



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:25 AM UTC

PDB ID : 8EOG / pdb_00008eog
EMDB ID : EMD-28375
Title : Structure of the human L-type voltage-gated calcium channel Cav1.2 complexed with L-leucine
Authors : Chen, Z.; Mondal, A.; Abderemane-Ali, F.; Minor, D.L.
Deposited on : 2022-10-03
Resolution : 3.30 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:

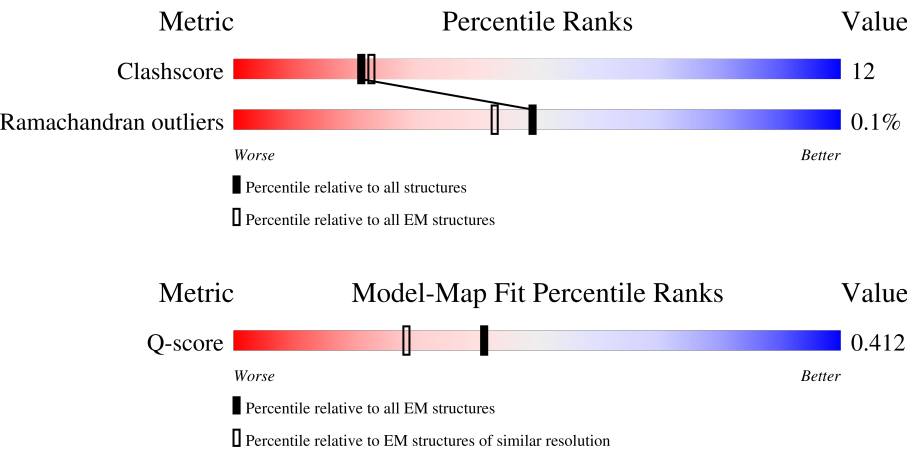
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.30 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	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1050	25% 76% 15% 9%
2	K	1499	58% 27% 15%
3	C	191	100% 68% 32%
4	A	3	33% 33% 33%
5	B	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	E	2	 50%50%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 19729 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

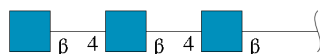
- Molecule 2 is a protein called Isoform 20 of Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	1270	Total	C	N	O	S	0	0
			10230	6729	1673	1761	67		

- 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



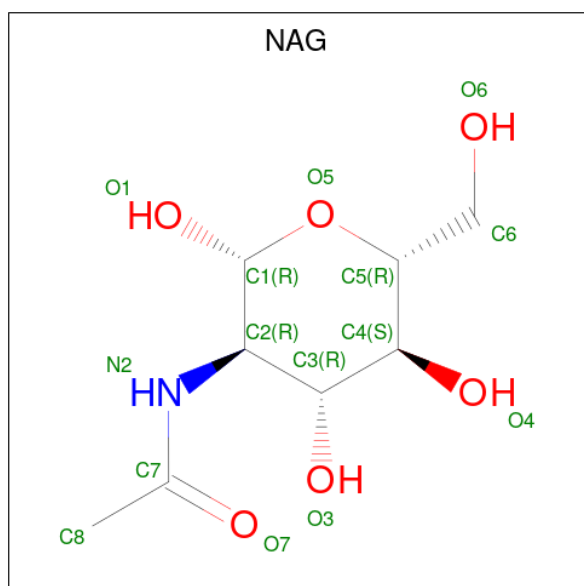
Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 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
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

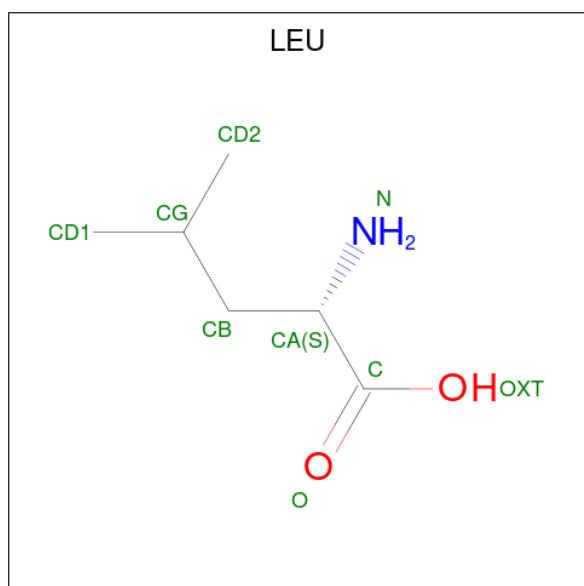
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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).

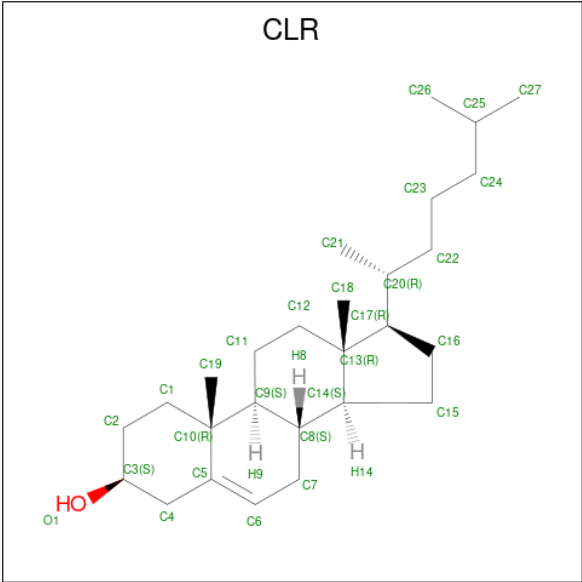
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Na	0
			1	1	

- Molecule 9 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).



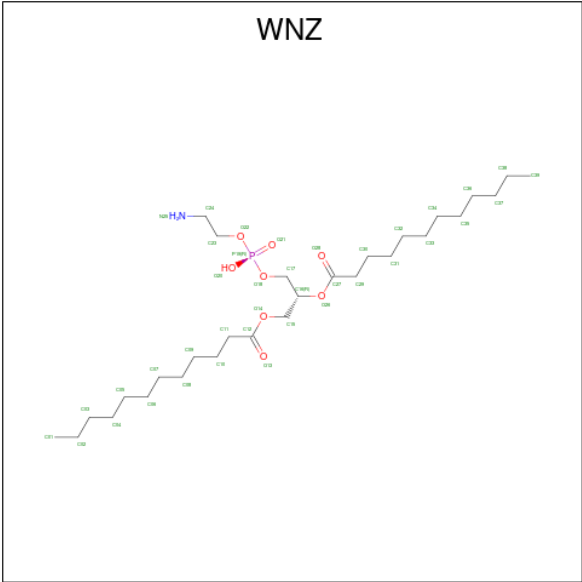
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			9	6	1	2	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



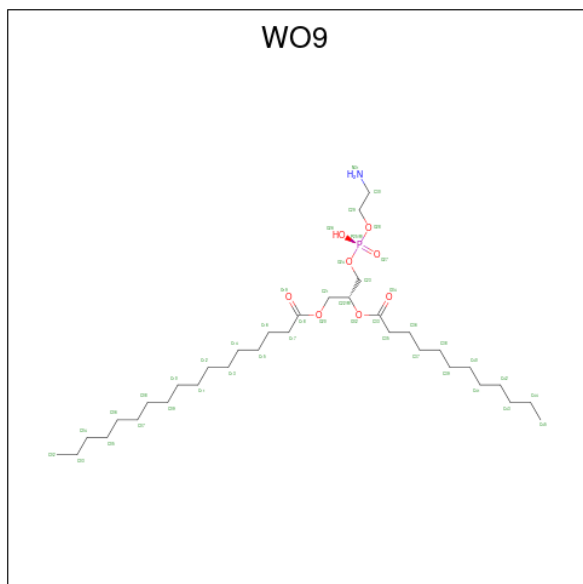
Mol	Chain	Residues	Atoms			AltConf
10	K	1	Total	C	O	0
			28	27	1	
10	K	1	Total	C	O	0
			28	27	1	
10	K	1	Total	C	O	0
			28	27	1	

- Molecule 11 is (2R)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(dodecanoyloxy)propyl dodecanoate (CCD ID: WNZ) (formula: C₂₉H₅₈NO₈P).



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

- Molecule 12 is (2R)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(dodecanoyloxy)propyl heptadecanoate (CCD ID: WO9) (formula: C₃₄H₆₈NO₈P).



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

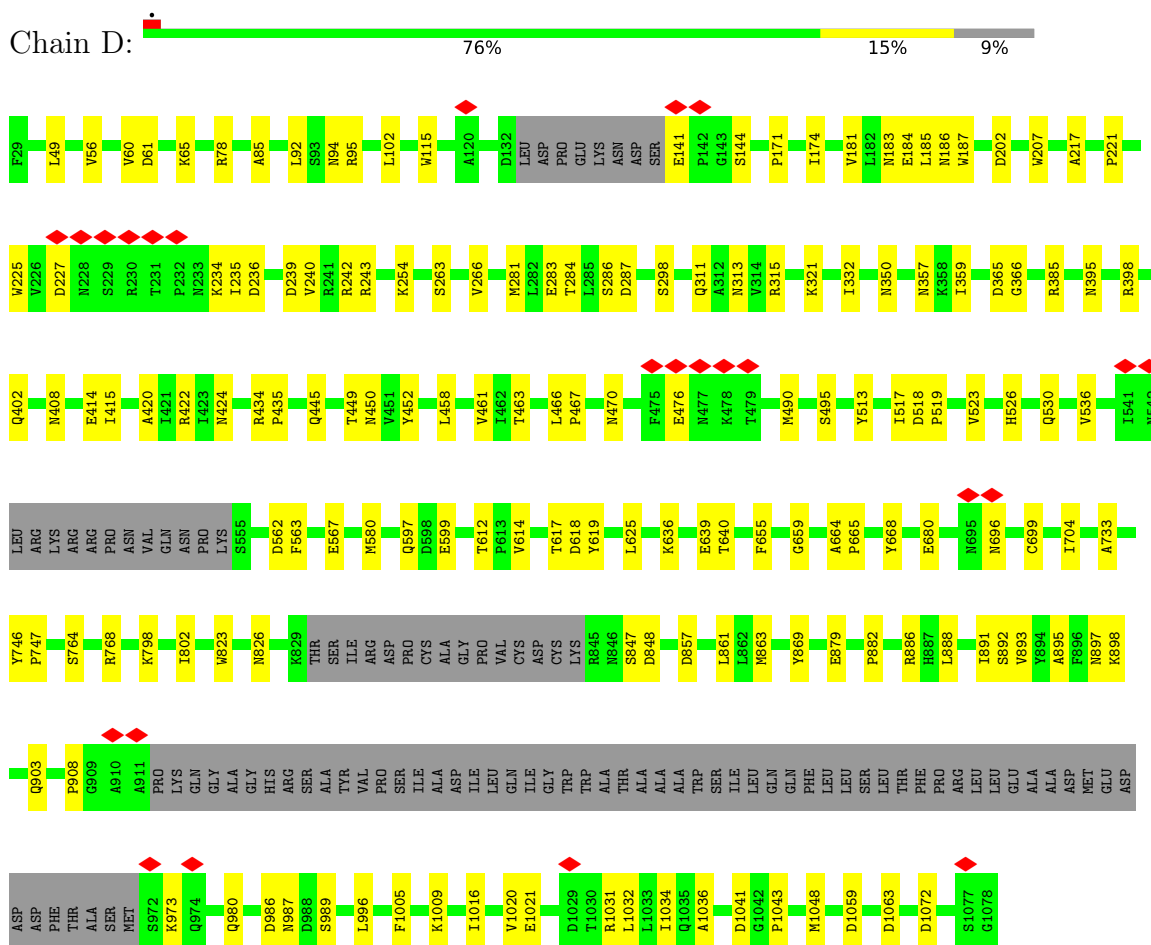
- Molecule 13 is water.

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

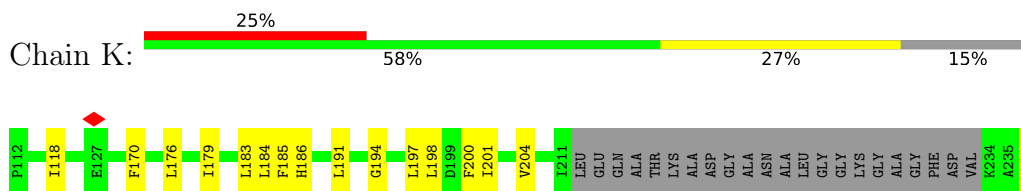
3 Residue-property plots

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

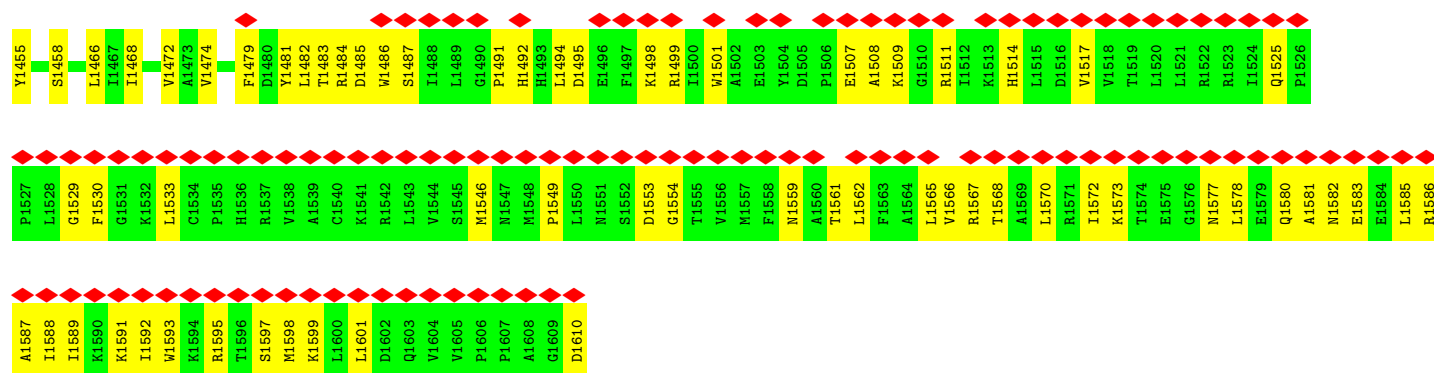
- Molecule 1: Voltage-dependent calcium channel subunit alpha-2/delta-1



