



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:07 PM UTC

PDB ID : 5GJE / pdb_00005gje
EMDB ID : EMD-9501
Title : Three-dimensional reconstruction of human LRP6 ectodomain complexed with Dkk1
Authors : Matoba, K.; Mihara, E.; Tamura-Kawakami, K.; Hirai, H.; Thompson, S.; Iwasaki, K.; Takagi, J.
Deposited on : 2016-06-29
Resolution : 21.00 Å (reported)
Based on initial models : 3S2K, 4DG6

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:

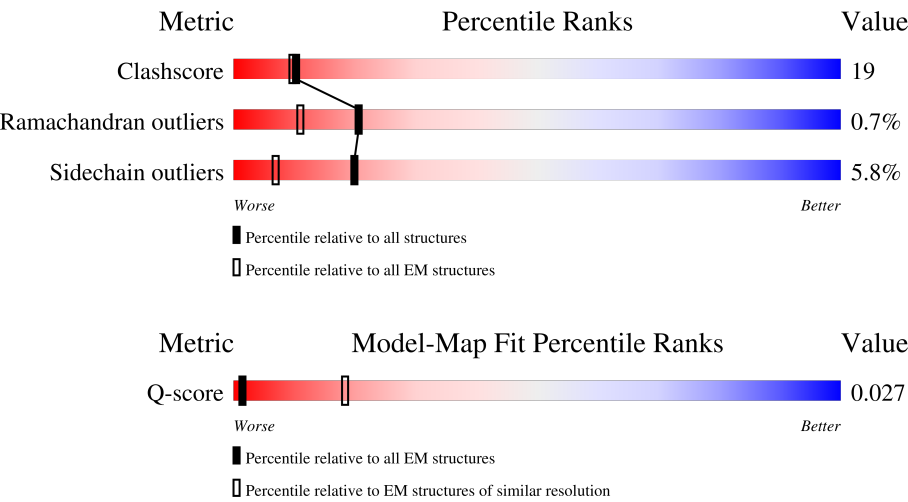
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 21.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11 (20.50 - 21.00)

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

Mol	Chain	Length	Quality of chain
1	A	611	47% 47% 6%
2	B	616	76% 21% ••
3	C	85	8% 69% 19% • 11%
4	D	2	100%

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Mol	Chain	Length	Quality of chain
4	E	2	 50%50%
4	F	2	 100%
4	H	2	 50%50%
5	G	3	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 10506 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	611	Total	C	N	O	S	0	0
			4856	3078	831	923	24		

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	606	Total	C	N	O	S	0	0
			4833	3033	856	919	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1062	ILE	VAL	engineered mutation	UNP O75581

- Molecule 3 is a protein called Dickkopf-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	76	Total	C	N	O	S	0	0
			596	362	123	101	10		

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



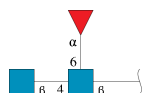
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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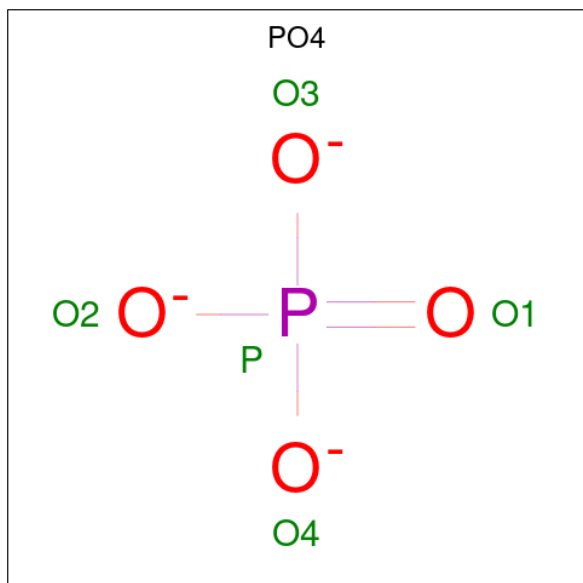
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	P	0
			5	4	1	
6	A	1	Total	O	P	0
			5	4	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	C	O	0
			6	3	3	

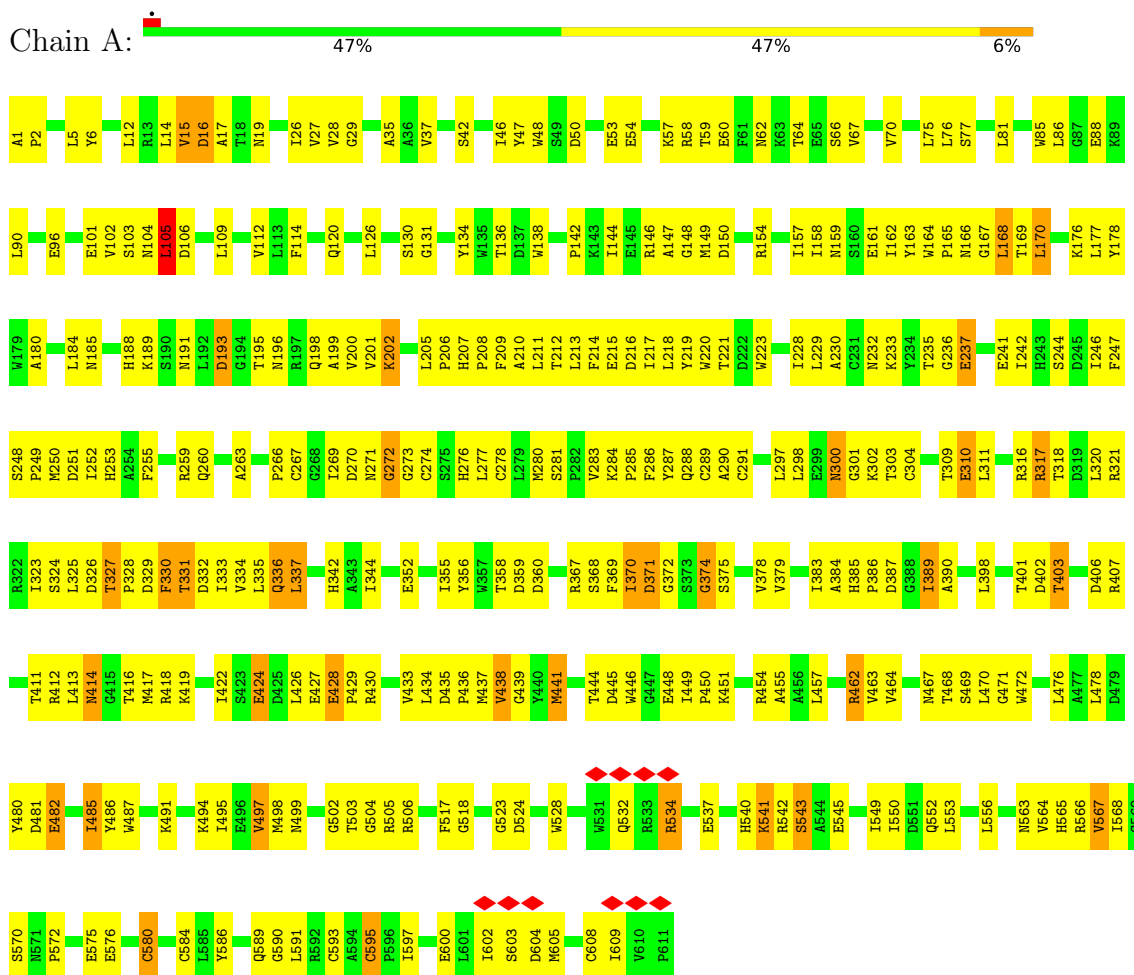
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	13	Total 13	O 13	0

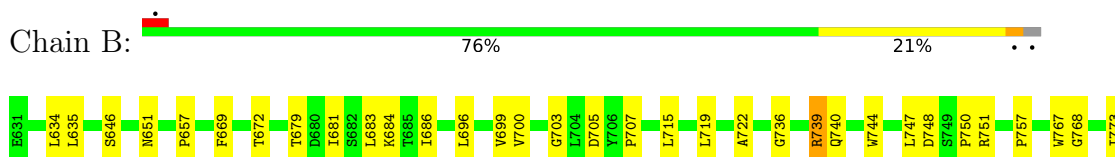
3 Residue-property plots

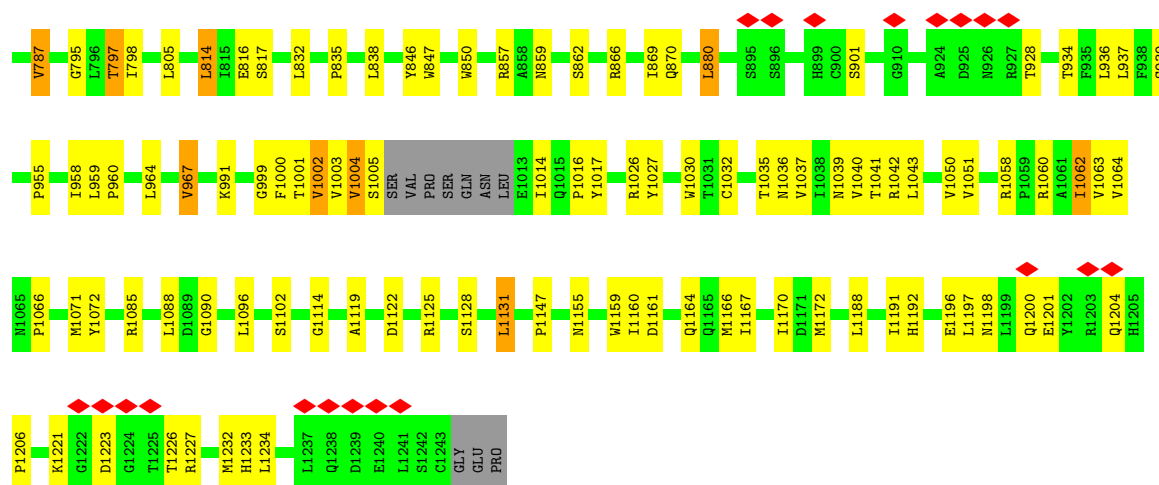
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Low-density lipoprotein receptor-related protein 6

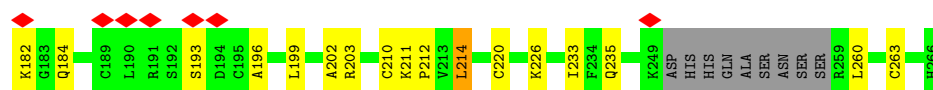


• Molecule 2: Low-density lipoprotein receptor-related protein 6





• Molecule 3: Dickkopf-related protein 1



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



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



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• 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5390	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; This was not done for RCT but for following single-particle reconstruction	Depositor
Microscope	HITACHI H-9500SD	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	80000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor
Maximum map value	1.038	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.198	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.2, 2.2, 2.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FUC, NAG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/4972	0.86	8/6766 (0.1%)
2	B	0.28	0/4934	0.70	0/6694
3	C	0.27	0/605	0.65	0/801
All	All	0.41	0/10511	0.78	8/14261 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	SER	CA-C-N	6.24	125.80	119.19
1	A	281	SER	C-N-CA	6.24	125.80	119.19
1	A	207	HIS	CA-C-N	5.70	125.46	119.76
1	A	207	HIS	C-N-CA	5.70	125.46	119.76
1	A	327	THR	CA-C-N	5.51	125.03	119.19
1	A	327	THR	C-N-CA	5.51	125.03	119.19
1	A	272	GLY	N-CA-C	-5.35	106.02	114.10
1	A	269	ILE	N-CA-C	-5.28	104.65	112.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	VAL	Peptide
1	A	374	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4856	0	4726	290	0
2	B	4833	0	4711	87	0
3	C	596	0	589	16	0
4	D	28	0	25	1	0
4	E	28	0	25	2	0
4	F	28	0	25	1	0
4	H	28	0	25	0	0
5	G	38	0	34	0	0
6	A	10	0	0	1	0
7	B	42	0	39	2	0
8	B	6	0	8	0	0
9	A	13	0	0	0	0
All	All	10506	0	10207	390	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 19.

