



## Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 08:31 AM EDT

PDB ID : 8EOG  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

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

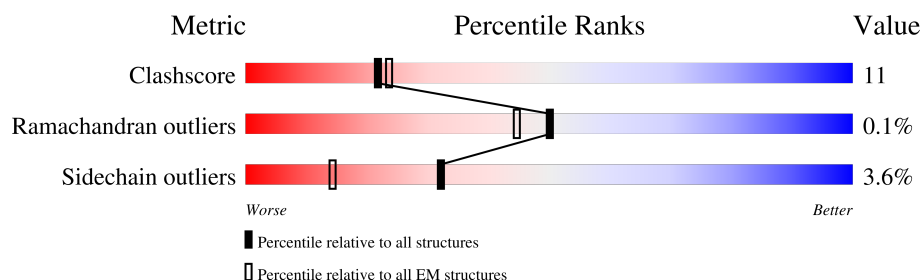
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	1050	
2	K	1499	
3	C	191	
4	A	3	
5	B	2	
5	E	2	

## 2 Entry composition

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

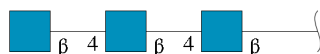
- Molecule 2 is a protein called Isoform 20 of Voltage-dependent L-type calcium channel subunit alpha-1C.

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.



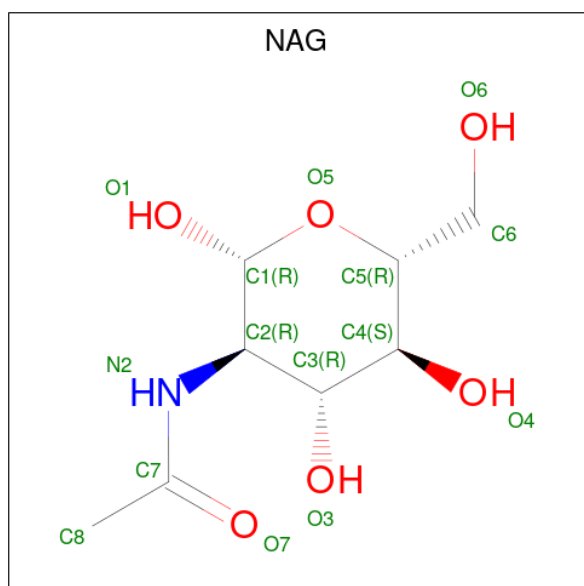
Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	3	Total	C	N	O	0	0
			42	24	3	15		

- 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 (three-letter code: 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	

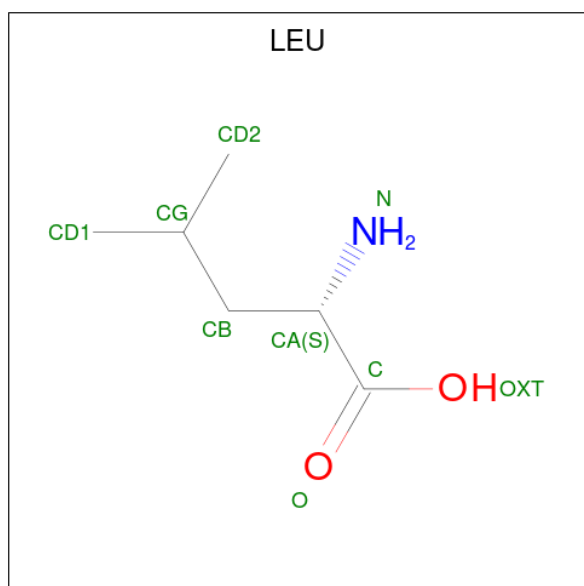
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-letter code: NA) (formula: Na).

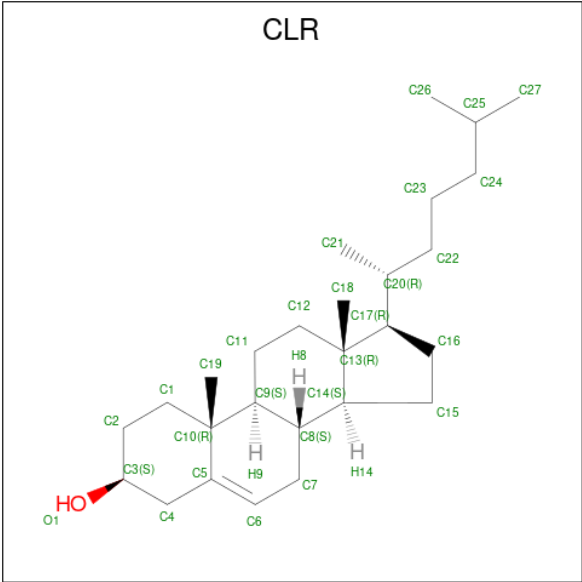
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Na	0
			1	1	

- Molecule 9 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



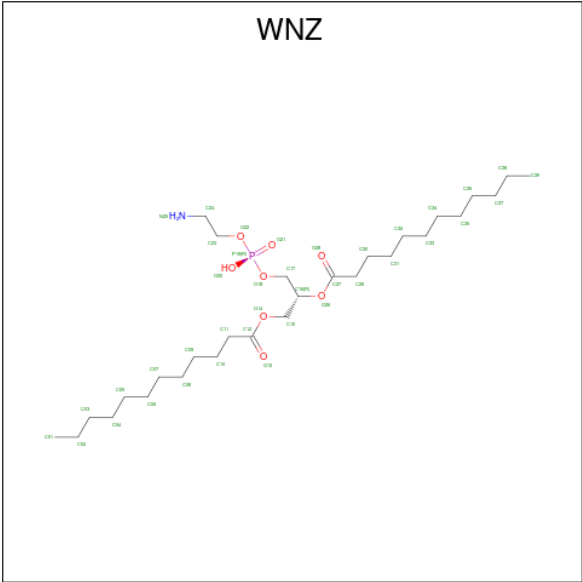
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			9	6	1	2	

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



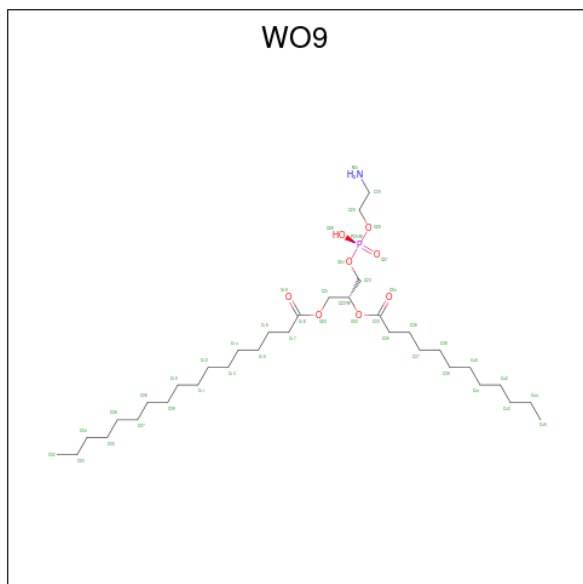
Mol	Chain	Residues	Atoms			AltConf
10	K	1	Total	C	O	0
			28	27	1	
10	K	1	Total	C	O	0
			28	27	1	
10	K	1	Total	C	O	0
			28	27	1	

- Molecule 11 is (2R)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(dodecanoyloxy)propyl dodecanoate (three-letter code: WNZ) (formula: C<sub>29</sub>H<sub>58</sub>NO<sub>8</sub>P).



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 (three-letter code: WO9) (formula: C<sub>34</sub>H<sub>68</sub>NO<sub>8</sub>P).



