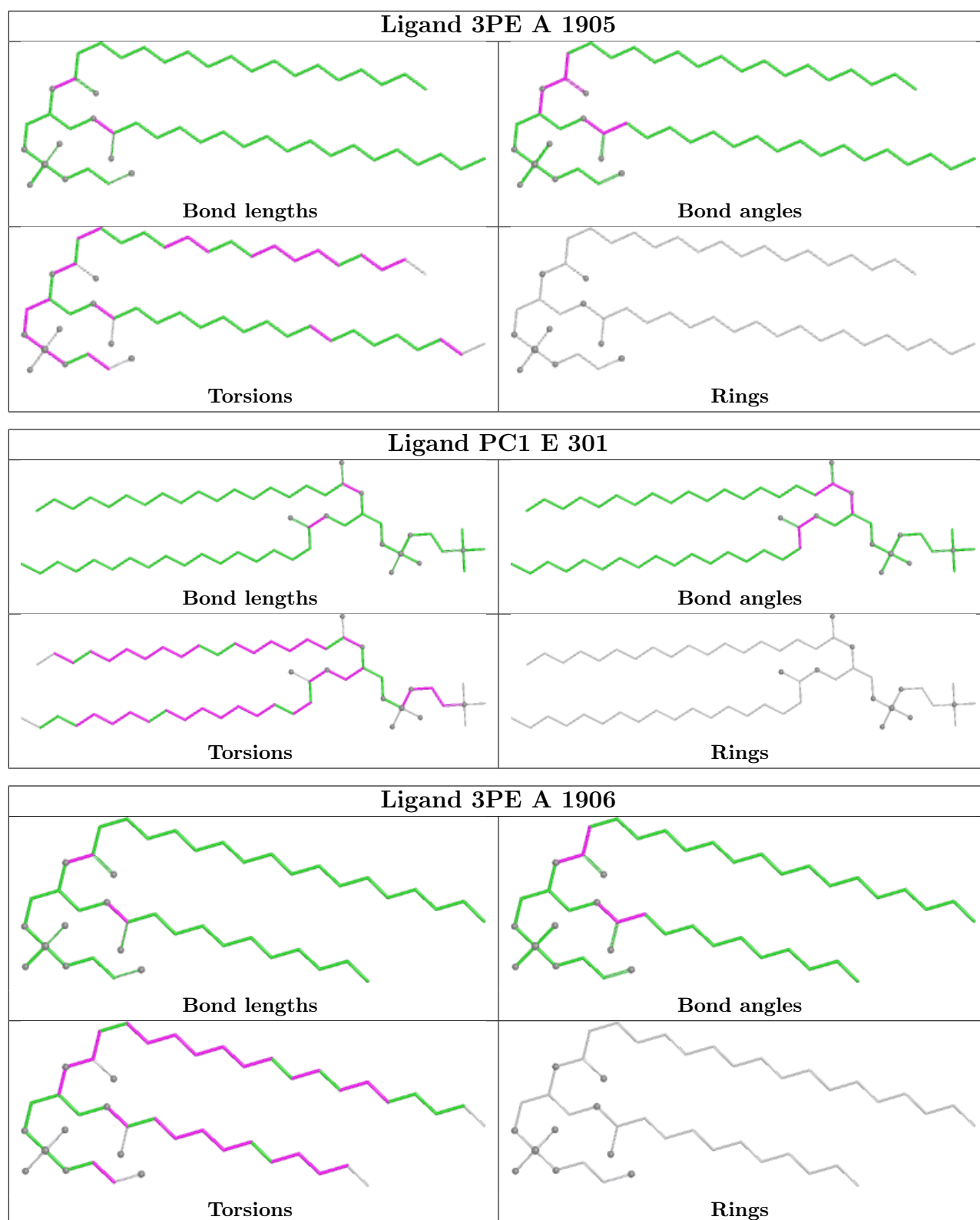
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