- Molecule 2: Isoform 20 of Voltage-dependent L-type calcium channel subunit alpha-1C







• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269802	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	35.807	Depositor
Minimum map value	-13.173	Depositor
Average map value	-0.061	Depositor
Map value standard deviation	0.915	Depositor
Recommended contour level	6.4	Depositor
Map size (Å)	372.504, 372.504, 372.504	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8466, 0.8466, 0.8466	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, NAG, CA, WNZ, WO9

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	0.12	0/7792	0.29	0/10569
2	K	0.12	0/10473	0.34	1/14203 (0.0%)
3	C	0.09	0/1544	0.26	0/2088
All	All	0.12	0/19809	0.32	1/26860 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	626	ARG	N-CA-C	-5.14	104.61	111.24

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	7428	117	0
2	K	10230	0	10445	309	0
3	C	1518	0	1567	43	0
4	A	42	0	37	7	0
5	B	28	0	25	3	0
5	E	28	0	25	6	0
6	D	70	0	65	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	K	2	0	0	0	0
8	D	1	0	0	0	0
9	D	9	0	10	0	0
10	K	84	0	138	7	0
11	K	39	0	0	0	0
12	K	44	0	0	0	0
13	K	3	0	0	0	0
All	All	19729	0	19740	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (471) 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:826:ASN:HD21	5:E:1:NAG:C1	1.48	1.26
1:D:826:ASN:ND2	5:E:1:NAG:C1	2.30	0.94
1:D:897:ASN:ND2	5:B:1:NAG:C1	2.32	0.92
2:K:611:MET:HE3	2:K:612:SER:H	1.44	0.83
1:D:49:LEU:HB2	5:E:2:NAG:O7	1.78	0.83
2:K:623:ARG:O	2:K:626:ARG:HB2	1.79	0.82
2:K:909:PHE:HB3	2:K:1005:PRO:HG3	1.63	0.79
2:K:623:ARG:HA	2:K:626:ARG:HD2	1.65	0.77
2:K:1081:VAL:HG22	2:K:1082:ASP:H	1.50	0.77
2:K:572:LEU:HA	2:K:575:MET:HG2	1.68	0.75
2:K:1222:GLU:HA	2:K:1225:MET:HE3	1.70	0.74
1:D:217:ALA:HB2	1:D:240:VAL:HG21	1.72	0.72
2:K:625:LEU:O	2:K:628:PHE:HB3	1.90	0.72
3:C:211:ARG:HG3	3:C:212:ILE:HG13	1.70	0.71
3:C:251:GLN:HA	3:C:254:ILE:HB	1.70	0.71
2:K:1582:ASN:HA	2:K:1586:ARG:HG2	1.72	0.71
1:D:470:ASN:HD22	4:A:1:NAG:C1	2.04	0.71
1:D:897:ASN:HB3	5:B:1:NAG:H83	1.73	0.71
1:D:115:TRP:NE1	4:A:3:NAG:H5	2.07	0.70
2:K:745:LEU:O	2:K:748:PHE:HB3	1.91	0.69
2:K:1219:THR:O	2:K:1222:GLU:HB3	1.93	0.69
1:D:882:PRO:HB3	1:D:1032:LEU:HA	1.74	0.69
2:K:1112:SER:HB2	2:K:1153:ILE:HG21	1.74	0.68
1:D:94:ASN:ND2	6:D:1101:NAG:O5	2.28	0.67
2:K:913:SER:HA	2:K:917:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:PRO:HG2	3:C:287:PRO:HB3	1.77	0.67
2:K:1578:LEU:HA	2:K:1581:ALA:HB3	1.76	0.67
2:K:297:THR:HA	2:K:313:PRO:HD2	1.76	0.66
1:D:466:LEU:HD12	1:D:467:PRO:HD2	1.78	0.66
2:K:1566:VAL:O	2:K:1570:LEU:N	2.27	0.65
1:D:94:ASN:HD21	6:D:1101:NAG:C1	2.10	0.65
2:K:118:ILE:HD11	2:K:176:LEU:HB2	1.78	0.65
2:K:1010:ASN:HB2	2:K:1015:LEU:HD13	1.77	0.65
2:K:620:ARG:O	2:K:624:LEU:N	2.30	0.64
1:D:470:ASN:ND2	4:A:1:NAG:C1	2.60	0.64
2:K:599:GLY:HA3	2:K:622:VAL:HG11	1.79	0.64
2:K:927:SER:O	2:K:931:HIS:N	2.28	0.64
2:K:442:THR:HG21	2:K:582:ALA:HB2	1.79	0.63
2:K:1588:ILE:HG22	2:K:1595:ARG:HG2	1.81	0.63
2:K:1498:LYS:HA	2:K:1501:TRP:HD1	1.64	0.63
2:K:1511:ARG:HE	2:K:1553:ASP:HB3	1.64	0.62
2:K:640:LEU:O	2:K:644:LEU:HG	2.00	0.62
2:K:1220:TYR:O	2:K:1223:TYR:HB2	2.00	0.62
2:K:1498:LYS:O	2:K:1501:TRP:HB2	2.01	0.61
2:K:1581:ALA:O	2:K:1585:LEU:N	2.31	0.61
2:K:969:PHE:O	2:K:972:LEU:HB3	2.01	0.61
2:K:603:THR:O	2:K:606:VAL:HG22	2.01	0.60
2:K:1328:PHE:O	2:K:1331:PHE:HB2	2.02	0.60
2:K:1007:ARG:NH1	2:K:1010:ASN:OD1	2.34	0.60
2:K:596:VAL:O	2:K:600:ILE:N	2.34	0.60
2:K:296:LYS:HE3	2:K:315:PRO:HB3	1.83	0.60
2:K:1238:MET:HE1	10:K:1701:CLR:H20	1.83	0.60
2:K:1227:VAL:O	2:K:1230:LEU:HB3	2.01	0.60
2:K:540:THR:HG21	2:K:560:ASN:HB3	1.84	0.60
2:K:595:VAL:O	2:K:599:GLY:N	2.33	0.60
2:K:1266:MET:HG2	2:K:1270:LEU:HD12	1.84	0.60
1:D:235:ILE:HD12	2:K:1084:PRO:HG2	1.83	0.59
2:K:1225:MET:HA	2:K:1228:LEU:HB2	1.84	0.59
2:K:1346:ILE:O	2:K:1350:LEU:HD23	2.02	0.59
3:C:192:VAL:O	3:C:196:MET:HG2	2.03	0.59
2:K:1231:LEU:O	2:K:1234:ILE:HG13	2.03	0.59
2:K:1237:ALA:O	2:K:1240:HIS:ND1	2.36	0.59
2:K:1201:ARG:NH1	2:K:1203:ILE:O	2.34	0.58
3:C:178:ARG:HH21	3:C:286:ALA:HB3	1.68	0.58
1:D:239:ASP:OD2	1:D:422:ARG:NH1	2.36	0.58
1:D:60:VAL:HG23	1:D:802:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ALA:HB1	1:D:614:VAL:HG12	1.85	0.58
3:C:232:PRO:HB2	3:C:247:ILE:HG21	1.86	0.58
1:D:470:ASN:ND2	4:A:1:NAG:O5	2.37	0.58
2:K:275:VAL:HA	2:K:395:PHE:HE2	1.68	0.58
2:K:1511:ARG:NH2	2:K:1553:ASP:O	2.36	0.58
2:K:1585:LEU:HD13	2:K:1610:ASP:HB3	1.86	0.58
1:D:286:SER:OG	1:D:287:ASP:N	2.36	0.57
2:K:296:LYS:HD2	2:K:315:PRO:HA	1.86	0.57
3:C:205:LYS:HA	3:C:209:ASP:HB2	1.85	0.57
2:K:194:GLY:O	2:K:197:LEU:HB3	2.05	0.57
2:K:421:PHE:HA	2:K:424:LEU:HB2	1.86	0.57
6:D:1105:NAG:H3	6:D:1105:NAG:H83	1.86	0.57
2:K:1468:ILE:O	2:K:1472:VAL:HG23	2.04	0.57
2:K:952:MET:O	2:K:953:THR:HG22	2.05	0.57
1:D:415:ILE:HG12	1:D:424:ASN:HD22	1.68	0.57
2:K:618:VAL:O	2:K:622:VAL:N	2.32	0.57
2:K:618:VAL:HA	2:K:621:CYS:HB3	1.86	0.57
2:K:1525:GLN:O	2:K:1529:GLY:N	2.38	0.57
1:D:886:ARG:NH2	1:D:1031:ARG:O	2.35	0.57
3:C:250:VAL:O	3:C:254:ILE:N	2.34	0.57
1:D:1043:PRO:HG2	1:D:1048:MET:HE2	1.87	0.57
2:K:426:GLU:O	2:K:430:LEU:N	2.30	0.57
2:K:1117:TRP:CD1	2:K:1118:PRO:HD3	2.39	0.56
2:K:1427:PRO:HA	2:K:1448:GLY:HA2	1.87	0.56
2:K:1018:VAL:HG21	2:K:1362:TYR:HB3	1.86	0.56
3:C:211:ARG:O	3:C:265:GLN:NE2	2.38	0.56
1:D:733:ALA:HA	1:D:747:PRO:HG2	1.86	0.56
1:D:115:TRP:CD1	4:A:3:NAG:H61	2.40	0.56
2:K:1215:VAL:O	2:K:1269:LYS:NZ	2.39	0.56
2:K:992:ASN:HA	2:K:996:ILE:HG23	1.88	0.55
1:D:1009:LYS:HG2	1:D:1016:ILE:HG22	1.87	0.55
2:K:311:ASP:OD1	2:K:311:ASP:N	2.38	0.55
3:C:339:GLU:HG3	3:C:345:ALA:HB2	1.86	0.55
2:K:1270:LEU:HA	2:K:1273:PHE:HB2	1.88	0.55
2:K:1486:TRP:HH2	2:K:1492:HIS:HB3	1.70	0.55
3:C:212:ILE:HG12	3:C:266:LEU:HB3	1.89	0.55
2:K:963:SER:OG	2:K:967:ASN:N	2.39	0.55
2:K:1006:LEU:O	2:K:1010:ASN:N	2.40	0.55
2:K:1370:LEU:HD22	2:K:1466:LEU:HD12	1.88	0.55
2:K:1514:HIS:HA	2:K:1517:VAL:HG22	1.89	0.55
1:D:1032:LEU:H	1:D:1032:LEU:HD23	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1209:GLN:HG2	2:K:1210:TYR:HD1	1.73	0.54
2:K:1577:ASN:HB2	2:K:1580:GLN:HE21	1.73	0.54
1:D:92:LEU:HD12	1:D:617:THR:HG21	1.88	0.54
2:K:1063:LYS:HB3	2:K:1068:GLU:HG3	1.89	0.54
1:D:227:ASP:HA	1:D:234:LYS:HE3	1.89	0.54
2:K:410:LYS:HZ1	2:K:753:VAL:HG13	1.72	0.54
2:K:1392:GLU:HG3	2:K:1420:ASP:HB3	1.88	0.54
1:D:879:GLU:HG2	1:D:1032:LEU:HD12	1.89	0.54
2:K:1597:SER:OG	2:K:1598:MET:N	2.41	0.54
2:K:537:ASN:HD21	2:K:623:ARG:HB3	1.72	0.54
1:D:141:GLU:OE2	1:D:144:SER:OG	2.25	0.53
2:K:648:VAL:HA	2:K:651:ILE:HG12	1.90	0.53
2:K:1530:PHE:HE2	2:K:1533:LEU:HB3	1.73	0.53
1:D:61:ASP:O	1:D:65:LYS:N	2.40	0.53
2:K:748:PHE:HA	2:K:1158:MET:HE1	1.91	0.53
2:K:197:LEU:O	2:K:201:ILE:HD12	2.07	0.53
2:K:331:VAL:HG23	2:K:333:LYS:HG2	1.91	0.53
2:K:989:SER:HA	2:K:993:VAL:HG22	1.90	0.53
2:K:1000:LEU:HD23	2:K:1003:LEU:HD13	1.90	0.53
3:C:182:LEU:HG	3:C:290:VAL:HB	1.90	0.53
2:K:1129:THR:HG22	2:K:1130:GLU:H	1.74	0.53
1:D:895:ALA:HB2	1:D:986:ASP:HB2	1.91	0.53
2:K:546:TYR:N	2:K:1099:ASP:OD1	2.42	0.53
1:D:359:ILE:HG22	1:D:385:ARG:HB2	1.90	0.53
1:D:513:TYR:OH	1:D:567:GLU:OE2	2.24	0.53
2:K:1006:LEU:HA	2:K:1009:ILE:HG12	1.90	0.53
2:K:1495:ASP:O	2:K:1498:LYS:HB2	2.09	0.53
2:K:185:PHE:CE1	2:K:191:LEU:HB3	2.44	0.52
2:K:901:ILE:HA	2:K:904:ASN:HD21	1.74	0.52
1:D:668:TYR:HB3	1:D:704:ILE:HD11	1.90	0.52
2:K:617:SER:O	2:K:621:CYS:N	2.33	0.52
2:K:1081:VAL:HG22	2:K:1082:ASP:N	2.23	0.52