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:NE2	1:A:337:LEU:H	1.40	1.20
1:A:389:ILE:HD11	1:A:398:LEU:HD11	1.49	0.94
1:A:336:GLN:NE2	1:A:337:LEU:N	2.21	0.88
1:A:162:ILE:HB	1:A:165:PRO:HG3	1.56	0.88
2:B:773:ILE:HB	2:B:787:VAL:HG13	1.57	0.86
1:A:437:MET:HE3	1:A:570:SER:H	1.41	0.84
1:A:549:ILE:HG13	1:A:550:ILE:HG22	1.61	0.82
1:A:597:ILE:HD12	1:A:597:ILE:H	1.44	0.82
1:A:274:CYS:HG	1:A:289:CYS:HG	1.19	0.81
1:A:193:ASP:HB2	1:A:195:THR:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:ALA:HB3	3:C:211:LYS:HD2	1.64	0.79
1:A:273:GLY:HA3	1:A:278:CYS:HB2	1.65	0.78
1:A:288:GLN:NE2	1:A:289:CYS:H	1.82	0.78
1:A:336:GLN:CD	1:A:337:LEU:H	1.93	0.76
1:A:335:LEU:HD23	1:A:335:LEU:H	1.49	0.76
1:A:157:ILE:HG13	1:A:158:ILE:H	1.50	0.76
1:A:321:ARG:HG2	1:A:335:LEU:HB3	1.67	0.75
1:A:291:CYS:HG	1:A:304:CYS:HG	1.10	0.73
1:A:454:ARG:HG2	1:A:455:ALA:N	2.04	0.72
1:A:136:THR:HG22	1:A:144:ILE:HG12	1.72	0.71
2:B:1058:ARG:HG3	2:B:1058:ARG:HH11	1.54	0.71
1:A:228:ILE:HD12	1:A:244:SER:HB3	1.72	0.71
1:A:580:CYS:HB3	1:A:593:CYS:HB3	1.73	0.70
1:A:218:LEU:O	1:A:230:ALA:HA	1.92	0.70
1:A:170:LEU:HD23	1:A:170:LEU:H	1.56	0.70
1:A:330:PHE:O	1:A:332:ASP:N	2.25	0.69
4:F:1:NAG:O3	4:F:2:NAG:H2	1.92	0.69
1:A:370:ILE:HG22	1:A:371:ASP:H	1.58	0.69
1:A:497:VAL:HG12	1:A:498:MET:H	1.57	0.68
1:A:310:GLU:HB2	1:A:325:LEU:HB2	1.74	0.68
1:A:468:THR:HG22	3:C:226:LYS:HD2	1.76	0.68
1:A:266:PRO:HB2	1:A:287:TYR:HB3	1.74	0.68
1:A:288:GLN:HE21	1:A:289:CYS:H	1.40	0.68
2:B:869:ILE:HG22	2:B:870:GLN:HG2	1.76	0.67
1:A:1:ALA:HB1	1:A:17:ALA:O	1.96	0.65
3:C:199:LEU:HD23	3:C:212:PRO:HA	1.78	0.65
1:A:211:LEU:HD12	1:A:219:TYR:O	1.97	0.64
1:A:176:LYS:HZ1	1:A:198:GLN:HE22	1.45	0.64
1:A:437:MET:O	1:A:438:VAL:HB	1.98	0.64
1:A:411:THR:HG22	1:A:418:ARG:HA	1.79	0.64
1:A:523:GLY:O	1:A:524:ASP:HB3	1.97	0.64
1:A:416:THR:HG22	1:A:417:MET:HG3	1.80	0.64
1:A:336:GLN:O	1:A:337:LEU:HB2	1.98	0.64
1:A:157:ILE:HG13	1:A:158:ILE:N	2.14	0.63
1:A:427:GLU:HG3	1:A:451:LYS:HE3	1.80	0.63
1:A:191:ASN:HB2	1:A:195:THR:OG1	1.98	0.63
1:A:235:THR:HG23	1:A:237:GLU:H	1.64	0.63
1:A:589:GLN:HG2	1:A:590:GLY:H	1.63	0.63
1:A:131:GLY:O	1:A:148:GLY:HA2	1.99	0.63
3:C:196:ALA:HB3	3:C:199:LEU:HD12	1.80	0.63
1:A:166:ASN:CG	1:A:167:GLY:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HA	1:A:47:TYR:O	1.99	0.62
1:A:335:LEU:H	1:A:335:LEU:CD2	2.13	0.62
1:A:263:ALA:O	4:D:1:NAG:H62	1.99	0.62
1:A:60:GLU:HG2	1:A:66:SER:HB3	1.82	0.62
1:A:370:ILE:HG22	1:A:371:ASP:N	2.14	0.62
2:B:1032:CYS:SG	2:B:1035:THR:HG22	2.40	0.61
1:A:291:CYS:HG	1:A:304:CYS:CB	2.14	0.61
1:A:372:GLY:C	1:A:374:GLY:H	2.08	0.61
1:A:220:TRP:NE1	1:A:229:LEU:HD13	2.16	0.60
1:A:540:HIS:HB3	1:A:543:SER:HB3	1.83	0.60
1:A:101:GLU:CD	1:A:112:VAL:HG22	2.26	0.59
1:A:161:GLU:O	1:A:161:GLU:HG3	2.03	0.59
2:B:669:PHE:HD2	2:B:880:LEU:HD11	1.67	0.59
1:A:498:MET:SD	1:A:502:GLY:HA2	2.42	0.59
1:A:429:PRO:HA	1:A:445:ASP:HB3	1.85	0.59
3:C:182:LYS:HE3	3:C:193:SER:O	2.03	0.58
2:B:798:ILE:HG12	2:B:805:LEU:CD2	2.34	0.58
1:A:159:ASN:HA	1:A:162:ILE:HD11	1.85	0.58
2:B:795:GLY:O	2:B:797:THR:HG22	2.04	0.58
2:B:880:LEU:C	2:B:880:LEU:HD23	2.28	0.58
2:B:936:LEU:HD21	2:B:1191:ILE:CG1	2.33	0.58
1:A:532:GLN:O	1:A:534:ARG:HG2	2.03	0.57
1:A:441:MET:HB3	1:A:457:LEU:HD23	1.86	0.57
1:A:454:ARG:HH21	1:A:463:VAL:HG21	1.68	0.57
2:B:715:LEU:HD12	2:B:757:PRO:HB2	1.86	0.57
1:A:524:ASP:HA	1:A:541:LYS:NZ	2.19	0.57
1:A:158:ILE:N	1:A:158:ILE:HD12	2.20	0.57
1:A:499:ASN:ND2	1:A:504:GLY:N	2.53	0.57
2:B:679:THR:HG22	2:B:686:ILE:HG12	1.87	0.57
1:A:358:THR:HB	1:A:386:PRO:HB2	1.87	0.56
2:B:1035:THR:HG23	2:B:1037:VAL:HG22	1.86	0.56
1:A:291:CYS:SG	1:A:297:LEU:HD13	2.45	0.56
1:A:147:ALA:HB2	1:A:154:ARG:HA	1.88	0.56
1:A:241:GLU:HG3	1:A:241:GLU:O	2.05	0.56
2:B:934:THR:HG22	2:B:1196:GLU:H	1.70	0.56
2:B:1160:ILE:HD12	2:B:1188:LEU:HB3	1.88	0.56
1:A:199:ALA:HB1	1:A:202:LYS:HB3	1.87	0.56
1:A:130:SER:OG	1:A:131:GLY:N	2.39	0.56
1:A:176:LYS:NZ	1:A:198:GLN:HE22	2.03	0.56
2:B:747:LEU:HD22	2:B:750:PRO:HG3	1.87	0.56
1:A:166:ASN:HB3	1:A:180:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:HIS:HB2	1:A:403:THR:HB	1.87	0.56
1:A:300:ASN:N	1:A:300:ASN:HD22	2.03	0.55
1:A:602:ILE:HG22	1:A:603:SER:N	2.20	0.55
2:B:1221:LYS:HE3	2:B:1227:ARG:CG	2.37	0.55
1:A:329:ASP:O	1:A:331:THR:N	2.40	0.55
1:A:330:PHE:C	1:A:332:ASP:H	2.15	0.55
2:B:1072:TYR:CE1	2:B:1085:ARG:HD3	2.42	0.55
2:B:1119:ALA:HB1	2:B:1147:PRO:HB2	1.89	0.54
1:A:446:TRP:CZ2	1:A:472:TRP:HB3	2.42	0.54
1:A:580:CYS:SG	1:A:584:CYS:HB2	2.47	0.54
1:A:15:VAL:O	1:A:16:ASP:HB2	2.07	0.54
1:A:370:ILE:CG2	1:A:371:ASP:H	2.15	0.54
2:B:744:TRP:CE2	2:B:955:PRO:HD3	2.43	0.54
1:A:170:LEU:HD23	1:A:170:LEU:N	2.21	0.54
1:A:298:LEU:HB2	1:A:300:ASN:ND2	2.23	0.54
1:A:2:PRO:HB3	1:A:214:PHE:CD2	2.43	0.54
1:A:270:ASP:C	1:A:272:GLY:H	2.16	0.54
2:B:1014:ILE:HG22	2:B:1016:PRO:HD3	1.90	0.54
1:A:327:THR:HB	1:A:328:PRO:HD2	1.90	0.54
1:A:335:LEU:CD2	1:A:335:LEU:N	2.71	0.54
1:A:468:THR:CG2	3:C:226:LYS:HD2	2.37	0.54
2:B:939:SER:HB2	2:B:967:VAL:HG21	1.89	0.54
2:B:937:LEU:O	2:B:1192:HIS:N	2.39	0.53
2:B:1200:GLN:HE22	2:B:1204:GLN:HE21	1.55	0.53
1:A:284:LYS:HB2	1:A:285:PRO:HD3	1.90	0.53
1:A:316:ARG:NH1	1:A:321:ARG:HH21	2.06	0.53
1:A:271:ASN:ND2	1:A:273:GLY:O	2.40	0.53
1:A:468:THR:HG21	3:C:226:LYS:HE2	1.90	0.53
1:A:524:ASP:HA	1:A:541:LYS:HD2	1.91	0.53
2:B:1114:GLY:HA2	2:B:1131:LEU:HD22	1.89	0.53
2:B:703:GLY:HA2	2:B:958:ILE:HD12	1.91	0.53
1:A:216:ASP:O	1:A:233:LYS:HB2	2.09	0.53
2:B:646:SER:HB2	2:B:651:ASN:HD22	1.74	0.53
1:A:330:PHE:C	1:A:332:ASP:N	2.66	0.53
1:A:468:THR:CG2	3:C:226:LYS:CE	2.87	0.53
1:A:478:LEU:HD23	1:A:480:TYR:CE1	2.44	0.53
1:A:289:CYS:SG	1:A:302:LYS:HG2	2.49	0.52
2:B:773:ILE:HB	2:B:787:VAL:CG1	2.36	0.52
1:A:498:MET:HG2	1:A:499:ASN:O	2.09	0.52
1:A:602:ILE:HD11	1:A:609:ILE:HG12	1.91	0.52
1:A:26:ILE:HG22	1:A:26:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HG21	1:A:387:ASP:HA	1.91	0.52
1:A:485:ILE:HG23	1:A:498:MET:HB3	1.91	0.52
3:C:214:LEU:HD23	3:C:220:CYS:HB3	1.91	0.52
1:A:437:MET:HE3	1:A:570:SER:N	2.18	0.52
1:A:178:TYR:CD1	1:A:189:LYS:HB2	2.45	0.52
1:A:471:GLY:HA3	1:A:491:LYS:HB3	1.91	0.52
2:B:1001:THR:CG2	2:B:1004:VAL:HG22	2.40	0.52
1:A:321:ARG:HG2	1:A:335:LEU:CB	2.39	0.51
1:A:602:ILE:HG22	1:A:603:SER:H	1.75	0.51
1:A:138:TRP:CD1	1:A:138:TRP:C	2.87	0.51
1:A:170:LEU:HB3	1:A:177:LEU:HD13	1.93	0.51
1:A:213:LEU:HD12	1:A:213:LEU:C	2.35	0.51
1:A:164:TRP:N	1:A:165:PRO:HD3	2.26	0.51
1:A:60:GLU:HB2	1:A:64:THR:HG21	1.93	0.51
1:A:320:LEU:O	1:A:335:LEU:HB2	2.10	0.51
1:A:426:LEU:HD13	1:A:448:GLU:OE1	2.11	0.51
1:A:220:TRP:CE2	1:A:229:LEU:HB2	2.46	0.51
1:A:291:CYS:CB	1:A:304:CYS:HG	2.24	0.51
1:A:136:THR:HG23	1:A:168:LEU:HD22	1.93	0.51
1:A:144:ILE:HD13	1:A:168:LEU:HD11	1.92	0.51
1:A:148:GLY:C	1:A:150:ASP:H	2.19	0.50
1:A:235:THR:HG23	1:A:237:GLU:HB2	1.93	0.50
2:B:859:ASN:HB3	2:B:862:SER:HB3	1.92	0.50
1:A:216:ASP:C	1:A:233:LYS:HB2	2.36	0.50
1:A:580:CYS:CB	1:A:593:CYS:HG	2.20	0.50
2:B:722:ALA:HB1	2:B:750:PRO:HB2	1.94	0.50
1:A:524:ASP:HA	1:A:541:LYS:CD	2.41	0.50
1:A:540:HIS:CB	1:A:543:SER:HB3	2.41	0.50
1:A:46:ILE:O	1:A:58:ARG:HA	2.11	0.50
1:A:486:TYR:OH	1:A:541:LYS:HG3	2.11	0.50
1:A:595:CYS:HG	1:A:608:CYS:HG	0.51	0.50
1:A:273:GLY:HA3	1:A:278:CYS:CB	2.38	0.49
2:B:1221:LYS:HE3	2:B:1227:ARG:HG2	1.93	0.49
1:A:138:TRP:HB3	1:A:165:PRO:HD2	1.94	0.49
1:A:436:PRO:HA	1:A:457:LEU:HD11	1.94	0.49
1:A:553:LEU:HD23	1:A:556:LEU:HD21	1.93	0.49
1:A:563:ASN:HB3	1:A:566:ARG:HB3	1.94	0.49
1:A:126:LEU:HD22	1:A:149:MET:HE3	1.93	0.49
1:A:384:ALA:O	1:A:386:PRO:HD3	2.12	0.49
1:A:335:LEU:HD23	1:A:335:LEU:N	2.18	0.49
1:A:457:LEU:HB2	1:A:586:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:PHE:CE1	1:A:528:TRP:HB2	2.47	0.49
2:B:1050:VAL:HG12	2:B:1232:MET:HG3	1.95	0.49
2:B:1058:ARG:HG3	2:B:1058:ARG:NH1	2.25	0.49
2:B:1159:TRP:HZ3	2:B:1170:ILE:HG23	1.78	0.49
2:B:1160:ILE:HG22	2:B:1167:ILE:HG12	1.95	0.49
1:A:57:LYS:HA	1:A:70:VAL:HG23	1.94	0.49
1:A:58:ARG:NH1	1:A:105:LEU:O	2.45	0.49
1:A:246:ILE:O	1:A:249:PRO:HD3	2.13	0.49
1:A:481:ASP:C	1:A:482:GLU:HG2	2.37	0.49
1:A:104:ASN:HD21	1:A:109:LEU:HD12	1.78	0.49
1:A:316:ARG:HH11	1:A:321:ARG:HH21	1.61	0.49
2:B:669:PHE:CD2	2:B:880:LEU:HD11	2.45	0.49
1:A:383:ILE:HG23	1:A:386:PRO:HG3	1.93	0.48
1:A:390:ALA:HB1	1:A:434:LEU:HG	1.94	0.48
1:A:283:VAL:HG12	1:A:285:PRO:HD2	1.95	0.48
1:A:355:ILE:O	1:A:367:ARG:HA	2.13	0.48
2:B:1198:ASN:HB3	2:B:1201:GLU:HB3	1.95	0.48
1:A:298:LEU:HB2	1:A:300:ASN:HD21	1.77	0.48
1:A:572:PRO:HD2	1:A:586:TYR:CE2	2.48	0.48
2:B:964:LEU:HD22	2:B:967:VAL:HG12	1.95	0.48
2:B:1064:VAL:C	2:B:1066:PRO:HD3	2.38	0.48
1:A:19:ASN:HD22	1:A:242:ILE:HG23	1.78	0.48
1:A:406:ASP:HA	1:A:429:PRO:HD2	1.96	0.48
1:A:534:ARG:HA	1:A:553:LEU:O	2.13	0.48
2:B:635:LEU:HB2	2:B:880:LEU:HD22	1.95	0.48