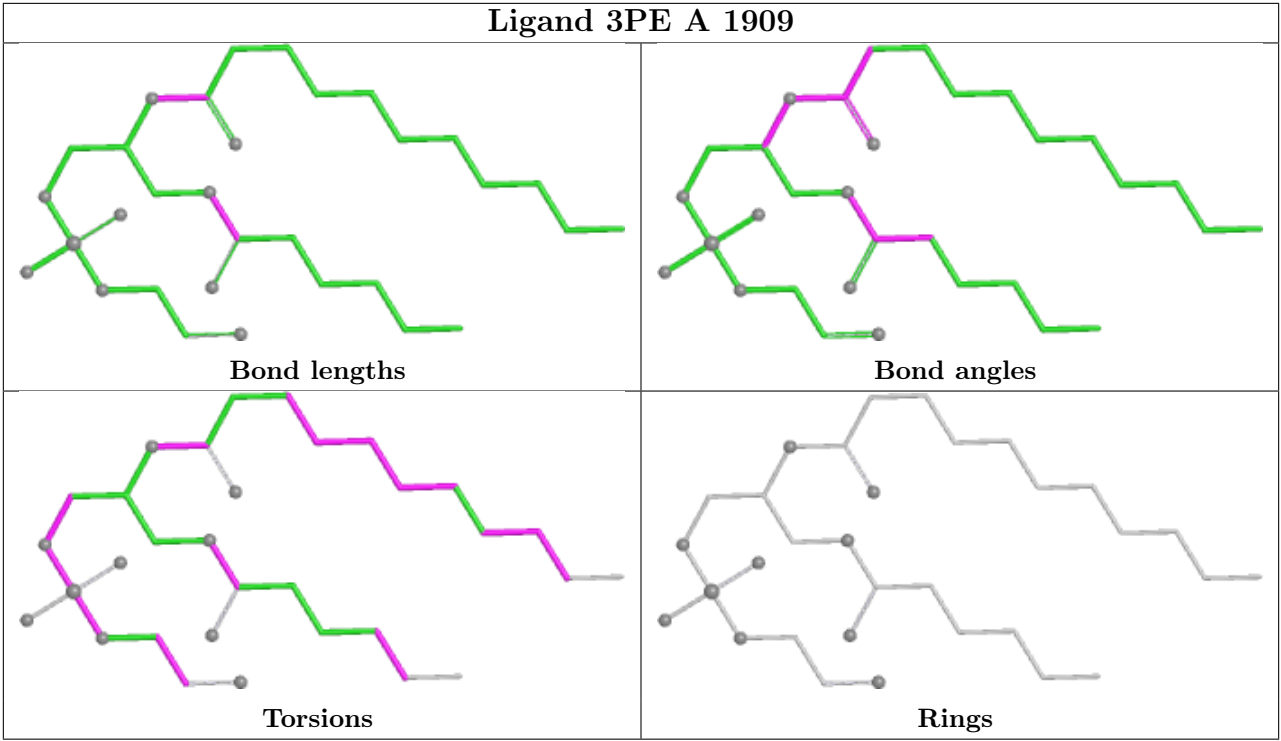












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1036:ASN	C	1037:ASN	N	1.04

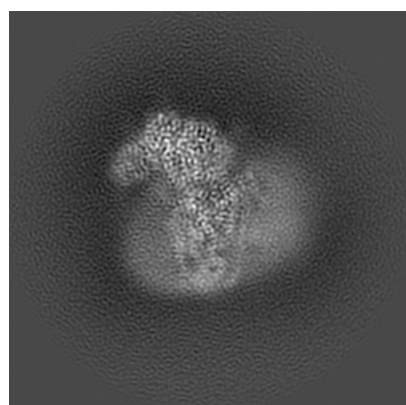
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22424. These allow visual inspection of the internal detail of the map and identification of artifacts.

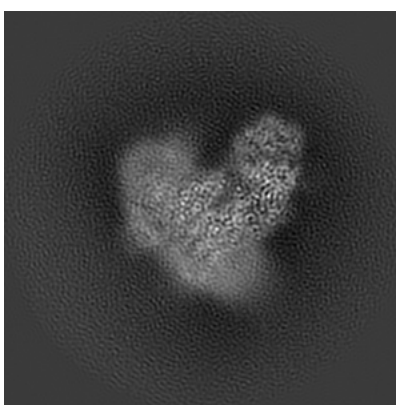
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

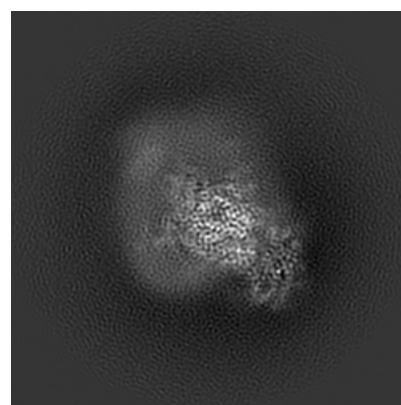
#### 6.1.1 Primary map



X



Y

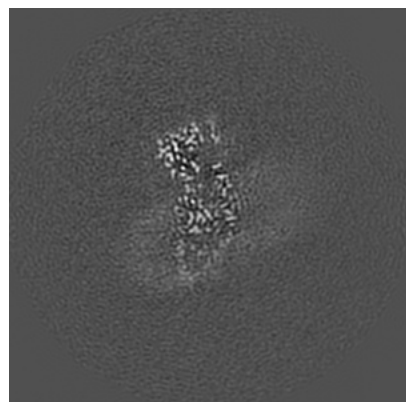


Z

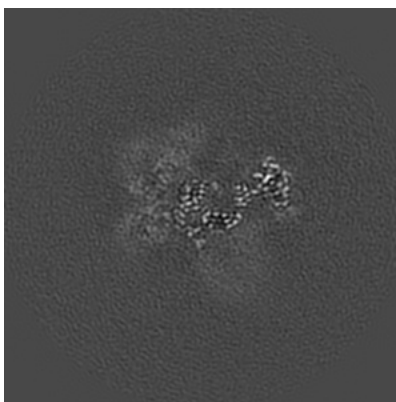
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