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

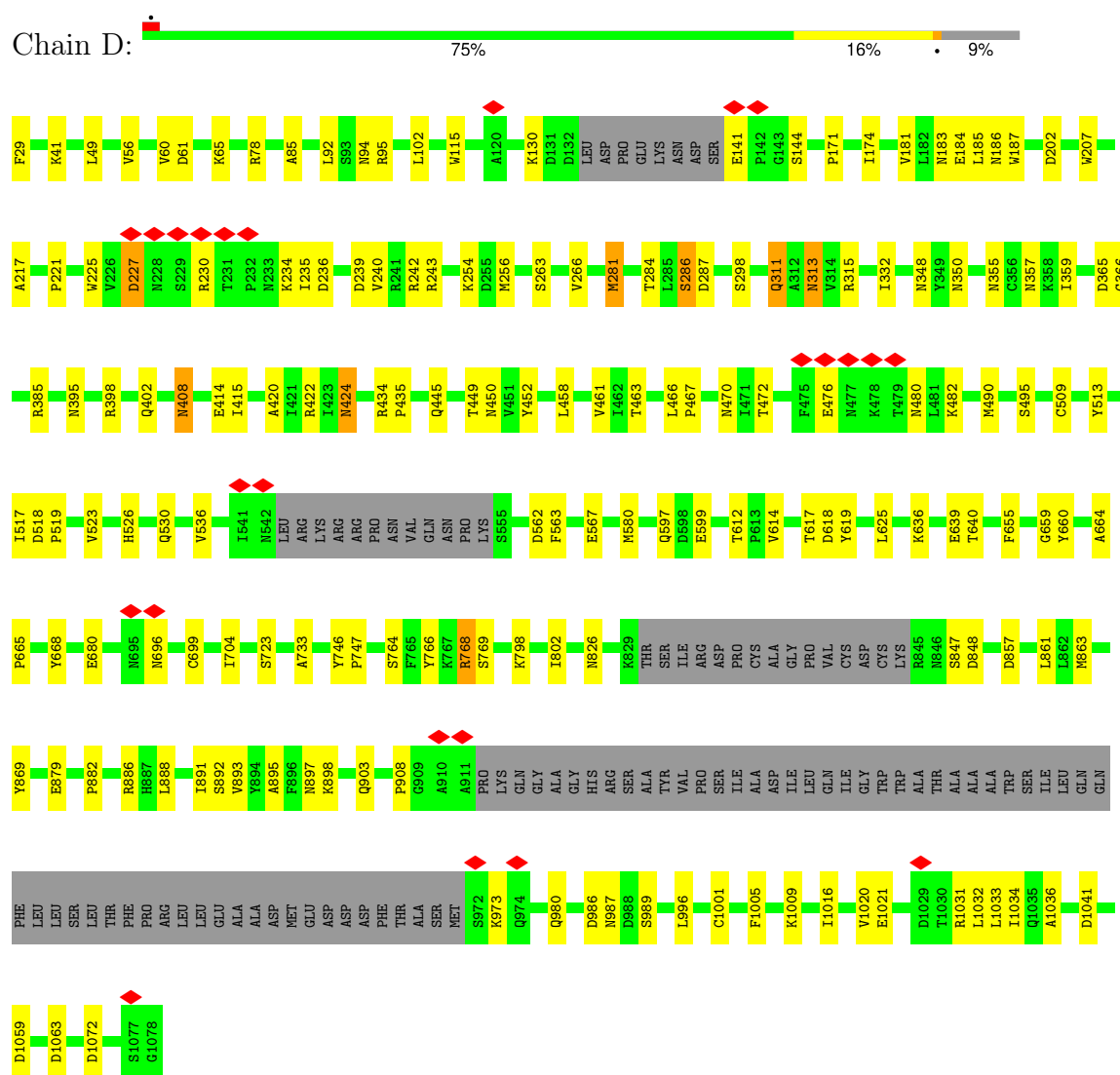
- Molecule 13 is water.

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

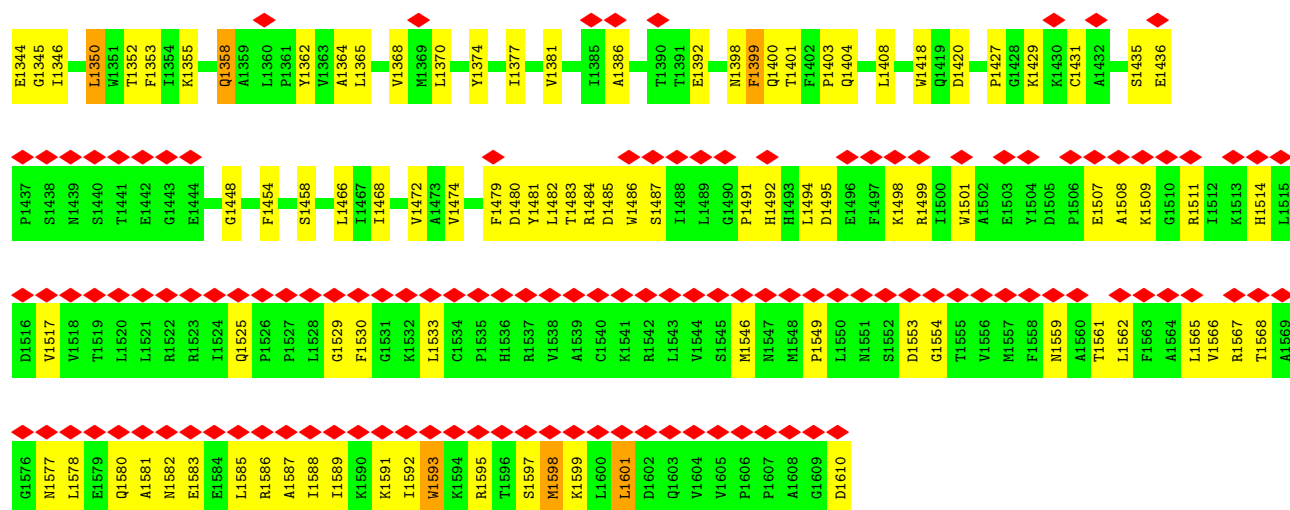


- Molecule 2: Isoform 20 of Voltage-dependent L-type calcium channel subunit alpha-1C









• 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-(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

Chain E:



MAG1  
MAG2

## 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: CA, NAG, WO9, CLR, WNZ, NA

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	0.26	0/7792	0.48	0/10569
2	K	0.25	0/10473	0.48	0/14203
3	C	0.23	0/1544	0.48	0/2088
All	All	0.25	0/19809	0.48	0/26860

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	7428	114	0
2	K	10230	0	10445	293	0
3	C	1518	0	1567	42	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
7	D	1	0	0	0	0
7	K	2	0	0	0	0
8	D	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	451	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 11.

All (451) 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
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
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:452:TYR:HH	1:D:463:THR:HG1	1.42	0.63
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:1238:MET:HE2	10:K:1701:CLR:H183	1.84	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: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:286:SER:OG	1:D:287:ASP:N	2.36	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:N	2:K:311:ASP:OD1	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
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
2:K:410:LYS:HZ1	2:K:753:VAL:HG13	1.73	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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:1224:LEU:O	2:K:1227:VAL:HG22	2.12	0.49
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:1205:LYS:HD2	2:K:1207:GLN:HG2	1.94	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
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:1507:GLU:HG2	2:K:1508:ALA:H	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:513:TYR:OH	1:D:567:GLU:OE2	2.24	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
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:D:183:ASN:O	1:D:184:GLU:C	2.53	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:624:LEU:C	2:K:626:ARG:H	2.20	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: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: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: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
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
2:K:1358:GLN:H	2:K:1358:GLN:CD	2.20	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:1191:GLU:O	2:K:1195:LYS:NZ	2.44	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:K:347:ASP:HB2	2:K:1240:HIS:HB2	2.00	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:1002:VAL:C	2:K:1005:PRO:HD2	2.39	0.43
2:K:1401:THR:HG22	2:K:1403:PRO:HD2	2.00	0.43
2:K:611:MET:HE3	2:K:612:SER:H	1.83	0.42
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:1485:ASP:OD1	2:K:1487:SER:OG	2.33	0.42
1:D:888:LEU:O	1:D:893:VAL:HG12	2.19	0.42
2:K:167:LEU:O	2:K:171:THR:OG1	2.27	0.42
1:D:141:GLU:OE2	1:D:144:SER:OG	2.25	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
2:K:604:ILE:O	2:K:607:GLU:HB2	2.20	0.42
2:K:624:LEU:C	2:K:626:ARG:N	2.73	0.42
2:K:1100:ASN:HD21	10:K:1702:CLR:H121	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:102:LEU:HB3	1:D:490:MET:HE2	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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:611:MET:HB3	2:K:611:MET:HE2	1.92	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: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
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

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:630:ILE:C	2:K:632:ARG:H	2.24	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:1010:ASN:OD1	2:K:1010:ASN:C	2.60	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%)	44	71
3	C	189/191 (99%)	186 (98%)	3 (2%)	0	100	100
All	All	2394/2740 (87%)	2211 (92%)	180 (8%)	3 (0%)	50	76

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 ⓘ

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	846/926 (91%)	820 (97%)	26 (3%)	35	61
2	K	1123/1319 (85%)	1077 (96%)	46 (4%)	26	54
3	C	172/172 (100%)	168 (98%)	4 (2%)	45	68
All	All	2141/2417 (89%)	2065 (96%)	76 (4%)	32	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	PHE
1	D	41	LYS
1	D	130	LYS
1	D	227	ASP
1	D	230	ARG
1	D	256	MET
1	D	281	MET
1	D	286	SER
1	D	311	GLN
1	D	313	ASN
1	D	348	ASN
1	D	355	ASN
1	D	408	ASN
1	D	424	ASN
1	D	472	THR
1	D	480	ASN
1	D	482	LYS
1	D	509	CYS
1	D	660	TYR
1	D	723	SER
1	D	766	TYR
1	D	768	ARG
1	D	769	SER
1	D	863	MET
1	D	1001	CYS
1	D	1033	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	123	TRP
2	K	137	ASN
2	K	138	CYS
2	K	190	TYR
2	K	197	LEU
2	K	199	ASP
2	K	200	PHE
2	K	290	PHE
2	K	443	GLN
2	K	528	TRP
2	K	554	GLU
2	K	576	TYR
2	K	594	PHE
2	K	621	CYS
2	K	626	ARG
2	K	629	LYS
2	K	649	ARG
2	K	754	ASP
2	K	921	ASP
2	K	929	ARG
2	K	955	TYR
2	K	995	LYS
2	K	1004	ARG
2	K	1080	GLU
2	K	1083	HIS
2	K	1094	SER
2	K	1098	PHE
2	K	1200	ARG
2	K	1202	TYR
2	K	1223	TYR
2	K	1241	TYR
2	K	1262	PHE
2	K	1278	TYR
2	K	1328	PHE
2	K	1332	ARG
2	K	1342	ARG
2	K	1350	LEU
2	K	1353	PHE
2	K	1358	GLN
2	K	1374	TYR
2	K	1399	PHE
2	K	1408	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	1480	ASP
2	K	1593	TRP
2	K	1598	MET
2	K	1601	LEU
3	C	177	MET
3	C	202	ASP
3	C	203	PHE
3	C	320	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	94	ASN
1	D	113	HIS
1	D	483	ASN
1	D	826	ASN
2	K	325	GLN
2	K	924	GLN
2	K	1100	ASN
2	K	1380	GLN
2	K	1398	ASN
2	K	1400	GLN
2	K	1580	GLN