1:A:468:THR:HG21	3:C:226:LYS:CE	2.43	0.48
1:A:469:SER:O	1:A:470:LEU:HD12	2.14	0.48
2:B:699:VAL:HG13	2:B:736:GLY:CA	2.44	0.48
1:A:14:LEU:HD21	1:A:255:PHE:CD1	2.49	0.47
2:B:751:ARG:HG2	2:B:767:TRP:CZ2	2.48	0.47
2:B:1051:VAL:O	2:B:1090:GLY:HA3	2.14	0.47
1:A:14:LEU:HD11	1:A:255:PHE:CE1	2.49	0.47
1:A:437:MET:O	1:A:438:VAL:CB	2.59	0.47
1:A:27:VAL:HG11	1:A:46:ILE:HD12	1.97	0.47
1:A:277:LEU:HB2	1:A:290:ALA:HB3	1.95	0.47
2:B:1027:TYR:CE1	2:B:1042:ARG:HG2	2.50	0.47
1:A:157:ILE:C	1:A:158:ILE:HD12	2.39	0.47
1:A:232:ASN:HB2	1:A:235:THR:O	2.13	0.47
1:A:367:ARG:O	1:A:375:SER:HA	2.14	0.47
1:A:505:ARG:O	1:A:506:ARG:HB3	2.14	0.47
2:B:1005:SER:HB2	2:B:1014:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1026:ARG:O	2:B:1043:LEU:HD13	2.14	0.47
1:A:356:TYR:OH	1:A:413:LEU:HB3	2.15	0.47
1:A:426:LEU:HB3	1:A:448:GLU:OE1	2.15	0.47
2:B:699:VAL:HG12	2:B:700:VAL:HG23	1.97	0.47
2:B:748:ASP:OD2	2:B:768:GLY:HA3	2.15	0.47
2:B:1071:MET:HB3	2:B:1088:LEU:HD23	1.95	0.47
2:B:1233:HIS:CE1	2:B:1234:LEU:HG	2.50	0.47
1:A:372:GLY:C	1:A:374:GLY:N	2.72	0.47
1:A:201:VAL:HG22	1:A:236:GLY:HA2	1.96	0.47
1:A:134:TYR:CE1	1:A:146:ARG:HG3	2.50	0.47
1:A:163:TYR:HB3	1:A:184:LEU:HG	1.97	0.47
2:B:936:LEU:HD21	2:B:1191:ILE:HD11	1.95	0.47
1:A:450:PRO:HG2	1:A:470:LEU:O	2.15	0.46
1:A:589:GLN:HG2	1:A:590:GLY:N	2.28	0.46
2:B:857:ARG:HG2	2:B:869:ILE:HD11	1.96	0.46
1:A:300:ASN:ND2	1:A:301:GLY:N	2.63	0.46
1:A:401:THR:HB	1:A:429:PRO:HB2	1.97	0.46
7:B:1305:NAG:O7	7:B:1305:NAG:H3	2.15	0.46
1:A:104:ASN:C	1:A:106:ASP:H	2.24	0.46
1:A:309:THR:H	1:A:326:ASP:CG	2.23	0.46
1:A:166:ASN:HD21	1:A:209:PHE:C	2.23	0.46
2:B:1001:THR:HG21	2:B:1004:VAL:HG22	1.98	0.46
1:A:336:GLN:CD	1:A:337:LEU:N	2.67	0.46
1:A:468:THR:CG2	3:C:226:LYS:NZ	2.78	0.46
1:A:59:THR:HG22	1:A:67:VAL:HA	1.98	0.46
1:A:114:PHE:CD1	1:A:154:ARG:HD2	2.51	0.46
1:A:369:PHE:N	1:A:374:GLY:HA3	2.31	0.46
1:A:383:ILE:CG2	1:A:386:PRO:HG3	2.46	0.46
2:B:1017:TYR:CE2	2:B:1060:ARG:HB3	2.51	0.46
1:A:427:GLU:HG3	1:A:451:LYS:CE	2.45	0.46
1:A:603:SER:HA	1:A:605:MET:HE3	1.98	0.46
2:B:1102:SER:HB3	2:B:1122:ASP:HB2	1.97	0.46
1:A:59:THR:HG22	1:A:66:SER:O	2.17	0.45
1:A:75:LEU:O	1:A:76:LEU:HD23	2.16	0.45
1:A:166:ASN:ND2	1:A:208:PRO:O	2.48	0.45
1:A:435:ASP:O	1:A:437:MET:O	2.33	0.45
2:B:850:TRP:CH2	3:C:233:ILE:HD13	2.51	0.45
7:B:1304:NAG:O7	7:B:1304:NAG:H3	2.16	0.45
1:A:467:ASN:HB2	4:E:1:NAG:N2	2.30	0.45
1:A:499:ASN:ND2	1:A:504:GLY:CA	2.79	0.45
2:B:1206:PRO:HB2	2:B:1226:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:GLN:O	3:C:210:CYS:HB2	2.16	0.45
1:A:317:ARG:HG3	1:A:342:HIS:CD2	2.52	0.45
1:A:120:GLN:HB2	1:A:138:TRP:O	2.16	0.45
1:A:469:SER:C	1:A:470:LEU:HD12	2.41	0.45
1:A:497:VAL:HG12	1:A:498:MET:N	2.28	0.45
1:A:215:GLU:O	1:A:217:ILE:HG13	2.17	0.45
1:A:270:ASP:O	1:A:272:GLY:N	2.45	0.45
1:A:428:GLU:HA	1:A:429:PRO:HD3	1.71	0.45
1:A:209:PHE:CZ	1:A:250:MET:HE3	2.52	0.45
1:A:542:ARG:O	1:A:543:SER:CB	2.63	0.45
3:C:214:LEU:HB3	3:C:263:CYS:SG	2.56	0.45
2:B:681:ILE:HG22	2:B:707:PRO:HD2	1.99	0.45
1:A:138:TRP:HA	1:A:142:PRO:HA	1.99	0.45
1:A:369:PHE:H	1:A:374:GLY:HA3	1.82	0.45
2:B:686:ILE:HG21	2:B:719:LEU:HD21	1.98	0.45
1:A:414:ASN:OD1	1:A:414:ASN:N	2.45	0.44
2:B:739:ARG:HG3	2:B:740:GLN:N	2.31	0.44
2:B:832:LEU:CB	2:B:835:PRO:HG3	2.47	0.44
1:A:35:ALA:O	1:A:251:ASP:HB2	2.17	0.44
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.76	0.44
1:A:102:VAL:HG22	1:A:103:SER:N	2.32	0.44
1:A:291:CYS:CB	1:A:304:CYS:SG	3.05	0.44
1:A:321:ARG:CZ	1:A:335:LEU:HD13	2.46	0.44
1:A:524:ASP:HA	1:A:541:LYS:HZ2	1.82	0.44
1:A:53:GLU:O	1:A:54:GLU:C	2.60	0.44
2:B:991:LYS:O	2:B:999:GLY:HA2	2.17	0.44
1:A:5:LEU:HD13	1:A:14:LEU:HG	2.00	0.44
1:A:384:ALA:HB3	1:A:402:ASP:OD1	2.18	0.44
1:A:480:TYR:C	1:A:482:GLU:H	2.26	0.44
1:A:86:LEU:HD23	1:A:280:MET:HE2	1.99	0.44
1:A:206:PRO:C	1:A:208:PRO:HD3	2.43	0.44
1:A:285:PRO:O	1:A:286:PHE:HB2	2.18	0.44
1:A:300:ASN:HD22	1:A:300:ASN:H	1.64	0.44
1:A:316:ARG:HD3	1:A:321:ARG:HE	1.83	0.44
1:A:166:ASN:CG	1:A:167:GLY:N	2.74	0.43
1:A:169:THR:O	1:A:177:LEU:HD12	2.18	0.43
1:A:221:THR:HG21	1:A:249:PRO:HB2	1.99	0.43
1:A:389:ILE:HG12	1:A:390:ALA:N	2.32	0.43
2:B:1062:ILE:HG13	2:B:1063:VAL:N	2.32	0.43
1:A:336:GLN:HB3	1:A:337:LEU:HD22	1.99	0.43
1:A:476:LEU:HD11	1:A:485:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:ARG:HG2	3:C:235:GLN:OE1	2.18	0.43
1:A:62:ASN:O	1:A:64:THR:HG22	2.19	0.43
1:A:323:ILE:HG22	1:A:324:SER:O	2.18	0.43
1:A:553:LEU:O	1:A:556:LEU:HG	2.18	0.43
1:A:424:GLU:HG3	1:A:462:ARG:HH22	1.84	0.43
2:B:1206:PRO:HB2	2:B:1226:THR:CG2	2.48	0.43
1:A:50:ASP:OD1	1:A:53:GLU:N	2.47	0.43
1:A:6:TYR:CE1	1:A:246:ILE:HG21	2.53	0.43
1:A:90:LEU:O	1:A:102:VAL:HA	2.19	0.43
1:A:158:ILE:N	1:A:158:ILE:CD1	2.80	0.43
2:B:859:ASN:CB	2:B:862:SER:HB3	2.49	0.43
2:B:1155:ASN:HA	2:B:1172:MET:HE2	2.01	0.43
1:A:19:ASN:HD21	1:A:242:ILE:HD13	1.83	0.43
1:A:342:HIS:O	1:A:359:ASP:HA	2.19	0.43
1:A:352:GLU:HA	1:A:352:GLU:OE1	2.18	0.43
1:A:210:ALA:HB3	1:A:252:ILE:HG22	1.99	0.43
1:A:223:TRP:CD1	1:A:248:SER:HA	2.54	0.43
1:A:277:LEU:CB	1:A:290:ALA:HB3	2.49	0.43
2:B:1164:GLN:HB3	2:B:1166:MET:HE2	2.00	0.43
1:A:317:ARG:HB3	1:A:318:THR:HG23	2.01	0.43
1:A:499:ASN:HB2	1:A:504:GLY:H	1.84	0.43
2:B:859:ASN:CG	2:B:862:SER:HB3	2.44	0.43
2:B:901:SER:CB	2:B:928:THR:HA	2.49	0.43
1:A:5:LEU:O	1:A:252:ILE:HA	2.19	0.42
1:A:200:VAL:HG12	1:A:201:VAL:HG23	2.01	0.42
1:A:266:PRO:HD3	1:A:280:MET:HE1	2.01	0.42
2:B:814:LEU:HD13	2:B:816:GLU:HG3	2.00	0.42
3:C:199:LEU:HD23	3:C:212:PRO:CA	2.47	0.42
1:A:518:GLY:O	1:A:528:TRP:HA	2.19	0.42
2:B:847:TRP:HH2	2:B:866:ARG:HD2	1.84	0.42
1:A:214:PHE:O	1:A:217:ILE:HD12	2.19	0.42
2:B:747:LEU:HD23	2:B:747:LEU:HA	1.93	0.42
1:A:297:LEU:HD12	1:A:303:THR:O	2.19	0.42
2:B:991:LYS:HE3	2:B:1000:PHE:HB3	2.01	0.42
2:B:1035:THR:O	2:B:1037:VAL:HG13	2.19	0.42
1:A:138:TRP:CD2	1:A:164:TRP:HA	2.55	0.42
1:A:205:LEU:HB3	1:A:206:PRO:HD3	2.01	0.42
1:A:228:ILE:H	1:A:244:SER:CB	2.33	0.42
1:A:564:VAL:O	1:A:565:HIS:HB2	2.19	0.42
2:B:1030:TRP:CE2	2:B:1039:ASN:HB3	2.54	0.42
1:A:291:CYS:SG	1:A:304:CYS:CB	3.05	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:MET:C	1:A:439:GLY:H	2.27	0.42
1:A:247:PHE:O	1:A:248:SER:HB3	2.20	0.42
1:A:379:VAL:CG1	1:A:383:ILE:HD11	2.50	0.42
1:A:276:HIS:ND1	1:A:304:CYS:HB2	2.34	0.42
1:A:454:ARG:CG	1:A:455:ALA:N	2.81	0.42
2:B:1002:VAL:HG22	2:B:1003:VAL:HG23	2.02	0.42
2:B:1161:ASP:HB3	2:B:1164:GLN:HB2	2.02	0.42
1:A:185:ASN:N	1:A:185:ASN:HD22	2.18	0.42
1:A:430:ARG:HE	1:A:430:ARG:HB3	1.68	0.42
1:A:517:PHE:CZ	1:A:528:TRP:HB2	2.54	0.42
1:A:600:GLU:O	1:A:608:CYS:HA	2.20	0.42
1:A:604:ASP:O	1:A:605:MET:HB2	2.19	0.42
2:B:684:LYS:NZ	2:B:705:ASP:O	2.50	0.42
1:A:77:SER:HB2	1:A:96:GLU:CD	2.45	0.41
1:A:229:LEU:N	1:A:229:LEU:HD12	2.34	0.41
2:B:805:LEU:O	2:B:817:SER:HA	2.20	0.41
2:B:1223:ASP:OD1	2:B:1223:ASP:N	2.52	0.41
1:A:208:PRO:HA	1:A:221:THR:O	2.20	0.41
1:A:378:VAL:HG12	1:A:379:VAL:HG23	2.02	0.41
1:A:12:LEU:HD11	1:A:48:TRP:HB3	2.02	0.41
1:A:220:TRP:CZ2	1:A:229:LEU:HD22	2.56	0.41
2:B:1072:TYR:CZ	2:B:1085:ARG:HD3	2.55	0.41
1:A:212:THR:CG2	1:A:219:TYR:HB2	2.49	0.41
1:A:591:LEU:C	1:A:591:LEU:HD12	2.46	0.41
2:B:635:LEU:HB2	2:B:880:LEU:CD2	2.50	0.41
2:B:1041:THR:HG22	2:B:1042:ARG:O	2.20	0.41
1:A:85:TRP:CD2	1:A:260:GLN:HB3	2.56	0.41
1:A:253:HIS:ND1	6:A:707:PO4:O3	2.52	0.41
1:A:575:GLU:O	1:A:576:GLU:C	2.64	0.41
1:A:259:ARG:HD2	1:A:259:ARG:HA	1.86	0.41
1:A:438:VAL:O	1:A:438:VAL:HG12	2.20	0.41
2:B:1066:PRO:HA	2:B:1088:LEU:HD11	2.02	0.41
1:A:503:THR:C	1:A:505:ARG:H	2.29	0.41
1:A:188:HIS:HB3	1:A:189:LYS:H	1.74	0.41
1:A:310:GLU:HB2	1:A:325:LEU:HD12	2.02	0.41
1:A:419:LYS:HZ2	1:A:419:LYS:HG2	1.77	0.41
2:B:838:LEU:HD12	2:B:846:TYR:O	2.21	0.41
2:B:1036:ASN:ND2	2:B:1058:ARG:HG2	2.35	0.41
1:A:487:TRP:HZ3	1:A:498:MET:HB2	1.85	0.40
4:E:1:NAG:O3	4:E:1:NAG:H83	2.21	0.40
1:A:16:ASP:OD2	1:A:19:ASN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:H	1:A:310:GLU:HG2	1.73	0.40
1:A:28:VAL:HG12	1:A:29:GLY:H	1.86	0.40
1:A:166:ASN:O	1:A:167:GLY:C	2.64	0.40
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.79	0.40
1:A:189:LYS:HE2	1:A:198:GLN:CD	2.47	0.40
1:A:311:LEU:HD12	1:A:324:SER:HA	2.02	0.40
1:A:567:VAL:HG13	1:A:568:ILE:N	2.37	0.40
2:B:959:LEU:HA	2:B:960:PRO:HD3	1.80	0.40
1:A:86:LEU:O	1:A:88:GLU:HG2	2.21	0.40
1:A:267:CYS:CB	1:A:278:CYS:HG	2.34	0.40
1:A:486:TYR:N	1:A:486:TYR:CD1	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	609/611 (100%)	505 (83%)	96 (16%)	8 (1%)	9	42
2	B	602/616 (98%)	559 (93%)	42 (7%)	1 (0%)	43	78
3	C	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
All	All	1283/1312 (98%)	1131 (88%)	143 (11%)	9 (1%)	20	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	VAL
1	A	543	SER
1	A	16	ASP
1	A	330	PHE
1	A	337	LEU
1	A	105	LEU

