



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:39 AM UTC

PDB ID : 8FD7 / pdb_00008fd7
EMDB ID : EMD-29004
Title : Structure of the human L-type voltage-gated calcium channel Cav1.2 complexed with gabapentin
Authors : Chen, Z.; Mondal, A.; Minor, D.L.
Deposited on : 2022-12-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

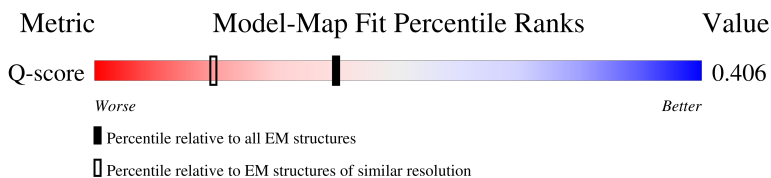
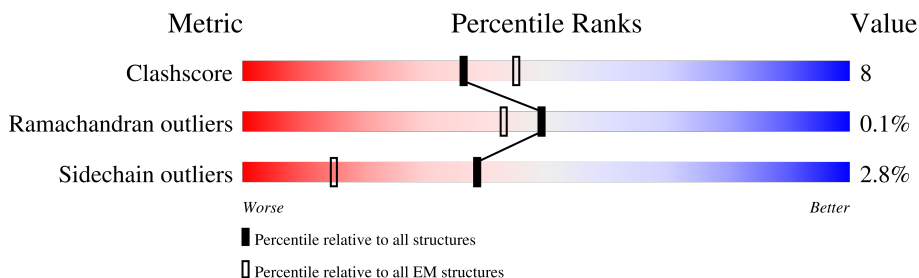
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	D	1105	
2	K	1648	
3	C	477	
4	F	2	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19701 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 calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	955	Total	C	N	O	S	0	0
			7630	4837	1282	1480	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P13806

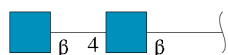
- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	1270	Total	C	N	O	S	0	0
			10227	6727	1673	1761	66		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	191	Total	C	N	O	S	0	0
			1518	964	266	280	8		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

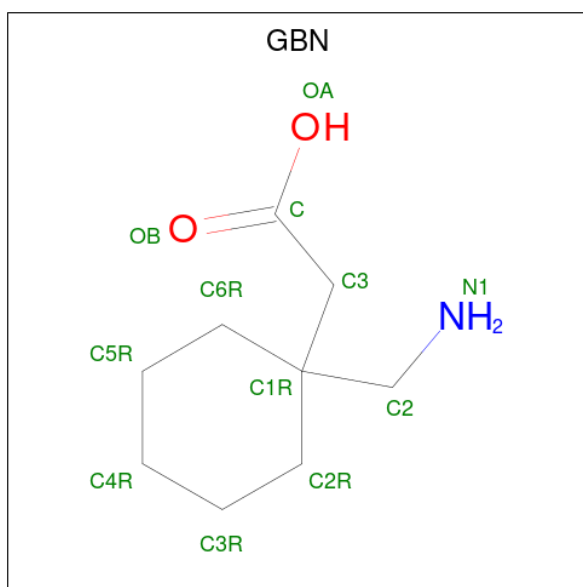
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is [1-(AMINOMETHYL)CYCLOHEXYL]ACETIC ACID (CCD ID: GBN) (formula: $C_9H_{17}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			12	9	1	2	

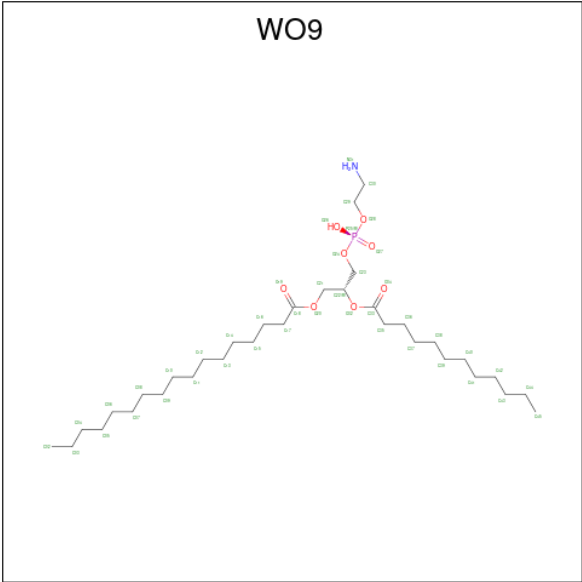
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Ca	0
			1	1	
7	K	2	Total	Ca	0
			2	2	

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

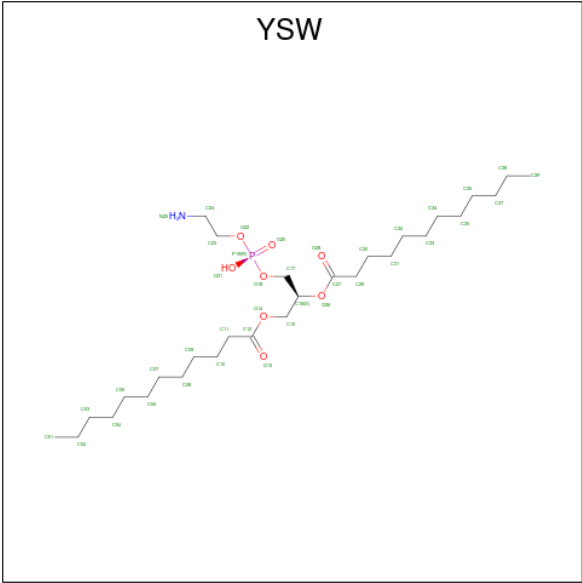
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Na	0
			1	1	

- Molecule 9 is (2R)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(dodecanoyloxy)propyl heptadecanoate (CCD ID: WO9) (formula: C₃₄H₆₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
9	K	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 10 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(dodecanoyloxy)propyl dodecanoate (CCD ID: YSW) (formula: C₂₉H₅₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
10	K	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 11 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
11	K	1	Total	C	O	0
			28	27	1	
11	K	1	Total	C	O	0
			28	27	1	
11	K	1	Total	C	O	0
			28	27	1	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	K	3	Total	O	0
			3	3	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	259107	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	65.419	Depositor
Minimum map value	-36.102	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	1.079	Depositor
Recommended contour level	7	Depositor
Map size (Å)	367.4, 367.4, 367.4	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	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: CLR, NA, WO9, GBN, NAG, CA, YSW

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	D	0.10	0/7792	0.27	0/10569
2	K	0.09	0/10470	0.26	0/14200
3	C	0.08	0/1544	0.21	0/2088
All	All	0.10	0/19806	0.26	0/26857

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	D	7630	0	7426	82	0
2	K	10227	0	10438	200	0
3	C	1518	0	1567	20	0
4	F	28	0	25	1	0
5	D	112	0	104	3	0
6	D	12	0	16	0	0
7	D	1	0	0	0	0
7	K	2	0	0	0	0
8	D	1	0	0	0	0
9	K	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	39	0	0	0	0
11	K	84	0	138	1	0
12	K	3	0	0	0	0
All	All	19701	0	19714	302	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 8.

