Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 07:01 PM JST

PDB ID	:	7DD6
EMDB ID	:	EMD-30645
Title	:	Structure of Ca2+/L-Trp-bonnd Calcium-Sensing Receptor in active state
Authors	:	Wen, T.L.; Yang, X.; Shen, Y.Q.
Deposited on	:	2020-10-27
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

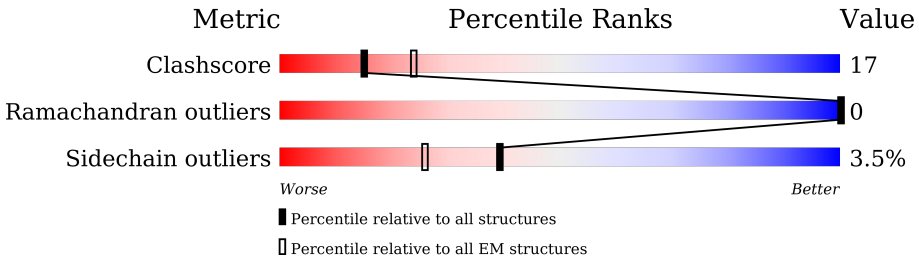
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1069	51% 22% 26%
1	B	1069	53% 21% 26%
2	C	2	50% 50%
2	D	2	100%
2	E	2	50% 50%
2	F	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12678 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 Calcium-sensing Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	791	Total 6209	C 4031	N 1003	O 1140	S 35	0	0
1	B	792	Total 6235	C 4048	N 1007	O 1145	S 35	0	0

- Molecule 2 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
2	C	2	Total 28	C 16	N 2	O 10	0	0
2	D	2	Total 28	C 16	N 2	O 10	0	0
2	E	2	Total 28	C 16	N 2	O 10	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0

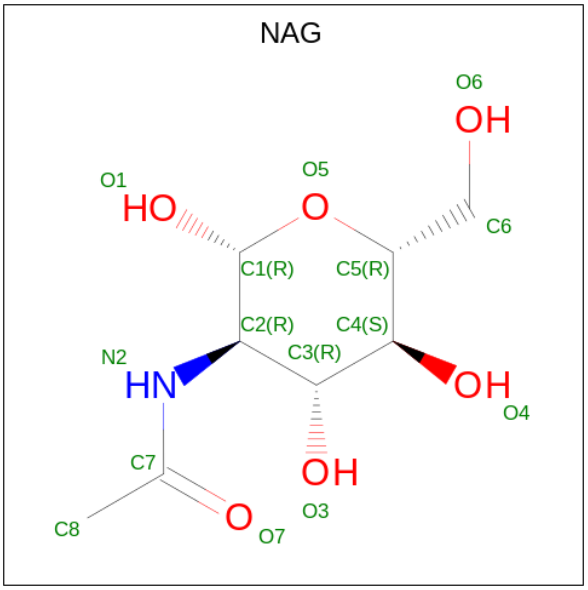
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Cl 1	0
3	B	1	Total 1	Cl 1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

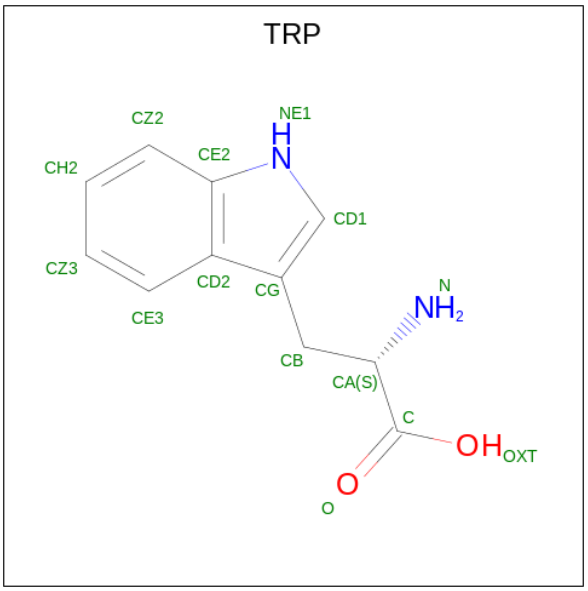
Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total Ca 3 3	0
4	B	3	Total Ca 3 3	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 42 24 3 15	0
5	A	1	Total C N O 42 24 3 15	0
5	A	1	Total C N O 42 24 3 15	0
5	B	1	Total C N O 42 24 3 15	0
5	B	1	Total C N O 42 24 3 15	0
5	B	1	Total C N O 42 24 3 15	0