### 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:

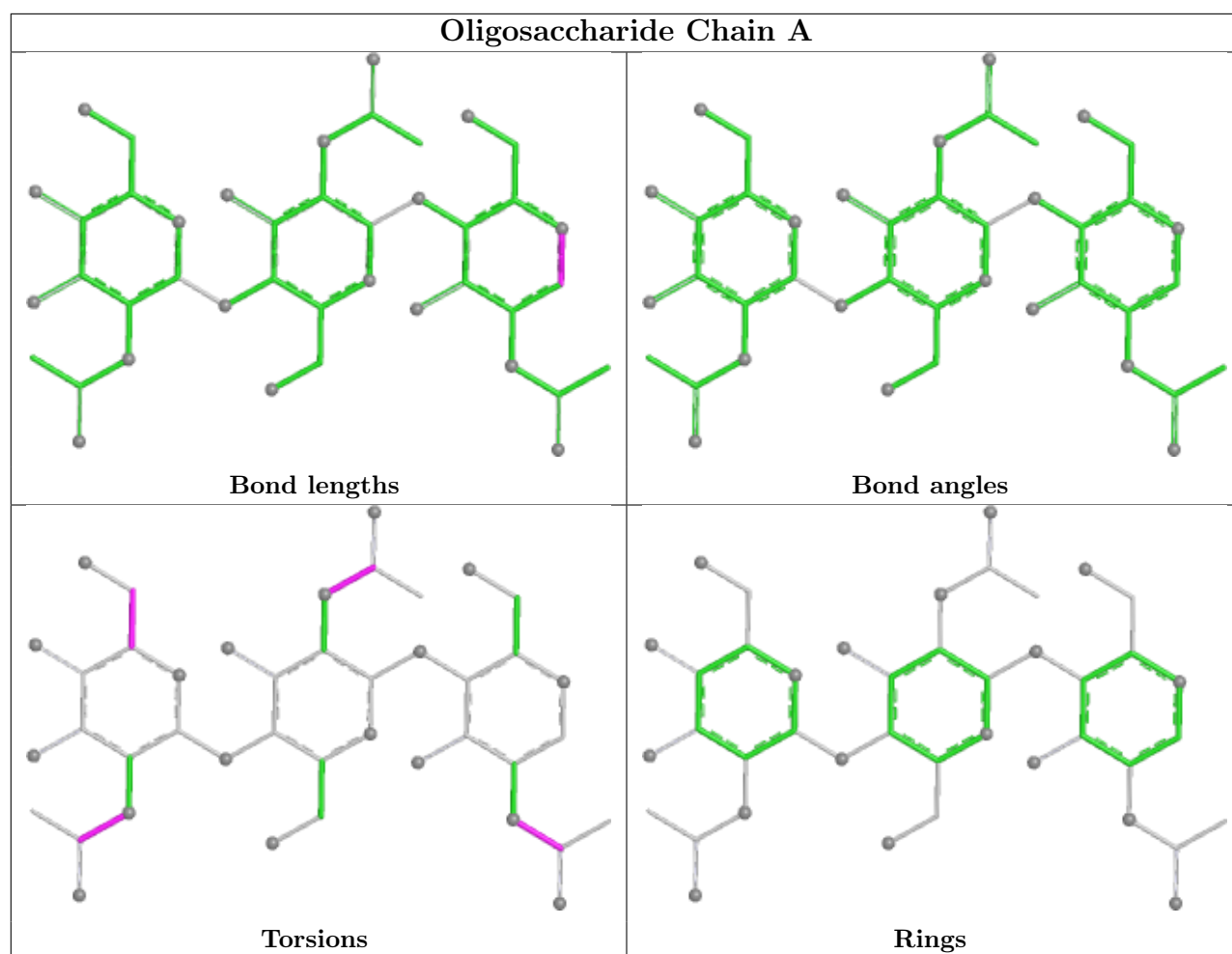
Mol	Chain	Res	Type	Atoms
4	A	3	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	A	3	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	3	NAG	C8-C7-N2-C2
4	A	3	NAG	O7-C7-N2-C2
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2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

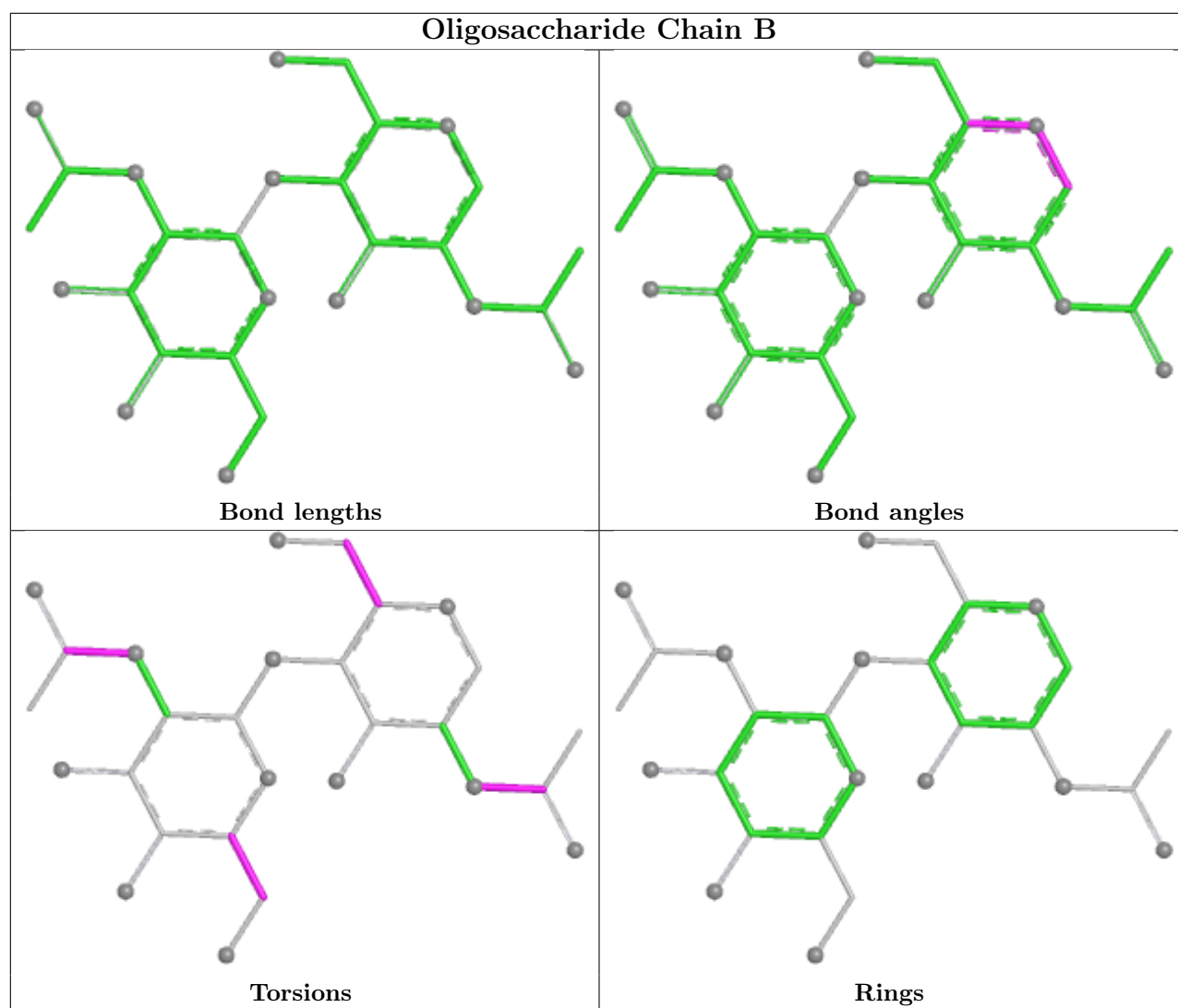
There are no ring outliers.