All (302) 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:D:210:PHE:HB2	1:D:490:MET:HE3	1.75	0.69
2:K:632:ARG:HH12	2:K:637:LEU:HB3	1.58	0.68
1:D:359:ILE:HG22	1:D:385:ARG:HB2	1.75	0.68
1:D:882:PRO:HB3	1:D:1032:LEU:HA	1.77	0.67
2:K:1511:ARG:NH2	2:K:1553:ASP:O	2.28	0.66
1:D:768:ARG:NH2	1:D:857:ASP:OD2	2.28	0.66
2:K:1222:GLU:O	2:K:1225:MET:HB3	1.96	0.66
1:D:662:PHE:HB2	1:D:743:THR:HG23	1.79	0.65
2:K:965:CYS:HB2	2:K:1007:ARG:HH11	1.60	0.65
1:D:59:LEU:HD23	1:D:800:VAL:HG11	1.79	0.64
2:K:1525:GLN:HG2	2:K:1527:PRO:HD2	1.79	0.64
1:D:706:ARG:NH1	1:D:710:ASP:OD1	2.30	0.64
2:K:1401:THR:HG22	2:K:1403:PRO:HD2	1.79	0.62
1:D:845:ARG:HD2	1:D:847:SER:HB2	1.80	0.62
1:D:1009:LYS:HG2	1:D:1016:ILE:HG22	1.82	0.61
2:K:1232:ASN:ND2	2:K:1255:ASN:OD1	2.33	0.61
2:K:611:MET:SD	2:K:612:SER:N	2.74	0.61
2:K:1573:LYS:HB3	2:K:1577:ASN:HB3	1.82	0.61
2:K:923:VAL:HG23	2:K:1435:SER:HB3	1.83	0.61
1:D:179:THR:O	1:D:183:ASN:ND2	2.31	0.61
2:K:274:LEU:HD13	2:K:1346:ILE:HD11	1.82	0.61
2:K:1547:ASN:ND2	2:K:1607:PRO:O	2.34	0.60
2:K:1239:GLN:HG3	2:K:1243:GLN:HB3	1.83	0.60
2:K:900:THR:O	2:K:904:ASN:ND2	2.34	0.60
2:K:1219:THR:HA	2:K:1222:GLU:HG2	1.82	0.60
2:K:1535:PRO:HD2	2:K:1539:ALA:HA	1.82	0.60
2:K:1557:MET:HG3	2:K:1559:ASN:H	1.67	0.60
2:K:314:SER:O	2:K:325:GLN:NE2	2.35	0.59
2:K:1588:ILE:HA	2:K:1592:ILE:HB	1.84	0.59
2:K:586:SER:HB3	2:K:589:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:403:VAL:HG12	2:K:749:LEU:HD13	1.85	0.59
2:K:1200:ARG:HD2	2:K:1509:LYS:HD3	1.83	0.59
1:D:92:LEU:HD12	1:D:617:THR:HG21	1.86	0.58
1:D:381:ASP:OD1	1:D:381:ASP:N	2.31	0.58
3:C:257:ILE:HD13	3:C:260:LEU:HD21	1.84	0.58
2:K:1583:GLU:HA	2:K:1587:ALA:HB3	1.84	0.58
2:K:186:HIS:HA	2:K:192:ARG:HD3	1.85	0.58
1:D:202:ASP:HB3	1:D:205:LEU:HD23	1.85	0.57
2:K:1511:ARG:HE	2:K:1553:ASP:HB3	1.68	0.57
3:C:213:SER:HB2	3:C:267:VAL:HG23	1.86	0.57
2:K:118:ILE:HG21	2:K:179:ILE:HG22	1.85	0.57
2:K:201:ILE:HA	2:K:204:VAL:HG12	1.87	0.56
2:K:446:ASP:O	2:K:516:LYS:NZ	2.36	0.56
2:K:557:ASP:HA	2:K:560:ASN:HD21	1.71	0.56
2:K:1117:TRP:CD1	2:K:1118:PRO:HD3	2.41	0.56
2:K:1520:LEU:HG	2:K:1523:ARG:HH12	1.70	0.55
1:D:597:GLN:NE2	1:D:762:GLU:O	2.39	0.55
1:D:849:VAL:HG13	1:D:850:MET:HG2	1.88	0.55
2:K:712:MET:HE2	2:K:730:CYS:HB2	1.87	0.55
2:K:1098:PHE:HA	2:K:1104:ALA:HB2	1.87	0.55
2:K:1582:ASN:HA	2:K:1586:ARG:HG2	1.89	0.55
2:K:294:MET:HE2	2:K:339:PRO:HG3	1.89	0.55
2:K:1093:ASN:ND2	2:K:1097:ASP:OD1	2.40	0.55
3:C:221:LEU:HB3	3:C:274:ILE:HD11	1.89	0.55
2:K:197:LEU:HD11	2:K:242:LEU:HD23	1.89	0.55
1:D:116:ARG:NH1	5:D:1201:NAG:O6	2.36	0.55
2:K:1275:PRO:HA	2:K:1278:TYR:HB3	1.88	0.55
2:K:1392:GLU:O	2:K:1397:ASN:ND2	2.38	0.55
2:K:1227:VAL:O	2:K:1230:LEU:HB3	2.07	0.55
2:K:1381:VAL:HG21	2:K:1451:PHE:HE1	1.71	0.55
2:K:901:ILE:HA	2:K:904:ASN:HD21	1.72	0.54
1:D:186:ASN:ND2	5:D:1201:NAG:O3	2.40	0.54
2:K:1511:ARG:NH1	2:K:1512:ILE:O	2.40	0.54
3:C:292:VAL:HB	3:C:337:LEU:HD12	1.88	0.54
2:K:401:LEU:HD11	2:K:1475:ILE:HG12	1.90	0.54
3:C:317:VAL:O	3:C:320:MET:HB3	2.07	0.54
2:K:627:ILE:O	2:K:630:ILE:HG13	2.08	0.54
2:K:1389:ASP:OD1	2:K:1395:ARG:NH2	2.40	0.54
2:K:405:SER:HB3	2:K:1482:LEU:HG	1.88	0.54
2:K:1572:ILE:HG23	2:K:1580:GLN:HE22	1.73	0.54
1:D:291:VAL:HG12	1:D:312:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASN:OD1	1:D:316:ASN:ND2	2.41	0.54
1:D:254:LYS:HA	1:D:357:ASN:HB2	1.89	0.53
2:K:299:TYR:HB2	2:K:333:LYS:HG3	1.90	0.53
2:K:663:ILE:HD13	2:K:696:LEU:HD21	1.91	0.53
3:C:291:PHE:HE1	3:C:325:LEU:HG	1.73	0.53
1:D:696:ASN:HB3	1:D:699:CYS:HB2	1.90	0.53
2:K:1581:ALA:HA	2:K:1584:GLU:HG2	1.90	0.53
2:K:1427:PRO:HA	2:K:1448:GLY:HA2	1.90	0.53
2:K:1031:ASN:HA	2:K:1034:ILE:HG12	1.90	0.53
1:D:38:TRP:HZ3	1:D:1019:MET:HE1	1.74	0.52
3:C:330:PRO:HA	3:C:333:PHE:HD2	1.75	0.52
2:K:1058:CYS:SG	2:K:1059:SER:N	2.81	0.52
2:K:624:LEU:O	2:K:627:ILE:HG12	2.09	0.52
2:K:1525:GLN:O	2:K:1529:GLY:N	2.43	0.52
2:K:1287:ASP:O	2:K:1290:ILE:HG13	2.10	0.52
2:K:1465:PHE:O	2:K:1468:ILE:HG12	2.10	0.52
1:D:884:LEU:O	1:D:888:LEU:HG	2.09	0.52
2:K:1336:LEU:HD12	2:K:1339:LEU:HD23	1.91	0.52
2:K:1588:ILE:O	2:K:1593:TRP:N	2.39	0.52
2:K:1106:MET:SD	2:K:1106:MET:N	2.79	0.52
1:D:370:ARG:HG3	1:D:400:PRO:HB3	1.92	0.51
2:K:1184:LYS:O	2:K:1188:GLN:NE2	2.42	0.51
2:K:1236:LEU:HA	2:K:1239:GLN:HE21	1.74	0.51
2:K:543:SER:OG	2:K:556:GLN:NE2	2.43	0.51
2:K:996:ILE:HG13	2:K:997:LEU:HD12	1.91	0.51
2:K:1230:LEU:O	2:K:1233:THR:OG1	2.28	0.51
1:D:154:ASP:OD2	1:D:163:TYR:OH	2.29	0.51
1:D:562:ASP:OD1	1:D:563:PHE:N	2.45	0.50
2:K:1093:ASN:OD1	2:K:1094:SER:N	2.39	0.50
2:K:1474:VAL:O	2:K:1478:ASN:ND2	2.44	0.50
2:K:551:TRP:HB2	2:K:552:LEU:HD12	1.92	0.50
2:K:912:LEU:HD13	2:K:1001:ARG:HH21	1.76	0.50
2:K:1063:LYS:HB3	2:K:1068:GLU:HG3	1.93	0.50
2:K:407:GLU:HB2	2:K:749:LEU:HD11	1.93	0.50
2:K:913:SER:HA	2:K:917:LEU:HD23	1.92	0.50
4:F:1:NAG:H61	4:F:2:NAG:HN2	1.75	0.50
1:D:275:ARG:HD2	1:D:325:ASN:HA	1.93	0.50
1:D:466:LEU:HD12	1:D:467:PRO:HD2	1.94	0.50
1:D:734:ARG:HG2	1:D:816:ILE:HG22	1.93	0.50
2:K:1578:LEU:HA	2:K:1581:ALA:HB3	1.92	0.50
2:K:632:ARG:HH21	2:K:635:ASN:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ASP:HB2	1:D:519:PRO:HD2	1.95	0.49
2:K:137:ASN:OD1	2:K:243:ARG:NH1	2.46	0.49
2:K:401:LEU:HD21	2:K:1475:ILE:HG12	1.95	0.49
2:K:1377:ILE:HG23	2:K:1455:TYR:HE2	1.77	0.49
3:C:186:SER:OG	3:C:318:GLN:OE1	2.27	0.49
2:K:583:TYR:O	2:K:589:ASN:ND2	2.46	0.49
1:D:523:VAL:HG11	1:D:526:HIS:HB2	1.95	0.49
2:K:931:HIS:CE1	2:K:935:ASN:HD21	2.31	0.49
3:C:339:GLU:HG3	3:C:345:ALA:HB2	1.95	0.49
1:D:571:ASP:O	1:D:575:GLU:HG2	2.13	0.48
2:K:439:ASP:O	2:K:443:GLN:N	2.41	0.48
2:K:1259:THR:HG22	2:K:1335:ARG:HH22	1.78	0.48
3:C:254:ILE:HG12	3:C:285:LEU:HD11	1.95	0.48
3:C:205:LYS:HA	3:C:209:ASP:HB2	1.95	0.48
1:D:39:VAL:HG21	1:D:1008:GLU:HG2	1.94	0.48
2:K:1112:SER:HB2	2:K:1153:ILE:HG21	1.95	0.48
2:K:443:GLN:HA	2:K:447:ILE:HB	1.95	0.48
2:K:1400:GLN:N	2:K:1400:GLN:OE1	2.46	0.48
2:K:927:SER:HB2	2:K:930:ASN:HB2	1.95	0.48
1:D:791:GLU:N	1:D:791:GLU:OE1	2.47	0.48
2:K:637:LEU:HG	2:K:640:LEU:HB3	1.95	0.48
2:K:1538:VAL:HB	2:K:1541:LYS:HB2	1.94	0.48
2:K:1254:LEU:HD23	2:K:1257:LEU:HD21	1.94	0.48
2:K:112:PRO:HD2	2:K:115:ARG:HE	1.78	0.47
2:K:1426:MET:HE2	2:K:1426:MET:HA	1.96	0.47
2:K:623:ARG:O	2:K:627:ILE:HG23	2.14	0.47
2:K:969:PHE:O	2:K:972:LEU:HB3	2.14	0.47
2:K:944:PHE:O	2:K:947:GLU:HG2	2.14	0.47
2:K:1117:TRP:CG	2:K:1118:PRO:HD3	2.49	0.47
1:D:783:ASN:OD1	1:D:783:ASN:N	2.48	0.47
1:D:579:LYS:HD2	1:D:611:TRP:HZ2	1.78	0.47
1:D:687:GLU:O	1:D:691:ARG:HG2	2.15	0.47
2:K:373:ASN:HB3	2:K:378:ARG:HG2	1.95	0.47
2:K:556:GLN:O	2:K:560:ASN:ND2	2.48	0.47
2:K:1610:ASP:N	2:K:1610:ASP:OD1	2.48	0.47
2:K:1518:VAL:O	2:K:1522:ARG:NH1	2.48	0.47
2:K:586:SER:HB3	2:K:589:ASN:ND2	2.30	0.47
1:D:857:ASP:OD1	1:D:1014:ASN:ND2	2.42	0.47
1:D:1001:CYS:SG	1:D:1002:SER:N	2.88	0.46
2:K:200:PHE:CE1	2:K:236:LEU:HB3	2.50	0.46
2:K:1127:SER:OG	2:K:1139:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1290:ILE:HD13	2:K:1335:ARG:HG2	1.96	0.46