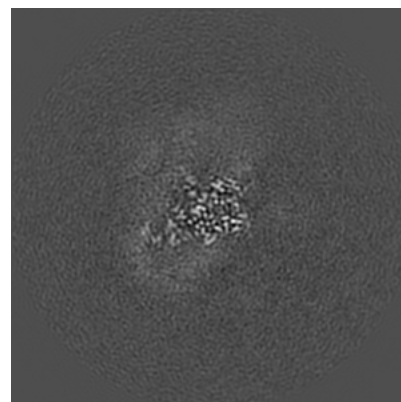
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

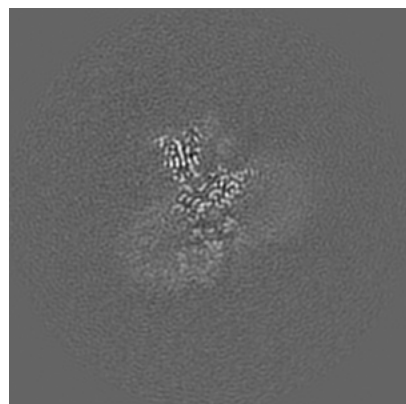


Z Index: 140

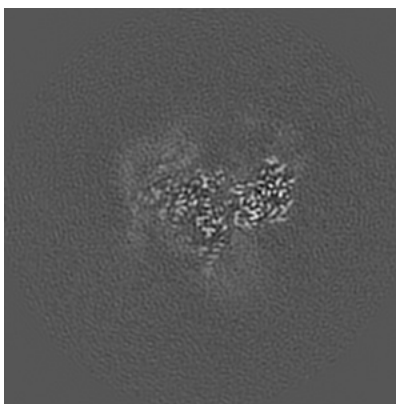
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

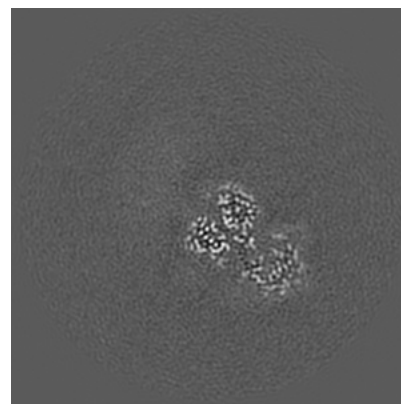
### 6.3.1 Primary map



X Index: 136



Y Index: 130

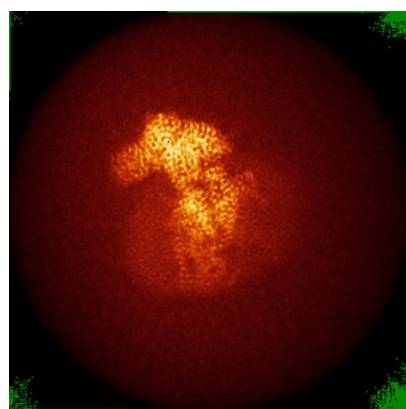


Z Index: 181

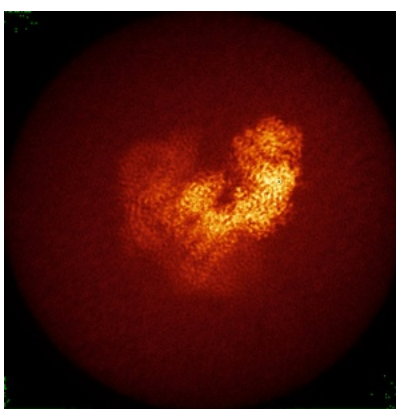
The images above show the largest variance slices of the map in three orthogonal directions.