1:D:420:ALA:HB1	1:D:424:ASN:HD21	1.74	0.52
3:C:213:SER:HB2	3:C:267:VAL:HG23	1.91	0.52
1:D:1072:ASP:N	1:D:1072:ASP:OD1	2.43	0.52
2:K:373:ASN:HB3	2:K:378:ARG:HG2	1.91	0.52
2:K:437:TYR:HB3	3:C:303:LEU:HD21	1.90	0.52
2:K:1499:ARG:CZ	2:K:1499:ARG:HA	2.39	0.52
2:K:600:ILE:O	2:K:603:THR:OG1	2.19	0.52
2:K:118:ILE:HG21	2:K:179:ILE:HG22	1.90	0.52
1:D:523:VAL:HG11	1:D:526:HIS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:TRP:HD1	4:A:3:NAG:H61	1.75	0.52
2:K:322:HIS:HB2	2:K:377:GLY:HA2	1.91	0.51
2:K:423:LYS:O	2:K:427:LYS:N	2.35	0.51
1:D:184:GLU:HA	1:D:187:TRP:CD1	2.45	0.51
2:K:200:PHE:CZ	2:K:236:LEU:HD12	2.45	0.51
2:K:1078:ASP:OD1	2:K:1078:ASP:N	2.40	0.51
2:K:1494:LEU:O	2:K:1498:LYS:N	2.42	0.51
1:D:449:THR:OG1	1:D:450:ASN:N	2.43	0.51
2:K:1127:SER:O	2:K:1139:ARG:NH2	2.44	0.51
1:D:183:ASN:O	1:D:184:GLU:C	2.53	0.51
2:K:1386:ALA:HB2	2:K:1431:CYS:SG	2.51	0.51
2:K:925:HIS:HA	2:K:1436:GLU:HA	1.91	0.51
1:D:519:PRO:HD3	1:D:618:ASP:O	2.10	0.51
1:D:398:ARG:O	1:D:402:GLN:NE2	2.43	0.50
2:K:1266:MET:HE3	2:K:1291:VAL:HG21	1.92	0.50
1:D:287:ASP:OD2	1:D:450:ASN:ND2	2.45	0.50
3:C:173:VAL:O	3:C:284:SER:OG	2.29	0.50
2:K:973:ASP:O	2:K:976:VAL:HB	2.11	0.50
2:K:1486:TRP:CH2	2:K:1492:HIS:HB3	2.46	0.50
2:K:1587:ALA:O	2:K:1591:LYS:N	2.29	0.50
1:D:115:TRP:CD1	4:A:3:NAG:H5	2.47	0.50
2:K:571:MET:HE2	2:K:600:ILE:HG21	1.92	0.50
3:C:216:ARG:HA	3:C:270:ASP:HB3	1.93	0.50
1:D:186:ASN:OD1	1:D:187:TRP:N	2.44	0.50
2:K:752:ALA:HA	2:K:1162:VAL:HG11	1.94	0.50
2:K:944:PHE:O	2:K:947:GLU:HG2	2.12	0.50
1:D:1034:ILE:HG22	1:D:1036:ALA:H	1.76	0.50
2:K:201:ILE:HA	2:K:204:VAL:HG12	1.93	0.50
2:K:1572:ILE:HG23	2:K:1580:GLN:HE22	1.77	0.50
3:C:304:ILE:HA	3:C:307:ARG:HG2	1.94	0.50
1:D:78:ARG:HH11	1:D:612:THR:HG22	1.76	0.49
2:K:1094:SER:O	2:K:1094:SER:OG	2.23	0.49
1:D:181:VAL:O	1:D:185:LEU:HD13	2.12	0.49
2:K:590:ARG:O	2:K:594:PHE:N	2.44	0.49
2:K:639:ASN:HD22	2:K:762:LEU:HD21	1.77	0.49
2:K:1039:LEU:HG	2:K:1156:PHE:HE2	1.77	0.49
2:K:1113:THR:HG21	2:K:1418:TRP:HZ2	1.76	0.49
1:D:102:LEU:HB3	1:D:490:MET:CE	2.42	0.49
1:D:1063:ASP:OD1	1:D:1063:ASP:N	2.43	0.49
2:K:624:LEU:C	2:K:626:ARG:H	2.20	0.49
2:K:1224:LEU:O	2:K:1227:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1256:MET:SD	2:K:1298:ILE:HG12	2.53	0.49
2:K:1127:SER:OG	2:K:1139:ARG:NH2	2.45	0.49
2:K:1358:GLN:H	2:K:1358:GLN:CD	2.20	0.49
2:K:1205:LYS:HD2	2:K:1207:GLN:HG2	1.94	0.49
3:C:178:ARG:O	3:C:356:TYR:OH	2.30	0.49
2:K:968:TYR:O	2:K:971:ILE:HG12	2.13	0.49
2:K:1298:ILE:O	2:K:1301:THR:OG1	2.31	0.49
1:D:461:VAL:HG12	1:D:495:SER:HA	1.94	0.49
1:D:996:LEU:HB2	1:D:1005:PHE:HE2	1.77	0.49
2:K:1287:ASP:O	2:K:1290:ILE:HG13	2.12	0.49
2:K:1157:MET:N	2:K:1157:MET:HE2	2.28	0.49
3:C:185:PRO:HD2	3:C:193:THR:HG23	1.94	0.49
1:D:857:ASP:OD1	1:D:857:ASP:N	2.42	0.49
2:K:347:ASP:N	2:K:347:ASP:OD1	2.45	0.49
2:K:418:ARG:HG2	2:K:418:ARG:HH11	1.78	0.49
2:K:1334:MET:HA	2:K:1334:MET:HE3	1.94	0.49
2:K:1507:GLU:HG2	2:K:1508:ALA:H	1.77	0.49
2:K:1595:ARG:NH1	2:K:1601:LEU:HB2	2.28	0.49
1:D:95:ARG:NH1	1:D:202:ASP:OD2	2.45	0.48
1:D:768:ARG:NH2	1:D:857:ASP:OD2	2.43	0.48
2:K:441:ILE:O	2:K:445:GLU:HB3	2.13	0.48
2:K:585:VAL:HA	2:K:590:ARG:HD2	1.95	0.48
2:K:1565:LEU:O	2:K:1568:THR:OG1	2.27	0.48
3:C:294:VAL:HG11	3:C:300:LEU:HB2	1.95	0.48
2:K:314:SER:N	2:K:323:GLY:O	2.45	0.48
1:D:639:GLU:OE2	1:D:640:THR:N	2.46	0.48
2:K:244:PRO:O	2:K:247:LEU:HB3	2.13	0.48
2:K:590:ARG:HA	2:K:593:CYS:HB2	1.93	0.48
2:K:1365:LEU:HA	2:K:1368:VAL:HG22	1.95	0.48
1:D:517:ILE:HD11	1:D:580:MET:HG3	1.95	0.48
2:K:401:LEU:HD21	2:K:1482:LEU:HB3	1.94	0.48
2:K:1484:ARG:NH1	2:K:1485:ASP:O	2.45	0.48
1:D:898:LYS:HA	1:D:980:GLN:O	2.14	0.48
2:K:1054:LYS:HG2	2:K:1129:THR:O	2.14	0.48
2:K:624:LEU:O	2:K:627:ILE:HG12	2.13	0.48
2:K:940:PHE:HB3	2:K:944:PHE:CZ	2.49	0.48
2:K:563:LEU:HA	2:K:566:LEU:HD12	1.96	0.48
2:K:1290:ILE:HD13	2:K:1335:ARG:HG2	1.96	0.48
2:K:1573:LYS:HB2	2:K:1577:ASN:HB3	1.94	0.48
2:K:1281:ASP:OD2	2:K:1284:ASN:N	2.47	0.48
2:K:1098:PHE:HA	2:K:1104:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1002:VAL:C	2:K:1005:PRO:HD2	2.39	0.47
2:K:1479:PHE:CD2	2:K:1483:THR:HG21	2.49	0.47
2:K:901:ILE:HA	2:K:904:ASN:ND2	2.29	0.47
2:K:952:MET:SD	2:K:952:MET:N	2.86	0.47
2:K:1100:ASN:ND2	2:K:1102:LEU:HB3	2.29	0.47
2:K:1586:ARG:O	2:K:1589:ILE:HG12	2.14	0.47
1:D:315:ARG:HH11	1:D:536:VAL:HG13	1.79	0.47
2:K:1484:ARG:HH12	2:K:1486:TRP:HE3	1.61	0.47
2:K:306:ASP:OD1	2:K:306:ASP:N	2.44	0.47
2:K:1200:ARG:HE	2:K:1200:ARG:HB3	1.49	0.47
2:K:170:PHE:HB3	2:K:198:LEU:HD11	1.95	0.47
2:K:437:TYR:HB3	3:C:303:LEU:HD11	1.97	0.47
2:K:527:TYR:O	2:K:530:VAL:HG12	2.15	0.47
2:K:621:CYS:O	2:K:624:LEU:HB2	2.15	0.47
2:K:624:LEU:C	2:K:626:ARG:N	2.73	0.47
2:K:1079:GLY:O	2:K:1080:GLU:HG3	2.15	0.47
2:K:1240:HIS:NE2	10:K:1701:CLR:H242	2.30	0.47
1:D:597:GLN:HB3	1:D:764:SER:HB2	1.95	0.47
1:D:1059:ASP:OD1	1:D:1059:ASP:N	2.41	0.47
2:K:970:ASN:OD1	2:K:971:ILE:N	2.48	0.47
2:K:1247:PHE:CE1	2:K:1251:MET:HE3	2.50	0.47
2:K:1601:LEU:H	2:K:1601:LEU:HD12	1.80	0.47
2:K:967:ASN:N	2:K:967:ASN:OD1	2.48	0.47
2:K:1369:MET:HE3	2:K:1369:MET:HB2	1.77	0.47
1:D:311:GLN:OE1	1:D:313:ASN:ND2	2.48	0.46
5:E:1:NAG:H4	5:E:2:NAG:N2	2.30	0.46
2:K:200:PHE:HZ	2:K:236:LEU:HD12	1.80	0.46
2:K:384:TYR:O	2:K:387:THR:OG1	2.28	0.46
2:K:415:ALA:HB3	2:K:416:LYS:HE2	1.96	0.46
2:K:433:ASP:OD1	2:K:434:LEU:N	2.49	0.46
3:C:217:VAL:HB	3:C:271:ALA:HA	1.97	0.46
1:D:281:MET:O	1:D:284:THR:OG1	2.28	0.46
1:D:746:TYR:HB3	1:D:747:PRO:HD3	1.97	0.46
2:K:526:PHE:HA	2:K:529:LEU:HD12	1.97	0.46
3:C:260:LEU:O	3:C:264:LEU:N	2.48	0.46
1:D:897:ASN:OD1	1:D:897:ASN:N	2.48	0.46
2:K:599:GLY:O	2:K:602:GLU:HB3	2.15	0.46
2:K:754:ASP:OD1	2:K:754:ASP:N	2.49	0.46
2:K:975:LEU:O	2:K:979:VAL:N	2.47	0.46
2:K:1135:ILE:HG22	2:K:1136:TYR:N	2.30	0.46
2:K:608:THR:O	2:K:609:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ASN:H	1:D:408:ASN:ND2	2.14	0.46
3:C:178:ARG:NH2	3:C:285:LEU:O	2.48	0.46
1:D:680:GLU:OE1	1:D:680:GLU:N	2.37	0.46
2:K:443:GLN:HA	2:K:447:ILE:HB	1.98	0.46
2:K:586:SER:HB3	2:K:589:ASN:HD21	1.80	0.46
2:K:945:THR:HG21	2:K:979:VAL:HG21	1.97	0.46
2:K:1092:GLU:N	2:K:1092:GLU:OE1	2.49	0.46
1:D:847:SER:OG	1:D:848:ASP:N	2.48	0.45
2:K:183:LEU:HD12	2:K:186:HIS:CE1	2.51	0.45
2:K:552:LEU:O	2:K:555:VAL:HB	2.16	0.45
2:K:1344:GLU:HG2	2:K:1345:GLY:H	1.80	0.45
2:K:1352:THR:HG21	2:K:1481:TYR:CD2	2.50	0.45
2:K:960:HIS:CE1	2:K:961:LYS:HG2	2.51	0.45
2:K:1163:GLY:O	2:K:1166:ILE:HG22	2.16	0.45
2:K:297:THR:OG1	2:K:298:CYS:N	2.48	0.45
2:K:299:TYR:HD2	2:K:333:LYS:HB2	1.81	0.45
3:C:174:VAL:HB	3:C:178:ARG:HH12	1.81	0.45
2:K:511:ARG:HB3	2:K:512:PHE:H	1.63	0.45
2:K:1126:ASP:HB2	2:K:1135:ILE:O	2.16	0.45
2:K:1256:MET:HE1	2:K:1298:ILE:HG23	1.97	0.45
1:D:562:ASP:OD1	1:D:563:PHE:N	2.49	0.45
2:K:321:GLY:HA2	2:K:324:ARG:NH2	2.31	0.45
2:K:1223:TYR:HA	2:K:1226:PHE:CD1	2.51	0.45
1:D:49:LEU:CB	5:E:2:NAG:O7	2.57	0.45
1:D:225:TRP:NE1	1:D:236:ASP:OD1	2.49	0.45
2:K:294:MET:HE1	2:K:371:TRP:HB3	1.99	0.45
2:K:923:VAL:HG23	2:K:1435:SER:HB3	1.99	0.45
2:K:1209:GLN:N	2:K:1209:GLN:OE1	2.50	0.45
2:K:1592:ILE:HG22	2:K:1593:TRP:CD1	2.51	0.45
2:K:299:TYR:HB2	2:K:333:LYS:HG3	1.98	0.45
2:K:1010:ASN:OD1	2:K:1010:ASN:C	2.60	0.45
2:K:1195:LYS:HA	2:K:1197:ARG:HH21	1.82	0.45
1:D:365:ASP:OD1	1:D:366:GLY:N	2.47	0.45
1:D:696:ASN:HB3	1:D:699:CYS:HB2	1.98	0.45
1:D:1031:ARG:HA	1:D:1031:ARG:NE	2.31	0.45
10:K:1702:CLR:H221	10:K:1702:CLR:H162	1.52	0.45
3:C:220:ASP:HA	3:C:273:THR:HG21	1.99	0.45