- Molecule 6 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



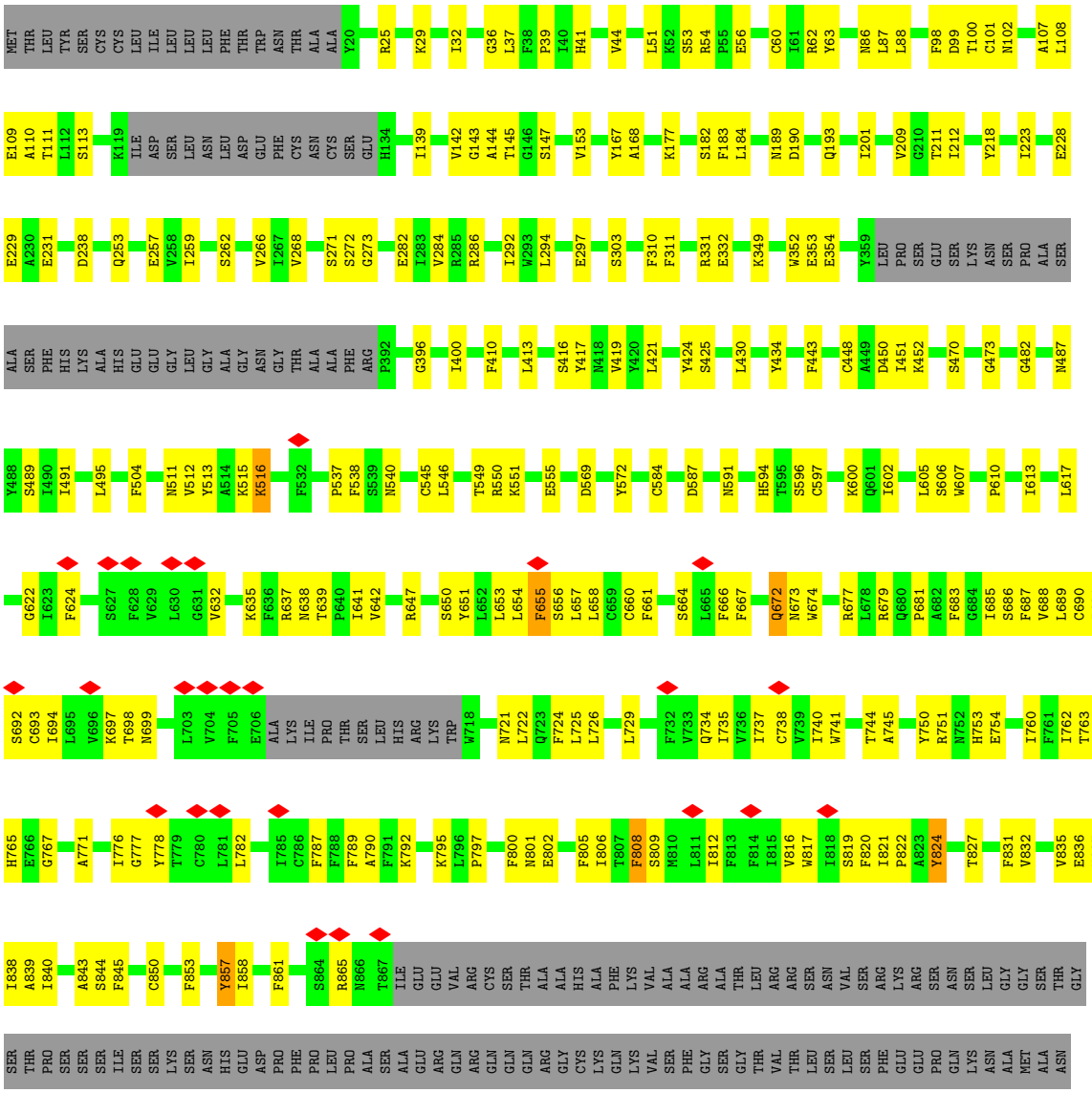
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	11	2	2	
6	B	1	Total	C	N	O	0
			15	11	2	2	

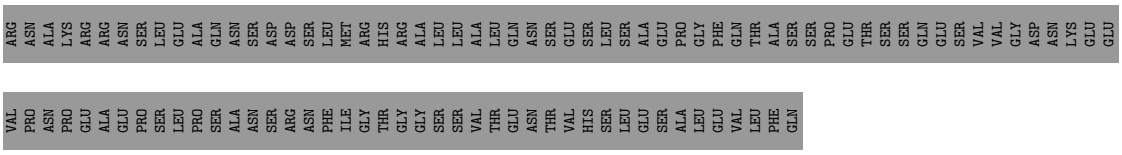
3 Residue-property plots (i)

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: Calcium-sensing Receptor

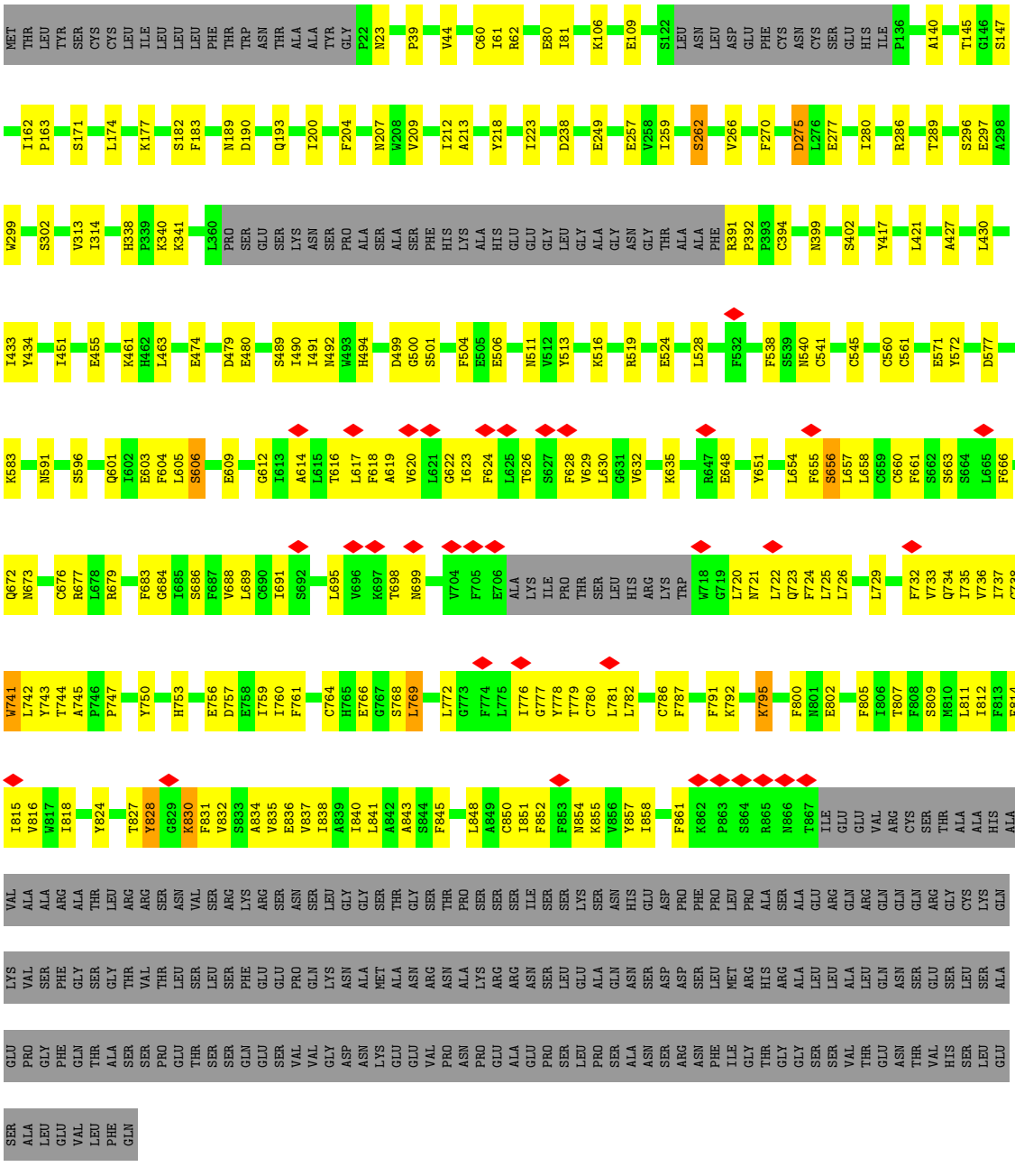
Chain A:





• Molecule 1: Calcium-sensing Receptor

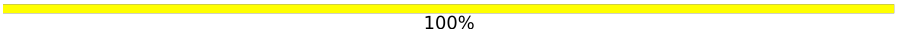
Chain B:



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

Chain C:

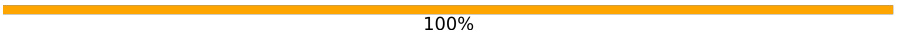
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

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

Chain E: 

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

Chain F: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.136	Depositor
Minimum map value	-1.794	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	283.92, 283.92, 283.92	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, NAG

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	0.40	0/6368	0.50	0/8648
1	B	0.40	0/6395	0.50	0/8683
All	All	0.40	0/12763	0.50	0/17331

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

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	6209	0	6018	207	0
1	B	6235	0	6055	206	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	42	0	39	0	0
6	A	15	0	9	1	0
6	B	15	0	9	1	0
All	All	12678	0	12269	412	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 17.

All (412) 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:B:623:ILE:CD1	1:B:661:PHE:HB3	1.50	1.38
1:A:827:THR:HG23	1:A:832:VAL:CG2	1.64	1.27
1:B:623:ILE:HD11	1:B:661:PHE:CB	1.63	1.26
1:A:60:CYS:SG	1:A:101:CYS:HB3	1.75	1.25
1:A:60:CYS:SG	1:A:101:CYS:CB	2.24	1.25
1:B:800:PHE:CE2	1:B:858:ILE:HG21	1.72	1.25
1:A:827:THR:CG2	1:A:832:VAL:CG2	2.24	1.15
1:A:545:CYS:SG	1:A:549:THR:HG21	1.87	1.15
1:B:827:THR:CG2	1:B:831:PHE:HB2	1.77	1.14
1:B:671:PRO:HB3	1:B:676:CYS:SG	1.88	1.13
1:B:623:ILE:CD1	1:B:661:PHE:CB	2.22	1.11
1:B:626:THR:O	1:B:629:VAL:HG12	1.48	1.11
1:A:685:ILE:O	1:A:689:LEU:HD13	1.50	1.10
1:A:751:ARG:HG2	1:A:762:ILE:HG12	1.28	1.08
1:A:827:THR:CG2	1:A:832:VAL:HG23	1.81	1.08
1:B:430:LEU:O	1:B:433:ILE:HG22	1.51	1.08
1:A:763:THR:HG22	1:A:764:CYS:H	1.21	1.05
1:B:827:THR:HG21	1:B:831:PHE:HB2	1.03	1.02
1:B:827:THR:HG21	1:B:831:PHE:CB	1.89	1.02
1:A:168:ALA:O	6:A:1108:TRP:HB2	1.59	1.01
1:B:541:CYS:HB3	1:B:561:CYS:HB3	1.42	0.99
1:A:827:THR:CG2	1:A:832:VAL:HG22	1.93	0.99
1:B:430:LEU:O	1:B:433:ILE:CG2	2.13	0.96
1:B:741:TRP:HZ2	1:B:768:SER:H	1.14	0.95
1:A:546:LEU:O	1:A:549:THR:HG22	1.66	0.95
1:B:855:LYS:HA	1:B:858:ILE:HG12	1.48	0.94
1:B:800:PHE:HE2	1:B:858:ILE:HG21	1.28	0.93
1:A:722:LEU:O	1:A:725:LEU:HB3	1.69	0.92
1:A:827:THR:HG23	1:A:832:VAL:HG23	0.92	0.92
1:A:417:TYR:CZ	1:A:421:LEU:HD11	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CE1	1:A:836:GLU:HA	2.03	0.91
1:A:763:THR:HG22	1:A:764:CYS:N	1.85	0.91
1:A:569:ASP:OD1	1:A:594:HIS:HE1	1.52	0.91
1:A:687:PHE:CE1	1:A:691:ILE:HD11	2.06	0.91
1:B:800:PHE:CE2	1:B:858:ILE:HD13	2.07	0.90
1:A:569:ASP:OD1	1:A:594:HIS:CE1	2.25	0.89
1:B:626:THR:O	1:B:629:VAL:CG1	2.20	0.88
1:B:800:PHE:HE2	1:B:858:ILE:HD13	1.39	0.87
1:A:60:CYS:HG	1:A:101:CYS:CB	1.77	0.87
1:A:417:TYR:O	1:A:421:LEU:HD13	1.75	0.85
1:B:832:VAL:O	1:B:835:VAL:HG12	1.78	0.83
1:B:800:PHE:CE2	1:B:858:ILE:CG2	2.60	0.83
1:B:541:CYS:CB	1:B:561:CYS:HB3	2.07	0.83
1:A:857:TYR:O	1:A:861:PHE:HB2	1.77	0.82
1:B:430:LEU:C	1:B:433:ILE:HG22	2.00	0.82
1:A:685:ILE:O	1:A:689:LEU:CD1	2.28	0.82
1:B:800:PHE:HE2	1:B:858:ILE:CD1	1.92	0.81
1:B:741:TRP:CH2	1:B:766:GLU:CB	2.64	0.81
1:A:687:PHE:CZ	1:A:691:ILE:HD11	2.14	0.80
1:A:545:CYS:SG	1:A:549:THR:CG2	2.69	0.79