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

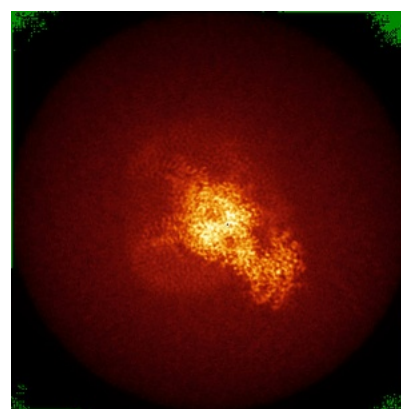
### 6.4.1 Primary map



X



Y

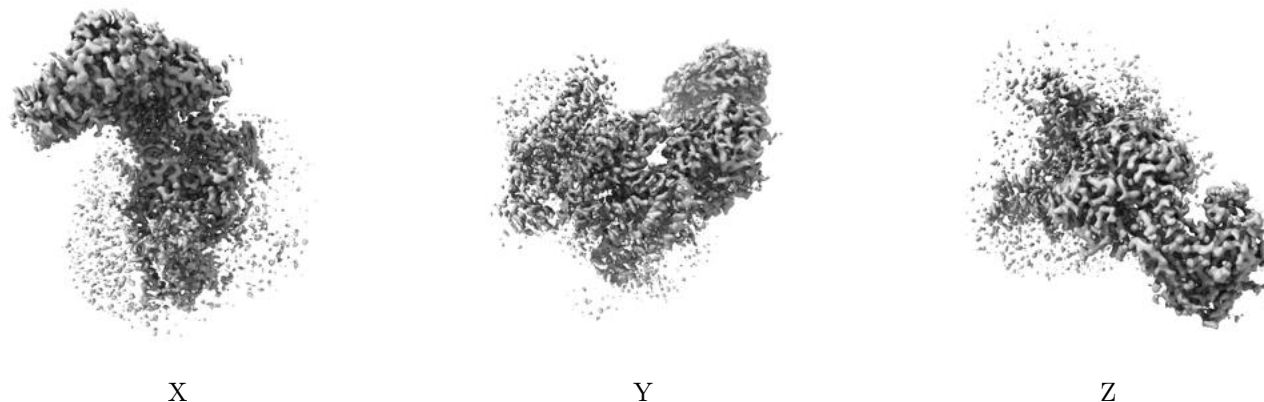


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

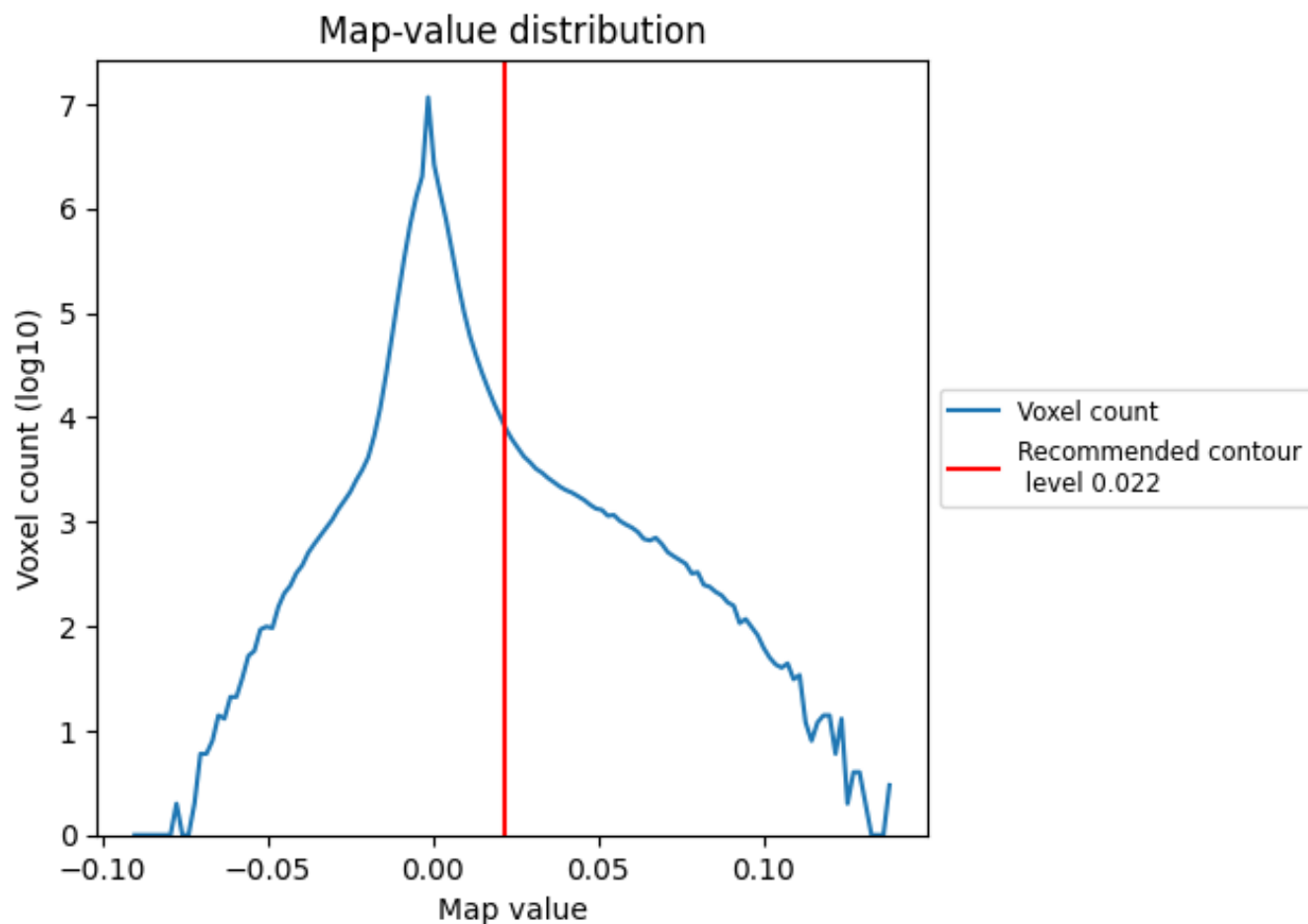
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