1:D:530:GLN:O	1:D:903:GLN:NE2	2.49	0.45
2:K:630:ILE:C	2:K:632:ARG:H	2.24	0.45
2:K:1507:GLU:HG2	2:K:1508:ALA:N	2.32	0.45
1:D:636:LYS:HB3	1:D:636:LYS:HE2	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:923:VAL:HG11	2:K:1400:GLN:HG2	1.98	0.45
2:K:1499:ARG:HA	2:K:1499:ARG:NE	2.32	0.45
1:D:234:LYS:HD2	1:D:234:LYS:HA	1.78	0.44
1:D:254:LYS:HA	1:D:357:ASN:HB2	1.99	0.44
1:D:892:SER:O	1:D:892:SER:OG	2.25	0.44
2:K:943:ILE:HG13	2:K:944:PHE:N	2.32	0.44
1:D:414:GLU:O	1:D:424:ASN:ND2	2.51	0.44
2:K:403:VAL:HG12	2:K:749:LEU:HD13	1.99	0.44
2:K:686:ARG:HD2	2:K:686:ARG:HA	1.74	0.44
2:K:1278:TYR:O	2:K:1284:ASN:ND2	2.50	0.44
2:K:949:ILE:O	2:K:952:MET:HG2	2.16	0.44
2:K:1203:ILE:HG23	2:K:1213:TRP:CD2	2.52	0.44
3:C:224:ALA:HA	3:C:247:ILE:HD11	1.99	0.44
3:C:358:ARG:HA	3:C:358:ARG:NE	2.32	0.44
2:K:348:ASN:HD21	10:K:1701:CLR:H181	1.83	0.44
2:K:1191:GLU:O	2:K:1195:LYS:NZ	2.44	0.44
2:K:1209:GLN:HG2	2:K:1210:TYR:CD1	2.52	0.44
3:C:202:ASP:HA	3:C:205:LYS:HE2	2.00	0.44
2:K:236:LEU:HD22	2:K:236:LEU:H	1.83	0.44
2:K:348:ASN:OD1	2:K:349:PHE:N	2.44	0.44
1:D:207:TRP:CE3	1:D:221:PRO:HD2	2.53	0.44
2:K:413:GLU:C	2:K:415:ALA:H	2.25	0.44
2:K:1398:ASN:HD22	2:K:1404:GLN:HE22	1.65	0.44
3:C:266:LEU:HD12	3:C:267:VAL:H	1.82	0.44
1:D:263:SER:O	1:D:266:VAL:HG22	2.18	0.44
2:K:333:LYS:O	2:K:335:GLY:N	2.50	0.44
2:K:575:MET:SD	2:K:575:MET:N	2.91	0.44
2:K:1010:ASN:CB	2:K:1015:LEU:HD13	2.48	0.44
3:C:320:MET:HA	3:C:323:ASP:OD2	2.17	0.44
1:D:395:ASN:N	1:D:395:ASN:OD1	2.51	0.43
2:K:1491:PRO:HA	2:K:1494:LEU:HD13	2.00	0.43
3:C:226:ARG:HH22	3:C:251:GLN:HE22	1.66	0.43
2:K:1454:PHE:O	2:K:1458:SER:OG	2.29	0.43
3:C:254:ILE:HA	3:C:257:ILE:HB	2.01	0.43
2:K:1374:TYR:O	2:K:1455:TYR:OH	2.35	0.43
2:K:1587:ALA:HB1	2:K:1591:LYS:HB3	2.00	0.43
2:K:340:LYS:HA	2:K:340:LYS:HD3	1.84	0.43
2:K:1238:MET:HE2	2:K:1238:MET:HA	1.99	0.43
2:K:1377:ILE:O	2:K:1381:VAL:HG12	2.18	0.43
3:C:343:GLU:O	3:C:347:GLU:HG2	2.17	0.43
2:K:921:ASP:C	2:K:924:GLN:HE22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:563:LEU:HD23	2:K:566:LEU:HD12	2.01	0.43
1:D:987:ASN:OD1	1:D:989:SER:OG	2.34	0.43
1:D:102:LEU:HB3	1:D:490:MET:HE2	2.01	0.43
2:K:347:ASP:HB2	2:K:1240:HIS:HB2	2.00	0.43
1:D:823:TRP:CD1	1:D:863:MET:HE1	2.53	0.43
2:K:560:ASN:O	2:K:563:LEU:HB2	2.19	0.43
2:K:655:LEU:HD23	2:K:655:LEU:HA	1.88	0.43
2:K:1331:PHE:HA	2:K:1334:MET:HG2	2.01	0.43
2:K:271:ILE:O	2:K:275:VAL:HG23	2.19	0.43
2:K:972:LEU:HB2	2:K:1004:ARG:NH1	2.34	0.43
2:K:1401:THR:HG22	2:K:1403:PRO:HD2	2.00	0.43
2:K:1364:ALA:O	2:K:1368:VAL:HG13	2.19	0.42
3:C:217:VAL:HG11	3:C:221:LEU:HD11	2.00	0.42
1:D:618:ASP:OD1	1:D:618:ASP:N	2.36	0.42
2:K:570:GLU:O	2:K:573:LEU:HB3	2.19	0.42
2:K:625:LEU:C	2:K:628:PHE:HB3	2.43	0.42
2:K:1485:ASP:OD1	2:K:1487:SER:OG	2.33	0.42
1:D:283:GLU:OE2	1:D:321:LYS:NZ	2.43	0.42
1:D:888:LEU:O	1:D:893:VAL:HG12	2.19	0.42
2:K:939:VAL:O	2:K:943:ILE:HG23	2.20	0.42
2:K:1154:ALA:O	2:K:1158:MET:N	2.52	0.42
1:D:171:PRO:HG2	1:D:174:ILE:HG12	2.02	0.42
1:D:452:TYR:OH	1:D:463:THR:OG1	2.21	0.42
2:K:604:ILE:O	2:K:607:GLU:HB2	2.20	0.42
2:K:1100:ASN:HD21	10:K:1702:CLR:H121	1.83	0.42
2:K:1135:ILE:HG22	2:K:1136:TYR:H	1.84	0.42
2:K:1599:LYS:HE3	2:K:1599:LYS:HB2	1.93	0.42
1:D:94:ASN:ND2	6:D:1101:NAG:C1	2.78	0.42
2:K:275:VAL:HA	2:K:395:PHE:CE2	2.53	0.42
2:K:348:ASN:HD21	10:K:1701:CLR:H152	1.83	0.42
2:K:442:THR:O	2:K:447:ILE:HG12	2.19	0.42
2:K:1583:GLU:HA	2:K:1587:ALA:HB3	2.01	0.42
1:D:599:GLU:N	1:D:599:GLU:OE1	2.52	0.42
1:D:908:PRO:HD3	1:D:973:LYS:HA	2.02	0.42
2:K:295:HIS:HB2	2:K:1241:TYR:OH	2.19	0.42
2:K:940:PHE:HA	2:K:943:ILE:HG12	2.02	0.42
2:K:1051:PHE:HA	2:K:1054:LYS:HD2	2.00	0.42
3:C:254:ILE:HG12	3:C:285:LEU:HD21	2.00	0.42
2:K:287:LEU:HD12	2:K:287:LEU:HA	1.80	0.42
2:K:1398:ASN:HD22	2:K:1404:GLN:NE2	2.18	0.42
2:K:1466:LEU:HD23	2:K:1466:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:995:LYS:HA	2:K:998:ARG:HE	1.85	0.42
2:K:1015:LEU:HG	2:K:1019:VAL:HB	2.02	0.42
2:K:1610:ASP:N	2:K:1610:ASP:OD1	2.52	0.42
3:C:204:LEU:O	3:C:209:ASP:N	2.53	0.42
1:D:664:ALA:HA	1:D:665:PRO:HD3	1.91	0.42
2:K:1507:GLU:HB2	2:K:1509:LYS:HE2	2.02	0.42
3:C:282:LYS:HD2	3:C:282:LYS:HA	1.74	0.42
3:C:309:LYS:HA	3:C:309:LYS:HD3	1.88	0.42
1:D:56:VAL:HG11	1:D:798:LYS:HG2	2.02	0.41
1:D:242:ARG:HE	1:D:242:ARG:HB3	1.72	0.41
1:D:518:ASP:HB2	1:D:519:PRO:HD2	2.02	0.41
2:K:1177:TYR:CZ	2:K:1178:LYS:HG2	2.55	0.41
2:K:1239:GLN:HG3	2:K:1243:GLN:HB3	2.01	0.41
2:K:1399:PHE:HD1	2:K:1399:PHE:O	2.03	0.41
2:K:1561:THR:O	2:K:1565:LEU:HG	2.19	0.41
2:K:1567:ARG:HG2	2:K:1572:ILE:HB	2.02	0.41
3:C:175:PRO:O	3:C:178:ARG:NH1	2.53	0.41
1:D:614:VAL:HG22	1:D:619:TYR:O	2.20	0.41
1:D:897:ASN:HD22	5:B:1:NAG:C1	2.26	0.41
2:K:622:VAL:HA	2:K:625:LEU:HG	2.02	0.41
2:K:1274:LYS:O	2:K:1277:HIS:N	2.51	0.41
2:K:1546:MET:SD	2:K:1561:THR:HA	2.61	0.41
3:C:317:VAL:HA	3:C:320:MET:SD	2.61	0.41
1:D:891:ILE:O	1:D:892:SER:HB3	2.19	0.41
2:K:533:LEU:HD23	2:K:533:LEU:HA	1.90	0.41
3:C:191:GLU:O	3:C:195:MET:HB2	2.20	0.41
3:C:338:ASP:OD1	3:C:338:ASP:N	2.53	0.41
1:D:298:SER:HB3	1:D:332:ILE:HG12	2.02	0.41
1:D:350:ASN:ND2	6:D:1103:NAG:O5	2.53	0.41
1:D:625:LEU:HD12	1:D:625:LEU:HA	1.93	0.41
2:K:269:LEU:HD23	2:K:270:HIS:H	1.85	0.41
2:K:1344:GLU:OE1	2:K:1344:GLU:N	2.54	0.41
10:K:1703:CLR:H162	10:K:1703:CLR:H222	1.72	0.41
2:K:1103:ALA:C	2:K:1105:MET:H	2.27	0.41
2:K:1225:MET:O	2:K:1229:ILE:HG22	2.19	0.41
2:K:1549:PRO:O	2:K:1554:GLY:HA2	2.21	0.41
2:K:397:LEU:HD21	2:K:1474:VAL:HG11	2.03	0.41
2:K:586:SER:OG	2:K:587:LEU:N	2.53	0.41
2:K:627:ILE:O	2:K:630:ILE:HG12	2.21	0.41
2:K:683:GLN:NE2	2:K:684:THR:O	2.54	0.41
2:K:921:ASP:HB3	2:K:924:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1429:LYS:HA	2:K:1429:LYS:HD3	1.92	0.41
1:D:183:ASN:O	1:D:186:ASN:N	2.53	0.41
1:D:434:ARG:HB2	1:D:435:PRO:HD3	2.02	0.41
2:K:966:ARG:HH11	2:K:1007:ARG:HH21	1.69	0.41
2:K:974:LEU:O	2:K:977:VAL:HG12	2.21	0.41
2:K:1156:PHE:O	2:K:1160:ILE:HG23	2.20	0.41
2:K:1174:GLU:HA	2:K:1177:TYR:HB3	2.01	0.41
1:D:445:GLN:OE1	1:D:445:GLN:N	2.54	0.41
1:D:655:PHE:O	1:D:659:GLY:N	2.53	0.41
2:K:444:ALA:O	2:K:448:ASP:HB2	2.21	0.41
2:K:1060:ASP:N	2:K:1060:ASP:OD1	2.52	0.41
2:K:1269:LYS:HA	2:K:1269:LYS:HD3	1.72	0.41
2:K:1559:ASN:O	2:K:1562:LEU:HD23	2.21	0.41
5:E:1:NAG:H4	5:E:2:NAG:C7	2.51	0.41
1:D:861:LEU:HD21	1:D:869:TYR:HB3	2.03	0.41
1:D:1041:ASP:OD1	1:D:1041:ASP:N	2.43	0.41
2:K:634:TRP:HZ3	2:K:637:LEU:HB2	1.86	0.41
2:K:1081:VAL:CG2	2:K:1082:ASP:H	2.25	0.41
2:K:1213:TRP:CZ2	2:K:1273:PHE:HA	2.56	0.41
2:K:696:LEU:HD23	2:K:696:LEU:HA	1.93	0.40
2:K:912:LEU:HD12	2:K:913:SER:N	2.36	0.40
2:K:921:ASP:OD1	2:K:921:ASP:N	2.54	0.40
2:K:945:THR:O	2:K:949:ILE:HG12	2.21	0.40
2:K:1274:LYS:HB2	2:K:1274:LYS:HE3	1.72	0.40
1:D:476:GLU:OE1	1:D:476:GLU:N	2.52	0.40
1:D:1020:VAL:HG13	1:D:1021:GLU:O	2.21	0.40
2:K:1005:PRO:HA	2:K:1008:ALA:HB3	2.02	0.40
2:K:1355:LYS:HA	2:K:1355:LYS:HD2	1.69	0.40
1:D:243:ARG:HA	1:D:243:ARG:HD2	1.84	0.40
2:K:184:LEU:HD12	2:K:184:LEU:HA	1.89	0.40
2:K:1031:ASN:O	2:K:1034:ILE:HG12	2.21	0.40
2:K:1206:ASN:OD1	2:K:1209:GLN:NE2	2.55	0.40
1:D:184:GLU:HA	1:D:187:TRP:NE1	2.36	0.40
1:D:207:TRP:HE1	1:D:458:LEU:HD22	1.86	0.40
2:K:418:ARG:HG2	2:K:418:ARG:NH1	2.36	0.40
2:K:630:ILE:C	2:K:632:ARG:N	2.80	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	D	945/1050 (90%)	892 (94%)	53 (6%)	0	100	100
2	K	1260/1499 (84%)	1133 (90%)	124 (10%)	3 (0%)	43	71
3	C	189/191 (99%)	186 (98%)	3 (2%)	0	100	100
All	All	2394/2740 (87%)	2211 (92%)	180 (8%)	3 (0%)	49	75