1:D:1005:PHE:HB3	1:D:1020:VAL:HG23	1.97	0.46
2:K:1542:ARG:HA	2:K:1546:MET:HB3	1.96	0.46
2:K:397:LEU:HD13	2:K:1471:PHE:CD1	2.50	0.46
2:K:1135:ILE:HG22	2:K:1136:TYR:H	1.81	0.46
2:K:1286:PHE:HZ	2:K:1334:MET:HB3	1.80	0.46
1:D:639:GLU:HB3	1:D:642:THR:HG22	1.97	0.46
2:K:586:SER:H	2:K:590:ARG:HB2	1.81	0.46
2:K:1231:LEU:O	2:K:1234:ILE:HG12	2.14	0.46
2:K:1577:ASN:HD22	2:K:1580:GLN:NE2	2.13	0.46
1:D:598:ASP:OD1	1:D:764:SER:OG	2.22	0.46
1:D:857:ASP:OD1	1:D:857:ASP:N	2.49	0.46
2:K:1125:ILE:HD11	2:K:1143:SER:HB3	1.98	0.46
2:K:1357:PHE:HA	2:K:1360:LEU:HB3	1.97	0.46
3:C:276:HIS:HE1	3:C:324:LYS:HG3	1.80	0.46
2:K:420:ASP:HA	2:K:423:LYS:HZ2	1.81	0.46
1:D:210:PHE:HD1	1:D:490:MET:HG2	1.81	0.46
2:K:241:VAL:O	2:K:244:PRO:HD2	2.15	0.46
2:K:1114:PHE:HE1	2:K:1150:ILE:HD12	1.80	0.46
3:C:211:ARG:O	3:C:265:GLN:NE2	2.49	0.46
2:K:123:TRP:CD1	2:K:125:PRO:HD2	2.50	0.46
2:K:1530:PHE:HE2	2:K:1533:LEU:HB3	1.81	0.46
1:D:231:THR:HG23	1:D:234:LYS:HB2	1.98	0.45
1:D:267:SER:HB3	1:D:329:ALA:HB3	1.98	0.45
1:D:746:TYR:HB3	1:D:747:PRO:HD3	1.97	0.45
2:K:1392:GLU:HG3	2:K:1420:ASP:HB3	1.99	0.45
2:K:1591:LYS:O	2:K:1594:LYS:NZ	2.42	0.45
1:D:668:TYR:O	1:D:699:CYS:HB3	2.17	0.45
1:D:710:ASP:HB3	1:D:738:THR:HG21	1.99	0.45
2:K:408:PHE:O	2:K:411:GLU:HG3	2.16	0.45
2:K:971:ILE:HD12	2:K:974:LEU:HD23	1.99	0.45
2:K:1081:VAL:HG22	2:K:1082:ASP:H	1.81	0.45
2:K:1507:GLU:HB2	2:K:1509:LYS:HG2	1.98	0.45
3:C:315:LEU:HA	3:C:318:GLN:HB3	1.98	0.45
2:K:1584:GLU:HG3	2:K:1585:LEU:HG	1.98	0.44
1:D:234:LYS:HA	1:D:234:LYS:HD2	1.79	0.44
1:D:725:GLN:HB3	1:D:728:ILE:HD11	1.99	0.44
1:D:482:LYS:HD3	5:D:1204:NAG:H4	1.98	0.44
2:K:441:ILE:O	2:K:445:GLU:HB3	2.17	0.44
2:K:544:GLU:HA	2:K:548:GLN:HE22	1.83	0.44
1:D:861:LEU:HD21	1:D:869:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:647:SER:O	2:K:651:ILE:HG12	2.18	0.44
1:D:519:PRO:HD3	1:D:618:ASP:O	2.18	0.44
2:K:1094:SER:O	2:K:1096:PHE:N	2.50	0.44
2:K:1263:THR:O	2:K:1266:MET:HG3	2.17	0.44
3:C:216:ARG:HA	3:C:270:ASP:HB3	2.00	0.44
2:K:1199:LEU:H	2:K:1499:ARG:HH22	1.64	0.44
1:D:266:VAL:O	1:D:270:THR:HG23	2.18	0.43
3:C:232:PRO:O	3:C:251:GLN:NE2	2.51	0.43
2:K:1065:THR:HG22	2:K:1132:LYS:HE2	2.00	0.43
2:K:1604:VAL:C	2:K:1607:PRO:HD2	2.43	0.43
3:C:321:ALA:HA	3:C:324:LYS:HG2	1.99	0.43
2:K:1595:ARG:HD2	2:K:1601:LEU:HD13	1.99	0.43
1:D:997:ASP:OD1	1:D:997:ASP:N	2.47	0.43
2:K:440:TRP:HE1	3:C:342:LEU:N	2.16	0.43
2:K:925:HIS:CD2	2:K:925:HIS:H	2.36	0.43
2:K:1219:THR:O	2:K:1223:TYR:N	2.47	0.43
1:D:256:MET:O	1:D:291:VAL:HA	2.19	0.43
2:K:188:ASN:O	2:K:192:ARG:HG2	2.18	0.43
2:K:1115:GLU:HB3	2:K:1419:GLN:HE22	1.83	0.43
2:K:1377:ILE:O	2:K:1381:VAL:HG12	2.19	0.43
2:K:917:LEU:HD21	2:K:1001:ARG:HD3	2.00	0.43
1:D:297:ASN:O	1:D:297:ASN:ND2	2.51	0.43
2:K:442:THR:HB	2:K:578:LEU:HD12	2.00	0.43
2:K:534:VAL:HG21	2:K:630:ILE:HG12	1.99	0.43
1:D:888:LEU:O	1:D:893:VAL:HG12	2.19	0.43
2:K:322:HIS:CG	2:K:377:GLY:HA2	2.53	0.43
2:K:599:GLY:HA3	2:K:622:VAL:HG11	2.01	0.43
2:K:1203:ILE:HG23	2:K:1213:TRP:CD2	2.53	0.43
2:K:1548:MET:SD	2:K:1548:MET:N	2.92	0.43
2:K:1567:ARG:HG2	2:K:1572:ILE:HB	2.00	0.43
2:K:1200:ARG:O	2:K:1508:ALA:HB3	2.19	0.43
2:K:1384:LYS:HG3	2:K:1446:PRO:HB2	2.01	0.43
2:K:275:VAL:HG22	2:K:395:PHE:CD2	2.54	0.43
2:K:1167:VAL:HG13	2:K:1170:GLN:HE21	1.84	0.43
2:K:1365:LEU:HA	2:K:1368:VAL:HG22	2.00	0.43
2:K:1488:ILE:HG13	2:K:1489:LEU:H	1.84	0.43
2:K:749:LEU:HD12	2:K:749:LEU:HA	1.90	0.42
2:K:1469:ASN:O	2:K:1472:VAL:HG22	2.18	0.42
2:K:1585:LEU:HB2	2:K:1586:ARG:HE	1.84	0.42
1:D:884:LEU:HA	1:D:996:LEU:HD11	2.01	0.42
2:K:929:ARG:HH21	2:K:932:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:TRP:CE3	1:D:746:TYR:HB2	2.54	0.42
1:D:895:ALA:HB2	1:D:986:ASP:HB2	2.01	0.42
2:K:544:GLU:HA	2:K:548:GLN:NE2	2.34	0.42
2:K:593:CYS:HA	2:K:596:VAL:HG22	2.01	0.42
2:K:1096:PHE:HZ	2:K:1419:GLN:HB2	1.84	0.42
1:D:449:THR:HG22	1:D:463:THR:H	1.83	0.42
2:K:118:ILE:HD11	2:K:176:LEU:HB2	2.01	0.42
2:K:982:ILE:HB	2:K:990:ALA:HB2	2.02	0.42
2:K:1382:PHE:HE1	2:K:1449:SER:HB2	1.85	0.42
2:K:1395:ARG:H	2:K:1395:ARG:HE	1.66	0.42
1:D:159:ARG:HD3	1:D:223:SER:OG	2.19	0.42
1:D:668:TYR:HB3	1:D:704:ILE:HD11	2.02	0.42
2:K:348:ASN:OD1	2:K:349:PHE:N	2.42	0.42
2:K:898:ASN:ND2	2:K:899:ASP:H	2.17	0.42
1:D:298:SER:HB3	1:D:332:ILE:HG12	2.02	0.42
3:C:191:GLU:O	3:C:195:MET:HB2	2.19	0.42
1:D:867:ASP:HA	1:D:870:THR:HG22	2.02	0.42
2:K:902:PHE:HZ	2:K:1009:ILE:HG22	1.85	0.42
2:K:1386:ALA:HB2	2:K:1431:CYS:HA	2.02	0.42
2:K:1069:CYS:SG	2:K:1089:ARG:HD3	2.60	0.42
2:K:1512:ILE:HG13	2:K:1556:VAL:HB	2.00	0.42
1:D:587:GLU:HA	1:D:609:TYR:O	2.19	0.41
2:K:314:SER:N	2:K:323:GLY:O	2.46	0.41
2:K:522:LYS:HA	2:K:526:PHE:HB3	2.02	0.41
2:K:1054:LYS:HG2	2:K:1129:THR:O	2.20	0.41
1:D:161:VAL:HG12	1:D:223:SER:HB2	2.01	0.41
1:D:281:MET:O	1:D:284:THR:OG1	2.37	0.41
1:D:671:ASP:N	1:D:671:ASP:OD1	2.51	0.41
2:K:1464:ALA:O	2:K:1468:ILE:HG23	2.21	0.41
1:D:70:TYR:HB2	1:D:633:ILE:HG23	2.01	0.41
2:K:322:HIS:CD2	2:K:378:ARG:HG3	2.55	0.41
2:K:1234:ILE:HD12	11:K:1705:CLR:H21	2.02	0.41
2:K:1526:PRO:HB2	2:K:1527:PRO:HD3	2.02	0.41
1:D:379:ASN:ND2	1:D:408:ASN:OD1	2.52	0.41
1:D:570:ASN:HB3	1:D:573:LYS:HG2	2.01	0.41
2:K:617:SER:HA	2:K:620:ARG:HD2	2.01	0.41
2:K:923:VAL:HG11	2:K:1385:ILE:HG22	2.02	0.41
2:K:1181:GLU:OE1	2:K:1187:ARG:NE	2.54	0.41
2:K:1203:ILE:HG12	2:K:1213:TRP:CZ3	2.56	0.41
3:C:176:SER:HB2	3:C:261:ALA:HB1	2.02	0.41
2:K:1547:ASN:HD22	2:K:1549:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:194:GLY:O	2:K:198:LEU:HG	2.21	0.41
2:K:1523:ARG:HD3	2:K:1523:ARG:H	1.85	0.41
1:D:896:PHE:HA	1:D:982:GLN:O	2.21	0.41
1:D:896:PHE:HB3	1:D:983:TYR:CE2	2.55	0.41
1:D:1034:ILE:HG22	1:D:1036:ALA:H	1.86	0.41
2:K:196:ASN:HA	2:K:199:ASP:OD2	2.21	0.41
2:K:557:ASP:HA	2:K:560:ASN:ND2	2.35	0.41
2:K:1274:LYS:HD3	2:K:1274:LYS:HA	1.94	0.41
2:K:1507:GLU:H	2:K:1507:GLU:CD	2.29	0.41
2:K:748:PHE:HB2	2:K:1158:MET:HG2	2.03	0.41
2:K:947:GLU:HA	2:K:950:LEU:HG	2.03	0.41
1:D:127:TYR:HB2	1:D:147:ILE:HB	2.02	0.40
2:K:608:THR:O	2:K:609:LYS:HG2	2.21	0.40
2:K:1398:ASN:HD22	2:K:1404:GLN:NE2	2.19	0.40
1:D:207:TRP:NE1	1:D:458:LEU:HD22	2.36	0.40
1:D:866:HIS:C	1:D:868:ASP:H	2.28	0.40
2:K:200:PHE:HZ	2:K:236:LEU:HD12	1.86	0.40
2:K:1344:GLU:HG2	2:K:1345:GLY:H	1.86	0.40
1:D:857:ASP:HB3	1:D:985:PHE:CE2	2.56	0.40
2:K:198:LEU:HA	2:K:201:ILE:HG22	2.03	0.40
2:K:262:ILE:O	2:K:266:VAL:HG23	2.21	0.40
2:K:181:TYR:HB3	2:K:184:LEU:HB3	2.04	0.40
2:K:296:LYS:NZ	2:K:334:PRO:HB3	2.36	0.40
2:K:401:LEU:HD12	2:K:1482:LEU:HD23	2.04	0.40
1:D:207:TRP:HE1	1:D:458:LEU:HD22	1.87	0.40
2:K:587:LEU:HG	2:K:588:PHE:HD1	1.85	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	D	945/1105 (86%)	897 (95%)	48 (5%)	0	100	100
2	K	1260/1648 (76%)	1163 (92%)	94 (8%)	3 (0%)	43	73
3	C	189/477 (40%)	184 (97%)	5 (3%)	0	100	100
All	All	2394/3230 (74%)	2244 (94%)	147 (6%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	1081	VAL
2	K	1095	LYS
2	K	380	TRP