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Mol	Chain	Res	Type
1	A	331	THR
1	A	370	ILE
2	B	657	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/527 (100%)	483 (92%)	44 (8%)	10	30
2	B	529/538 (98%)	510 (96%)	19 (4%)	31	52
3	C	66/74 (89%)	64 (97%)	2 (3%)	36	57
All	All	1122/1139 (98%)	1057 (94%)	65 (6%)	20	40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	105	LEU
1	A	168	LEU
1	A	170	LEU
1	A	193	ASP
1	A	196	ASN
1	A	202	LYS
1	A	237	GLU
1	A	300	ASN
1	A	310	GLU
1	A	317	ARG
1	A	333	ILE
1	A	334	VAL
1	A	336	GLN
1	A	360	ASP
1	A	368	SER
1	A	371	ASP
1	A	389	ILE
1	A	403	THR

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Mol	Chain	Res	Type
1	A	407	ARG
1	A	412	ARG
1	A	414	ASN
1	A	422	ILE
1	A	424	GLU
1	A	428	GLU
1	A	433	VAL
1	A	441	MET
1	A	444	THR
1	A	449	ILE
1	A	462	ARG
1	A	464	VAL
1	A	482	GLU
1	A	485	ILE
1	A	494	LYS
1	A	495	ILE
1	A	497	VAL
1	A	534	ARG
1	A	537	GLU
1	A	541	LYS
1	A	545	GLU
1	A	552	GLN
1	A	567	VAL
1	A	580	CYS
1	A	595	CYS
2	B	634	LEU
2	B	672	THR
2	B	683	LEU
2	B	696	LEU
2	B	739	ARG
2	B	787	VAL
2	B	797	THR
2	B	814	LEU
2	B	880	LEU
2	B	967	VAL
2	B	1002	VAL
2	B	1004	VAL
2	B	1040	VAL
2	B	1062	ILE
2	B	1096	LEU
2	B	1125	ARG
2	B	1128	SER

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Mol	Chain	Res	Type
2	B	1131	LEU
2	B	1197	LEU
3	C	214	LEU
3	C	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	166	ASN
1	A	185	ASN
1	A	196	ASN
1	A	198	GLN
1	A	258	GLN
1	A	271	ASN
1	A	288	GLN
1	A	300	ASN
1	A	336	GLN
1	A	499	ASN
1	A	563	ASN
2	B	738	HIS
2	B	813	ASN
2	B	899	HIS
2	B	902	HIS
2	B	986	GLN
2	B	1200	GLN
3	C	248	GLN
3	C	266	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

11 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	D	1	4,1	14,14,15	0.75	0	17,19,21	0.81	0
4	NAG	D	2	4	14,14,15	0.70	0	17,19,21	0.69	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.69	0	17,19,21	0.68	0
4	NAG	E	2	4	14,14,15	0.81	0	17,19,21	0.63	0
4	NAG	F	1	4,1	14,14,15	0.83	0	17,19,21	1.20	2 (11%)
4	NAG	F	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.66	0
5	NAG	G	1	5,2	14,14,15	0.50	0	17,19,21	0.65	0
5	NAG	G	2	5	14,14,15	0.47	0	17,19,21	0.69	0
5	FUC	G	3	5	10,10,11	0.65	0	14,14,16	0.62	0
4	NAG	H	1	2,4	14,14,15	0.51	0	17,19,21	1.31	1 (5%)
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	0.71	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	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	6/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
4	NAG	H	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	2.49	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C4-C3-C2	3.71	116.46	111.02
4	H	1	NAG	C1-O5-C5	3.27	116.57	112.19
4	D	2	NAG	C2-N2-C7	-2.24	119.90	122.90
4	F	1	NAG	C2-N2-C7	-2.17	120.00	122.90

There are no chirality outliers.