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

7 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	A	1	4	14,14,15	0.95	1 (7%)	17,19,21	0.58	0
4	NAG	A	2	4	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	A	3	4	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	B	1	5	14,14,15	0.50	0	17,19,21	0.73	1 (5%)
5	NAG	B	2	5	14,14,15	0.18	0	17,19,21	0.46	0
5	NAG	E	1	5	14,14,15	0.41	0	17,19,21	0.41	0
5	NAG	E	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.62	0

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	A	1	4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	NAG	A	3	4	-	4/6/23/26	0/1/1/1
5	NAG	B	1	5	-	4/6/23/26	0/1/1/1
5	NAG	B	2	5	-	4/6/23/26	0/1/1/1
5	NAG	E	1	5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	NAG	O5-C1	-3.25	1.38	1.43
5	E	2	NAG	C1-C2	2.44	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	C1-O5-C5	2.40	115.40	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

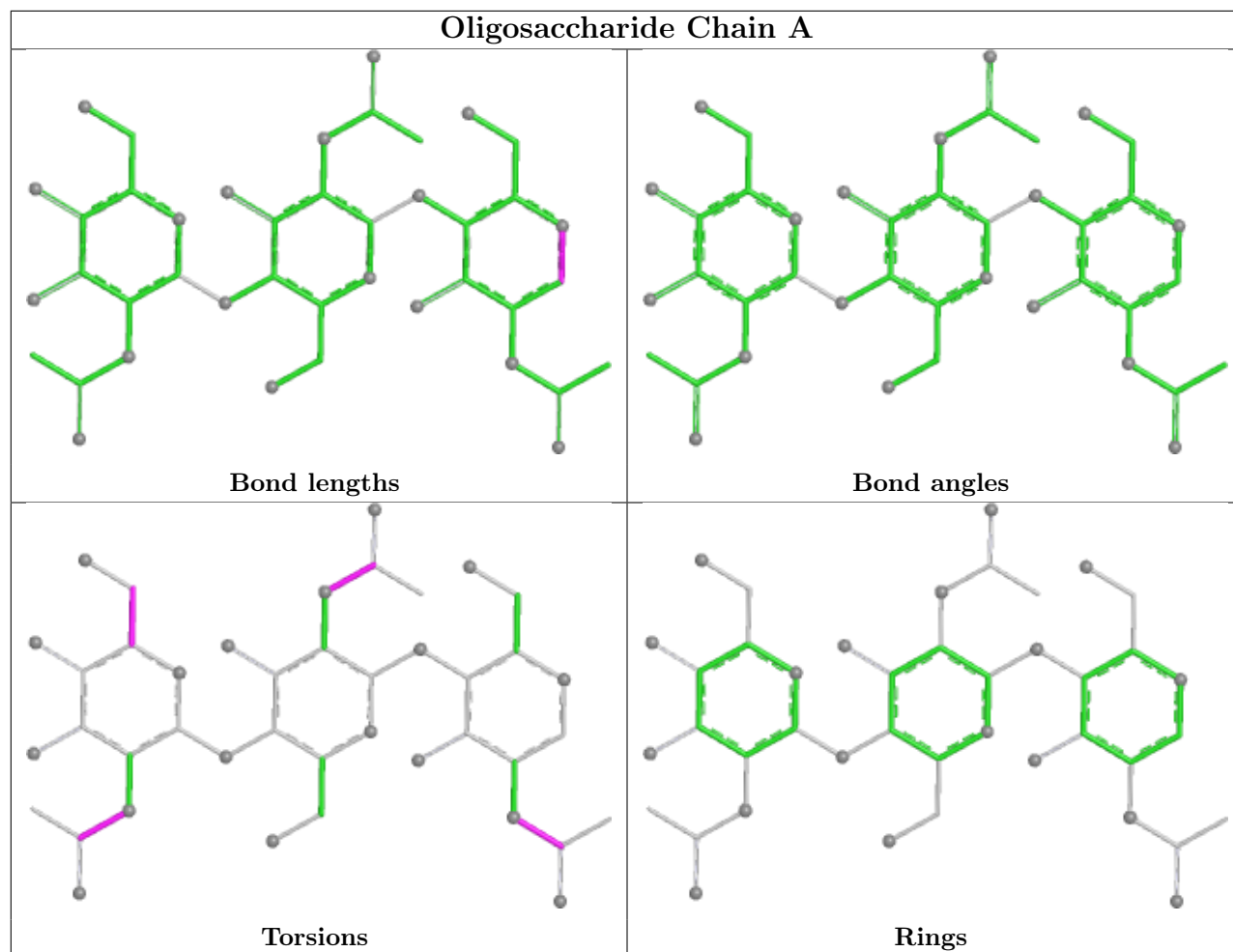
Mol	Chain	Res	Type	Atoms
4	A	3	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	A	3	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	3	NAG	C8-C7-N2-C2
4	A	3	NAG	O7-C7-N2-C2
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	B	1	NAG	C4-C5-C6-O6
5	B	2	NAG	O5-C5-C6-O6
5	B	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6

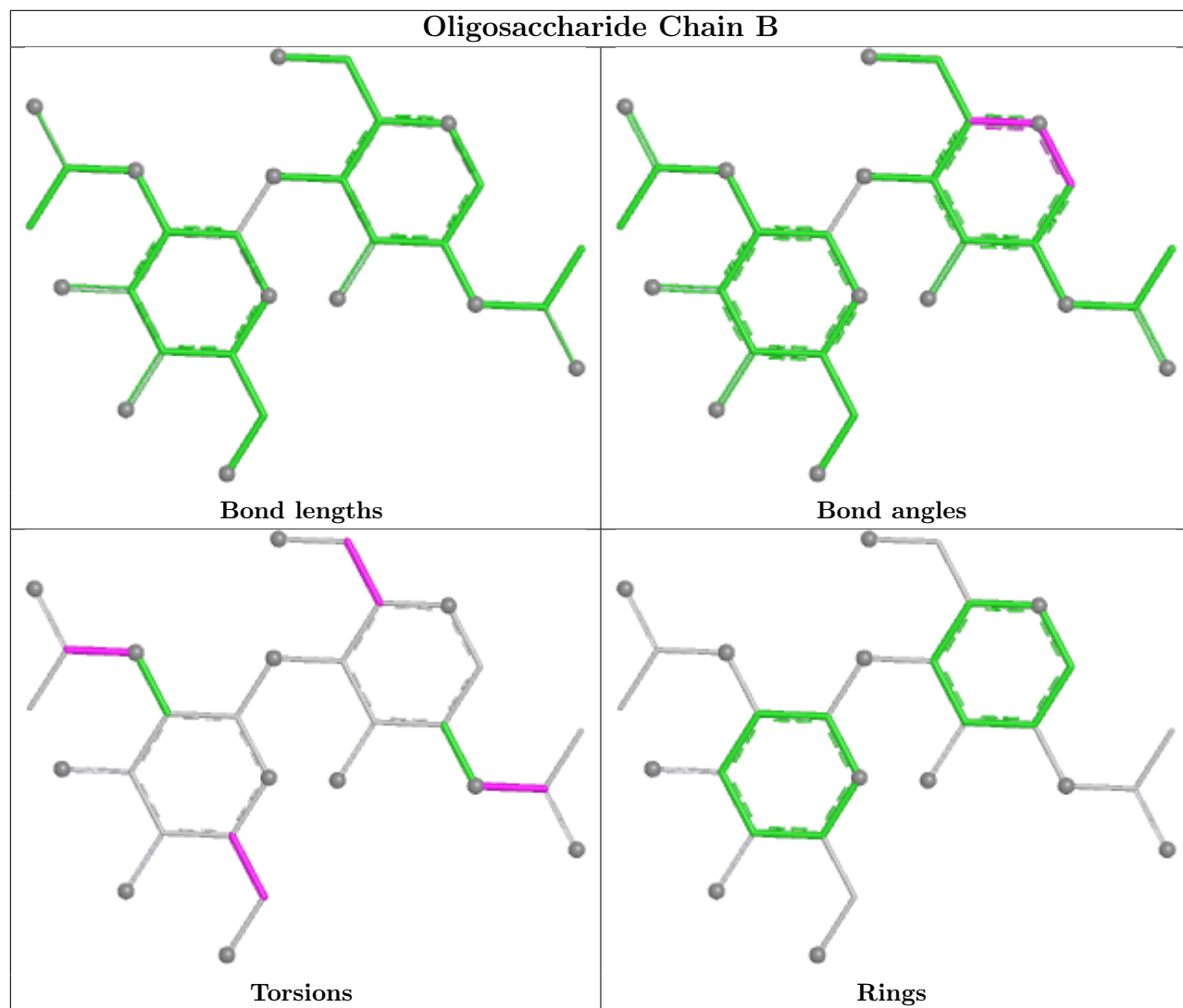
There are no ring outliers.

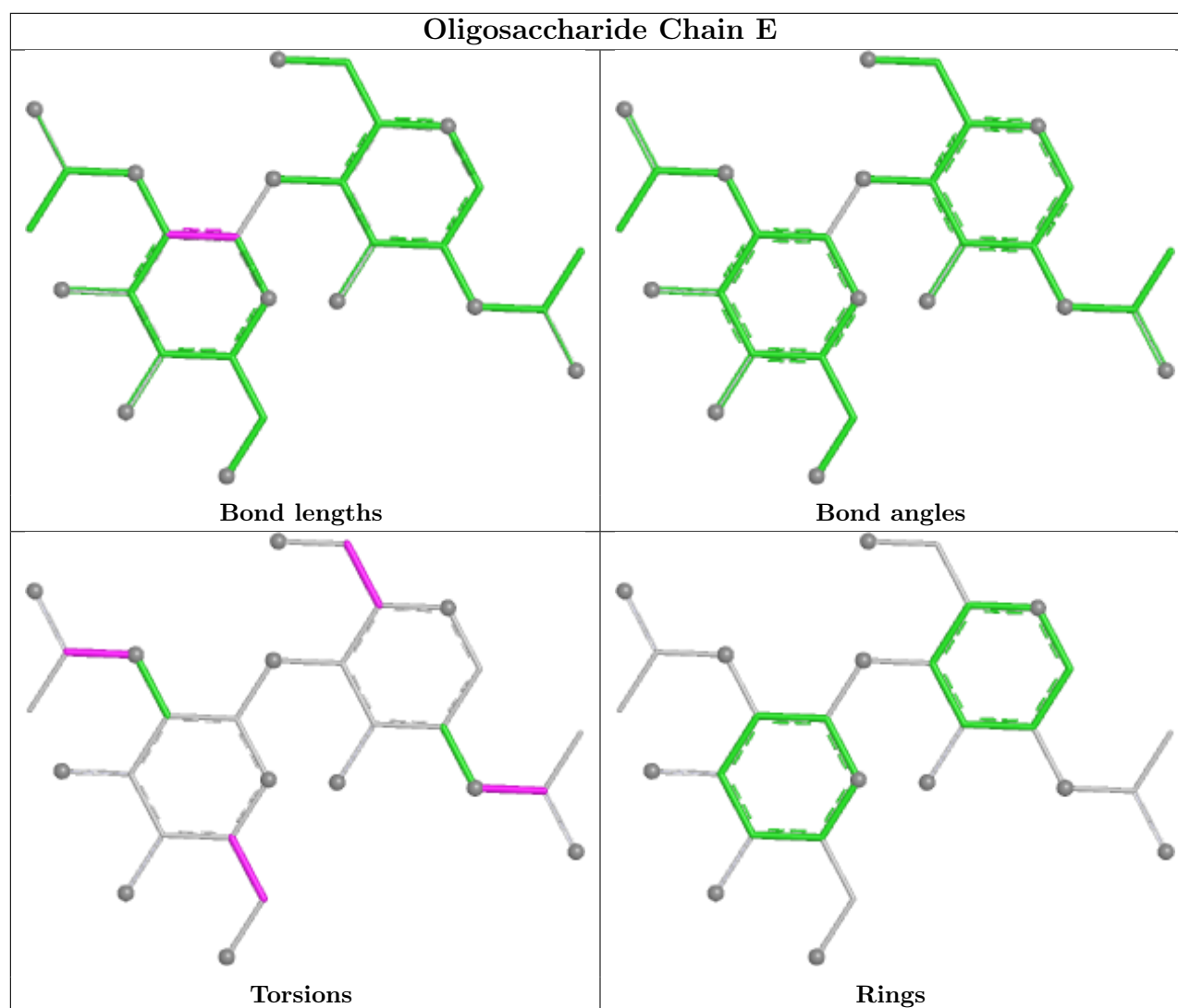
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	3	0
5	B	1	NAG	3	0
4	A	3	NAG	4	0
5	E	2	NAG	4	0
5	E	1	NAG	4	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	WO9	K	1705	-	43,43,43	0.98	4 (9%)	46,48,48	1.19	3 (6%)
10	CLR	K	1701	-	31,31,31	1.04	1 (3%)	48,48,48	0.70	0
9	LEU	D	1108	-	6,8,8	0.86	0	5,10,10	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLR	K	1702	-	31,31,31	1.05	0	48,48,48	0.66	0
6	NAG	D	1103	-	14,14,15	0.48	0	17,19,21	0.42	0
6	NAG	D	1101	-	14,14,15	0.24	0	17,19,21	0.58	0
6	NAG	D	1105	-	14,14,15	0.84	2 (14%)	17,19,21	1.70	3 (17%)
6	NAG	D	1104	-	14,14,15	0.32	0	17,19,21	0.39	0
6	NAG	D	1102	-	14,14,15	0.24	0	17,19,21	0.38	0
10	CLR	K	1703	-	31,31,31	1.05	1 (3%)	48,48,48	0.56	0
11	WNZ	K	1704	-	38,38,38	1.04	4 (10%)	41,43,43	1.20	3 (7%)

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
12	WO9	K	1705	-	-	26/47/47/47	-
10	CLR	K	1701	-	-	5/10/68/68	0/4/4/4
9	LEU	D	1108	-	-	5/8/8/8	-
10	CLR	K	1702	-	-	8/10/68/68	0/4/4/4
6	NAG	D	1103	-	-	4/6/23/26	0/1/1/1
6	NAG	D	1101	-	-	2/6/23/26	0/1/1/1
6	NAG	D	1105	-	-	6/6/23/26	0/1/1/1
6	NAG	D	1104	-	-	3/6/23/26	0/1/1/1
6	NAG	D	1102	-	-	2/6/23/26	0/1/1/1
10	CLR	K	1703	-	-	5/10/68/68	0/4/4/4
11	WNZ	K	1704	-	-	19/42/42/42	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	1705	WO9	O32-C22	-2.70	1.40	1.46
11	K	1704	WNZ	O14-C12	2.39	1.40	1.33
12	K	1705	WO9	O20-C18	2.36	1.40	1.33
11	K	1704	WNZ	O26-C16	-2.34	1.41	1.46
11	K	1704	WNZ	O26-C27	2.31	1.40	1.34
6	D	1105	NAG	O5-C1	2.27	1.47	1.43
11	K	1704	WNZ	O14-C15	-2.16	1.40	1.45
12	K	1705	WO9	O20-C21	-2.09	1.40	1.45
10	K	1703	CLR	C11-C9	2.06	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	1705	WO9	O32-C33	2.05	1.40	1.34
10	K	1701	CLR	C20-C17	2.03	1.57	1.54
6	D	1105	NAG	C1-C2	2.00	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1105	NAG	C2-N2-C7	4.66	129.15	122.90
6	D	1105	NAG	C1-O5-C5	4.24	117.87	112.19
12	K	1705	WO9	O32-C33-C35	3.99	120.11	111.48
11	K	1704	WNZ	O26-C27-C29	3.95	120.02	111.48
11	K	1704	WNZ	O14-C12-C11	2.73	120.17	111.83
12	K	1705	WO9	O20-C18-C17	2.73	120.15	111.83
11	K	1704	WNZ	O20-P19-O21	-2.47	100.94	112.44
12	K	1705	WO9	O26-P25-O27	-2.40	101.27	112.44
6	D	1105	NAG	C1-C2-N2	2.27	114.01	110.43