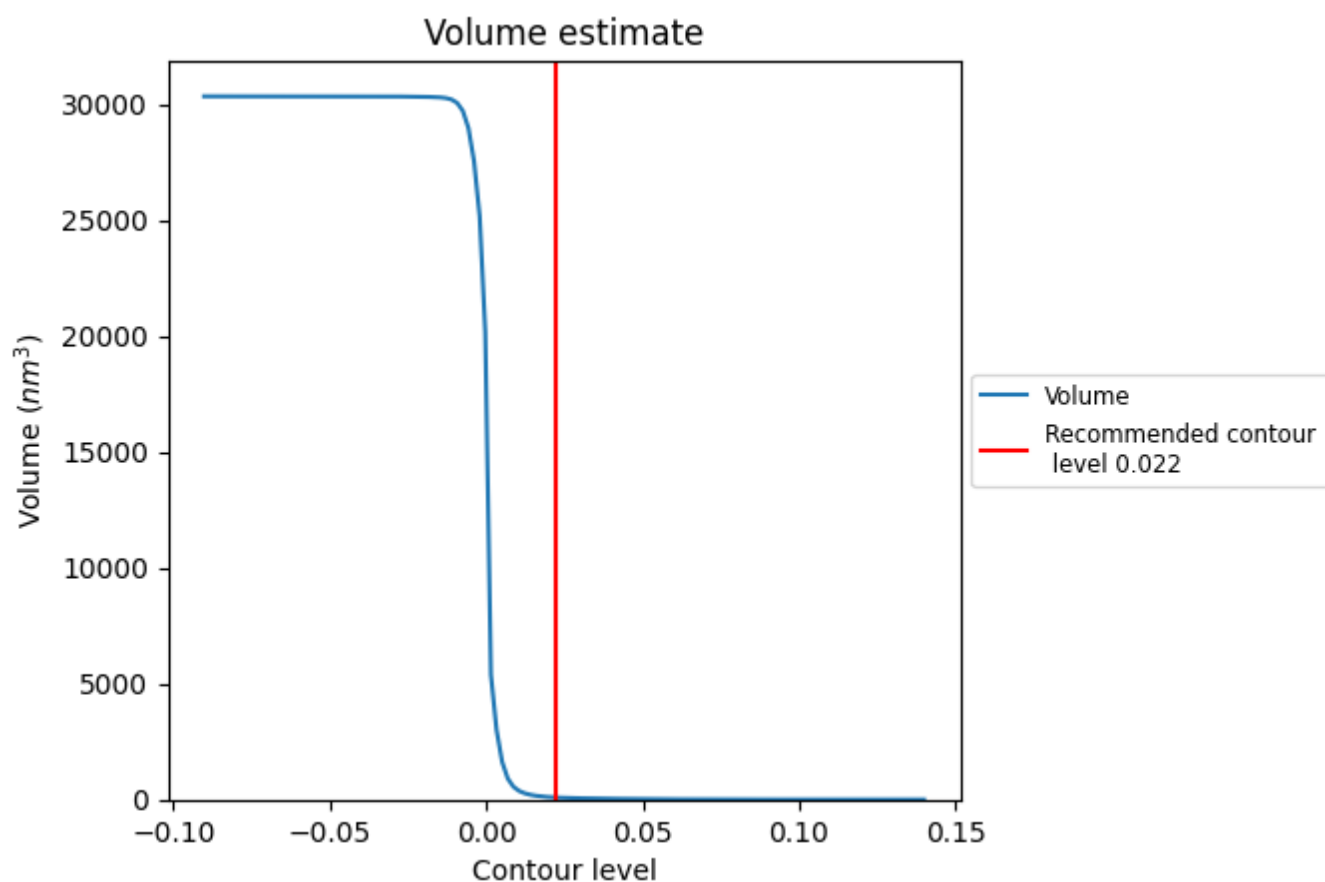
This section contains the results of statistical analysis of the map.