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	D	846/973 (87%)	820 (97%)	26 (3%)	35	64
2	K	1122/1437 (78%)	1089 (97%)	33 (3%)	37	66
3	C	172/420 (41%)	172 (100%)	0	100	100
All	All	2140/2830 (76%)	2081 (97%)	59 (3%)	38	66

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	41	LYS
1	D	56	VAL
1	D	104	LEU
1	D	108	LYS
1	D	125	VAL
1	D	182	LEU
1	D	185	LEU
1	D	205	LEU
1	D	270	THR
1	D	373	GLU

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Mol	Chain	Res	Type
1	D	381	ASP
1	D	650	LEU
1	D	671	ASP
1	D	678	ASN
1	D	688	PHE
1	D	736	VAL
1	D	743	THR
1	D	800	VAL
1	D	804	ILE
1	D	870	THR
1	D	880	ILE
1	D	889	VAL
1	D	996	LEU
1	D	1000	ASN
1	D	1001	CYS
1	D	1033	LEU
2	K	137	ASN
2	K	145	ILE
2	K	167	LEU
2	K	175	PHE
2	K	287	LEU
2	K	320	THR
2	K	331	VAL
2	K	345	ASN
2	K	399	LEU
2	K	570	GLU
2	K	600	ILE
2	K	611	MET
2	K	746	ASN
2	K	748	PHE
2	K	923	VAL
2	K	924	GLN
2	K	977	VAL
2	K	1002	VAL
2	K	1069	CYS
2	K	1081	VAL
2	K	1098	PHE
2	K	1100	ASN
2	K	1158	MET
2	K	1166	ILE
2	K	1222	GLU
2	K	1223	TYR

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Mol	Chain	Res	Type
2	K	1227	VAL
2	K	1236	LEU
2	K	1278	TYR
2	K	1346	ILE
2	K	1395	ARG
2	K	1399	PHE
2	K	1586	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	GLN
1	D	165	HIS
1	D	186	ASN
1	D	316	ASN
1	D	424	ASN
1	D	643	GLN
1	D	696	ASN
1	D	774	ASN
1	D	805	GLN
1	D	826	ASN
1	D	887	HIS
1	D	897	ASN
1	D	980	GLN
1	D	1000	ASN
2	K	325	GLN
2	K	373	ASN
2	K	556	GLN
2	K	560	ASN
2	K	694	GLN
2	K	741	ASN
2	K	892	GLN
2	K	894	HIS
2	K	904	ASN
2	K	931	HIS
2	K	935	ASN
2	K	1083	HIS
2	K	1087	GLN
2	K	1239	GLN
2	K	1358	GLN
2	K	1404	GLN
2	K	1478	ASN

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Mol	Chain	Res	Type
2	K	1580	GLN
3	C	276	HIS
3	C	348	HIS

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 ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	4	14,14,15	0.95	0	17,19,21	1.30	3 (17%)
4	NAG	F	2	4	14,14,15	1.04	1 (7%)	17,19,21	0.92	1 (5%)

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
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	2.28	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-O5-C5	2.72	115.83	112.19
4	F	2	NAG	C1-O5-C5	2.60	115.67	112.19
4	F	1	NAG	C3-C4-C5	2.47	114.71	110.23
4	F	1	NAG	O5-C1-C2	-2.35	107.65	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

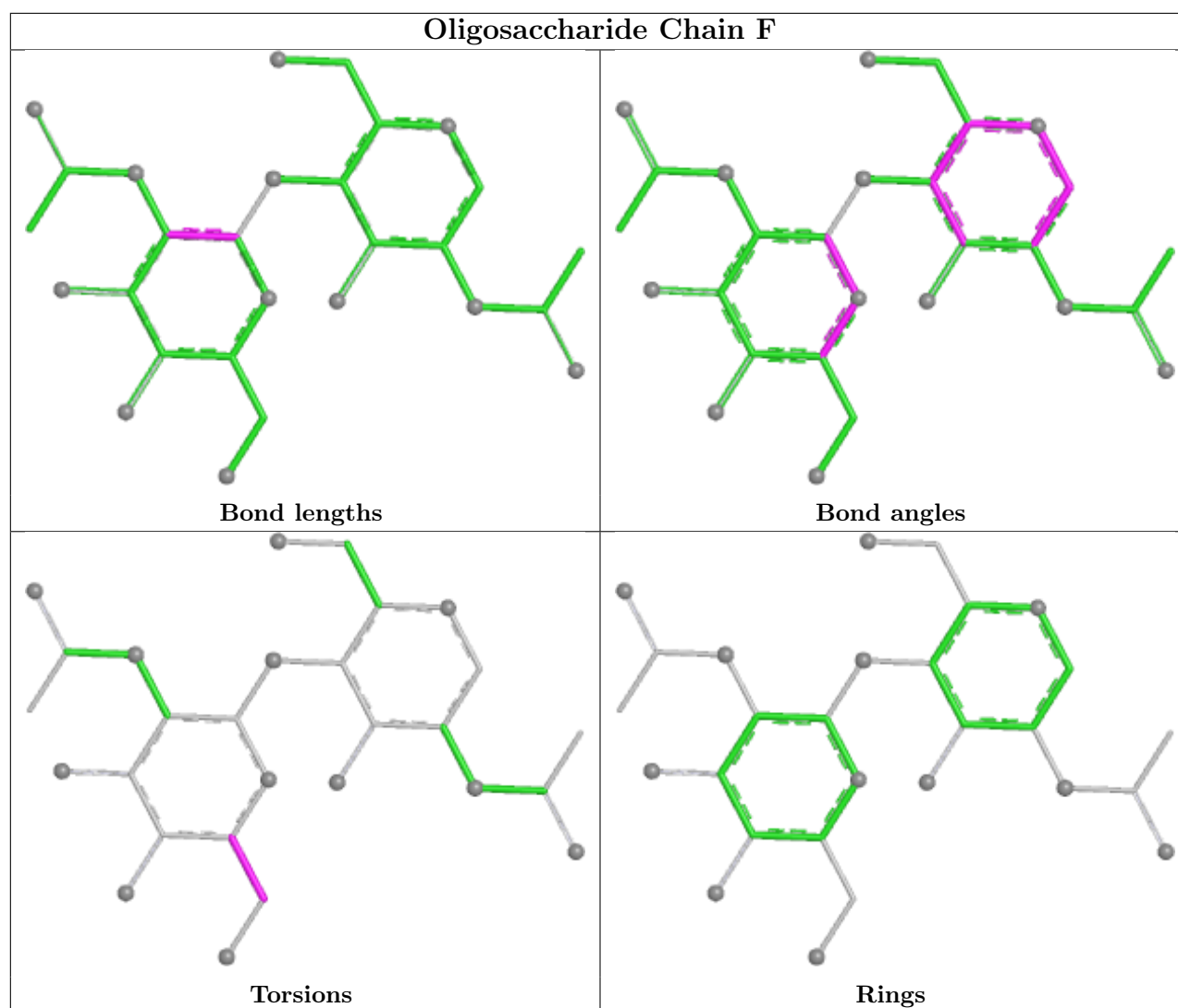
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	F	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	NAG	D	1203	1	14,14,15	1.07	1 (7%)	17,19,21	1.23	1 (5%)
11	CLR	K	1705	-	31,31,31	1.05	0	48,48,48	0.53	0
5	NAG	D	1207	-	14,14,15	1.01	1 (7%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	1204	1	14,14,15	1.03	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	D	1201	-	14,14,15	1.00	1 (7%)	17,19,21	0.91	1 (5%)
9	WO9	K	1701	-	43,43,43	2.20	11 (25%)	46,48,48	1.20	3 (6%)
11	CLR	K	1703	-	31,31,31	1.06	0	48,48,48	0.55	0
11	CLR	K	1704	-	31,31,31	1.05	0	48,48,48	0.60	0
5	NAG	D	1209	-	14,14,15	0.99	1 (7%)	17,19,21	1.06	1 (5%)
6	GBN	D	1202	-	11,12,12	0.99	1 (9%)	13,16,16	1.27	2 (15%)
5	NAG	D	1208	-	14,14,15	0.98	0	17,19,21	1.12	1 (5%)
10	YSW	K	1702	-	38,38,38	0.84	1 (2%)	41,43,43	0.98	2 (4%)
5	NAG	D	1206	-	14,14,15	0.99	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	D	1205	-	14,14,15	1.09	1 (7%)	17,19,21	1.09	2 (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	NAG	D	1203	1	-	0/6/23/26	0/1/1/1
11	CLR	K	1705	-	-	4/10/68/68	0/4/4/4
5	NAG	D	1207	-	-	2/6/23/26	0/1/1/1
5	NAG	D	1204	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1201	-	-	2/6/23/26	0/1/1/1
9	WO9	K	1701	-	-	11/47/47/47	-
11	CLR	K	1703	-	-	3/10/68/68	0/4/4/4
11	CLR	K	1704	-	-	7/10/68/68	0/4/4/4
5	NAG	D	1209	-	-	0/6/23/26	0/1/1/1
6	GBN	D	1202	-	-	2/8/18/18	0/1/1/1
5	NAG	D	1208	-	-	2/6/23/26	0/1/1/1
10	YSW	K	1702	-	-	26/42/42/42	-
5	NAG	D	1206	-	-	2/6/23/26	0/1/1/1
5	NAG	D	1205	-	-	3/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	1701	WO9	O20-C18	4.82	1.47	1.33
9	K	1701	WO9	O32-C33	4.54	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	1701	WO9	P25-O24	3.56	1.73	1.59
9	K	1701	WO9	P25-O28	3.54	1.73	1.59
9	K	1701	WO9	C35-C33	3.47	1.60	1.50
9	K	1701	WO9	C17-C18	3.47	1.60	1.50
9	K	1701	WO9	C23-C22	3.20	1.60	1.50
9	K	1701	WO9	C21-C22	3.15	1.60	1.50
9	K	1701	WO9	C30-C29	2.64	1.60	1.49
5	D	1205	NAG	C1-C2	2.46	1.55	1.52
9	K	1701	WO9	C36-C35	2.40	1.61	1.52
5	D	1204	NAG	C1-C2	2.36	1.55	1.52
9	K	1701	WO9	C16-C17	2.32	1.60	1.52
5	D	1203	NAG	C1-C2	2.32	1.55	1.52
5	D	1207	NAG	C1-C2	2.22	1.55	1.52
10	K	1702	YSW	C10-C11	-2.20	1.44	1.52
6	D	1202	GBN	OA-C	-2.19	1.23	1.30
5	D	1201	NAG	C1-C2	2.13	1.55	1.52
5	D	1209	NAG	C1-C2	2.05	1.55	1.52
5	D	1206	NAG	C1-C2	2.02	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	1701	WO9	O32-C33-C35	4.01	120.15	111.48
5	D	1203	NAG	C1-O5-C5	3.90	117.42	112.19
5	D	1204	NAG	C1-O5-C5	3.50	116.87	112.19
5	D	1208	NAG	C1-O5-C5	3.36	116.69	112.19
5	D	1209	NAG	C1-O5-C5	3.25	116.54	112.19
6	D	1202	GBN	OB-C-C3	-3.01	114.42	122.95
5	D	1206	NAG	C1-O5-C5	2.83	115.98	112.19
10	K	1702	YSW	O26-C27-C29	2.74	117.42	111.48
9	K	1701	WO9	O20-C18-C17	2.69	120.05	111.83
5	D	1205	NAG	C4-C3-C2	2.43	114.58	111.02
9	K	1701	WO9	O26-P25-O27	-2.41	101.25	112.44
10	K	1702	YSW	O21-P19-O22	2.38	118.36	107.57
5	D	1201	NAG	C1-O5-C5	2.38	115.37	112.19
5	D	1205	NAG	C2-N2-C7	2.35	126.04	122.90
5	D	1207	NAG	C1-O5-C5	2.13	115.04	112.19
6	D	1202	GBN	C2-C1R-C3	-2.05	108.13	110.49