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	1108	LEU	N-CA-CB-CG
9	D	1108	LEU	C-CA-CB-CG
10	K	1701	CLR	C13-C17-C20-C21
10	K	1701	CLR	C13-C17-C20-C22
10	K	1701	CLR	C16-C17-C20-C22
11	K	1704	WNZ	O22-C23-C24-N25
11	K	1704	WNZ	C29-C27-O26-C16
11	K	1704	WNZ	C17-O18-P19-O20
12	K	1705	WO9	O28-C29-C30-N31
12	K	1705	WO9	C23-O24-P25-O26
10	K	1701	CLR	C16-C17-C20-C21
10	K	1702	CLR	C13-C17-C20-C21
10	K	1703	CLR	C13-C17-C20-C21
11	K	1704	WNZ	O28-C27-O26-C16
10	K	1702	CLR	C21-C20-C22-C23
10	K	1702	CLR	C16-C17-C20-C21
10	K	1703	CLR	C16-C17-C20-C21
10	K	1702	CLR	C16-C17-C20-C22
10	K	1702	CLR	C13-C17-C20-C22
10	K	1703	CLR	C13-C17-C20-C22
10	K	1703	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
6	D	1103	NAG	O5-C5-C6-O6
6	D	1101	NAG	C4-C5-C6-O6
6	D	1103	NAG	C4-C5-C6-O6
11	K	1704	WNZ	C11-C12-O14-C15
10	K	1702	CLR	C17-C20-C22-C23
6	D	1101	NAG	O5-C5-C6-O6
12	K	1705	WO9	O20-C21-C22-O32
6	D	1103	NAG	C8-C7-N2-C2
6	D	1103	NAG	O7-C7-N2-C2
6	D	1104	NAG	C8-C7-N2-C2
6	D	1104	NAG	O7-C7-N2-C2
6	D	1105	NAG	C8-C7-N2-C2
6	D	1105	NAG	O7-C7-N2-C2
11	K	1704	WNZ	O13-C12-O14-C15
10	K	1702	CLR	C22-C23-C24-C25
10	K	1703	CLR	C20-C22-C23-C24
6	D	1104	NAG	O5-C5-C6-O6
12	K	1705	WO9	C17-C18-O20-C21
11	K	1704	WNZ	C29-C30-C31-C32
11	K	1704	WNZ	C03-C04-C05-C06
11	K	1704	WNZ	C02-C03-C04-C05
6	D	1105	NAG	C4-C5-C6-O6
12	K	1705	WO9	O19-C18-O20-C21
10	K	1702	CLR	C20-C22-C23-C24
12	K	1705	WO9	C08-C09-C10-C11
11	K	1704	WNZ	C07-C08-C09-C10
9	D	1108	LEU	CA-CB-CG-CD1
12	K	1705	WO9	C35-C33-O32-C22
11	K	1704	WNZ	C06-C07-C08-C09
11	K	1704	WNZ	C04-C05-C06-C07
12	K	1705	WO9	C39-C40-C41-C42
12	K	1705	WO9	O20-C21-C22-C23
6	D	1105	NAG	O5-C5-C6-O6
11	K	1704	WNZ	C15-C16-O26-C27
12	K	1705	WO9	C12-C13-C14-C15
12	K	1705	WO9	C38-C39-C40-C41
9	D	1108	LEU	CA-CB-CG-CD2
12	K	1705	WO9	C41-C42-C43-C44
12	K	1705	WO9	C14-C15-C16-C17
12	K	1705	WO9	O34-C33-O32-C22
12	K	1705	WO9	C21-C22-C23-O24
6	D	1102	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	K	1705	WO9	O32-C22-C23-O24
12	K	1705	WO9	C10-C11-C12-C13
11	K	1704	WNZ	C27-C29-C30-C31
12	K	1705	WO9	C33-C35-C36-C37
12	K	1705	WO9	C05-C06-C07-C08
11	K	1704	WNZ	O14-C15-C16-O26
11	K	1704	WNZ	O14-C15-C16-C17
11	K	1704	WNZ	C17-O18-P19-O21
11	K	1704	WNZ	C17-O18-P19-O22
12	K	1705	WO9	C23-O24-P25-O27
12	K	1705	WO9	C23-O24-P25-O28
12	K	1705	WO9	C29-O28-P25-O26
6	D	1102	NAG	O5-C5-C6-O6
12	K	1705	WO9	C11-C12-C13-C14
11	K	1704	WNZ	C01-C02-C03-C04
9	D	1108	LEU	OXT-C-CA-N
6	D	1105	NAG	C1-C2-N2-C7
6	D	1105	NAG	C3-C2-N2-C7
10	K	1701	CLR	C23-C24-C25-C26
12	K	1705	WO9	C15-C16-C17-C18
12	K	1705	WO9	C07-C08-C09-C10
12	K	1705	WO9	C22-C23-O24-P25

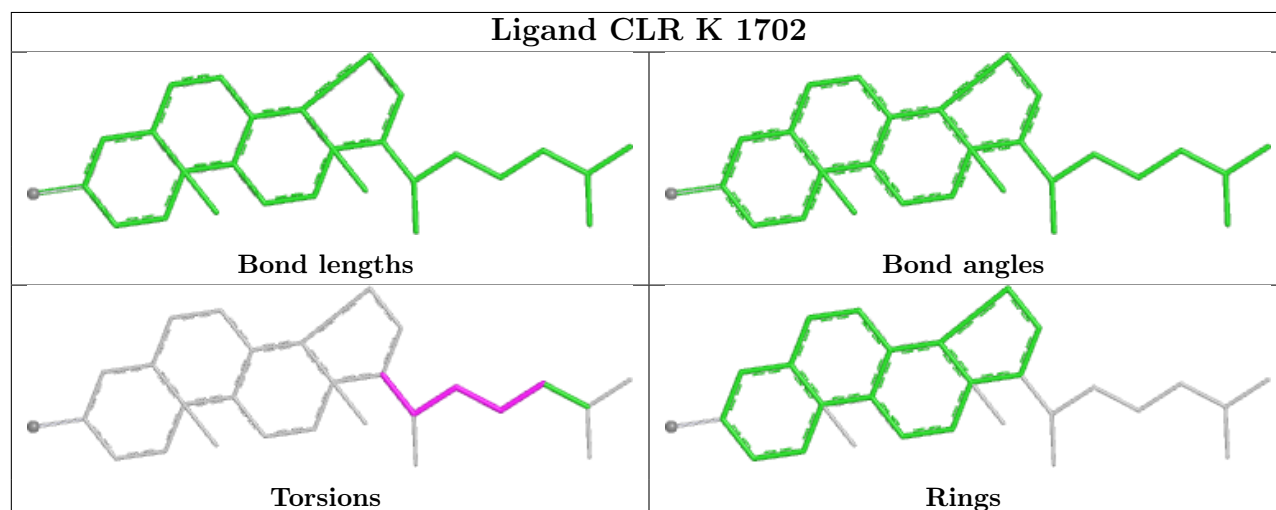
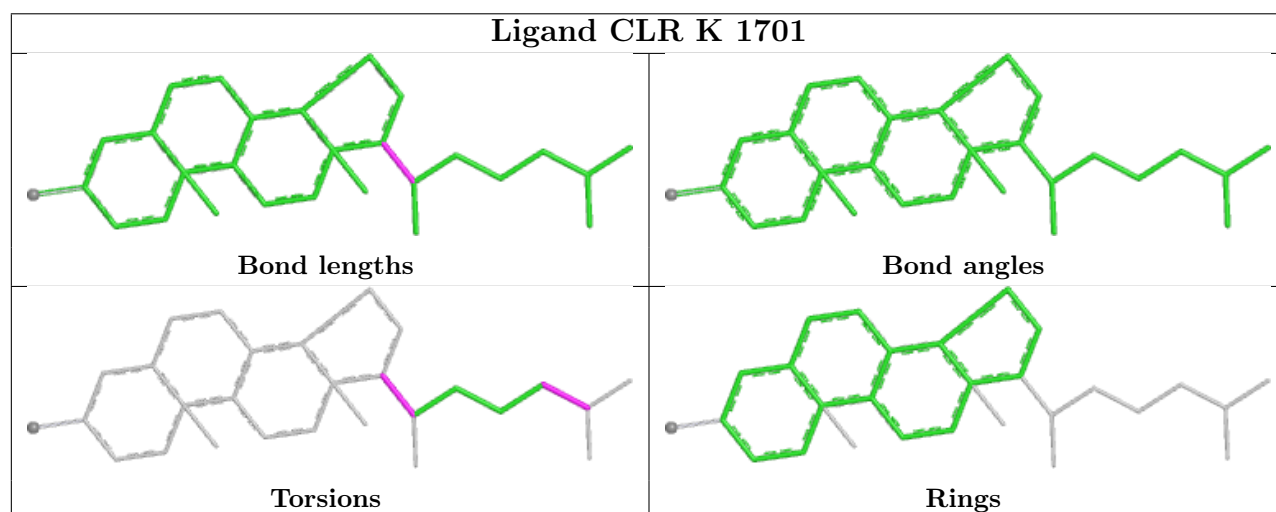
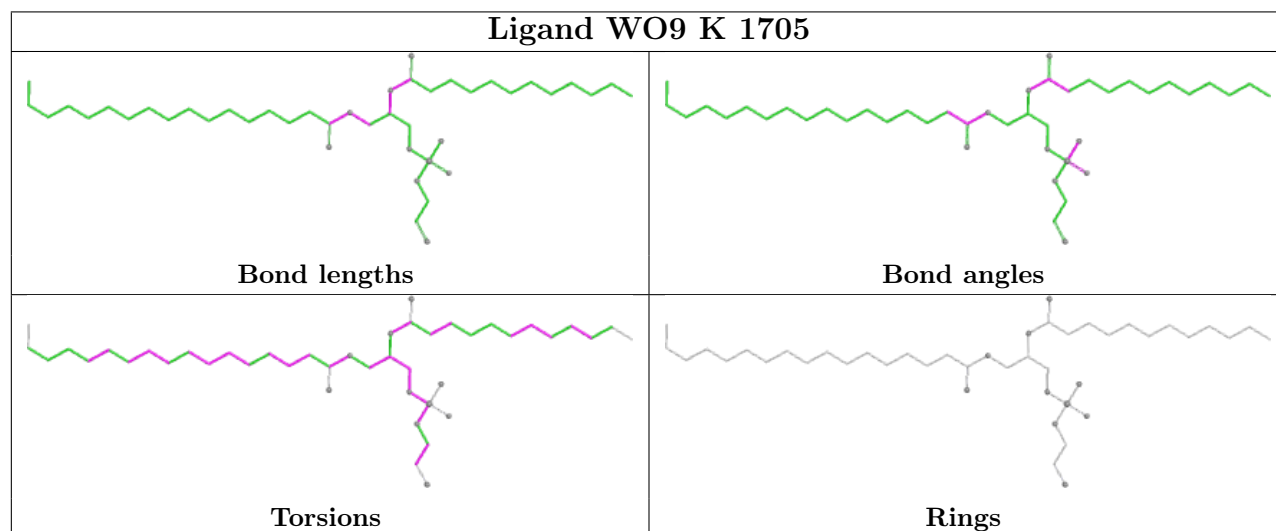
There are no ring outliers.

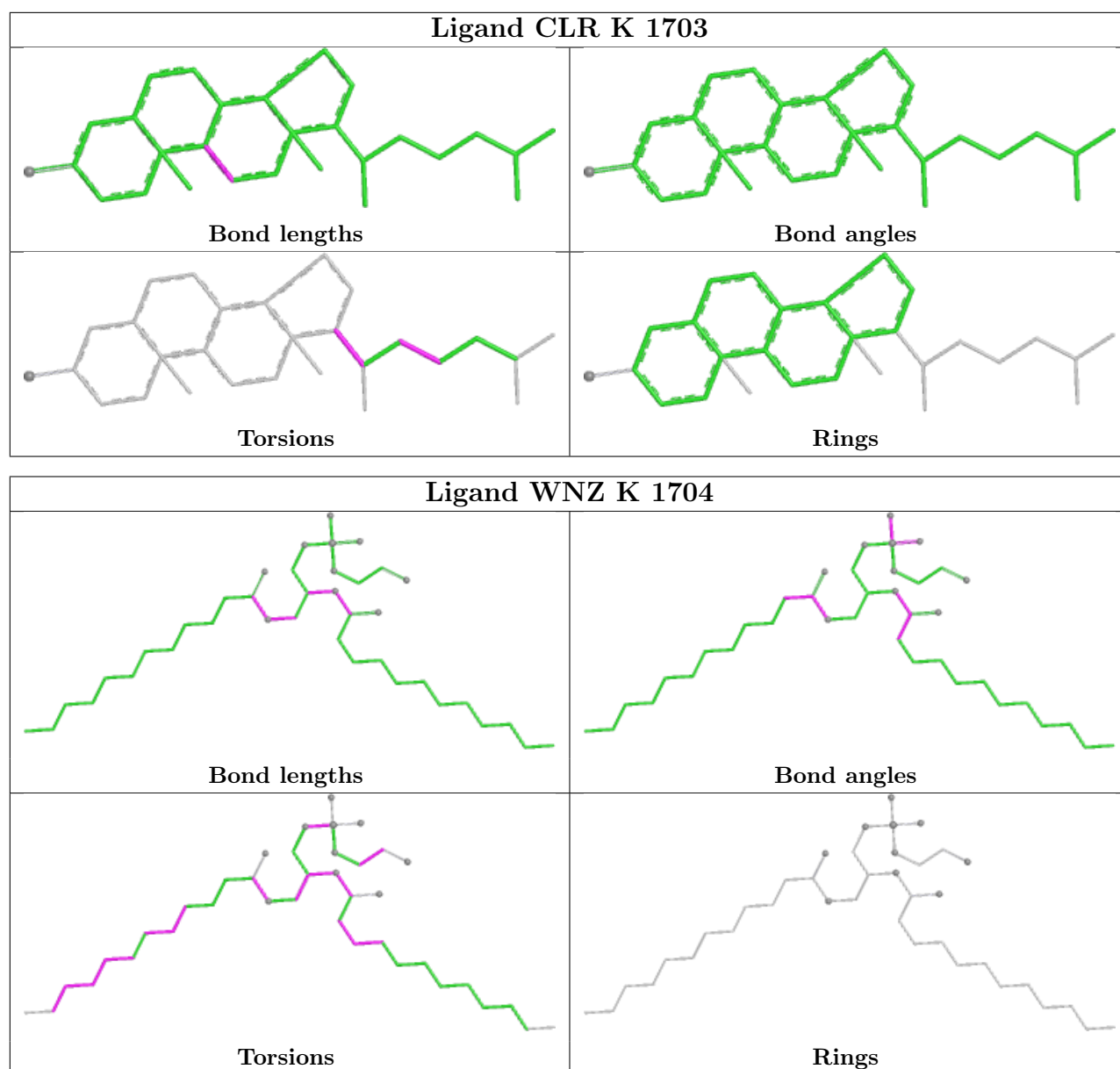
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	1701	CLR	4	0
10	K	1702	CLR	2	0
6	D	1103	NAG	1	0
6	D	1101	NAG	3	0
6	D	1105	NAG	1	0
10	K	1703	CLR	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 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.