### 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](#)

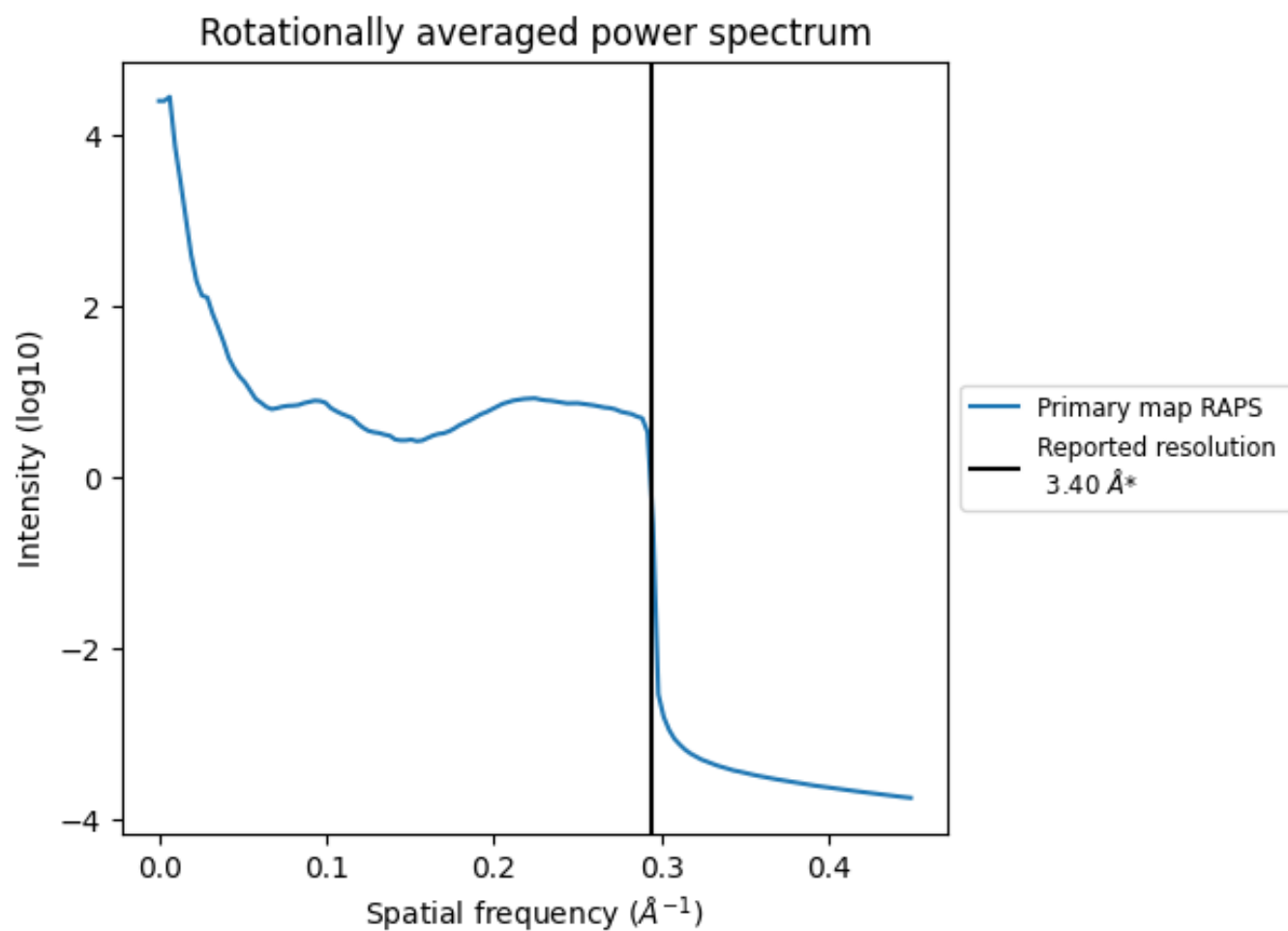


The volume at the recommended contour level is 91 nm<sup>3</sup>; this corresponds to an approximate mass of 82 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