1:A:763:THR:CG2	1:A:764:CYS:H	1.94	0.79
1:B:855:LYS:O	1:B:858:ILE:HG12	1.82	0.79
1:B:619:ALA:O	1:B:623:ILE:HG12	1.83	0.79
1:B:855:LYS:CA	1:B:858:ILE:HG12	2.15	0.77
1:B:854:ASN:O	1:B:858:ILE:HG23	1.85	0.77
1:A:60:CYS:SG	1:A:101:CYS:HB2	2.24	0.76
1:A:193:GLN:HE22	1:A:297:GLU:HB2	1.49	0.76
1:A:687:PHE:CE1	1:A:691:ILE:CD1	2.68	0.76
1:B:630:LEU:HD23	1:B:654:LEU:HD13	1.67	0.76
1:A:734:GLN:NE2	1:A:778:TYR:HD2	1.85	0.74
1:A:827:THR:HG21	1:A:832:VAL:HA	1.69	0.74
1:B:213:ALA:HB2	1:B:223:ILE:HG13	1.68	0.74
1:A:683:PHE:CE1	1:A:840:ILE:HB	2.22	0.74
1:A:32:ILE:HG23	1:A:139:ILE:HD13	1.68	0.74
1:A:642:VAL:HG23	1:A:865:ARG:CB	2.18	0.73
1:B:417:TYR:CE2	1:B:421:LEU:HD11	2.24	0.72
1:A:44:VAL:HA	1:A:60:CYS:HA	1.71	0.72
1:A:683:PHE:CZ	1:A:840:ILE:HG22	2.24	0.72
1:B:417:TYR:O	1:B:421:LEU:HD13	1.89	0.72
1:B:741:TRP:CE2	1:B:768:SER:HB3	2.26	0.71
1:B:800:PHE:CE2	1:B:858:ILE:CD1	2.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:VAL:HG21	1:A:843:ALA:HB2	1.73	0.70
1:A:513:TYR:HE2	2:C:1:NAG:HN2	1.38	0.70
1:B:623:ILE:HD11	1:B:661:PHE:HB3	0.73	0.70
1:A:413:LEU:HB3	1:A:416:SER:OG	1.91	0.70
1:B:741:TRP:NE1	1:B:768:SER:HB3	2.07	0.70
1:B:698:THR:HG22	1:B:699:ASN:N	2.07	0.70
1:B:855:LYS:HA	1:B:858:ILE:CG1	2.22	0.70
1:A:184:LEU:CD2	1:A:482:GLY:HA2	2.22	0.70
1:B:623:ILE:HD13	1:B:661:PHE:CB	2.20	0.70
1:A:189:ASN:OD1	1:A:190:ASP:N	2.25	0.69
1:A:656:SER:OG	1:A:690:CYS:SG	2.46	0.69
1:A:820:PHE:HE1	1:A:836:GLU:HA	1.57	0.69
1:B:827:THR:HG22	1:B:828:TYR:O	1.93	0.69
1:B:511:ASN:ND2	2:E:1:NAG:O5	2.26	0.69
1:A:751:ARG:HG2	1:A:762:ILE:CG1	2.15	0.68
1:A:253:GLN:NE2	1:A:282:GLU:OE2	2.26	0.68
1:A:683:PHE:CE1	1:A:840:ILE:CG2	2.78	0.67
1:A:253:GLN:OE1	1:A:286:ARG:NH1	2.26	0.67
1:B:541:CYS:SG	1:B:561:CYS:HB3	2.35	0.67
1:B:673:ASN:O	1:B:677:ARG:HB2	1.95	0.67
1:B:630:LEU:CD2	1:B:654:LEU:HD13	2.23	0.67
1:A:417:TYR:CE1	1:A:421:LEU:HD11	2.28	0.66
1:B:855:LYS:O	1:B:858:ILE:CG1	2.43	0.66
1:B:741:TRP:HH2	1:B:766:GLU:CB	2.05	0.66
1:A:737:ILE:O	1:A:740:ILE:HB	1.95	0.66
1:A:790:ALA:HB1	1:A:806:ILE:CD1	2.25	0.66
1:B:698:THR:HG22	1:B:699:ASN:H	1.60	0.66
1:A:683:PHE:HE1	1:A:840:ILE:HB	1.61	0.66
1:B:623:ILE:CD1	1:B:661:PHE:HB2	2.22	0.65
1:B:683:PHE:CE1	1:B:840:ILE:CG2	2.80	0.65
1:B:809:SER:OG	1:B:850:CYS:SG	2.49	0.65
1:B:189:ASN:OD1	1:B:190:ASP:N	2.30	0.65
1:B:193:GLN:HE22	1:B:297:GLU:HB2	1.62	0.65
1:B:147:SER:OG	6:B:1108:TRP:O	2.15	0.64
1:A:827:THR:HG22	1:A:832:VAL:HG22	1.79	0.64
1:A:820:PHE:CE1	1:A:835:VAL:HG12	2.33	0.63
1:B:671:PRO:HB3	1:B:676:CYS:HG	1.58	0.63
1:A:44:VAL:HG12	1:A:60:CYS:SG	2.38	0.63
1:A:591:ASN:ND2	1:A:596:SER:O	2.31	0.63
1:B:855:LYS:C	1:B:858:ILE:HG12	2.18	0.63
1:A:332:GLU:OE1	1:A:332:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:VAL:HG12	1:B:266:VAL:HB	1.82	0.62
1:B:571:GLU:HG2	1:B:583:LYS:HG2	1.82	0.62
1:B:683:PHE:CE1	1:B:840:ILE:HG22	2.35	0.62
1:A:602:ILE:HA	1:A:760:ILE:HG22	1.80	0.62
1:A:417:TYR:CE2	1:A:421:LEU:HD11	2.34	0.62
1:B:604:PHE:HA	1:B:830:LYS:HZ1	1.63	0.62
1:B:720:LEU:O	1:B:723:GLN:HG3	2.00	0.61
1:B:800:PHE:CD2	1:B:858:ILE:HG21	2.32	0.61
1:A:655:PHE:HA	1:A:658:LEU:HG	1.82	0.61
1:B:626:THR:C	1:B:629:VAL:HG12	2.19	0.61
1:B:800:PHE:HE2	1:B:858:ILE:CG2	2.05	0.60
1:B:735:ILE:O	1:B:738:CYS:HB3	2.02	0.60
1:A:698:THR:HG22	1:A:699:ASN:H	1.67	0.60
1:B:816:VAL:HG11	1:B:843:ALA:HB2	1.82	0.60
1:A:735:ILE:O	1:A:738:CYS:HB3	2.01	0.60
1:B:434:TYR:HB2	1:B:451:ILE:HD12	1.82	0.60