5 monomers are involved in 16 short contacts:

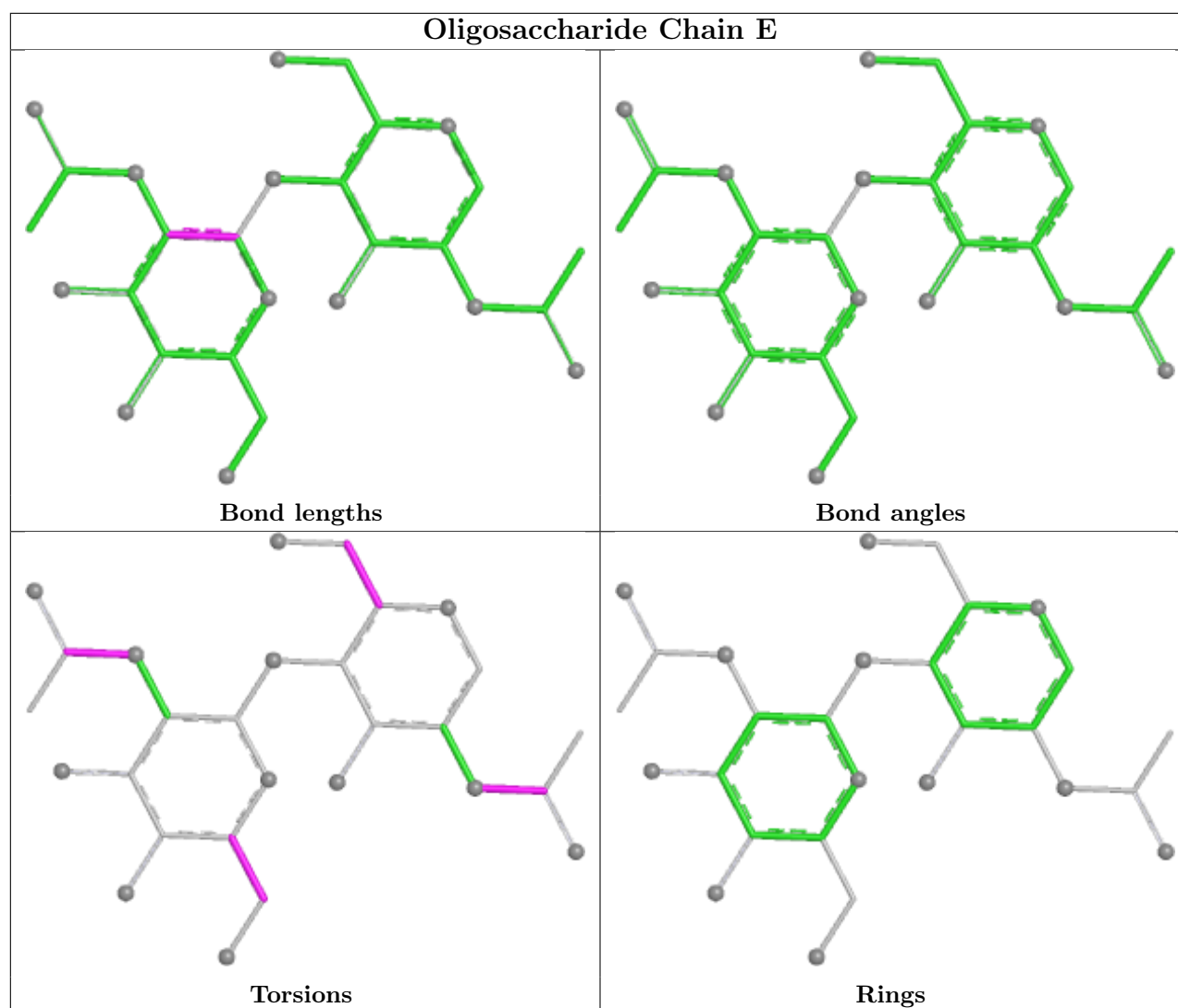
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	3	0
5	E	1	NAG	4	0
5	E	2	NAG	4	0
4	A	3	NAG	4	0
5	B	1	NAG	3	0

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	$\# Z  > 2$
10	CLR	K	1701	-	31,31,31	1.04	1 (3%)	48,48,48	0.70	0
12	WO9	K	1705	-	43,43,43	0.98	4 (9%)	46,48,48	1.19	3 (6%)
6	NAG	D	1103	-	14,14,15	0.48	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	WNZ	K	1704	-	38,38,38	1.04	4 (10%)	41,43,43	1.20	3 (7%)
6	NAG	D	1102	-	14,14,15	0.24	0	17,19,21	0.38	0
6	NAG	D	1105	-	14,14,15	0.84	2 (14%)	17,19,21	1.70	3 (17%)
6	NAG	D	1101	-	14,14,15	0.24	0	17,19,21	0.58	0
10	CLR	K	1703	-	31,31,31	1.05	1 (3%)	48,48,48	0.56	0
9	LEU	D	1108	-	6,8,8	0.86	0	5,10,10	0.85	0
6	NAG	D	1104	-	14,14,15	0.32	0	17,19,21	0.39	0
10	CLR	K	1702	-	31,31,31	1.05	0	48,48,48	0.66	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
10	CLR	K	1701	-	-	5/10/68/68	0/4/4/4
12	WO9	K	1705	-	-	26/47/47/47	-
6	NAG	D	1103	-	-	4/6/23/26	0/1/1/1
11	WNZ	K	1704	-	-	19/42/42/42	-
6	NAG	D	1102	-	-	2/6/23/26	0/1/1/1
6	NAG	D	1105	-	-	6/6/23/26	0/1/1/1
6	NAG	D	1101	-	-	2/6/23/26	0/1/1/1
10	CLR	K	1703	-	-	5/10/68/68	0/4/4/4
9	LEU	D	1108	-	-	5/8/8/8	-
6	NAG	D	1104	-	-	3/6/23/26	0/1/1/1
10	CLR	K	1702	-	-	8/10/68/68	0/4/4/4

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

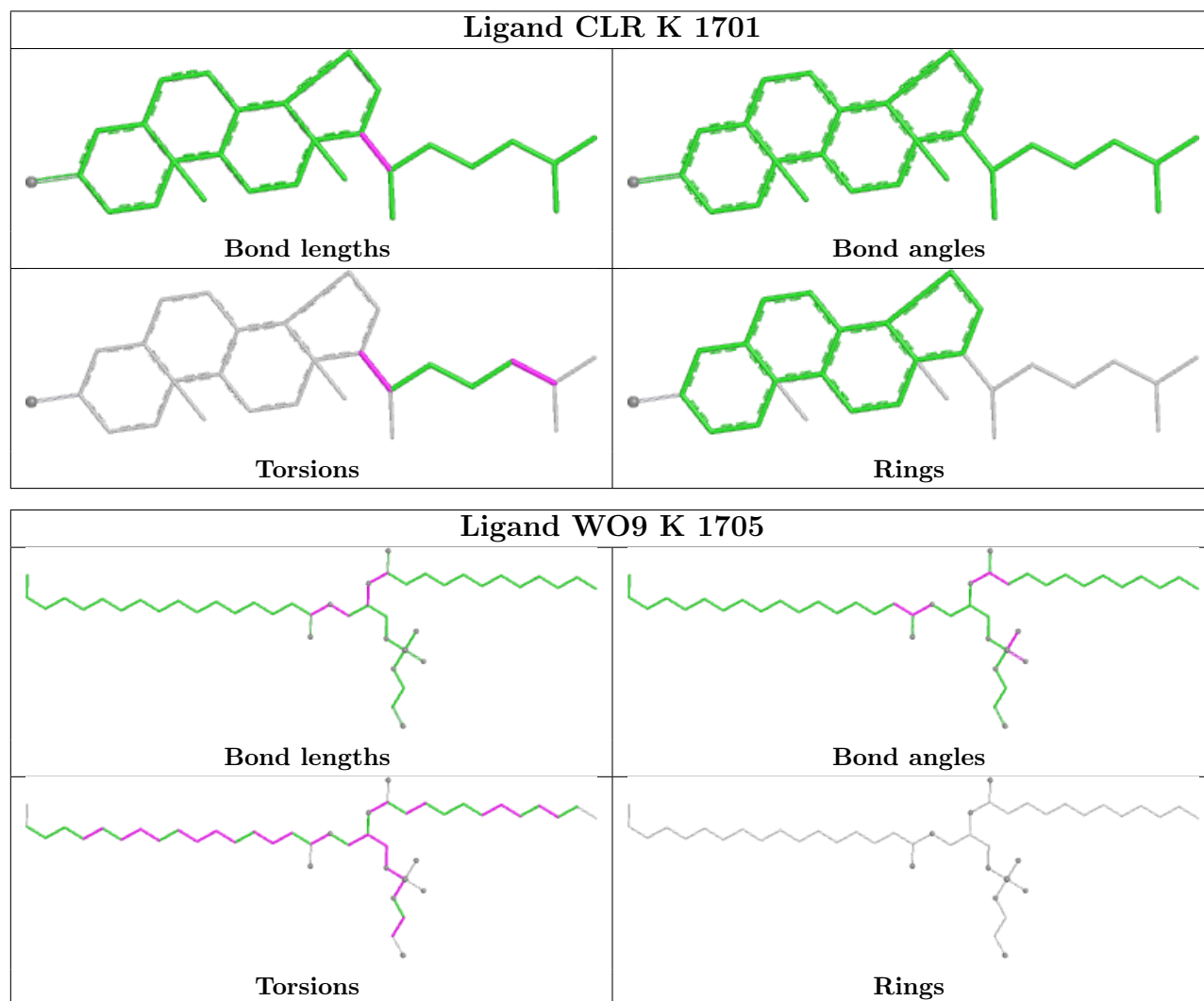
There are no ring outliers.