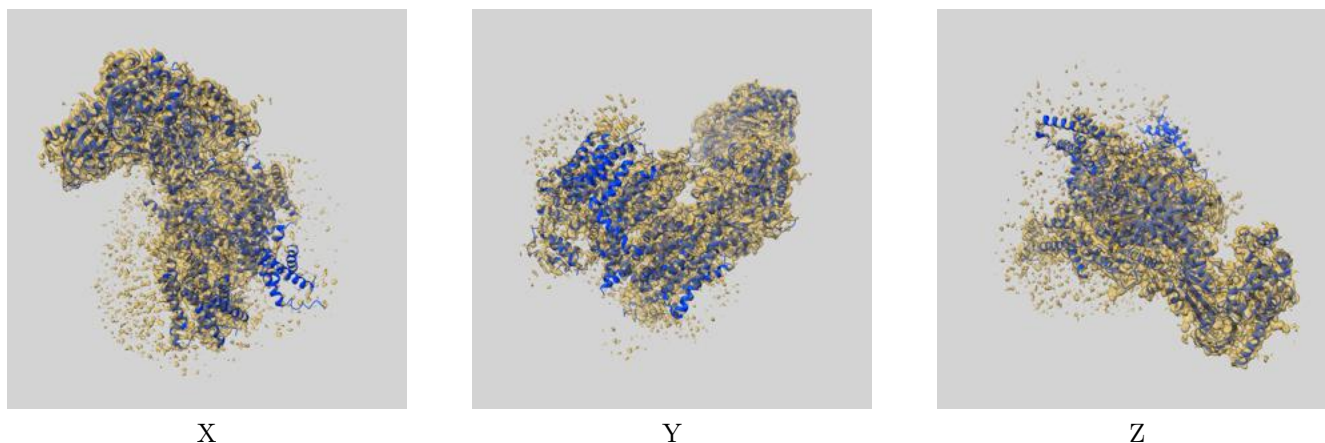
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

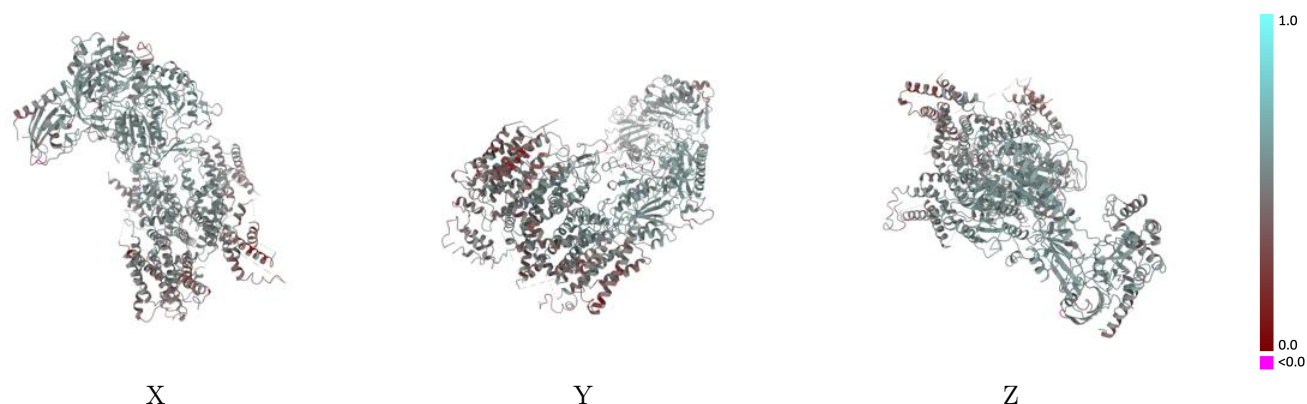
This section contains information regarding the fit between EMDB map EMD-22424 and PDB model 7JPV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



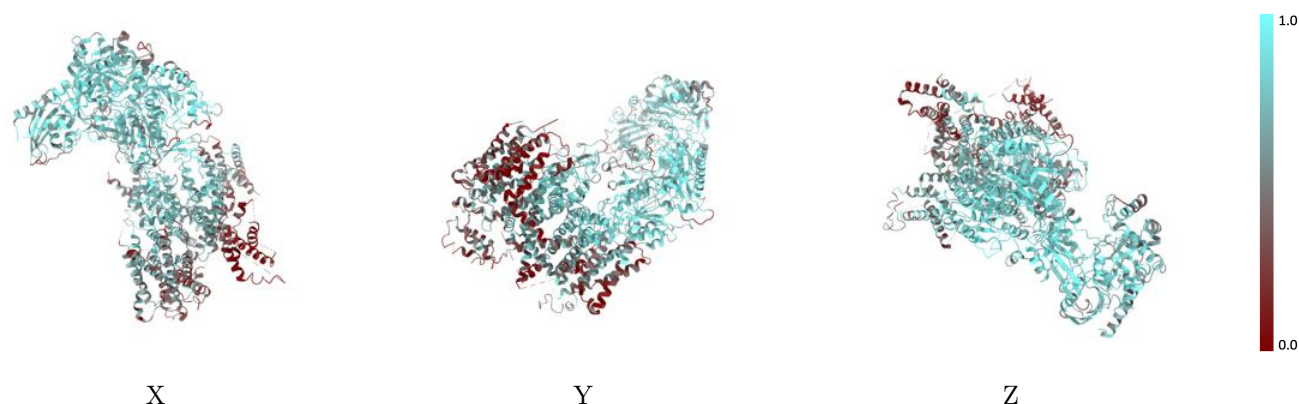
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