All (27) torsion outliers are listed below:

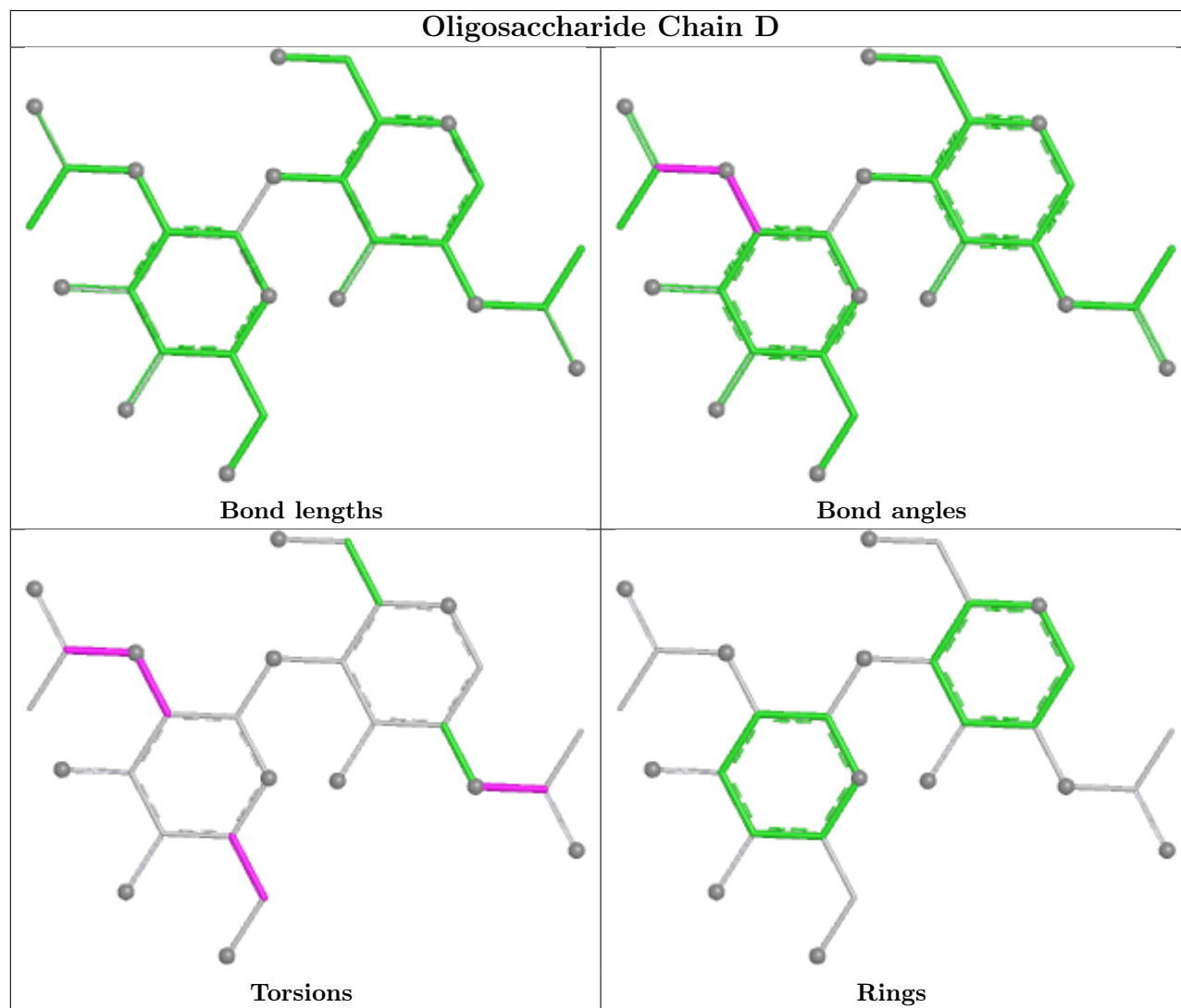
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C3-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6

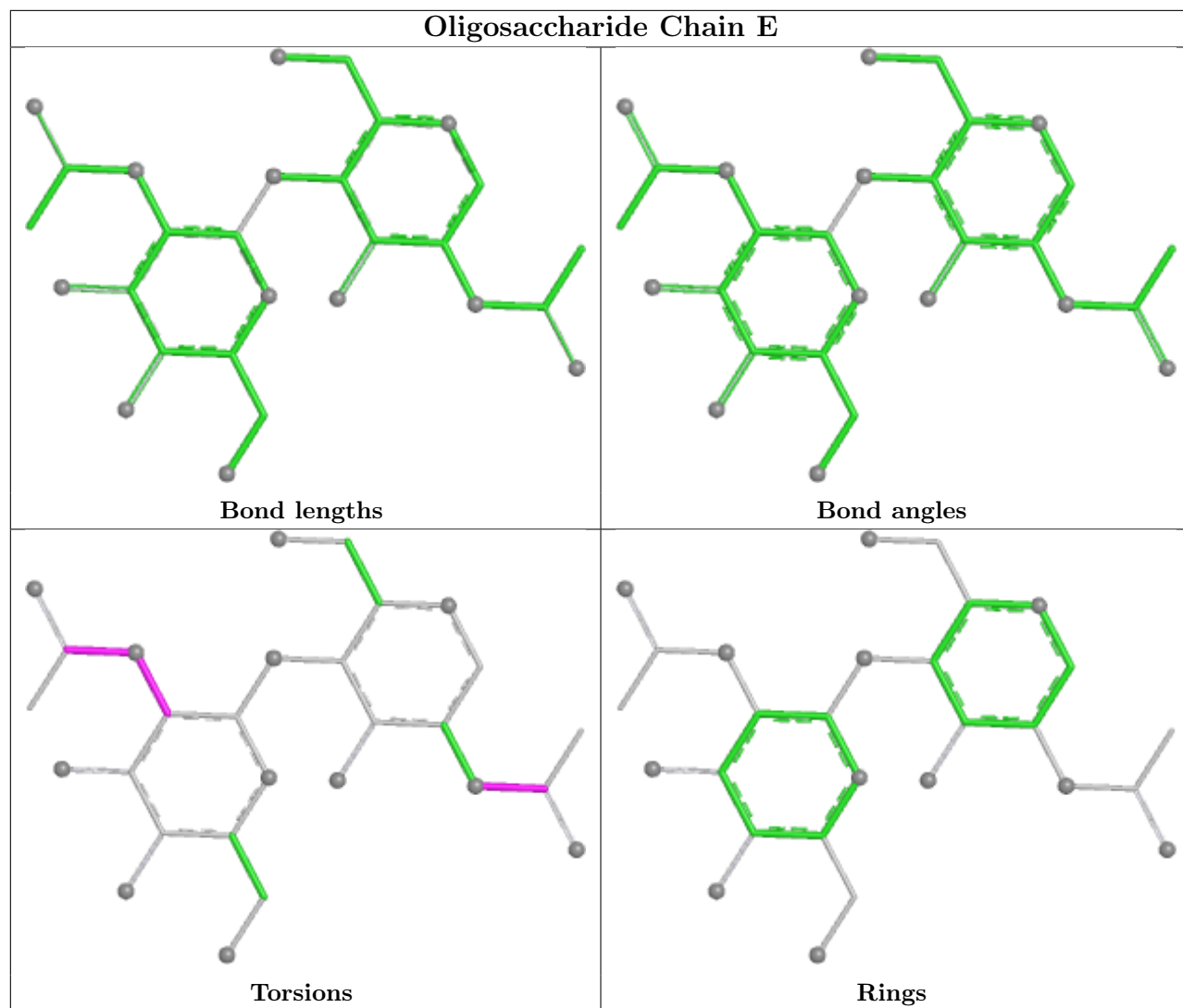
There are no ring outliers.

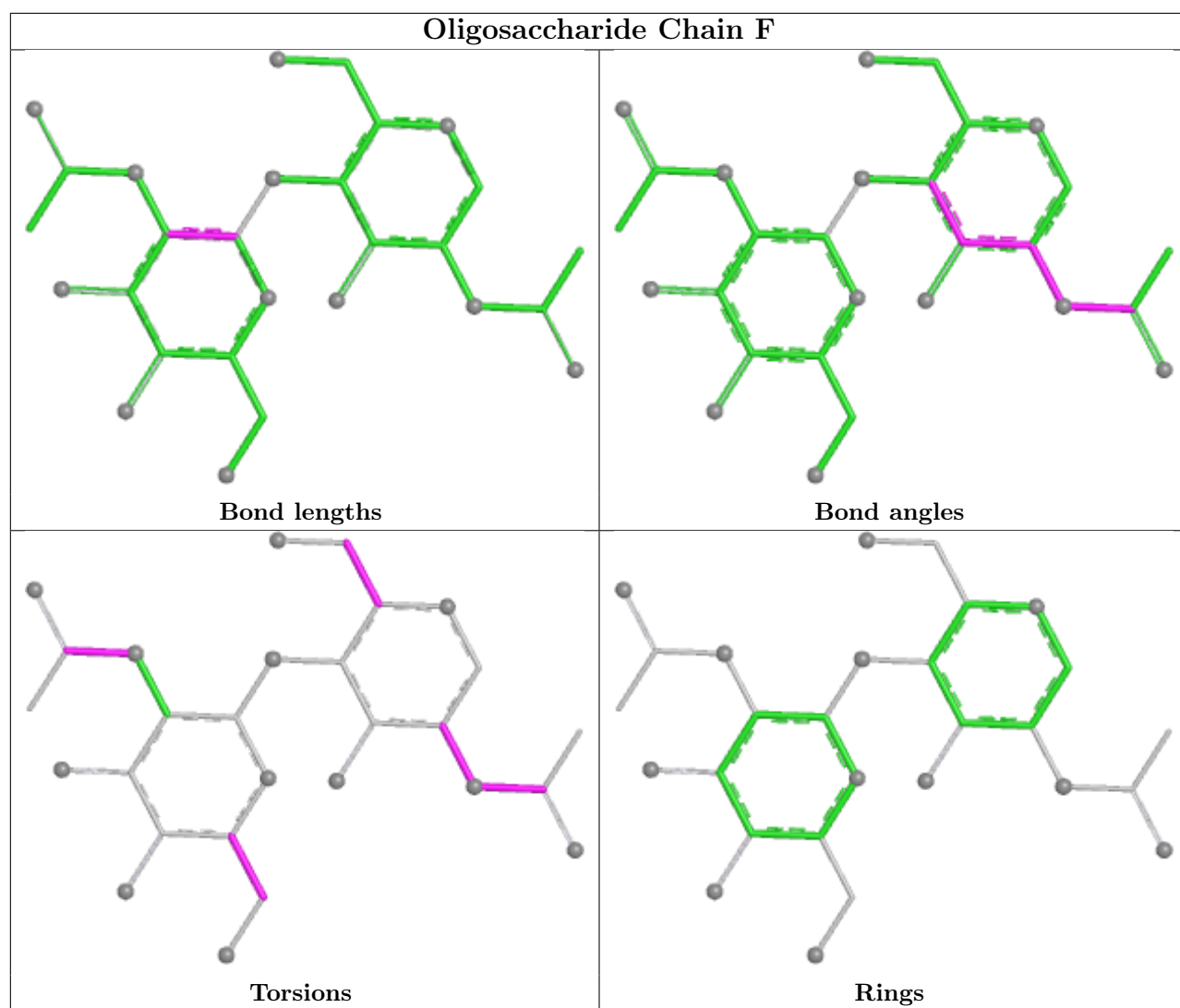
4 monomers are involved in 4 short contacts:

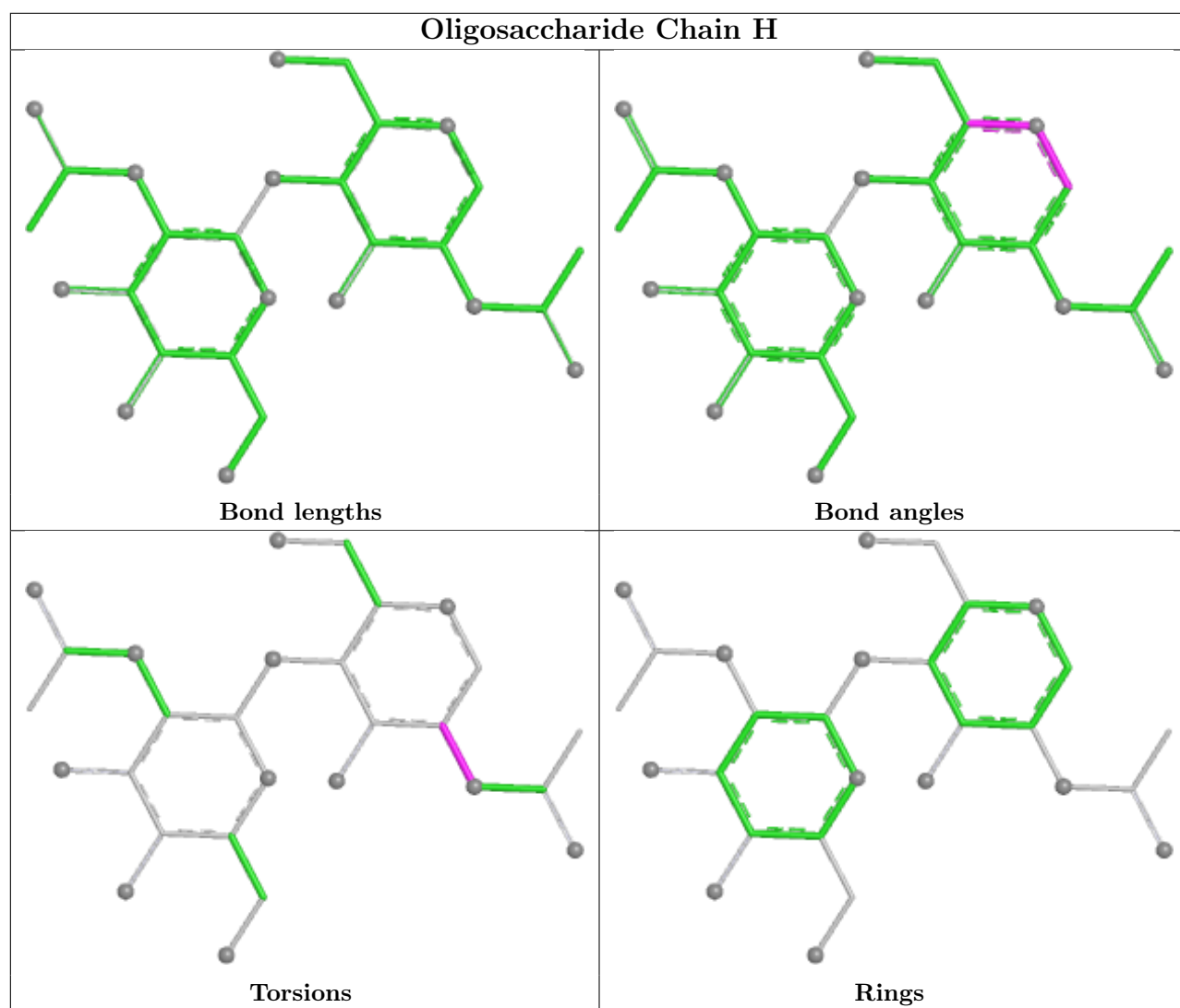
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	F	2	NAG	1	0
4	E	1	NAG	2	0
4	F	1	NAG	1	0

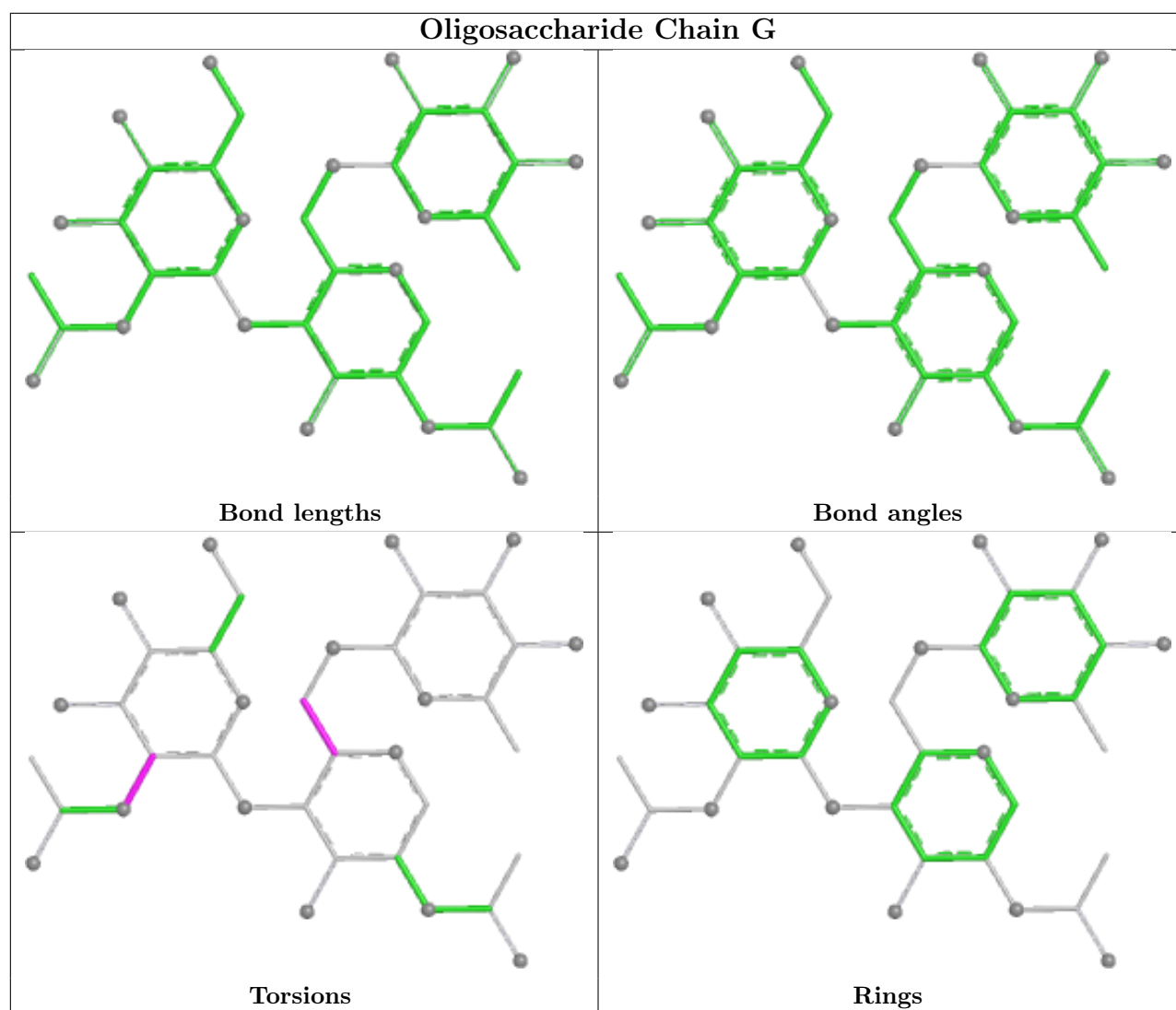
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z > 2$
6	PO4	A	708	-	4,4,4	1.67	0	6,6,6	0.45	0
7	NAG	B	1304	2	14,14,15	0.47	0	17,19,21	0.86	0
7	NAG	B	1306	2	14,14,15	0.49	0	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	1309	-	5,5,5	0.40	0	5,5,5	0.24	0
6	PO4	A	707	-	4,4,4	1.64	1 (25%)	6,6,6	0.46	0
7	NAG	B	1305	2	14,14,15	0.45	0	17,19,21	0.93	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1304	2	-	3/6/23/26	0/1/1/1
7	NAG	B	1305	2	-	2/6/23/26	0/1/1/1
7	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
8	GOL	B	1309	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	707	PO4	P-O2	-2.06	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1306	NAG	C1-O5-C5	2.15	115.07	112.19
7	B	1305	NAG	C2-N2-C7	2.07	125.67	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1304	NAG	C3-C2-N2-C7
7	B	1305	NAG	C3-C2-N2-C7
7	B	1304	NAG	O5-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	B	1306	NAG	C8-C7-N2-C2
7	B	1306	NAG	O7-C7-N2-C2
7	B	1305	NAG	O5-C5-C6-O6
8	B	1309	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	NAG	1	0
6	A	707	PO4	1	0
7	B	1305	NAG	1	0

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.

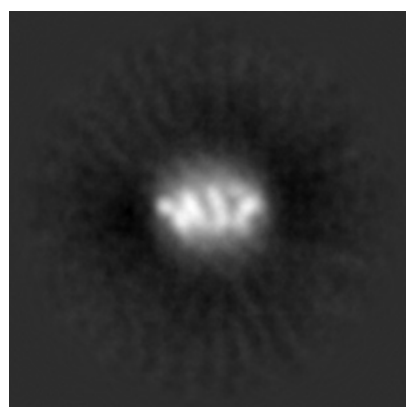
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9501. These allow visual inspection of the internal detail of the map and identification of artifacts.

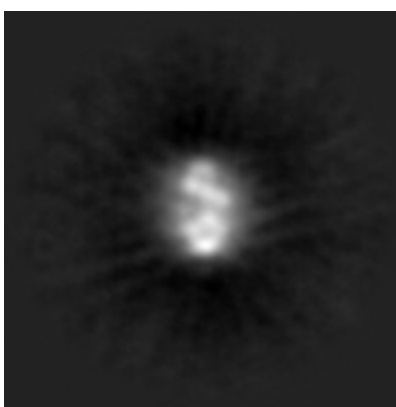
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

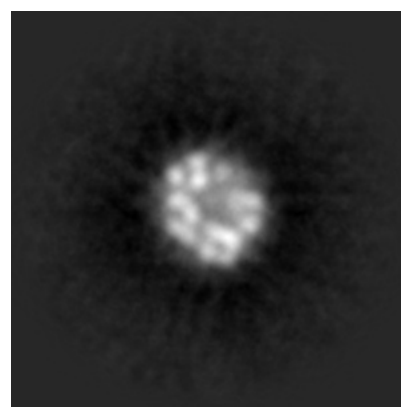
6.1.1 Primary map



X



Y

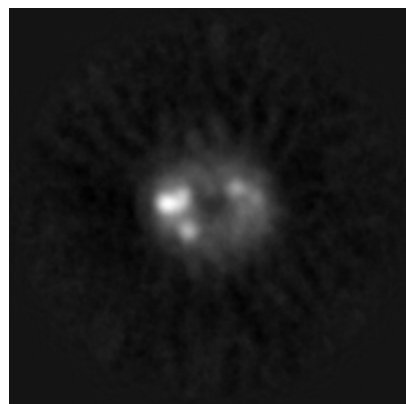


Z

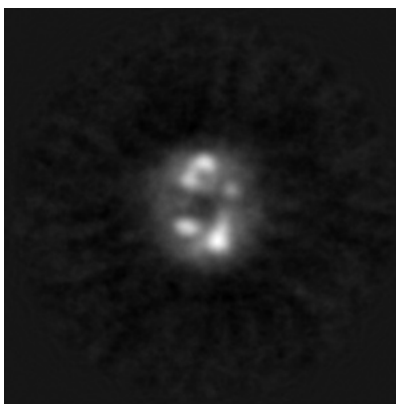
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

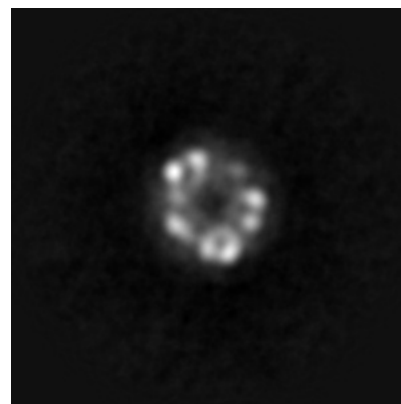
6.2.1 Primary map



X Index: 100



Y Index: 100

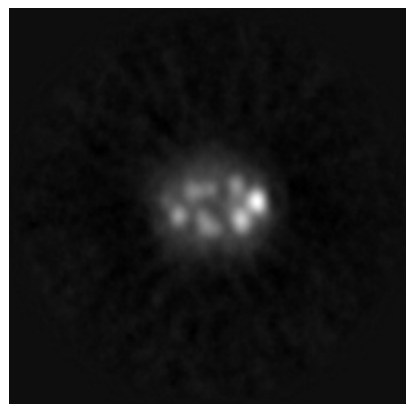


Z Index: 100

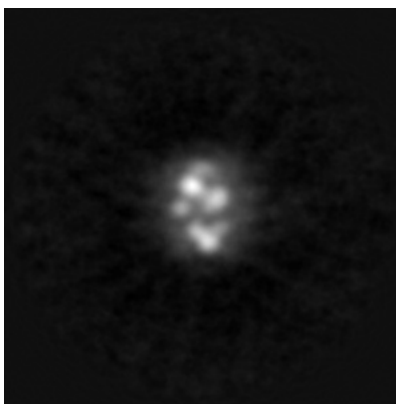
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

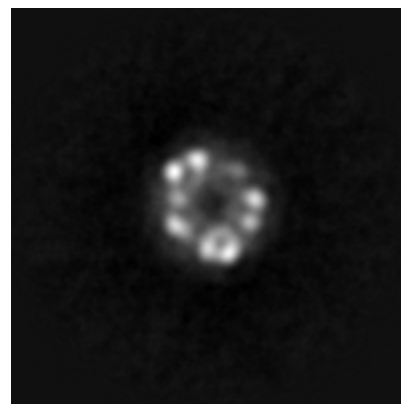
6.3.1 Primary map



X Index: 92



Y Index: 88



Z Index: 101

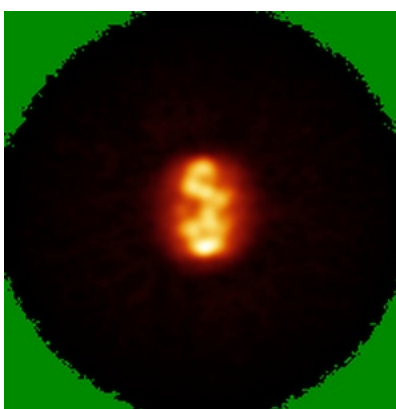
The images above show the largest variance slices of the map in three orthogonal directions.