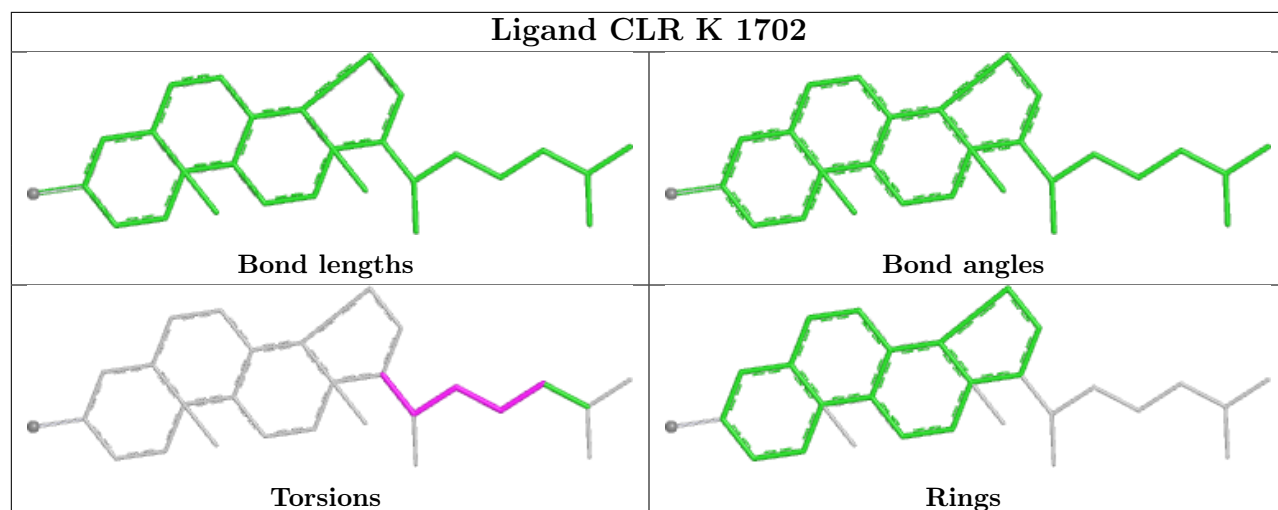
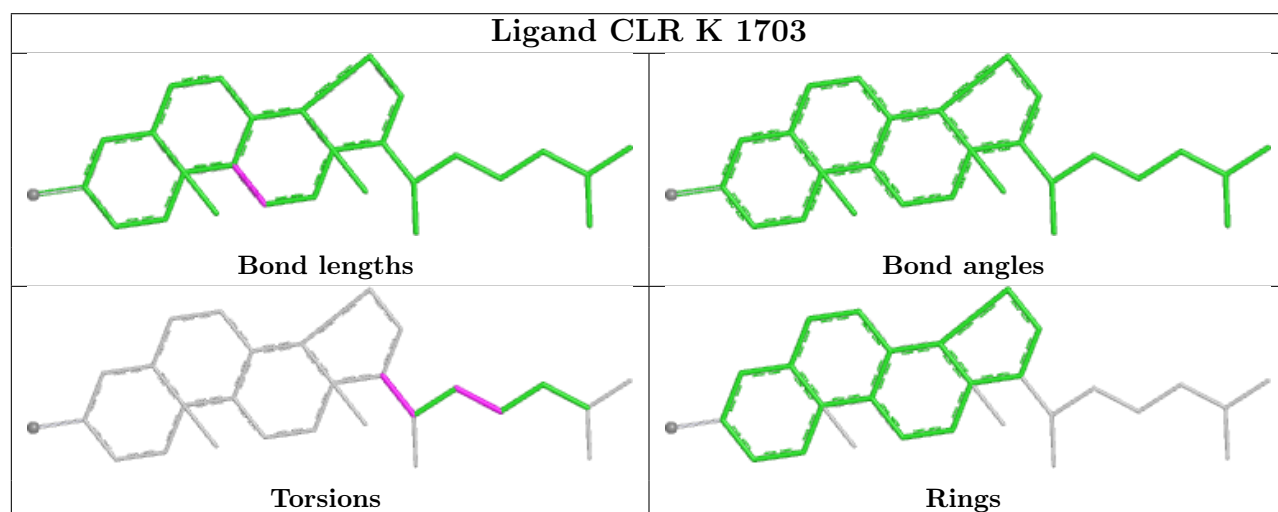
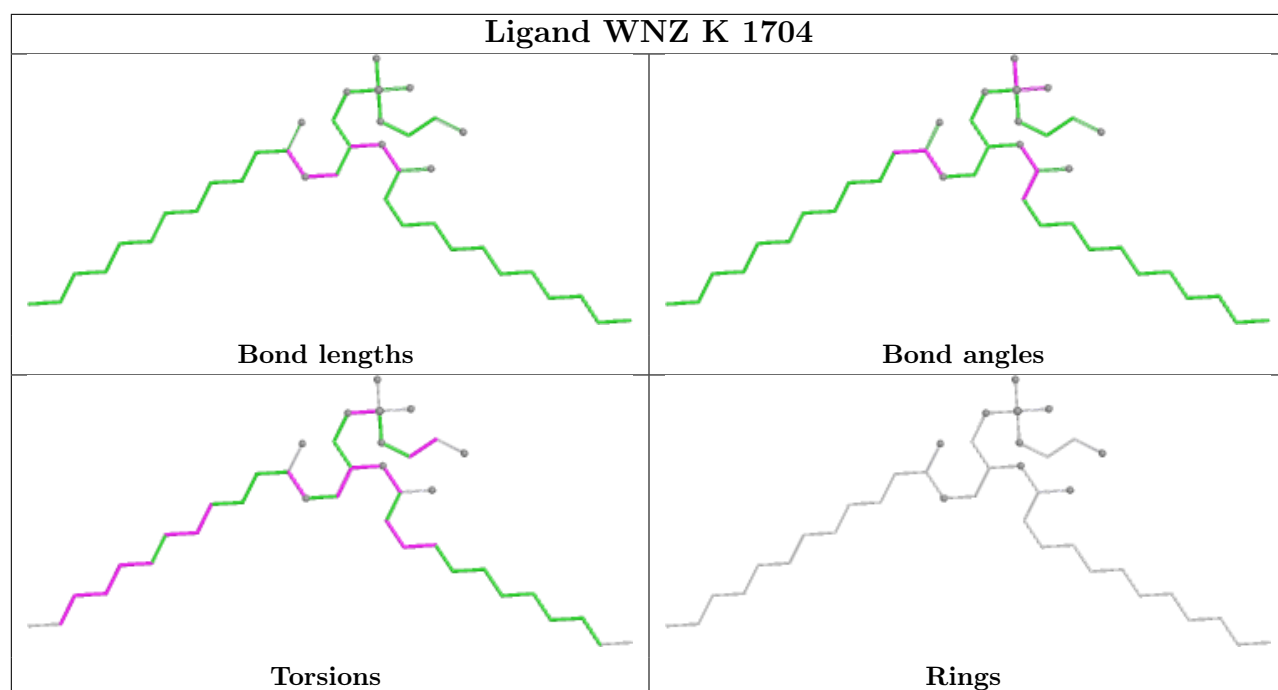
6 monomers are involved in 12 short contacts:

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



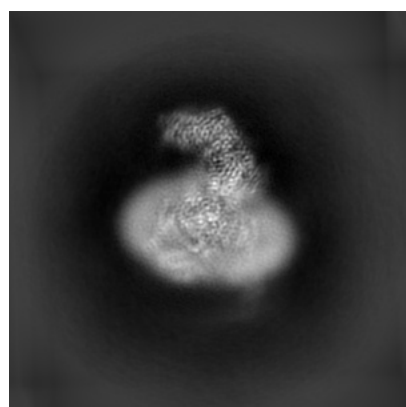
## 6 Map visualisation [i](#)

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.

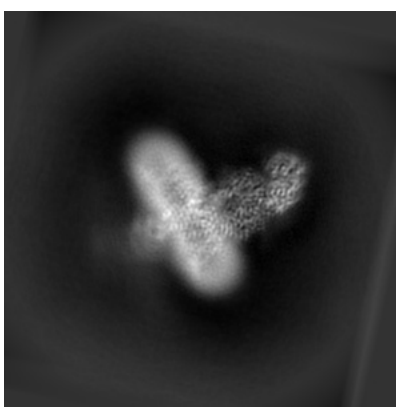
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

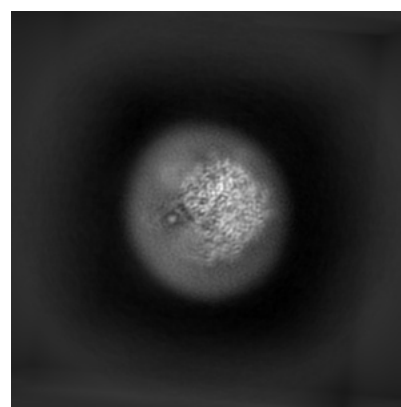
#### 6.1.1 Primary map



X



Y

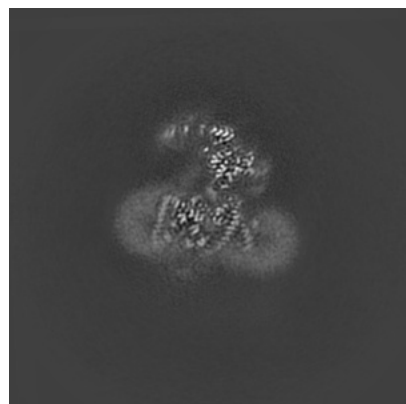


Z

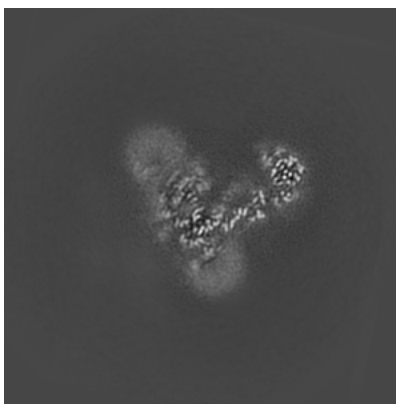
The images above show the map projected in three orthogonal directions.