1:A:88:LEU:HD21	1:A:430:LEU:HB3	1.83	0.59
1:A:778:TYR:CZ	1:A:782:LEU:HD11	2.38	0.59
1:A:257:GLU:OE1	1:A:286:ARG:NH2	2.35	0.59
1:A:491:ILE:HD12	1:A:504:PHE:HB3	1.84	0.59
1:B:732:PHE:O	1:B:735:ILE:HG22	2.02	0.59
1:A:837:VAL:O	1:A:840:ILE:HG13	2.02	0.59
1:B:39:PRO:HG3	1:B:145:THR:HG21	1.85	0.59
1:A:751:ARG:CG	1:A:762:ILE:HG12	2.20	0.58
1:B:601:GLN:HB3	1:B:759:ILE:HG12	1.84	0.58
1:A:639:THR:HG22	1:A:641:ILE:HG12	1.85	0.58
1:B:698:THR:CG2	1:B:699:ASN:H	2.16	0.58
1:B:430:LEU:CA	1:B:433:ILE:HG22	2.33	0.58
1:B:741:TRP:CZ2	1:B:768:SER:N	2.65	0.58
1:A:44:VAL:CG1	1:A:60:CYS:SG	2.91	0.58
1:B:623:ILE:HD13	1:B:661:PHE:CD2	2.39	0.58
1:A:667:PHE:HB2	1:A:837:VAL:HG21	1.85	0.58
1:A:820:PHE:HE1	1:A:836:GLU:CA	2.16	0.58
1:A:820:PHE:CD1	1:A:835:VAL:HG12	2.38	0.58
1:B:430:LEU:HA	1:B:433:ILE:HG22	1.86	0.58
1:A:60:CYS:HG	1:A:101:CYS:HB2	1.63	0.58
1:B:430:LEU:O	1:B:433:ILE:HG23	2.03	0.58
1:B:623:ILE:O	1:B:626:THR:OG1	2.15	0.57
1:B:62:ARG:NH2	1:B:277:GLU:OE1	2.37	0.57
1:B:528:LEU:O	1:B:528:LEU:HD12	2.04	0.57
1:A:584:CYS:CB	1:A:597:CYS:HG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:ILE:HD12	1:B:779:THR:CG2	2.35	0.57
1:A:331:ARG:NH1	1:A:410:PHE:O	2.37	0.57
1:B:814:PHE:O	1:B:818:ILE:HG13	2.04	0.57
1:A:587:ASP:O	1:A:600:LYS:N	2.33	0.57
1:B:741:TRP:NE1	1:B:768:SER:CB	2.67	0.57
1:B:832:VAL:O	1:B:835:VAL:CG1	2.50	0.56
1:B:741:TRP:HZ2	1:B:768:SER:N	1.96	0.56
1:A:41:HIS:ND1	1:A:62:ARG:O	2.29	0.56
1:B:632:VAL:HA	1:B:635:LYS:HD2	1.87	0.56
1:A:820:PHE:CE1	1:A:836:GLU:CA	2.83	0.56
1:B:541:CYS:SG	1:B:561:CYS:CB	2.93	0.56
1:A:184:LEU:HD23	1:A:482:GLY:CA	2.36	0.56
1:A:683:PHE:CZ	1:A:840:ILE:CG2	2.89	0.55
1:A:808:PHE:HB3	1:A:850:CYS:SG	2.46	0.55
1:B:629:VAL:HG21	1:B:852:PHE:CD1	2.41	0.55
1:B:733:VAL:O	1:B:736:VAL:HB	2.05	0.55
1:A:211:THR:HB	1:A:223:ILE:HD11	1.87	0.55
1:A:613:ILE:O	1:A:617:LEU:HG	2.07	0.55
1:A:487:ASN:OD1	1:A:512:VAL:HG12	2.06	0.55
1:B:695:LEU:HD13	1:B:786:CYS:HB2	1.88	0.55
1:B:296:SER:OG	1:B:297:GLU:N	2.40	0.55
1:B:491:ILE:HD12	1:B:504:PHE:HB3	1.89	0.55
1:A:778:TYR:O	1:A:782:LEU:HG	2.08	0.54
1:A:184:LEU:CD2	1:A:482:GLY:CA	2.85	0.54
1:A:683:PHE:CE1	1:A:840:ILE:CB	2.90	0.54
1:A:831:PHE:O	1:A:835:VAL:HG23	2.07	0.54
1:A:642:VAL:CG2	1:A:865:ARG:CB	2.84	0.54
1:A:688:VAL:O	1:A:692:SER:OG	2.23	0.54
1:B:417:TYR:CZ	1:B:421:LEU:HD11	2.41	0.54
1:A:434:TYR:HB2	1:A:451:ILE:HD12	1.89	0.54
1:B:776:ILE:HD12	1:B:777:GLY:N	2.22	0.54
1:B:204:PHE:HE1	1:B:524:GLU:OE1	1.90	0.54
1:A:209:VAL:HG12	1:A:266:VAL:HB	1.88	0.54
1:A:37:LEU:HB2	1:A:144:ALA:H	1.73	0.54
1:A:697:LYS:O	1:A:697:LYS:HG2	2.07	0.54
1:B:792:LYS:HE2	1:B:792:LYS:HA	1.90	0.54
1:B:722:LEU:O	1:B:725:LEU:HB3	2.08	0.53
1:A:721:ASN:O	1:A:724:PHE:HB2	2.09	0.53
1:B:698:THR:CG2	1:B:699:ASN:N	2.71	0.53
1:A:584:CYS:CB	1:A:597:CYS:SG	2.96	0.53
1:B:676:CYS:CB	1:B:764:CYS:HG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:THR:HG22	1:B:828:TYR:N	2.24	0.53
1:A:271:SER:OG	1:A:272:SER:N	2.42	0.53
1:A:443:PHE:HD2	1:A:448:CYS:HA	1.74	0.53
1:B:756:GLU:HG3	1:B:759:ILE:H	1.73	0.53
1:A:182:SER:O	1:A:182:SER:OG	2.27	0.52
1:A:212:ILE:HD11	1:A:259:ILE:HD11	1.91	0.52
1:A:776:ILE:HD13	1:A:817:TRP:HZ2	1.74	0.52
1:B:299:TRP:HA	1:B:302:SER:HB2	1.91	0.52
1:A:311:PHE:HE2	1:A:495:LEU:HB2	1.74	0.52
1:A:610:PRO:HA	1:A:613:ILE:HD12	1.90	0.52
1:B:753:HIS:HB3	1:B:760:ILE:HG12	1.90	0.52