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

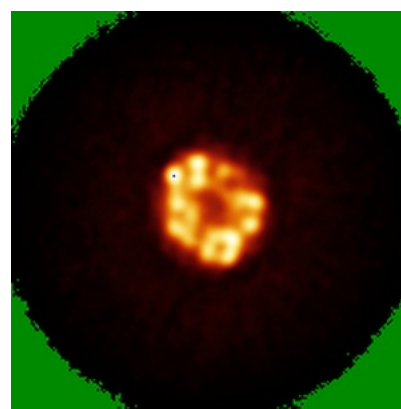
6.4.1 Primary map



X



Y

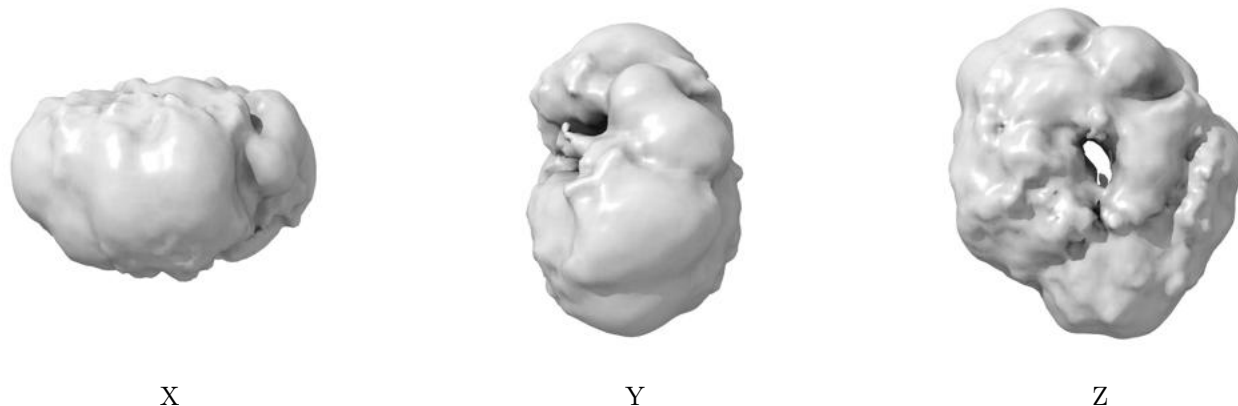


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

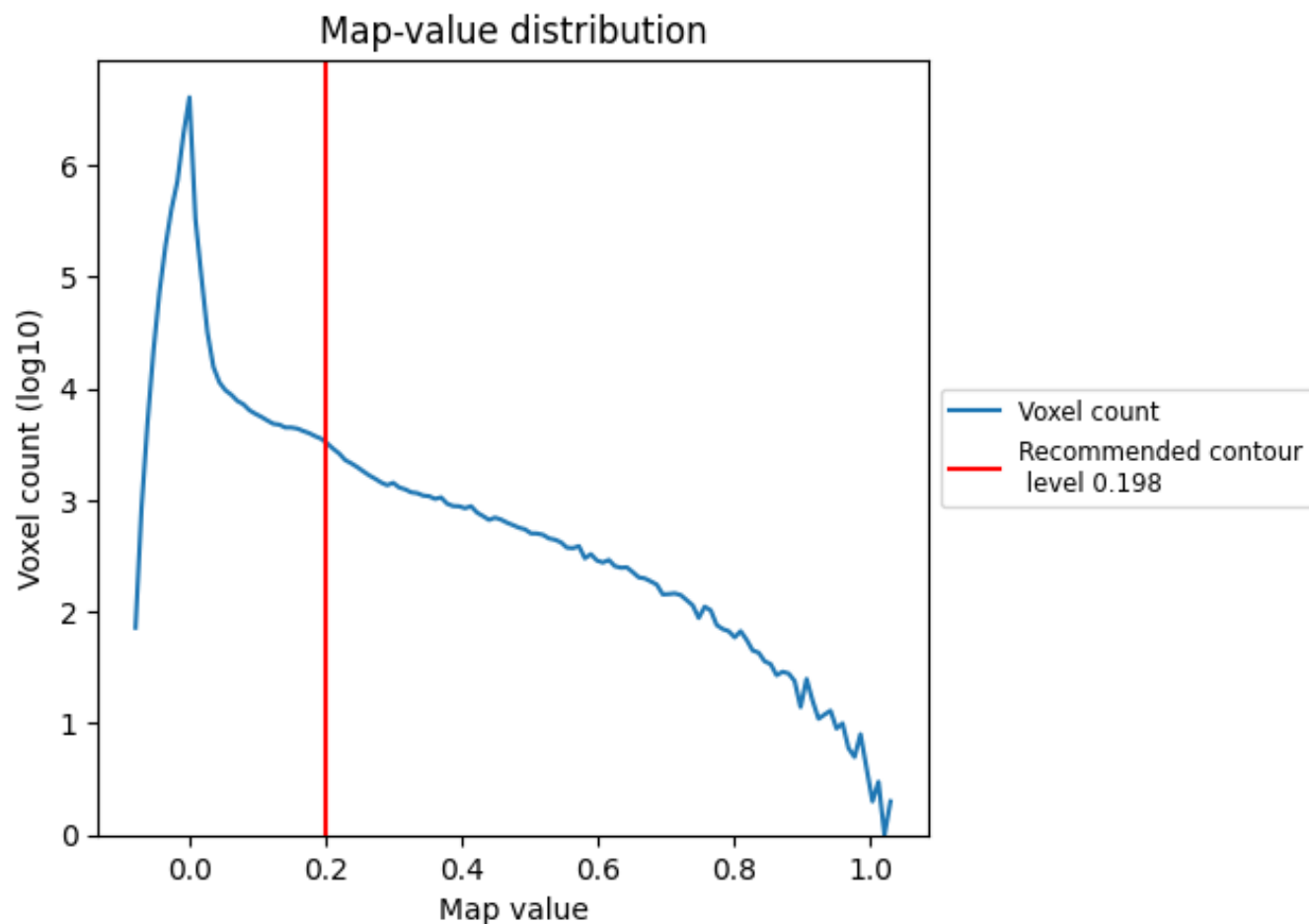
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

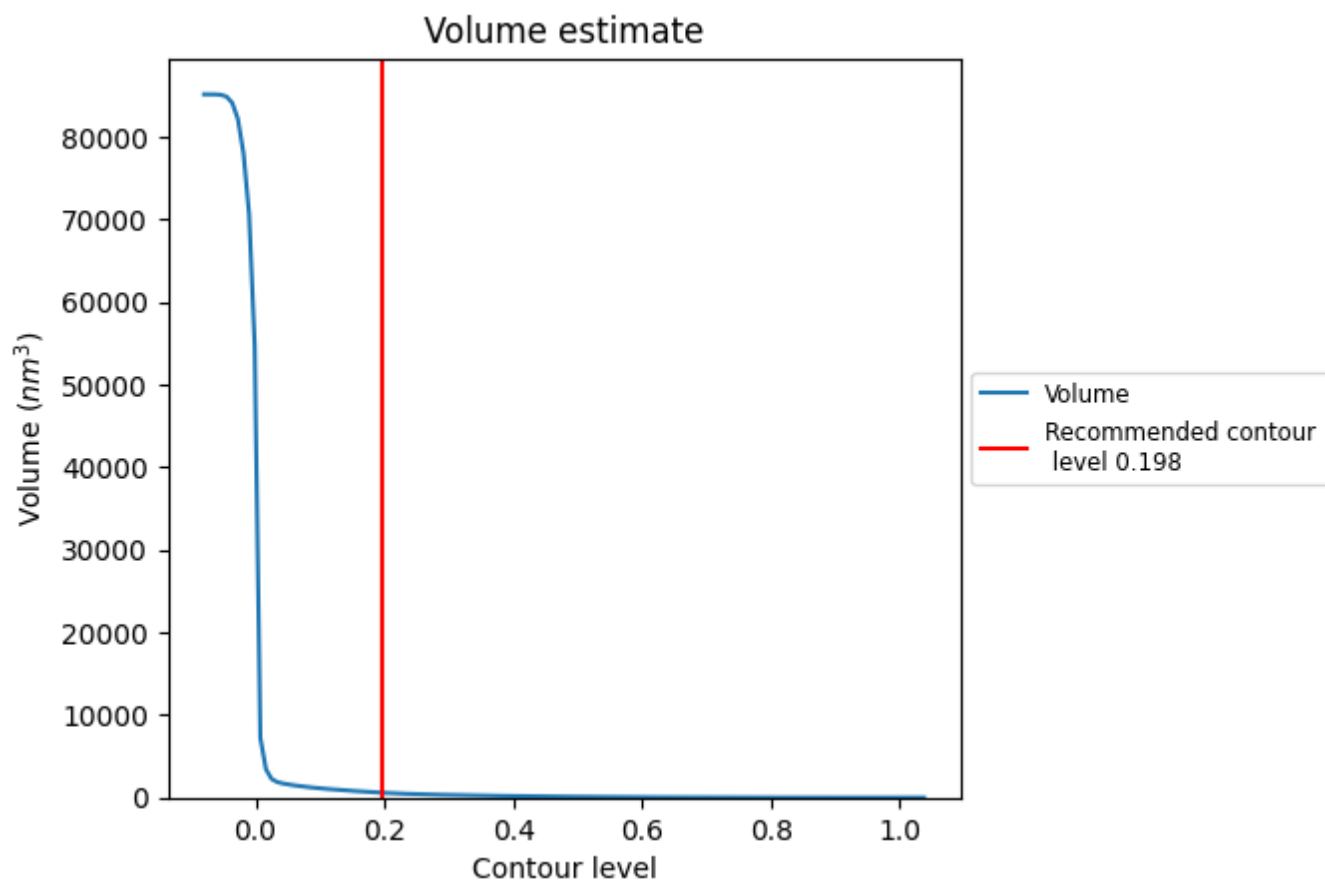
This section contains the results of statistical analysis of the map.

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.