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

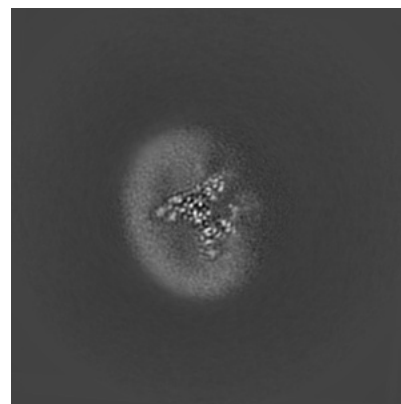
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

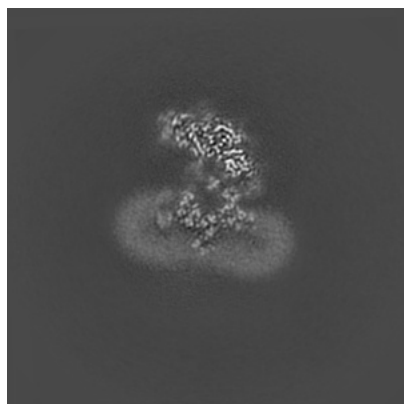


Z Index: 220

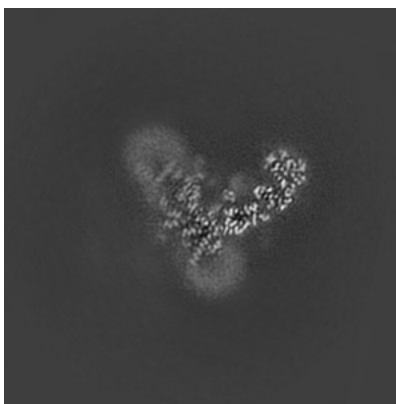
The images above show central slices of the map in three orthogonal directions.

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

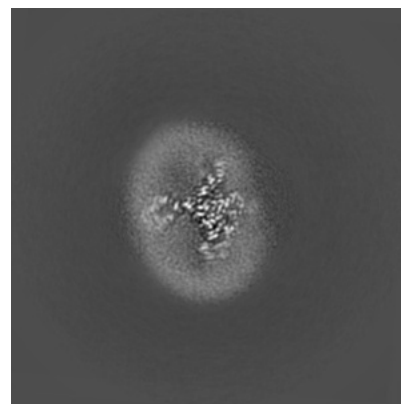
### 6.3.1 Primary map



X Index: 231



Y Index: 226

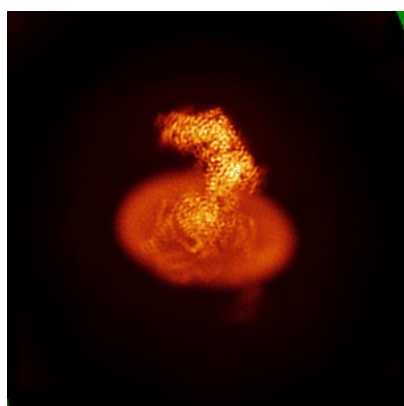


Z Index: 210

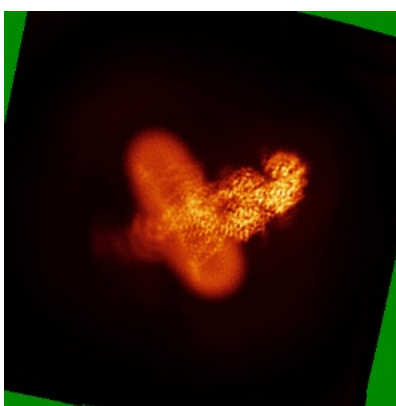
The images above show the largest variance slices of the map in three orthogonal directions.

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

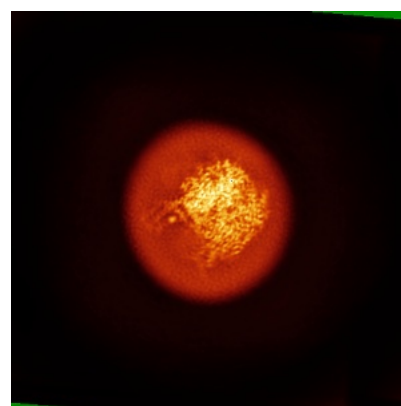
### 6.4.1 Primary map



X



Y

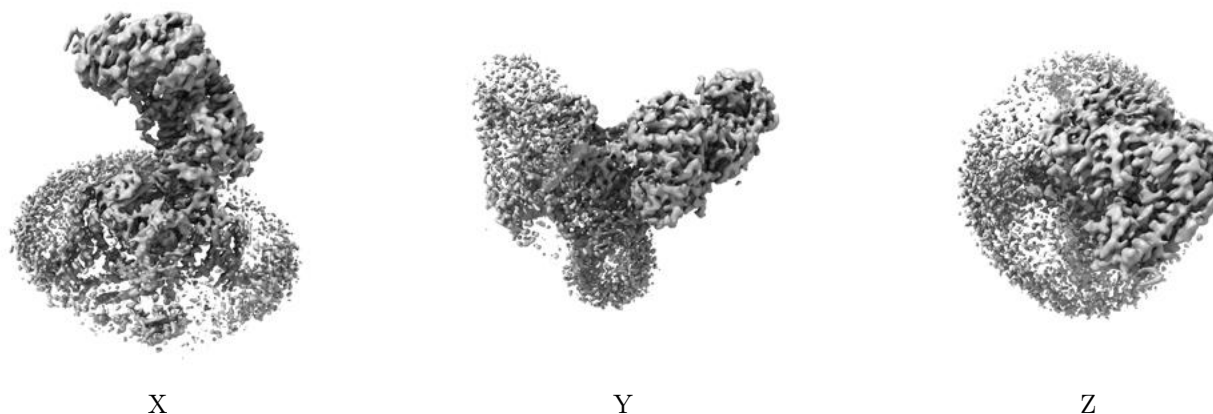


Z

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.

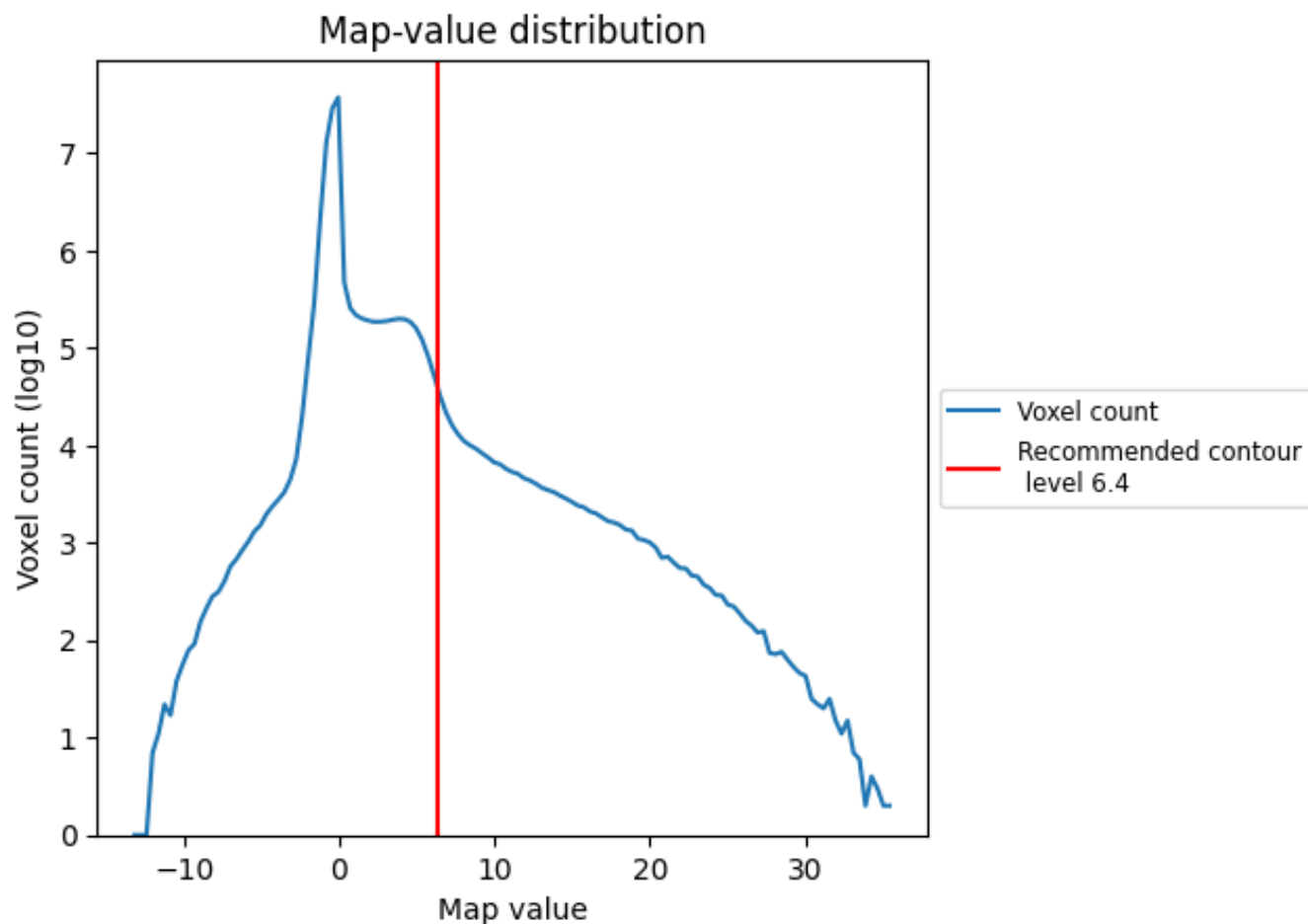
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