1:A:673:ASN:O	1:A:677:ARG:HB2	2.08	0.52
1:A:184:LEU:HD22	1:A:482:GLY:HA2	1.92	0.52
1:B:834:ALA:O	1:B:837:VAL:HG12	2.09	0.52
1:B:683:PHE:CZ	1:B:840:ILE:HG22	2.45	0.52
1:B:737:ILE:O	1:B:740:ILE:HB	2.10	0.52
1:B:787:PHE:CE1	1:B:811:LEU:HD21	2.45	0.52
1:A:741:TRP:HE1	1:A:771:ALA:HB3	1.75	0.51
1:B:212:ILE:HD11	1:B:259:ILE:HD11	1.90	0.51
1:B:538:PHE:HD1	2:F:1:NAG:H82	1.75	0.51
1:A:734:GLN:NE2	1:A:778:TYR:CD2	2.73	0.51
1:B:734:GLN:NE2	1:B:737:ILE:HB	2.25	0.51
2:F:1:NAG:O6	2:F:2:NAG:N2	2.43	0.51
1:B:670:GLU:OE2	1:B:672:GLN:NE2	2.44	0.51
1:A:606:SER:OG	1:A:607:TRP:N	2.43	0.51
1:B:479:ASP:OD1	1:B:480:GLU:N	2.42	0.51
1:B:684:GLY:O	1:B:688:VAL:HG22	2.11	0.51
1:A:632:VAL:HA	1:A:635:LYS:HD2	1.92	0.51
1:B:430:LEU:HA	1:B:433:ILE:CG2	2.40	0.51
1:A:790:ALA:HB1	1:A:806:ILE:HD12	1.92	0.50
1:A:177:LYS:NZ	1:A:183:PHE:O	2.35	0.50
1:A:417:TYR:O	1:A:421:LEU:CD1	2.52	0.50
1:B:855:LYS:HA	1:B:858:ILE:CD1	2.41	0.50
1:A:36:GLY:HA2	1:A:142:VAL:O	2.12	0.50
1:A:184:LEU:HD23	1:A:482:GLY:HA3	1.92	0.50
1:A:734:GLN:HB2	1:A:778:TYR:CE2	2.46	0.50
1:A:857:TYR:O	1:A:861:PHE:CB	2.55	0.50
1:B:807:THR:O	1:B:811:LEU:HG	2.11	0.50
1:A:400:ILE:HD12	1:A:400:ILE:H	1.76	0.50
1:B:622:GLY:O	1:B:626:THR:HG23	2.12	0.50
1:A:39:PRO:HG3	1:A:145:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:O	1:A:353:GLU:HG2	2.11	0.50
1:A:827:THR:HG21	1:A:832:VAL:CA	2.39	0.50
1:B:772:LEU:O	1:B:776:ILE:HG13	2.12	0.50
1:B:778:TYR:CZ	1:B:782:LEU:HD11	2.46	0.50
1:A:515:LYS:NZ	1:A:516:LYS:O	2.44	0.50
1:B:538:PHE:CZ	1:B:540:ASN:HB2	2.47	0.49
1:B:676:CYS:CB	1:B:764:CYS:SG	3.00	0.49
1:B:591:ASN:HB2	1:B:596:SER:O	2.12	0.49
1:B:617:LEU:HA	1:B:620:VAL:HG22	1.93	0.49
1:A:824:TYR:O	1:A:827:THR:HG22	2.13	0.49
1:B:660:CYS:SG	1:B:686:SER:OG	2.63	0.49
1:A:110:ALA:O	1:A:113:SER:OG	2.19	0.49
1:B:200:ILE:HD11	1:B:490:ILE:HD13	1.93	0.49
1:B:741:TRP:HA	1:B:744:THR:OG1	2.13	0.49
1:B:857:TYR:O	1:B:861:PHE:HB3	2.13	0.49
1:B:545:CYS:HB2	1:B:577:ASP:HA	1.94	0.49
1:B:399:ASN:HB3	1:B:402:SER:OG	2.12	0.49
1:A:584:CYS:HB3	1:A:597:CYS:SG	2.52	0.49
1:B:338:HIS:CD2	1:B:340:LYS:HB2	2.47	0.49
1:B:741:TRP:NE1	1:B:745:ALA:O	2.45	0.49
1:A:666:PHE:HD2	1:A:679:ARG:HA	1.77	0.49
1:B:726:LEU:O	1:B:729:LEU:HB3	2.13	0.49
1:A:820:PHE:HE1	1:A:836:GLU:N	2.10	0.48
1:A:268:VAL:HG22	1:A:294:LEU:HD12	1.94	0.48
1:A:821:ILE:HG23	1:A:822:PRO:HD3	1.96	0.48
1:B:655:PHE:O	1:B:658:LEU:HG	2.14	0.48
1:B:338:HIS:CD2	1:B:341:LYS:HD3	2.49	0.48
1:B:721:ASN:HA	1:B:724:PHE:CD2	2.48	0.48
1:B:204:PHE:CE1	1:B:524:GLU:OE2	2.67	0.48
1:B:606:SER:OG	1:B:609:GLU:N	2.46	0.48
1:B:614:ALA:O	1:B:617:LEU:HG	2.14	0.48
1:A:51:LEU:HB2	1:B:461:LYS:HD3	1.95	0.47
1:A:661:PHE:HE1	1:A:844:SER:HG	1.61	0.47
1:B:612:GLY:O	1:B:616:THR:HG22	2.14	0.47
1:A:60:CYS:CB	1:A:101:CYS:SG	3.02	0.47
1:B:44:VAL:HA	1:B:60:CYS:HA	1.96	0.47
1:B:726:LEU:H	1:B:726:LEU:HD22	1.80	0.47
1:A:672:GLN:OE1	1:A:674:TRP:HB2	2.14	0.47
1:A:111:THR:HG21	1:A:153:VAL:HG13	1.96	0.47
1:A:745:ALA:O	1:A:767:GLY:HA3	2.15	0.47
1:B:854:ASN:OD1	1:B:854:ASN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:SER:OG	1:A:273:GLY:N	2.48	0.46
1:B:666:PHE:HD2	1:B:679:ARG:HA	1.81	0.46
1:B:218:TYR:OH	1:B:296:SER:OG	2.33	0.46
1:A:661:PHE:O	1:A:664:SER:OG	2.25	0.46
1:A:681:PRO:O	1:A:685:ILE:HG12	2.16	0.46
1:A:853:PHE:O	1:A:857:TYR:HB3	2.15	0.46
1:B:257:GLU:OE2	1:B:286:ARG:NH2	2.30	0.46
1:A:201:ILE:HD13	1:A:209:VAL:HG11	1.98	0.46