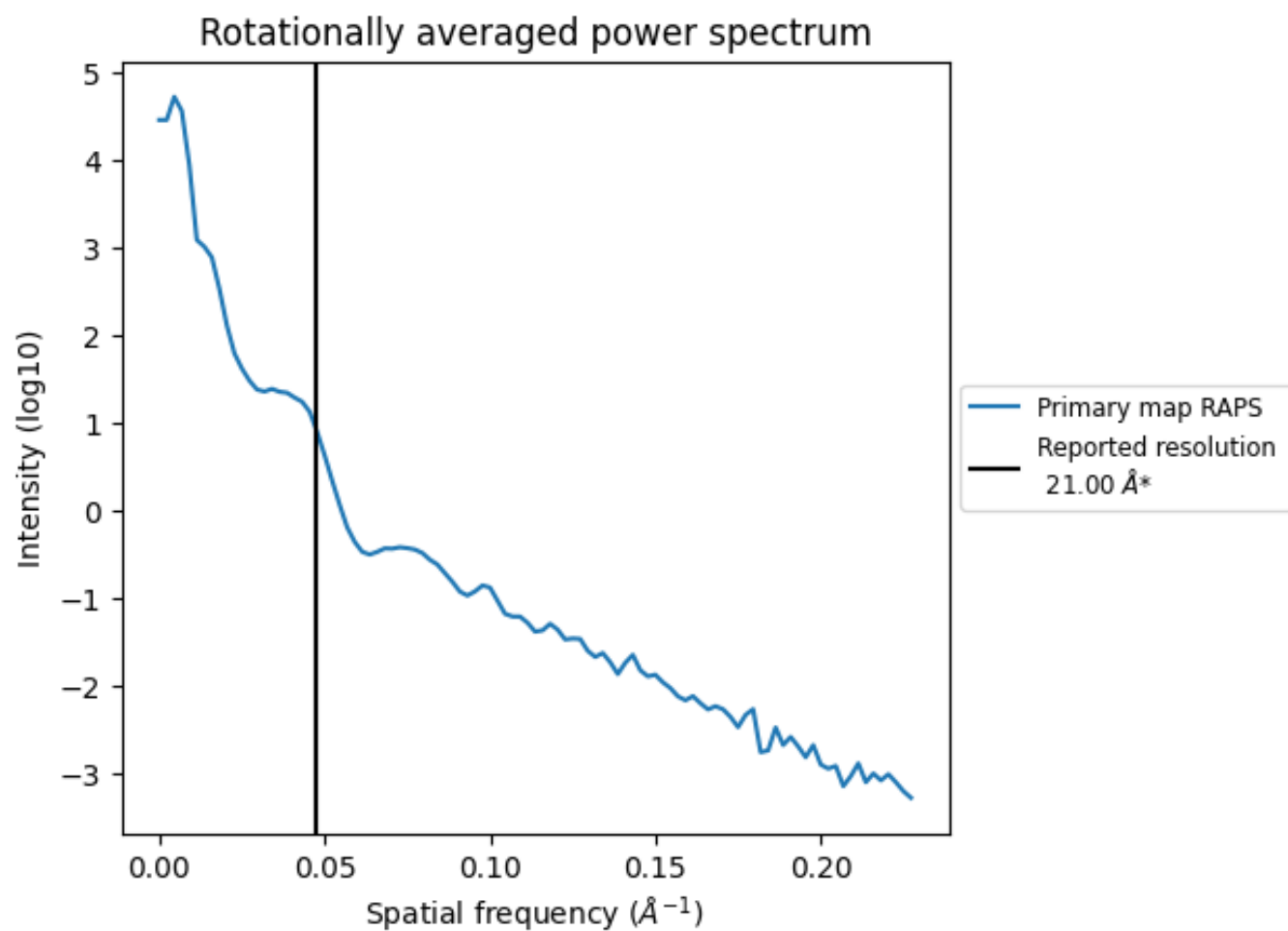
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 580 nm^3 ; this corresponds to an approximate mass of 524 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 0.048 $\text{\AA}^{-1}$

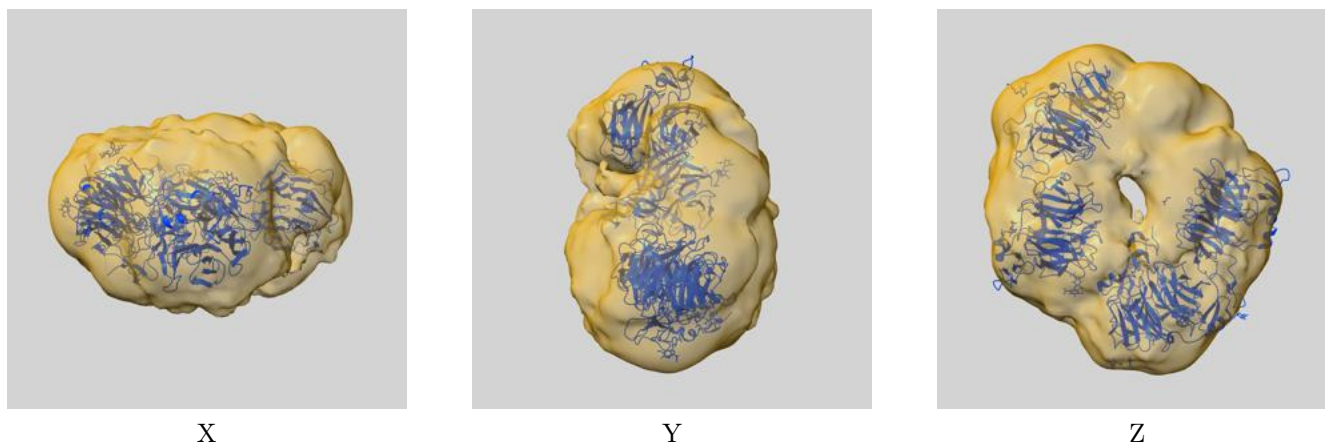
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

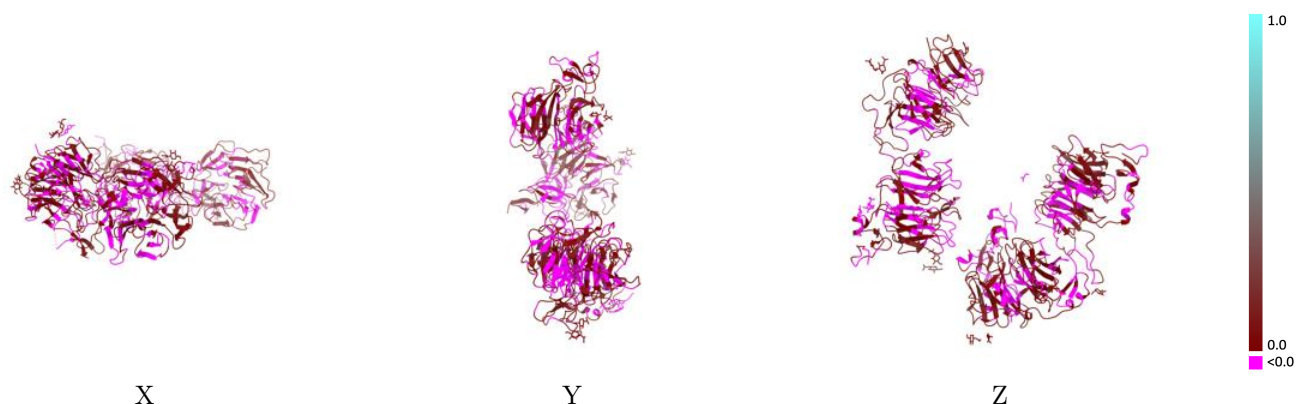
This section contains information regarding the fit between EMDB map EMD-9501 and PDB model 5GJE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



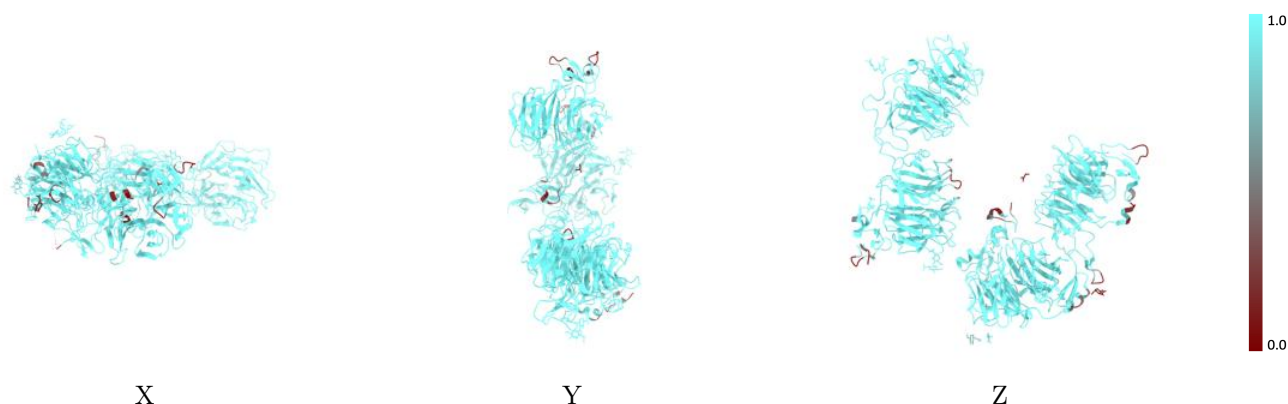
The images above show the 3D surface view of the map at the recommended contour level 0.198 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



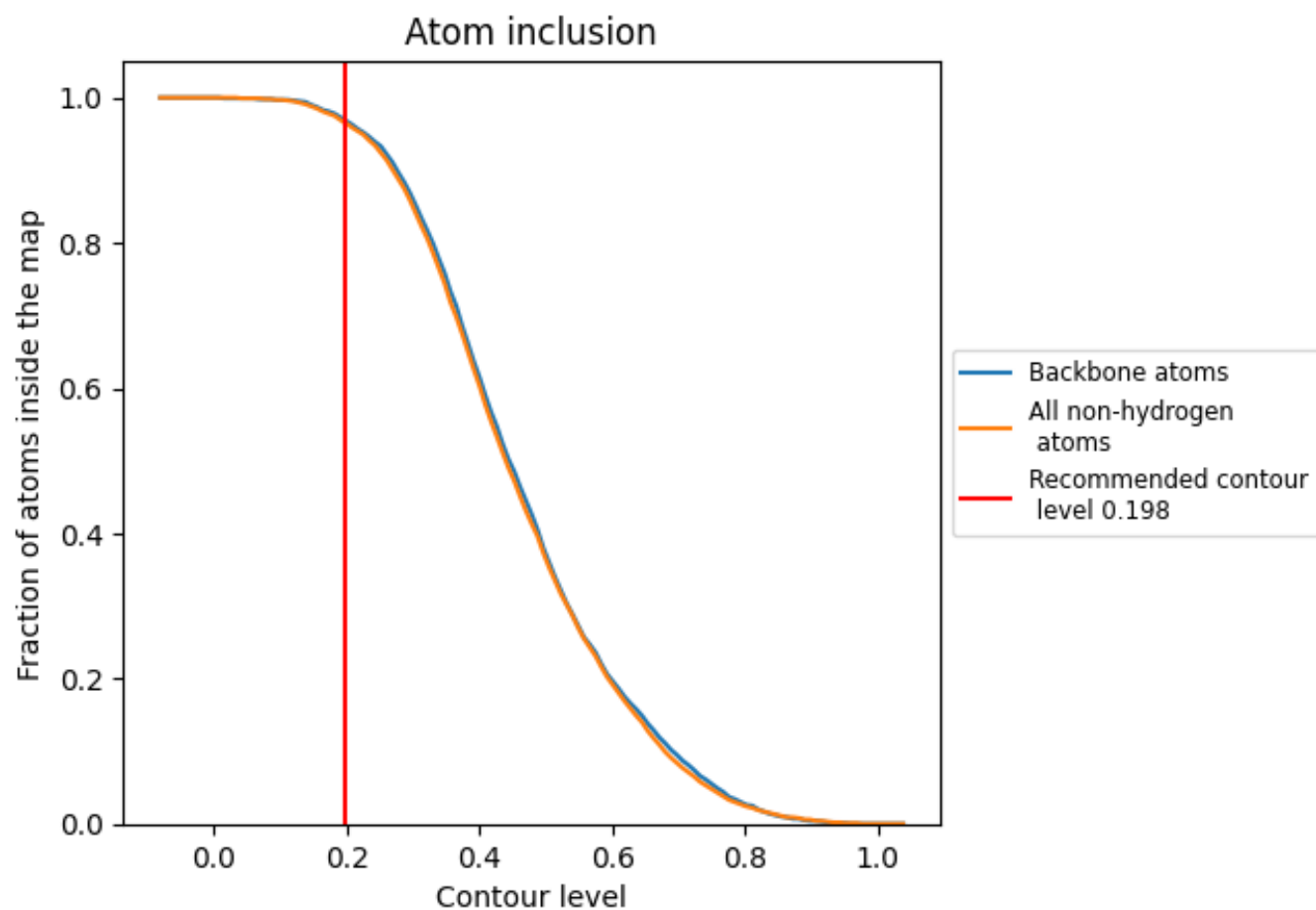
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.198).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.0270
A	0.9760	0.0280
B	0.9620	0.0300
C	0.9080	0.0010
D	0.9640	0.0480
E	1.0000	0.1780
F	1.0000	-0.0610
G	1.0000	-0.0050
H	1.0000	0.0410

1.0

0.0

<0.0