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	1701	WO9	C29-O28-P25-O27
10	K	1702	YSW	C17-O18-P19-O20
10	K	1702	YSW	C17-O18-P19-O21
10	K	1702	YSW	C17-O18-P19-O22
10	K	1702	YSW	O28-C27-O26-C16
11	K	1704	CLR	C17-C20-C22-C23
5	D	1201	NAG	C4-C5-C6-O6
5	D	1207	NAG	C4-C5-C6-O6
10	K	1702	YSW	C11-C12-O14-C15
9	K	1701	WO9	C35-C33-O32-C22
10	K	1702	YSW	C29-C27-O26-C16
10	K	1702	YSW	O13-C12-O14-C15
5	D	1207	NAG	O5-C5-C6-O6
5	D	1201	NAG	O5-C5-C6-O6
5	D	1208	NAG	O5-C5-C6-O6
11	K	1704	CLR	C21-C20-C22-C23
5	D	1208	NAG	C4-C5-C6-O6
5	D	1206	NAG	O5-C5-C6-O6
5	D	1206	NAG	C4-C5-C6-O6
9	K	1701	WO9	O34-C33-O32-C22
10	K	1702	YSW	C15-C16-O26-C27
11	K	1704	CLR	C22-C23-C24-C25
10	K	1702	YSW	C31-C32-C33-C34
9	K	1701	WO9	C41-C42-C43-C44
10	K	1702	YSW	C33-C34-C35-C36
10	K	1702	YSW	C02-C03-C04-C05
9	K	1701	WO9	C09-C10-C11-C12
10	K	1702	YSW	O26-C16-C17-O18
10	K	1702	YSW	C15-C16-C17-O18
10	K	1702	YSW	O14-C15-C16-C17
5	D	1205	NAG	C3-C2-N2-C7
10	K	1702	YSW	C05-C06-C07-C08
10	K	1702	YSW	C34-C35-C36-C37
10	K	1702	YSW	C03-C04-C05-C06
11	K	1704	CLR	C16-C17-C20-C21
10	K	1702	YSW	C01-C02-C03-C04
10	K	1702	YSW	C16-C17-O18-P19
11	K	1704	CLR	C13-C17-C20-C21
9	K	1701	WO9	C08-C09-C10-C11
11	K	1704	CLR	C13-C17-C20-C22
11	K	1704	CLR	C16-C17-C20-C22
5	D	1205	NAG	C1-C2-N2-C7
10	K	1702	YSW	C04-C05-C06-C07

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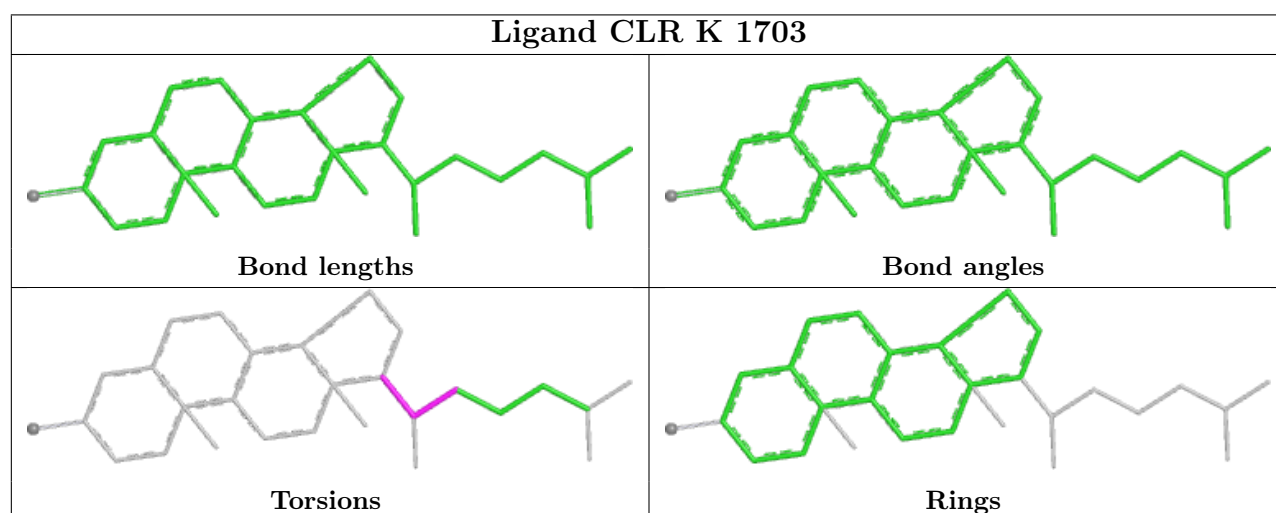
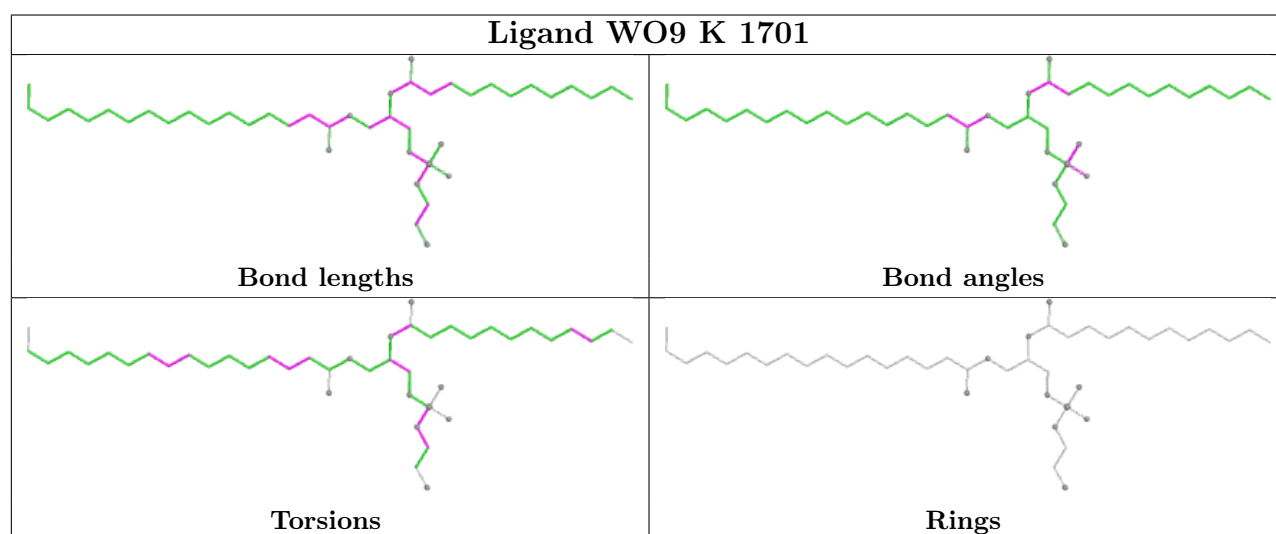
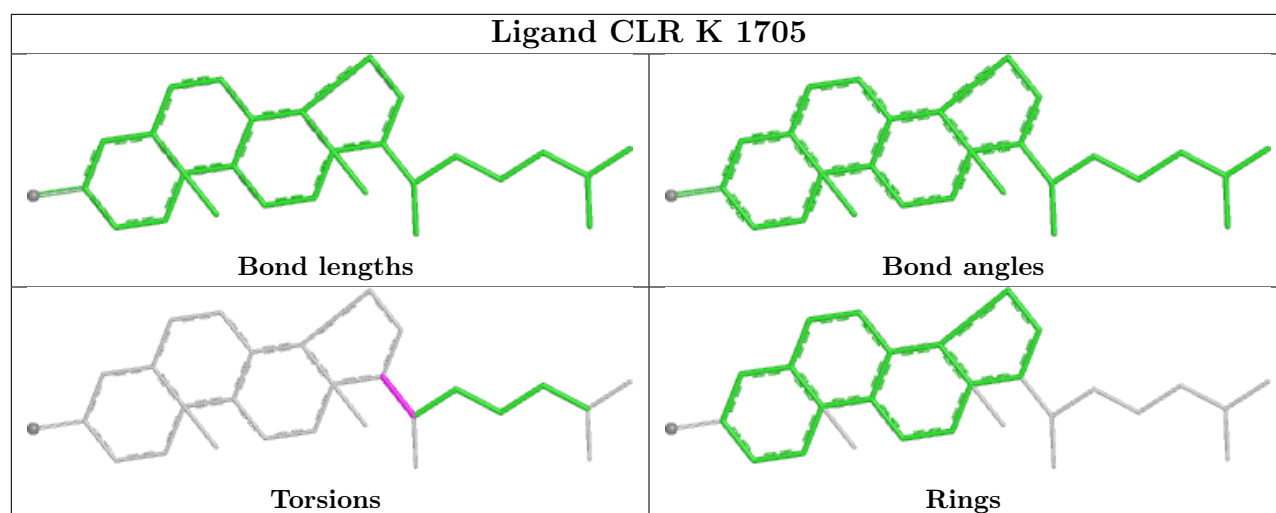
Mol	Chain	Res	Type	Atoms
11	K	1705	CLR	C13-C17-C20-C22
11	K	1705	CLR	C13-C17-C20-C21
9	K	1701	WO9	C30-C29-O28-P25
10	K	1702	YSW	O14-C15-C16-O26
9	K	1701	WO9	C14-C15-C16-C17
11	K	1705	CLR	C16-C17-C20-C22
11	K	1703	CLR	C21-C20-C22-C23
9	K	1701	WO9	O32-C22-C23-O24
11	K	1705	CLR	C16-C17-C20-C21
9	K	1701	WO9	C15-C16-C17-C18
10	K	1702	YSW	O22-C23-C24-N25
10	K	1702	YSW	C23-O22-P19-O21
10	K	1702	YSW	C35-C36-C37-C38
6	D	1202	GBN	OA-C-C3-C1R
10	K	1702	YSW	C32-C33-C34-C35
6	D	1202	GBN	OB-C-C3-C1R
5	D	1205	NAG	C4-C5-C6-O6
9	K	1701	WO9	C21-C22-C23-O24
11	K	1703	CLR	C16-C17-C20-C22
11	K	1703	CLR	C13-C17-C20-C21
10	K	1702	YSW	O26-C27-C29-C30