1:B:513:TYR:HE2	2:E:1:NAG:HN2	1.64	0.46
1:A:25:ARG:HD3	1:A:98:PHE:HE1	1.80	0.46
1:A:802:GLU:HA	1:A:805:PHE:HD2	1.80	0.46
1:B:781:LEU:HD12	1:B:782:LEU:HD23	1.96	0.46
1:B:629:VAL:HG21	1:B:852:PHE:HD1	1.80	0.45
1:B:666:PHE:HB3	1:B:679:ARG:CB	2.46	0.45
1:A:725:LEU:O	1:A:729:LEU:N	2.47	0.45
1:A:413:LEU:HB3	1:A:416:SER:HG	1.81	0.45
1:A:687:PHE:CE1	1:A:691:ILE:HD12	2.51	0.45
1:B:840:ILE:HG13	1:B:841:LEU:N	2.31	0.45
1:A:228:GLU:O	1:A:231:GLU:HG3	2.16	0.45
1:A:660:CYS:N	1:A:686:SER:OG	2.50	0.45
1:B:623:ILE:HD13	1:B:661:PHE:CG	2.51	0.45
1:B:626:THR:HG22	1:B:848:LEU:CD1	2.47	0.45
1:B:721:ASN:HA	1:B:724:PHE:HD2	1.81	0.45
1:A:253:GLN:O	1:A:257:GLU:HG2	2.16	0.45
1:B:648:GLU:HA	1:B:651:TYR:CD2	2.51	0.45
1:A:99:ASP:OD1	1:A:100:THR:N	2.50	0.45
1:A:657:LEU:HD12	1:A:690:CYS:SG	2.56	0.45
1:B:836:GLU:O	1:B:840:ILE:HG12	2.17	0.45
1:A:54:ARG:NH2	1:B:455:GLU:OE2	2.50	0.45
1:B:657:LEU:CD1	1:B:848:LEU:HB2	2.47	0.45
1:A:734:GLN:HB2	1:A:778:TYR:HE2	1.81	0.45
1:B:499:ASP:OD2	1:B:500:GLY:N	2.50	0.45
1:A:228:GLU:HG3	1:A:229:GLU:N	2.32	0.45
1:A:584:CYS:SG	1:A:597:CYS:CB	3.04	0.44
1:B:140:ALA:HB2	1:B:163:PRO:HG2	1.99	0.44
1:B:725:LEU:O	1:B:729:LEU:N	2.50	0.44
1:A:797:PRO:HA	1:A:801:ASN:HB2	2.00	0.44
1:A:647:ARG:O	1:A:650:SER:OG	2.31	0.44
1:B:193:GLN:HE22	1:B:297:GLU:H	1.64	0.44
1:B:289:THR:HG23	1:B:313:VAL:HA	1.99	0.44
1:B:499:ASP:OD2	1:B:501:SER:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:OG	1:A:218:TYR:HB2	2.17	0.44
1:A:605:LEU:HD23	1:A:605:LEU:HA	1.80	0.44
1:A:639:THR:CG2	1:A:641:ILE:HG23	2.47	0.44
1:A:292:ILE:HD11	1:A:537:PRO:HG2	2.00	0.44
1:A:487:ASN:ND2	1:A:511:ASN:OD1	2.51	0.44
1:A:776:ILE:HD12	1:A:777:GLY:N	2.32	0.44
1:B:61:ILE:HG13	1:B:62:ARG:H	1.82	0.44
1:A:653:LEU:HG	1:A:693:CYS:SG	2.58	0.44
1:B:656:SER:HB2	1:B:689:LEU:HD22	2.00	0.44
1:A:352:TRP:HE1	1:A:396:GLY:HA2	1.82	0.43
1:A:835:VAL:O	1:A:838:ILE:HG13	2.17	0.43
1:A:637:ARG:NH1	1:A:638:ASN:OD1	2.52	0.43
1:A:642:VAL:O	1:A:642:VAL:HG12	2.16	0.43
1:A:809:SER:HA	1:A:812:ILE:HD12	2.00	0.43
1:A:238:ASP:OD2	1:A:262:SER:HB2	2.18	0.43
1:A:789:PHE:HA	1:A:792:LYS:NZ	2.33	0.43
1:B:489:SER:OG	1:B:506:GLU:HG3	2.18	0.43
1:A:654:LEU:O	1:A:658:LEU:HG	2.18	0.43
1:A:790:ALA:CB	1:A:806:ILE:HD12	2.49	0.43
1:B:654:LEU:HD21	1:B:852:PHE:CE1	2.53	0.43
1:B:802:GLU:HA	1:B:805:PHE:HD2	1.84	0.43
1:A:452:LYS:HE3	1:A:452:LYS:HB3	1.86	0.43
1:A:470:SER:O	1:A:473:GLY:N	2.52	0.43
1:B:492:ASN:HD22	1:B:494:HIS:CD2	2.36	0.43
1:A:60:CYS:HB2	1:A:101:CYS:SG	2.59	0.43
1:B:827:THR:CG2	1:B:828:TYR:N	2.82	0.43
1:A:639:THR:HG22	1:A:641:ILE:HG23	2.01	0.43
1:A:685:ILE:C	1:A:689:LEU:HD13	2.33	0.43
1:A:726:LEU:HD22	1:A:726:LEU:H	1.83	0.43
1:A:550:ARG:NH2	1:A:551:LYS:O	2.52	0.42
1:B:778:TYR:O	1:B:782:LEU:HG	2.19	0.42
1:A:622:GLY:HA3	1:A:661:PHE:CE2	2.54	0.42
1:B:676:CYS:HB3	1:B:764:CYS:HG	1.84	0.42
1:A:538:PHE:CE1	1:A:540:ASN:HB2	2.54	0.42
1:B:193:GLN:HE22	1:B:297:GLU:N	2.16	0.42
1:B:280:ILE:HG23	1:B:314:ILE:HD11	2.01	0.42
1:B:791:PHE:O	1:B:795:LYS:NZ	2.52	0.42
1:A:44:VAL:HG13	1:A:60:CYS:SG	2.59	0.42
1:A:284:VAL:HG21	1:A:310:PHE:CD1	2.54	0.42
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.87	0.42
1:A:647:ARG:HB3	1:A:651:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLU:N	1:B:474:GLU:OE2	2.52	0.42
1:B:516:LYS:HG2	1:B:519:ARG:NH1	2.34	0.42
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.73	0.42