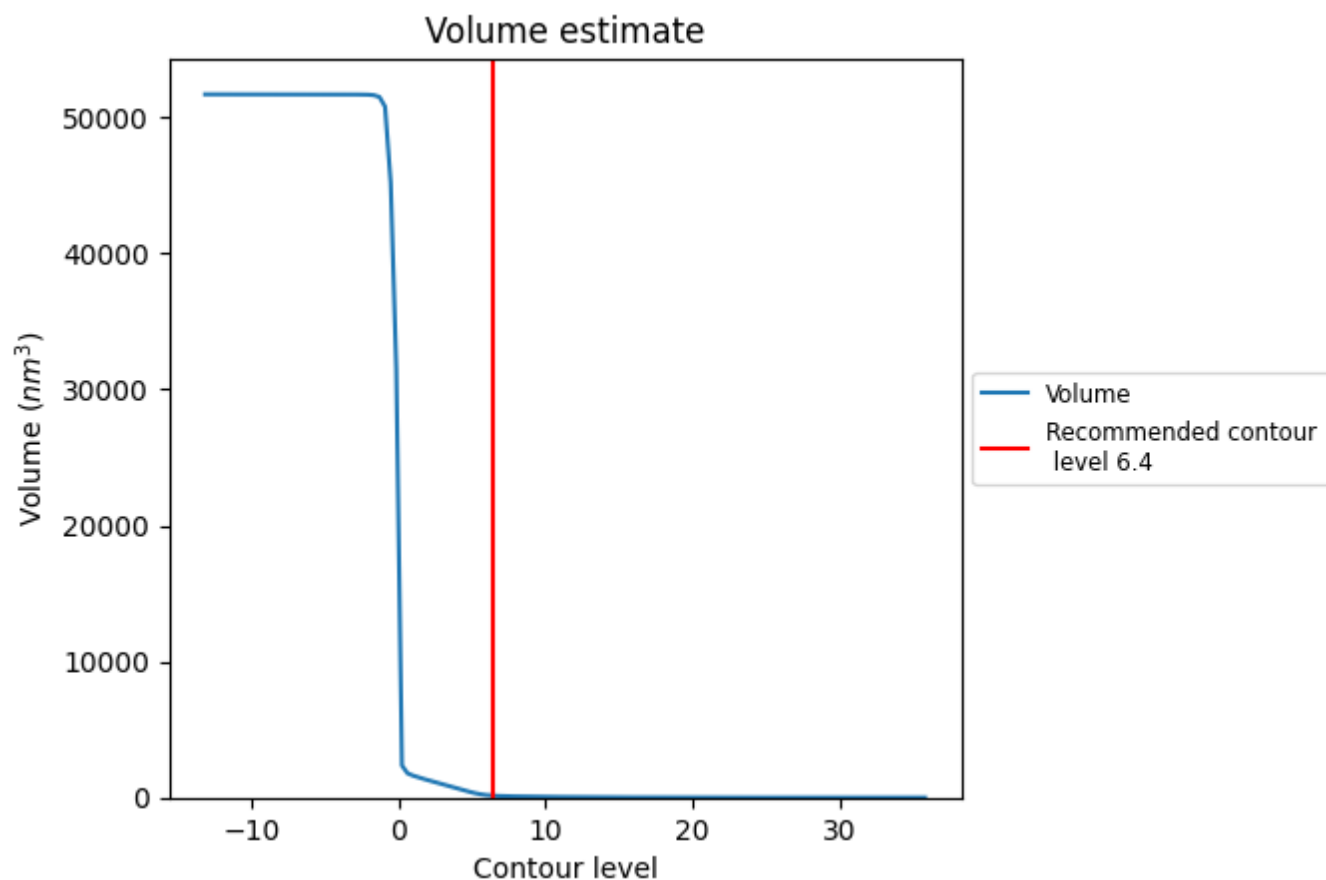
This section contains the results of statistical analysis of the map.

### 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.

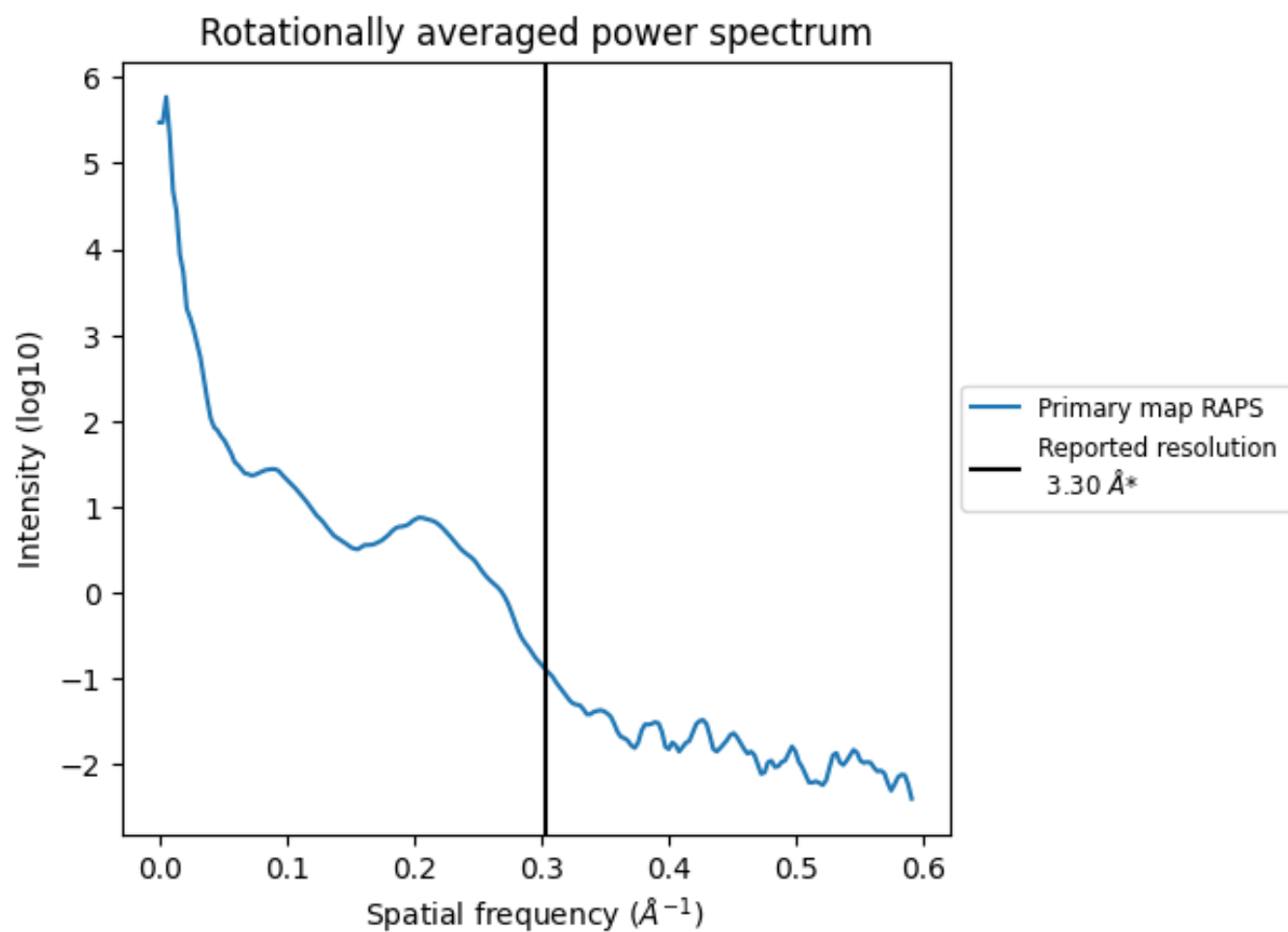
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141  $\text{nm}^3$ ; 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<sup>-1</sup>