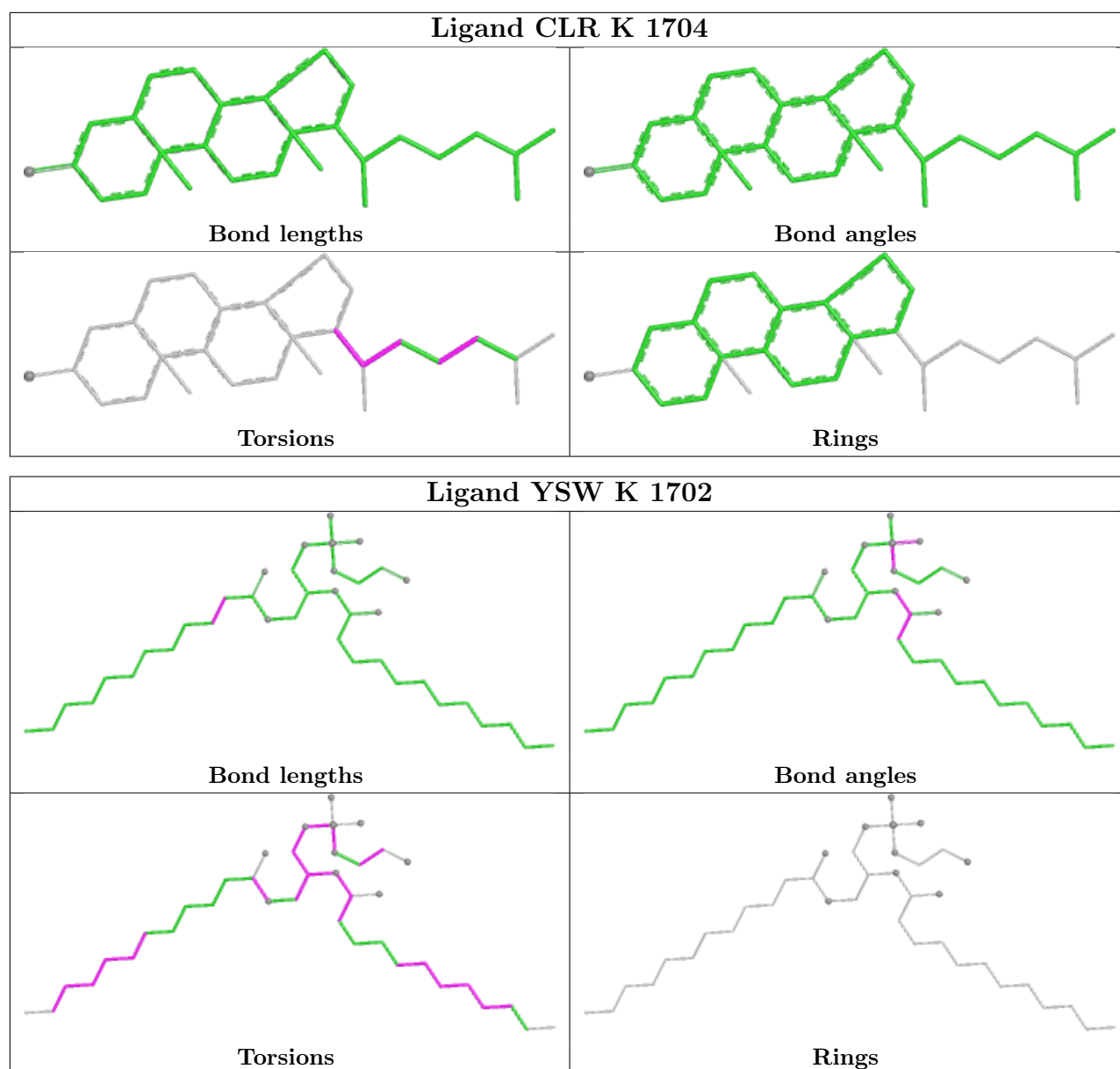
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1705	CLR	1	0
5	D	1204	NAG	1	0
5	D	1201	NAG	2	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.

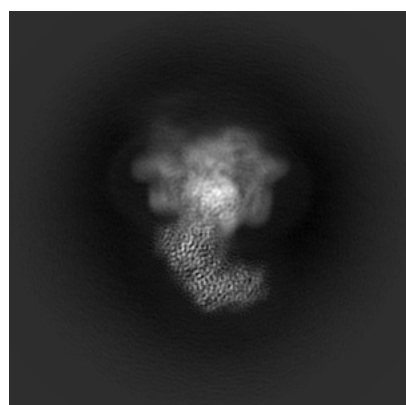
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29004. These allow visual inspection of the internal detail of the map and identification of artifacts.

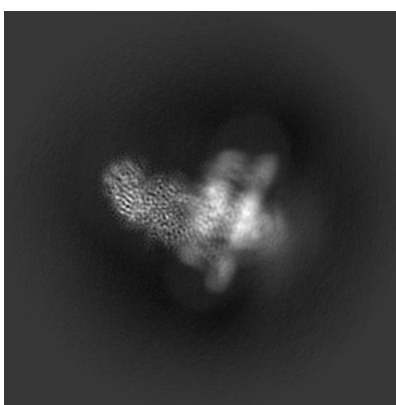
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

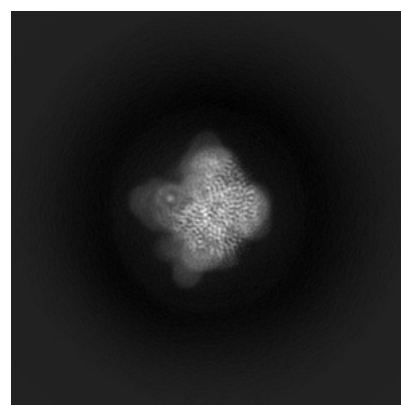
6.1.1 Primary map



X



Y

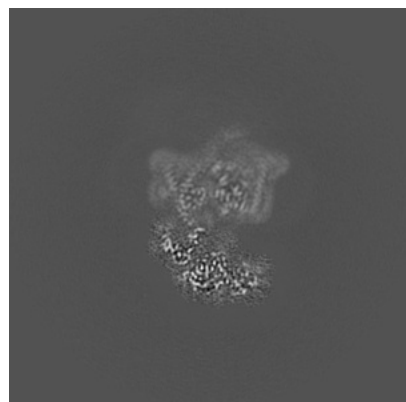


Z

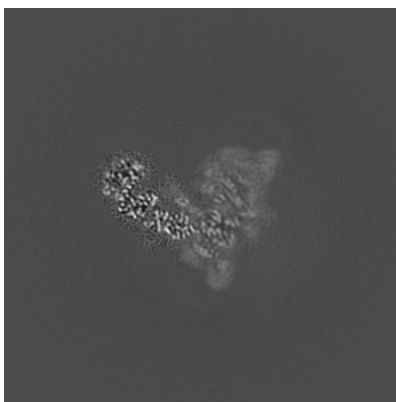
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

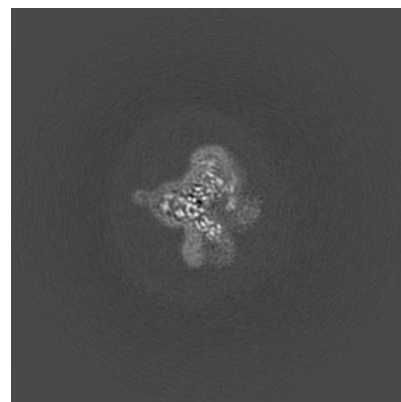
6.2.1 Primary map



X Index: 220



Y Index: 220

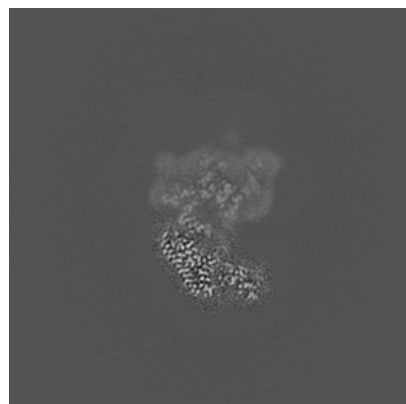


Z Index: 220

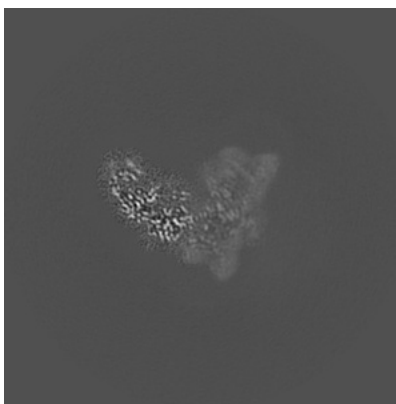
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

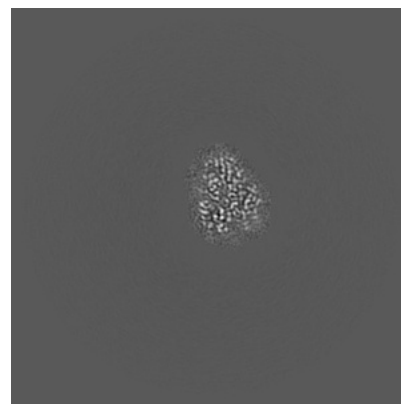
6.3.1 Primary map



X Index: 229



Y Index: 209

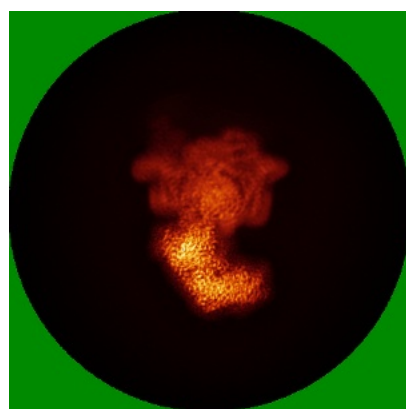


Z Index: 139

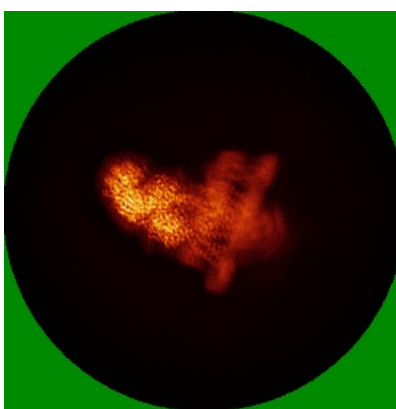
The images above show the largest variance slices of the map in three orthogonal directions.