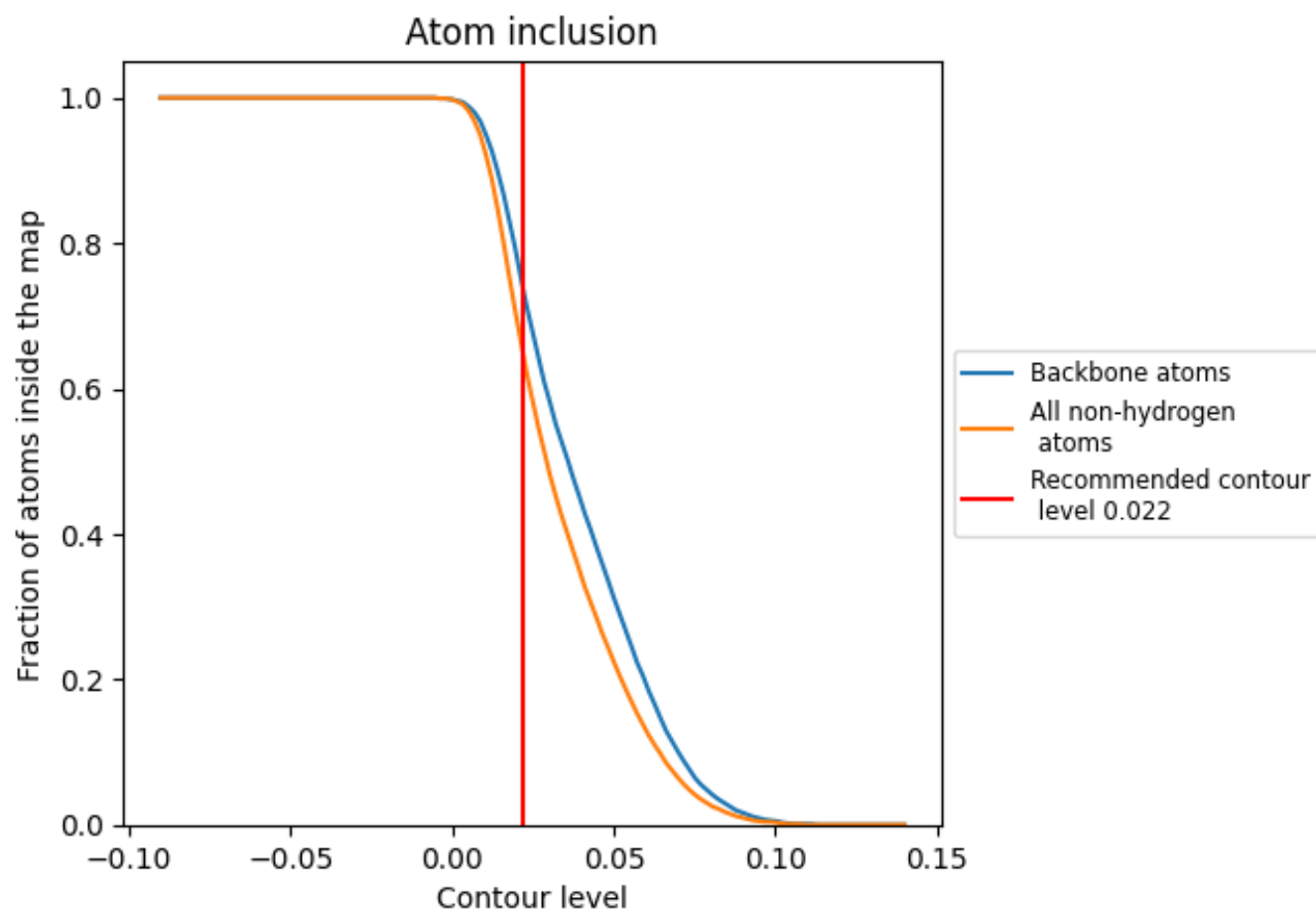
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6480	<div></div> 0.5070
A	<div></div> 0.5710	<div></div> 0.4920
E	<div></div> 0.4150	<div></div> 0.4490
F	<div></div> 0.7730	<div></div> 0.5330