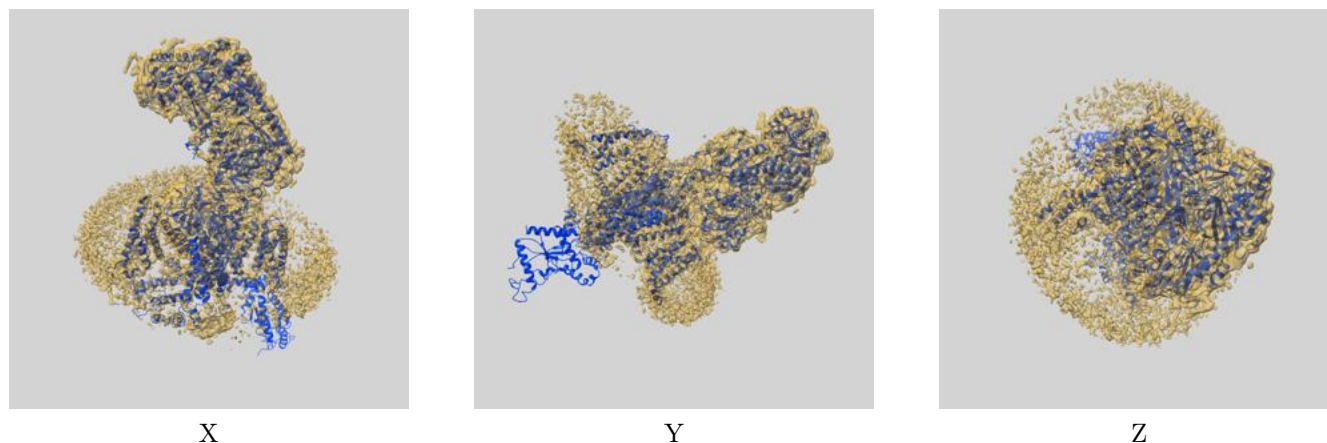
## 8 Fourier-Shell correlation

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

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

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

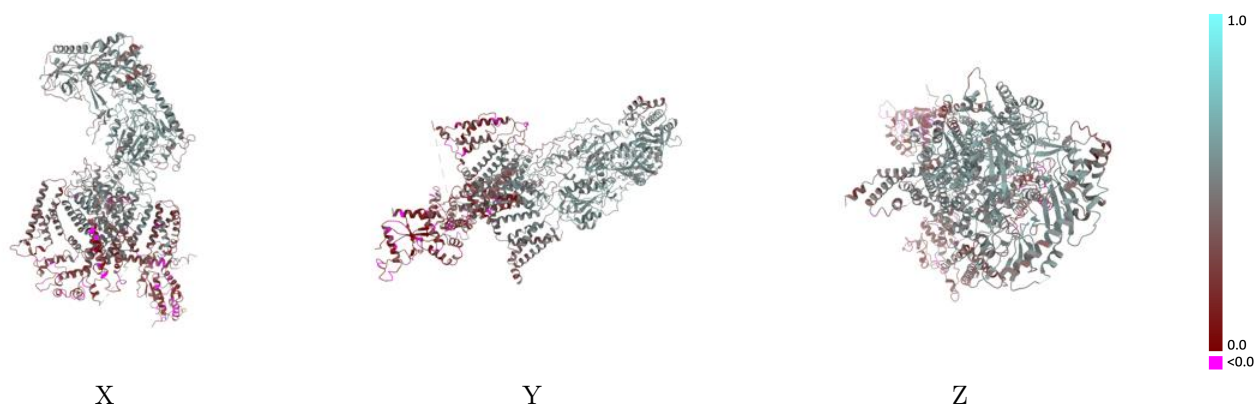
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 6.4 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.

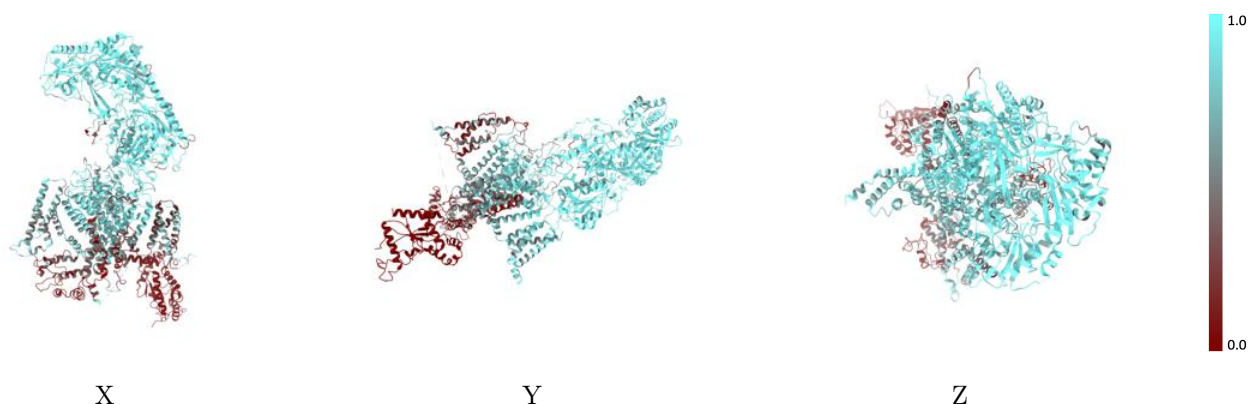


## 9.2 Q-score mapped to coordinate model [i](#)



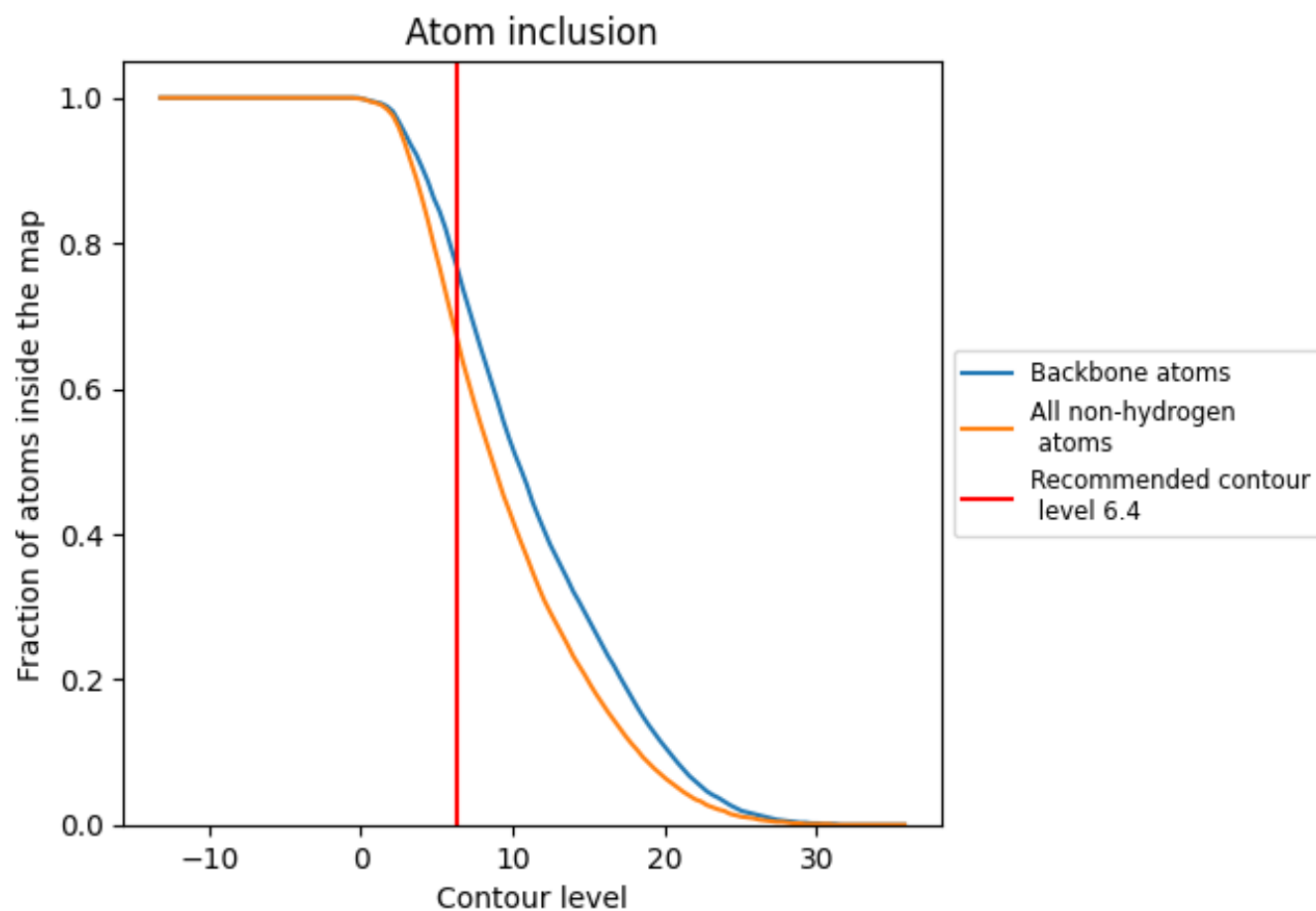
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (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	<div></div> 0.6650	<div></div> 0.4120
A	<div></div> 0.7620	<div></div> 0.4120
B	<div></div> 0.7860	<div></div> 0.4420
C	<div></div> 0.0010	<div></div> 0.1510
D	<div></div> 0.9020	<div></div> 0.5240
E	<div></div> 0.7860	<div></div> 0.3570
K	<div></div> 0.5850	<div></div> 0.3680

1.0

0.0

<0.0