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

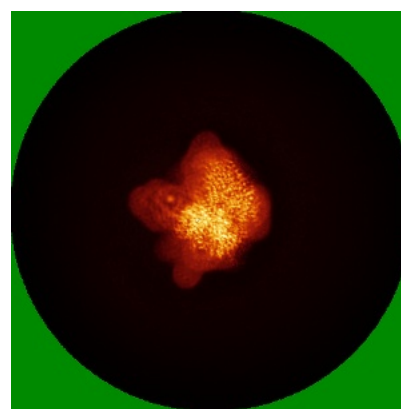
6.4.1 Primary map



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

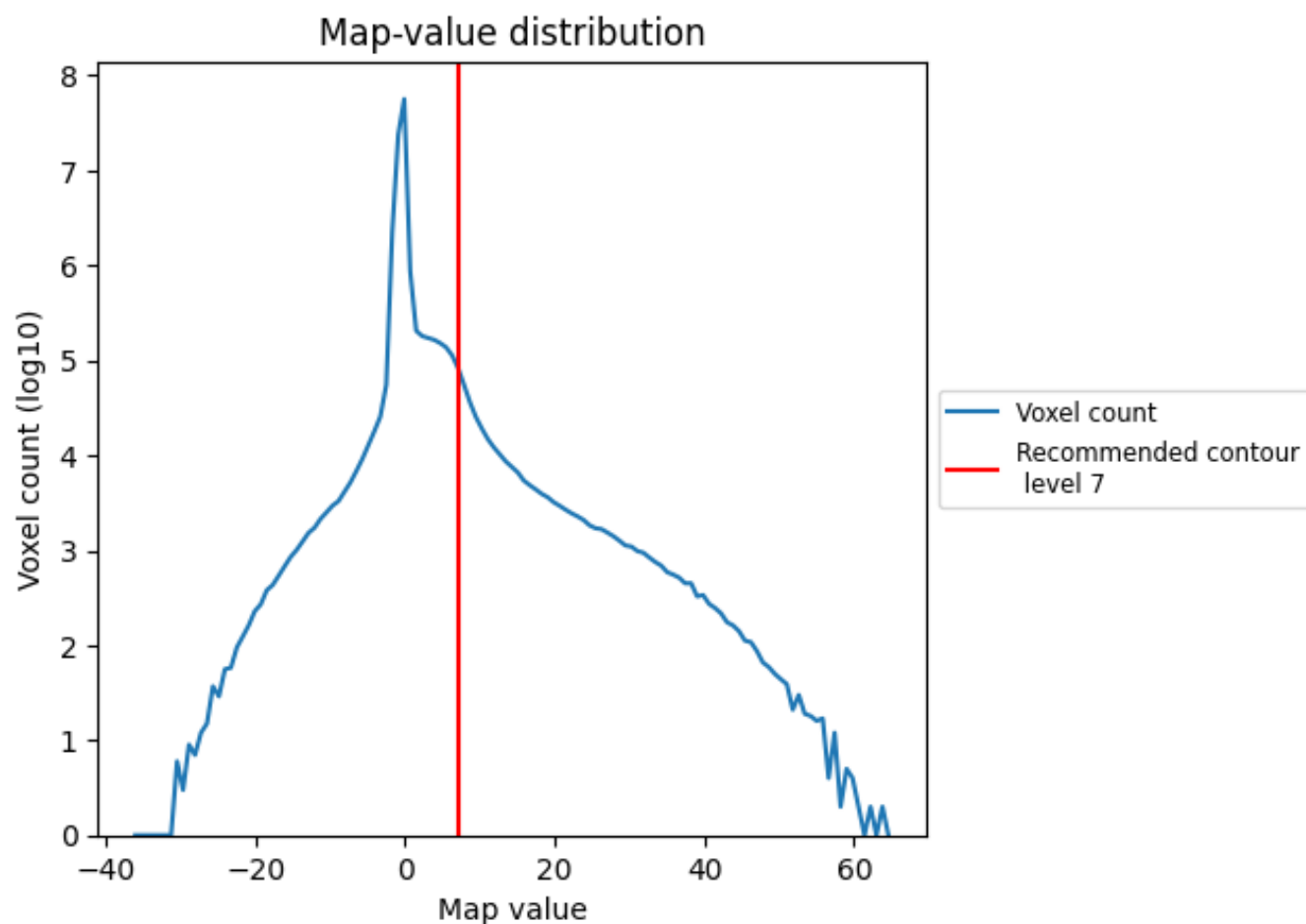
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

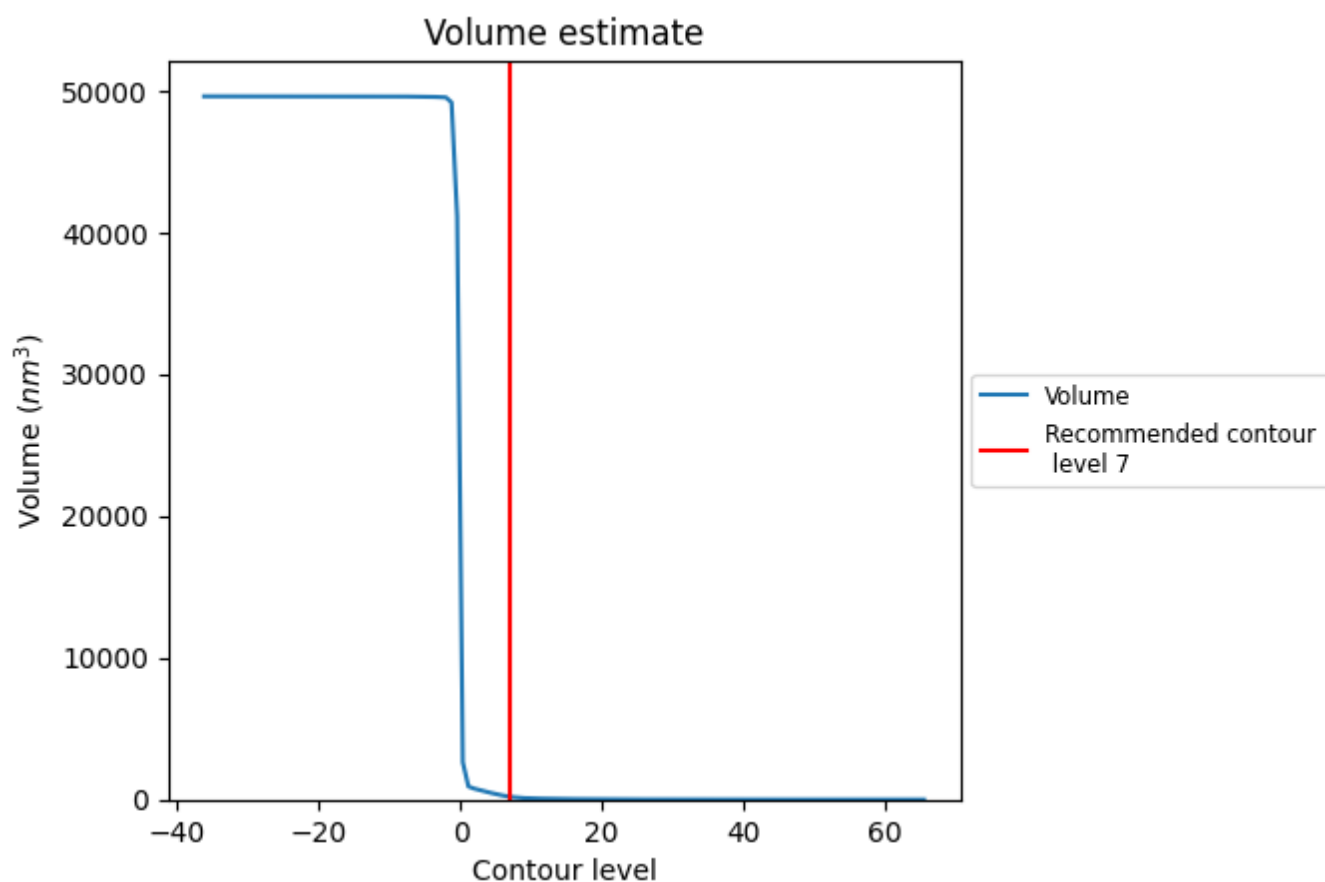
This section contains the results of statistical analysis of the map.

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.

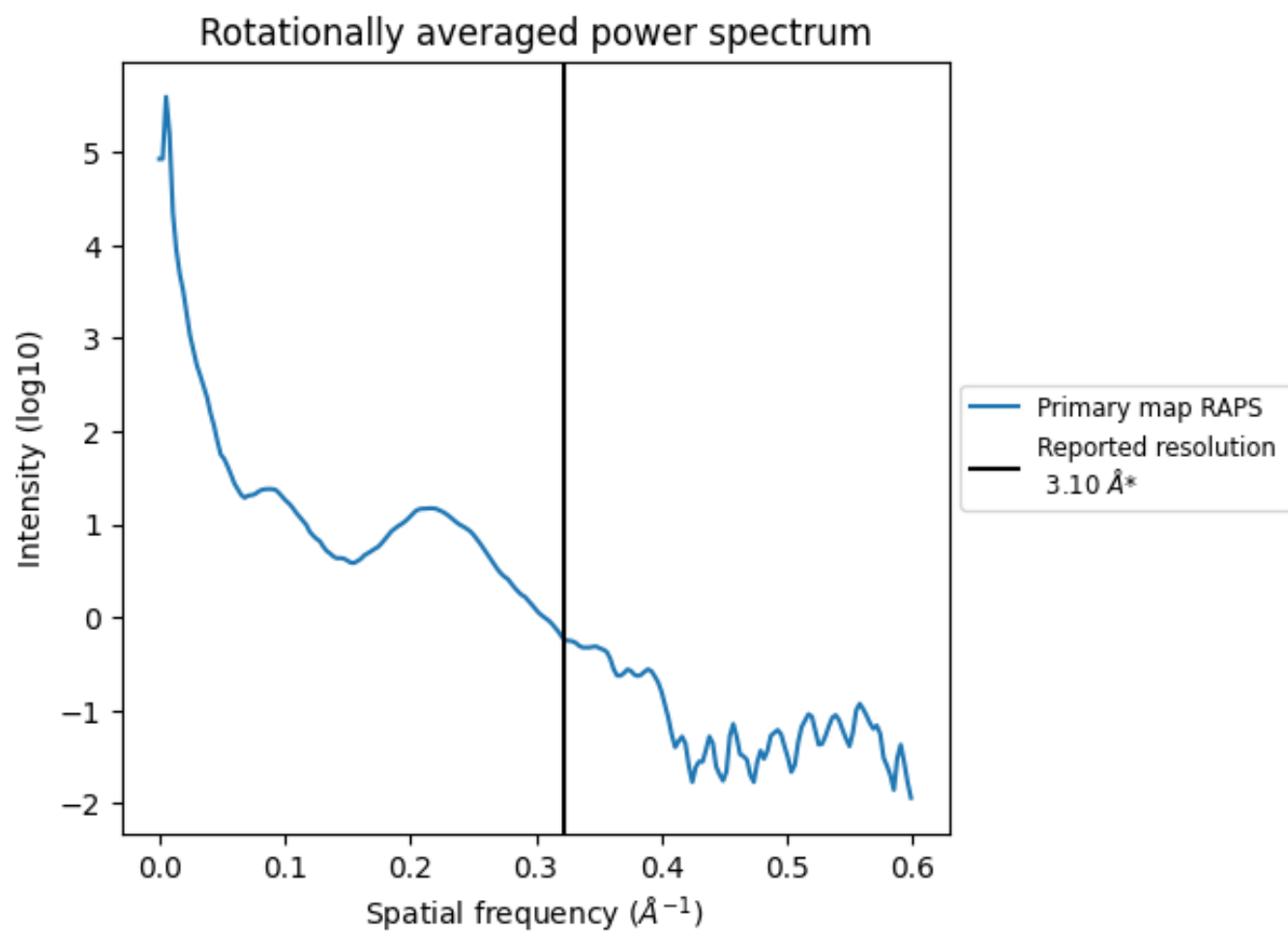
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 184 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 0.323 Å⁻¹