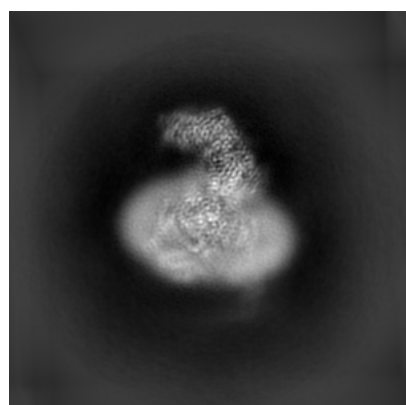
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28375. These allow visual inspection of the internal detail of the map and identification of artifacts.

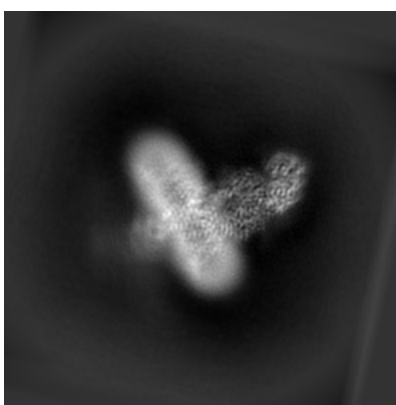
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

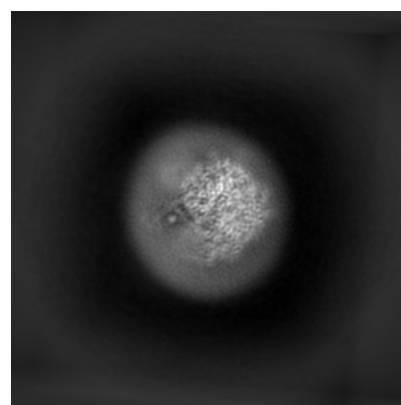
6.1.1 Primary map



X



Y

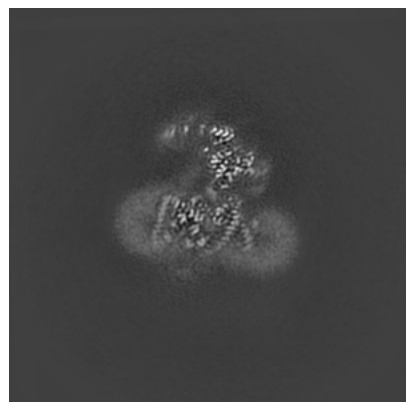


Z

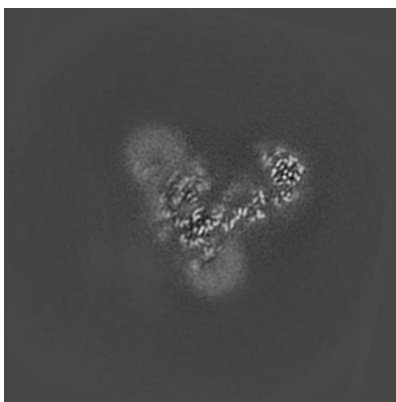
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

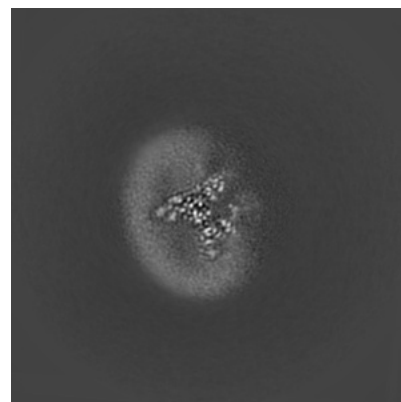
6.2.1 Primary map



X Index: 220



Y Index: 220

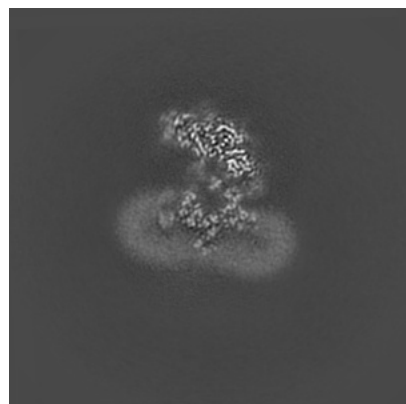


Z Index: 220

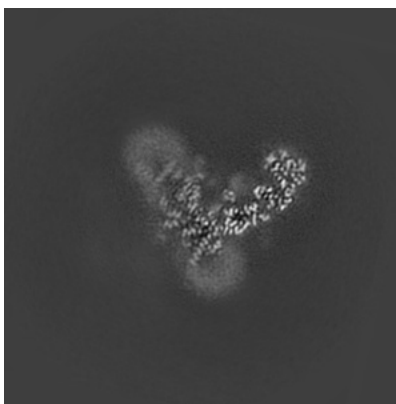
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

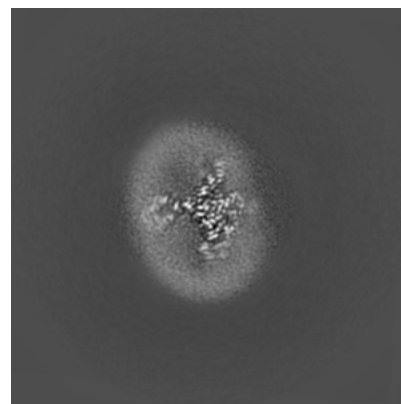
6.3.1 Primary map



X Index: 231



Y Index: 226

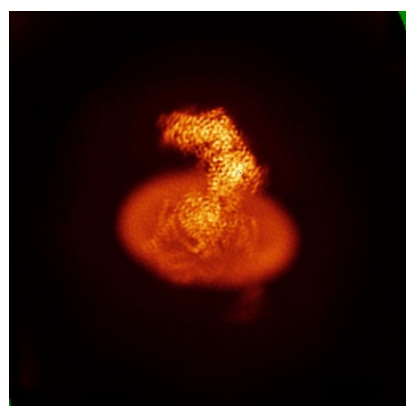


Z Index: 210

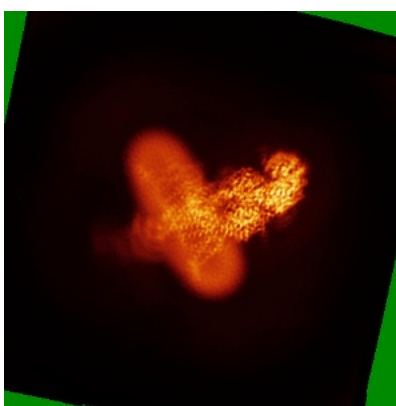
The images above show the largest variance slices of the map in three orthogonal directions.

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

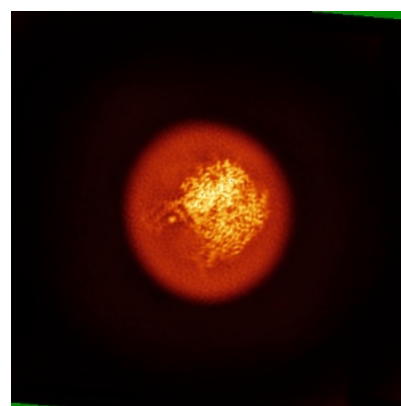
6.4.1 Primary map



X



Y

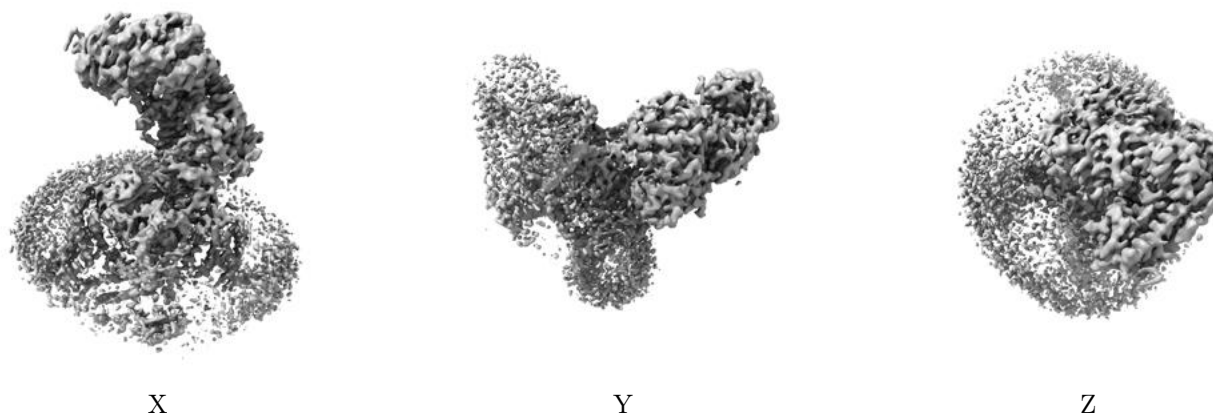


Z

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

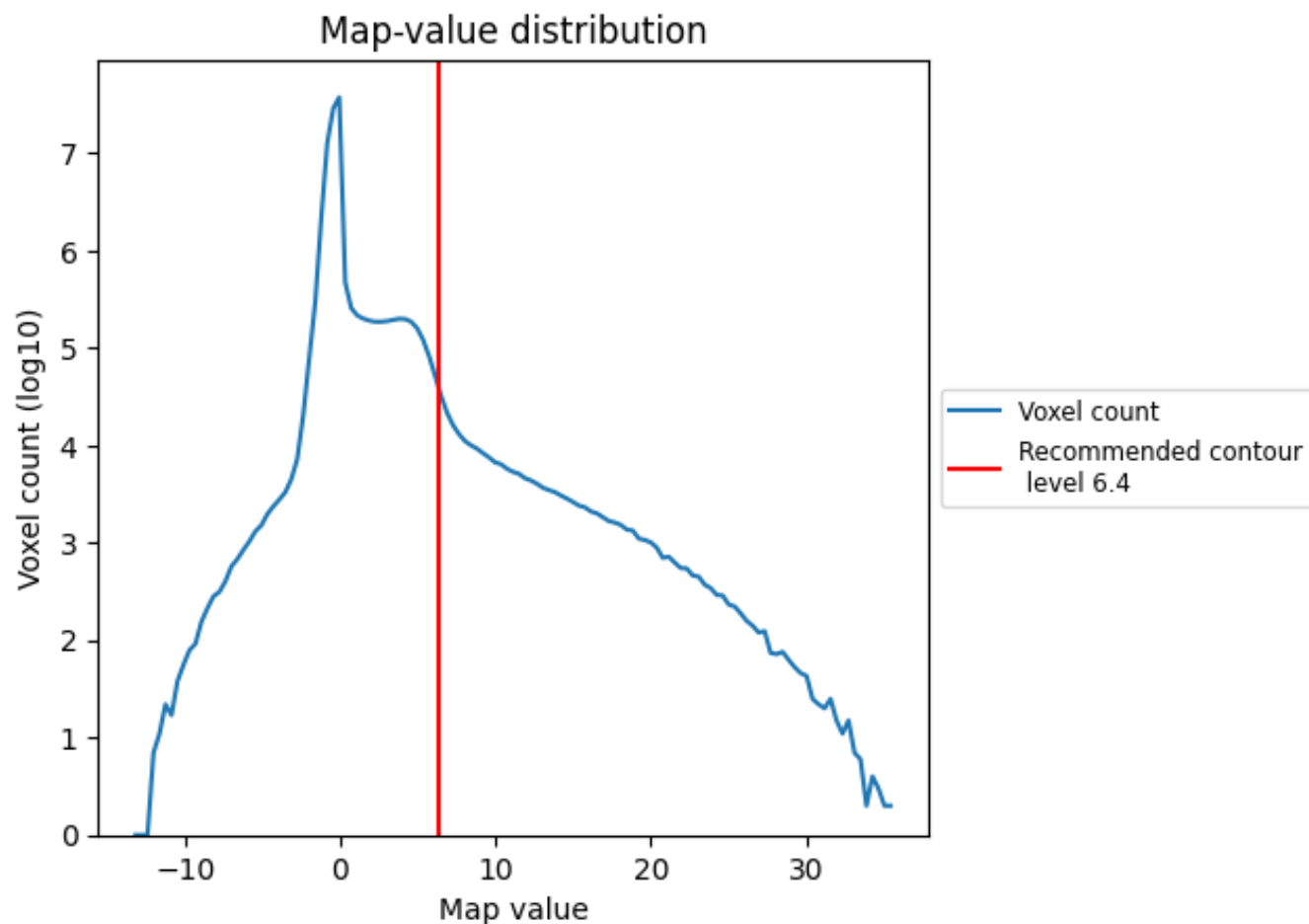
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