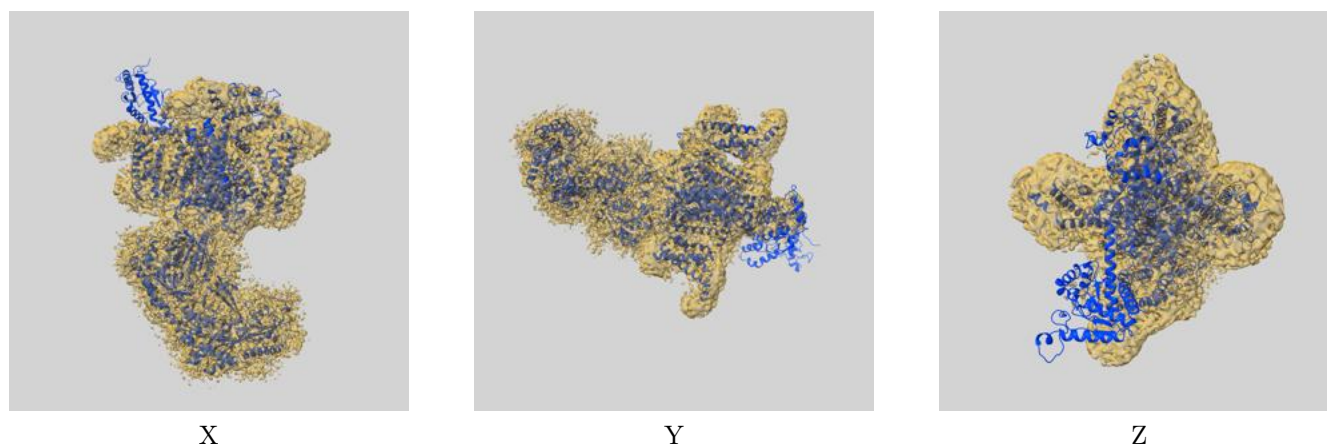
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

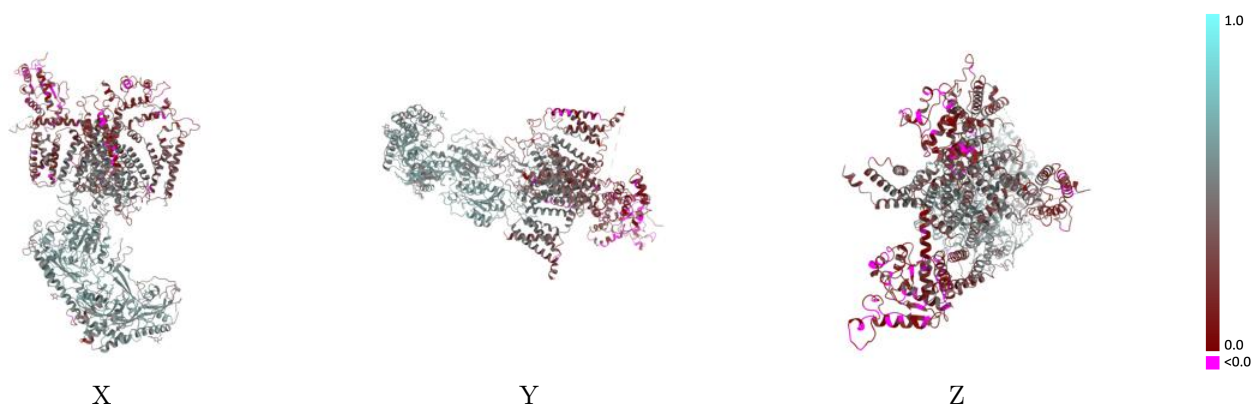
This section contains information regarding the fit between EMDB map EMD-29004 and PDB model 8FD7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



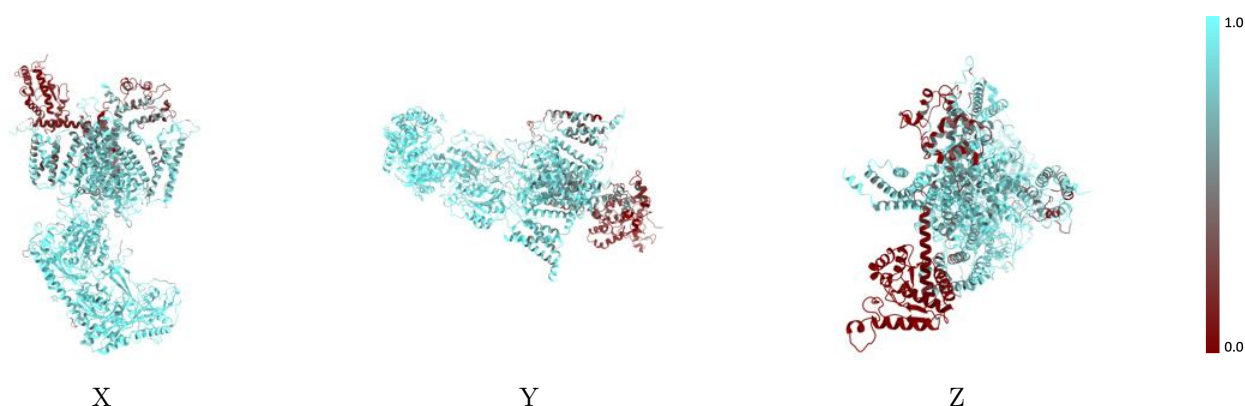
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



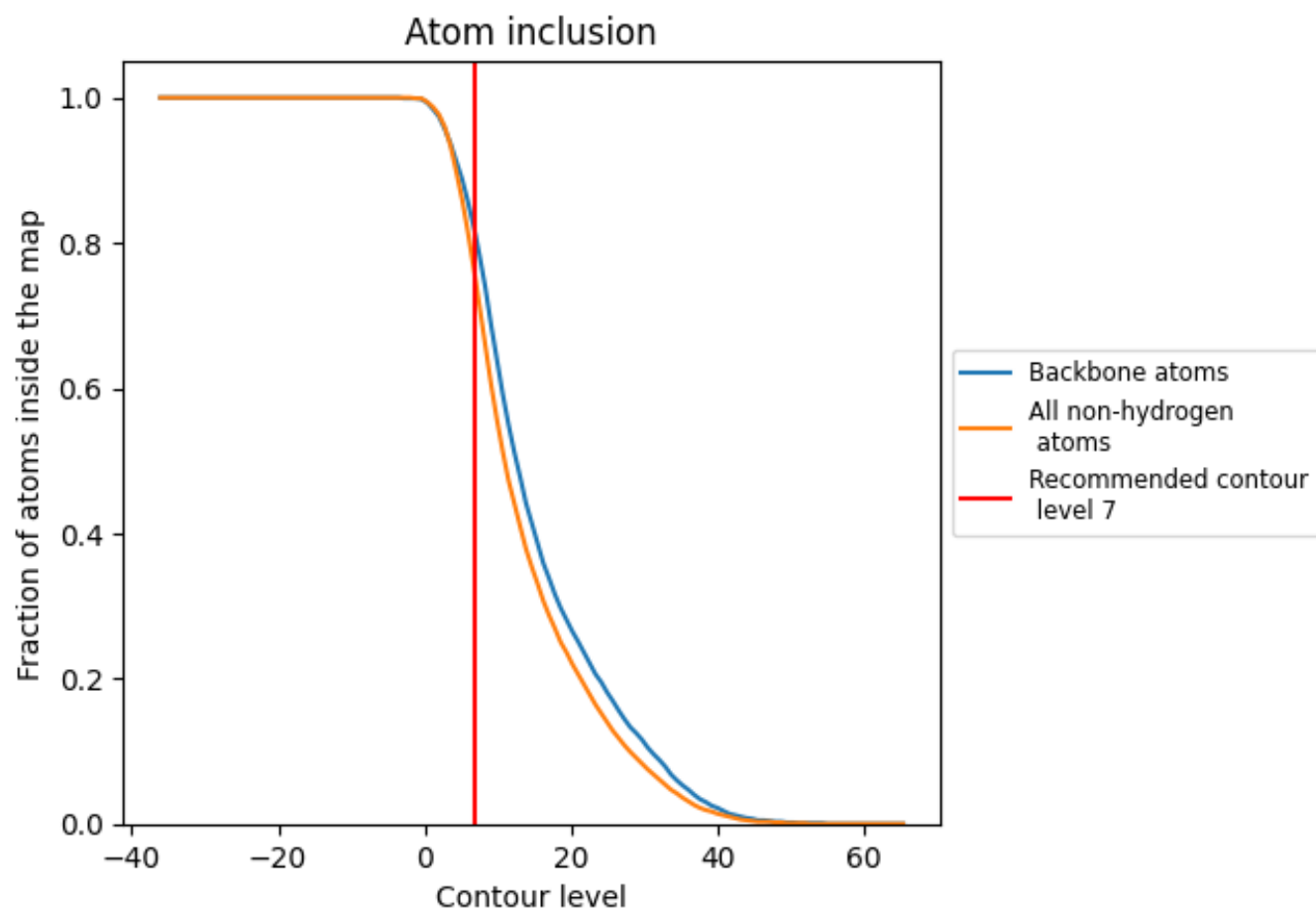
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.4060
C	0.0010	0.1270
D	0.9360	0.5500
F	0.9640	0.5320
K	0.7150	0.3380