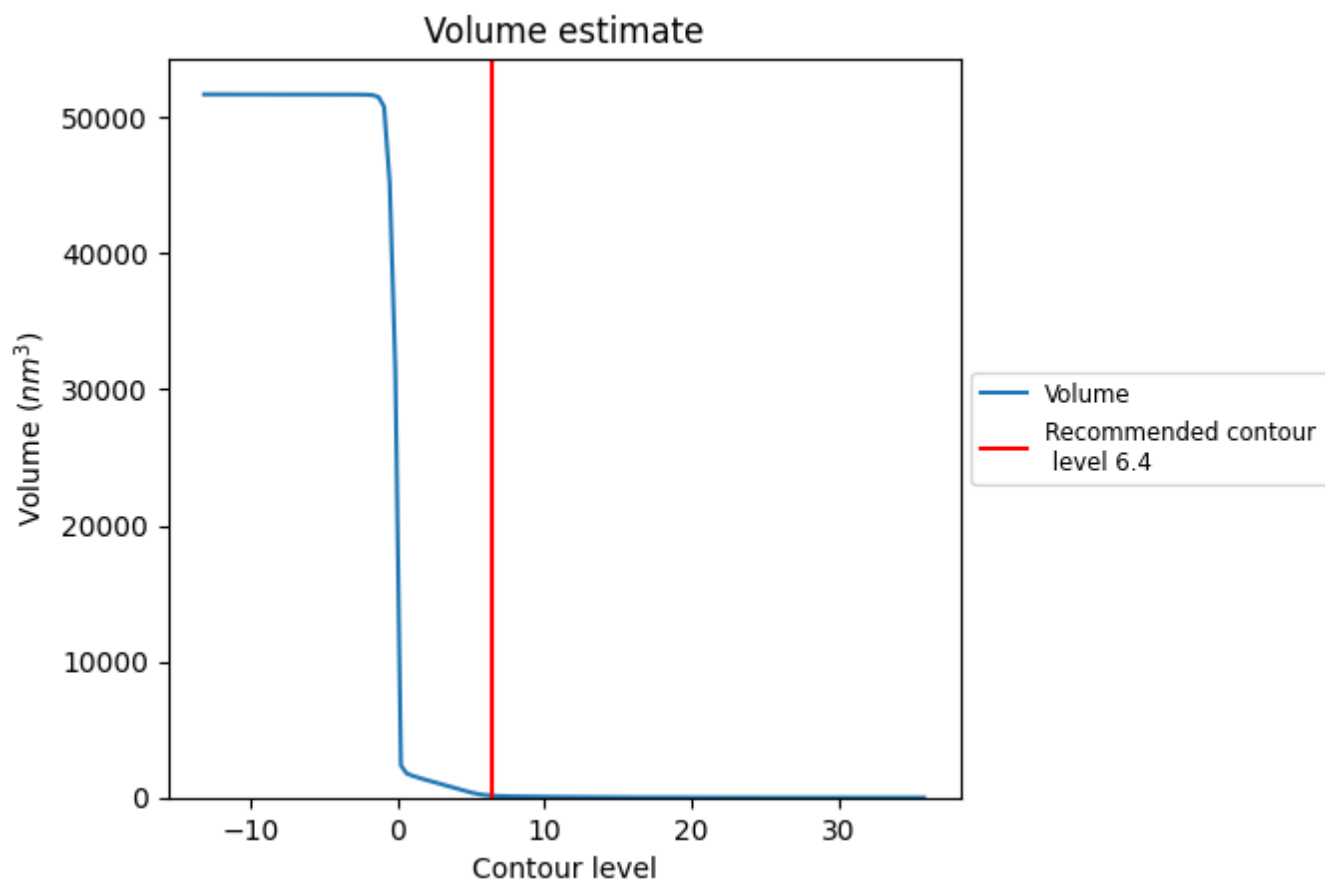
This section contains the results of statistical analysis of the map.

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.

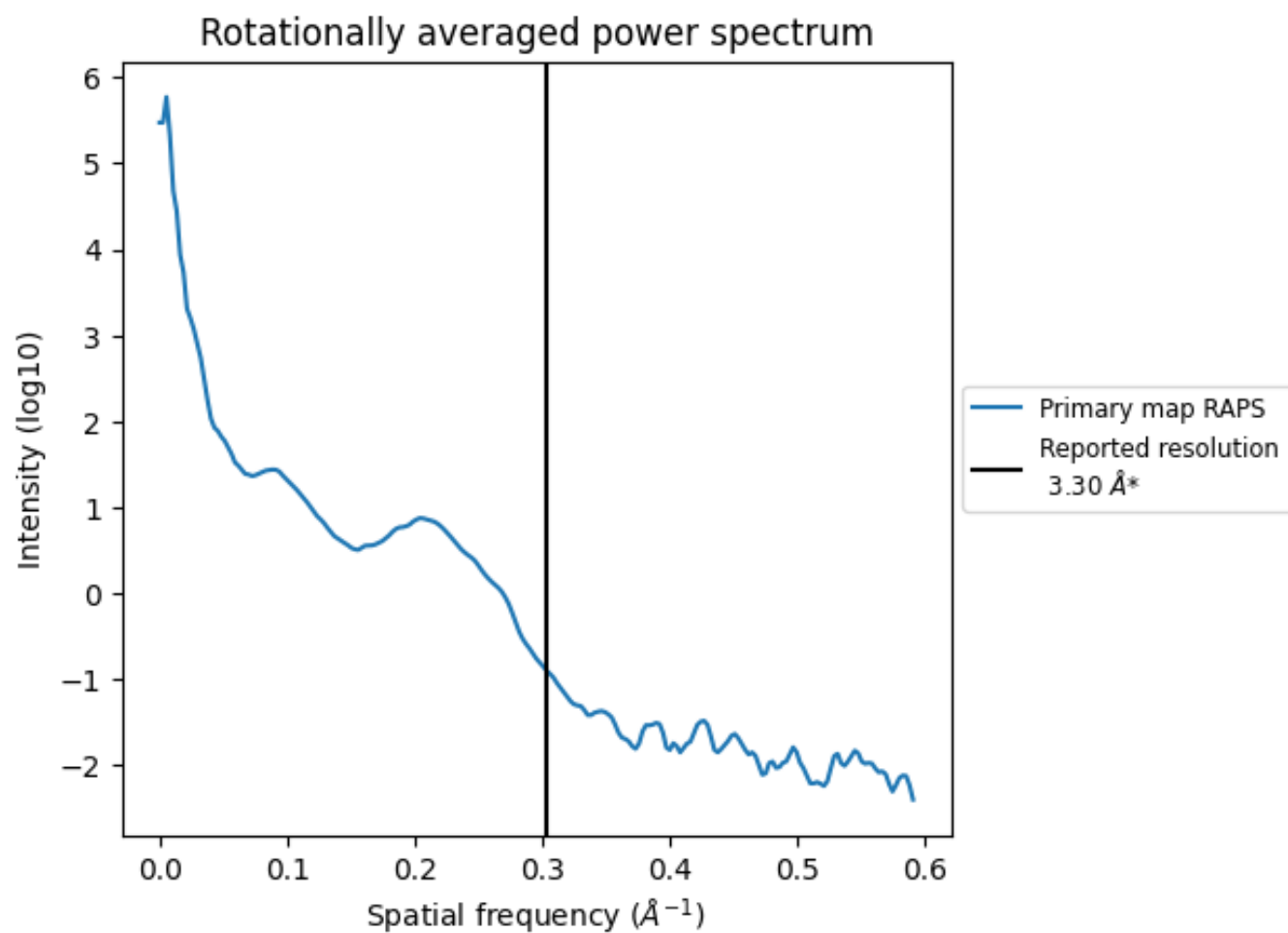
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm^3 ; this corresponds to an approximate mass of 127 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 0.303 Å⁻¹

8 Fourier-Shell correlation

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

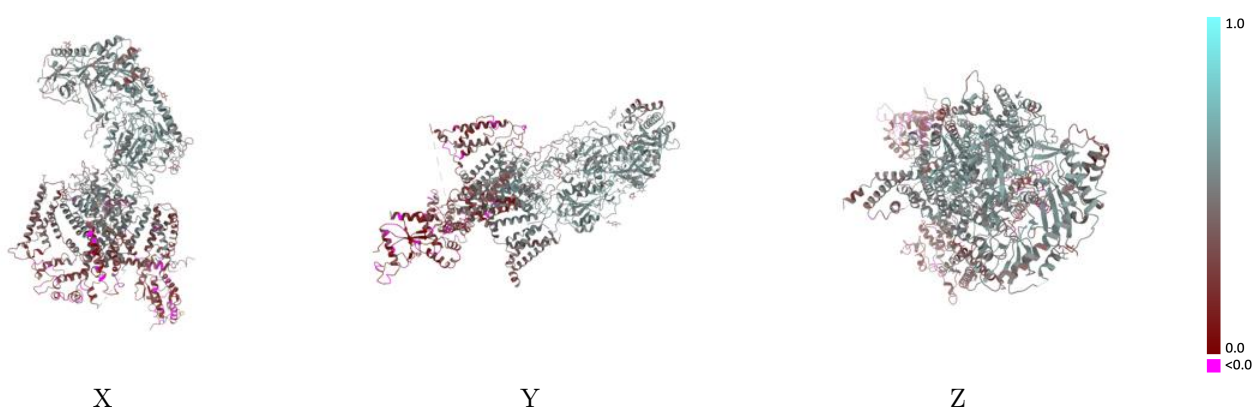
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28375 and PDB model 8EOG. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

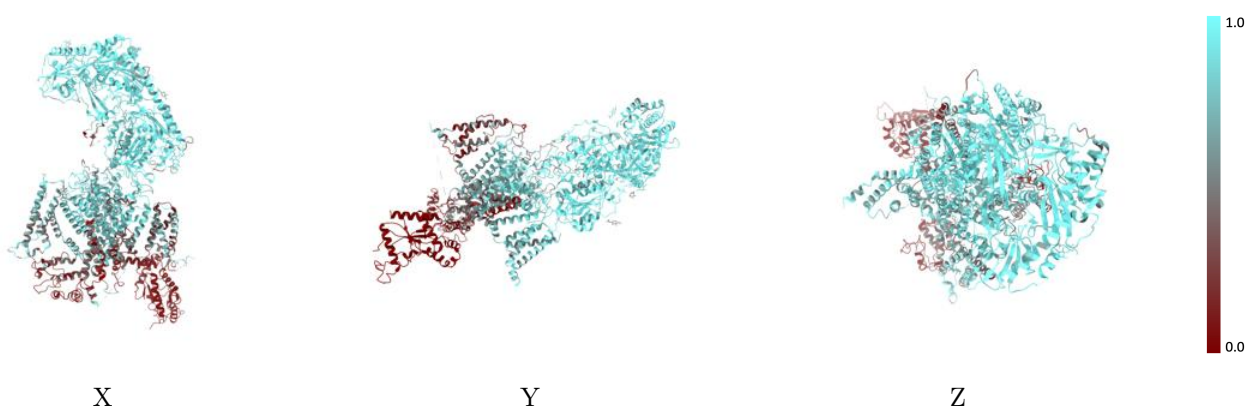
This section was not generated.

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



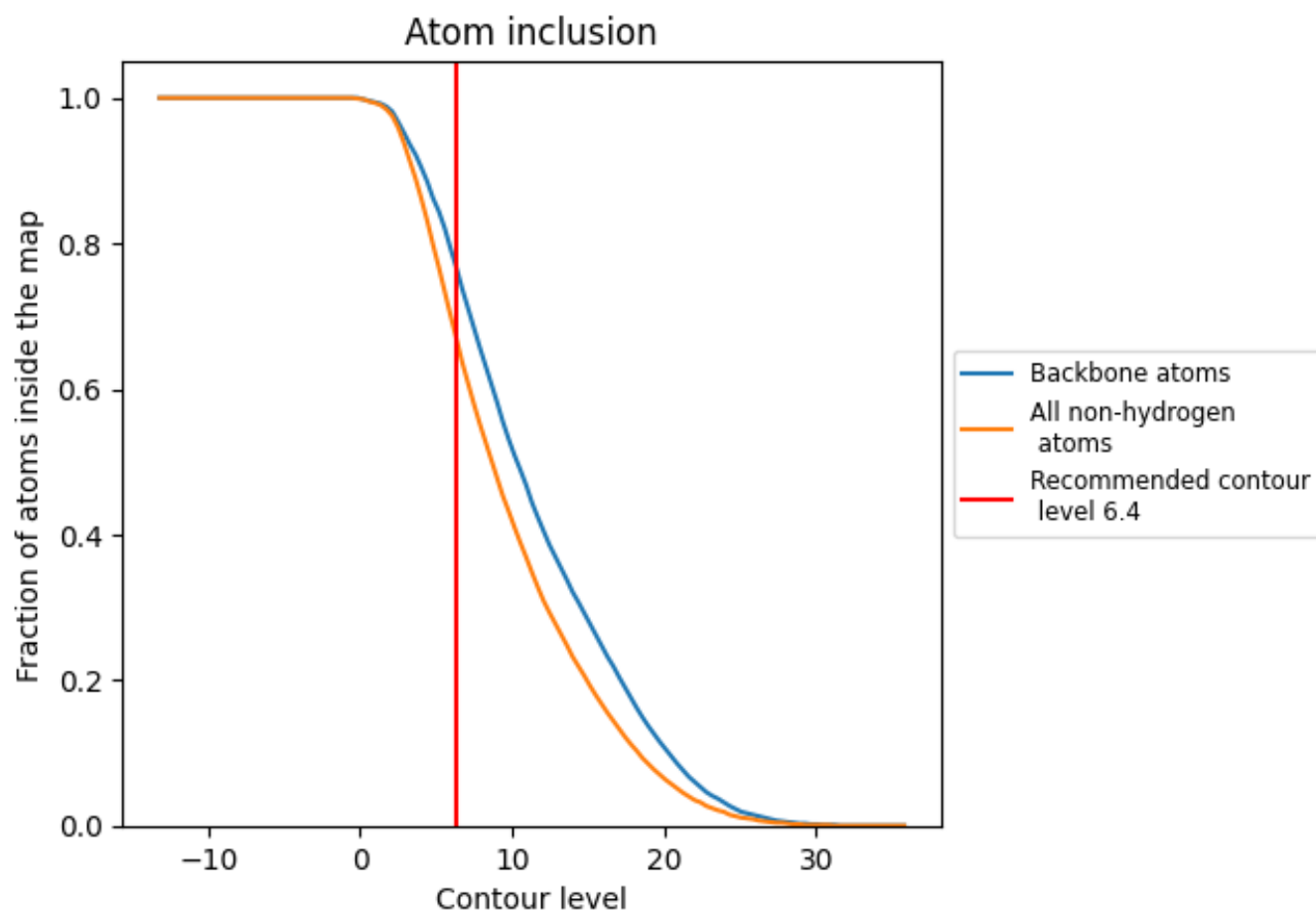
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 66% 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 (6.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.4120
A	0.7620	0.4120
B	0.7860	0.4420
C	0.0010	0.1510
D	0.9020	0.5240
E	0.7860	0.3570
K	0.5850	0.3680

1.0

0.0

<0.0