1:B:106:LYS:O	1:B:109:GLU:HG2	2.20	0.42
1:B:162:ILE:O	1:B:182:SER:OG	2.37	0.42
1:B:207:ASN:ND2	1:B:560:CYS:HB2	2.35	0.42
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.93	0.42
1:B:630:LEU:HD21	1:B:654:LEU:HB3	2.00	0.42
1:B:691:ILE:CD1	1:B:779:THR:HG22	2.49	0.42
1:B:812:ILE:HD12	1:B:815:ILE:HD11	2.02	0.42
1:B:837:VAL:HG13	1:B:838:ILE:N	2.34	0.42
1:A:143:GLY:HA2	1:A:167:TYR:CE2	2.54	0.42
1:A:538:PHE:CZ	1:A:540:ASN:HB2	2.55	0.42
1:B:275:ASP:OD1	1:B:275:ASP:N	2.53	0.42
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.75	0.42
1:B:238:ASP:OD2	1:B:262:SER:HB2	2.19	0.42
1:B:851:ILE:HG22	1:B:852:PHE:CD2	2.55	0.42
1:A:167:TYR:CD2	1:A:419:VAL:HG22	2.55	0.41
1:A:858:ILE:HD12	1:A:858:ILE:HA	1.84	0.41
1:B:734:GLN:HE21	1:B:737:ILE:HB	1.85	0.41
1:A:107:ALA:O	1:A:111:THR:HG23	2.20	0.41
1:A:450:ASP:OD2	1:A:450:ASP:N	2.53	0.41
1:B:688:VAL:HG11	1:B:778:TYR:HE2	1.85	0.41
1:A:740:ILE:O	1:A:744:THR:N	2.54	0.41
1:B:605:LEU:H	1:B:830:LYS:NZ	2.18	0.41
1:B:835:VAL:HG13	1:B:836:GLU:N	2.36	0.41
1:A:63:TYR:CD1	1:A:354:GLU:HG3	2.55	0.41
1:A:734:GLN:HE21	1:A:778:TYR:HD2	1.61	0.41
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.93	0.41
1:B:655:PHE:HA	1:B:658:LEU:CD2	2.50	0.41
1:A:753:HIS:CE1	1:A:754:GLU:OE2	2.74	0.41
1:B:182:SER:OG	1:B:182:SER:O	2.38	0.41
1:A:311:PHE:CE2	1:A:495:LEU:HB2	2.54	0.41
1:A:86:ASN:OD1	1:A:87:LEU:N	2.54	0.41
1:B:603:GLU:HB3	1:B:761:PHE:CD1	2.55	0.41
1:B:735:ILE:O	1:B:739:VAL:HG23	2.21	0.41
1:B:747:PRO:HA	1:B:766:GLU:HA	2.03	0.41
1:B:769:LEU:H	1:B:769:LEU:HD23	1.85	0.41
1:A:53:SER:OG	1:A:54:ARG:N	2.54	0.40
1:A:641:ILE:HG13	1:A:642:VAL:H	1.84	0.40
1:A:653:LEU:HD21	1:A:694:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:N	1:B:392:PRO:HD2	2.35	0.40
1:A:790:ALA:HB1	1:A:806:ILE:HD11	1.99	0.40
1:B:174:LEU:HD13	1:B:183:PHE:CZ	2.57	0.40
1:B:338:HIS:CD2	1:B:340:LYS:H	2.39	0.40
1:A:56:GLU:CD	1:A:56:GLU:H	2.25	0.40
1:B:249:GLU:H	1:B:249:GLU:CD	2.25	0.40
1:B:811:LEU:O	1:B:815:ILE:HG23	2.21	0.40
1:A:721:ASN:N	1:A:721:ASN:OD1	2.55	0.40
1:A:820:PHE:CD1	1:A:839:ALA:HB2	2.57	0.40
1:B:177:LYS:HD3	1:B:177:LYS:HA	1.88	0.40
1:B:742:LEU:HG	1:B:743:TYR:CE2	2.57	0.40
1:A:827:THR:HG21	1:A:832:VAL:CG2	2.37	0.40
1:B:81:ILE:HD13	1:B:427:ALA:HB2	2.04	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	783/1069 (73%)	740 (94%)	43 (6%)	0	100	100
1	B	784/1069 (73%)	744 (95%)	40 (5%)	0	100	100
All	All	1567/2138 (73%)	1484 (95%)	83 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	670/926 (72%)	647 (97%)	23 (3%)	37	70
1	B	675/926 (73%)	651 (96%)	24 (4%)	35	69
All	All	1345/1852 (73%)	1298 (96%)	47 (4%)	39	69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	102	ASN
1	A	109	GLU
1	A	303	SER
1	A	424	TYR
1	A	425	SER
1	A	489	SER
1	A	516	LYS
1	A	555	GLU
1	A	572	TYR
1	A	624	PHE
1	A	655	PHE
1	A	672	GLN
1	A	750	TYR
1	A	765	HIS
1	A	787	PHE
1	A	795	LYS
1	A	800	PHE
1	A	808	PHE
1	A	819	SER
1	A	824	TYR
1	A	845	PHE
1	A	857	TYR
1	B	23	ASN
1	B	80	GLU
1	B	171	SER
1	B	262	SER
1	B	270	PHE
1	B	275	ASP
1	B	394	CYS
1	B	572	TYR
1	B	606	SER
1	B	618	PHE

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Mol	Chain	Res	Type
1	B	624	PHE
1	B	628	PHE
1	B	656	SER
1	B	663	SER
1	B	741	TRP
1	B	750	TYR
1	B	757	ASP
1	B	769	LEU
1	B	780	CYS
1	B	795	LYS
1	B	824	TYR
1	B	828	TYR
1	B	830	LYS
1	B	845	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	594	HIS
1	A	734	GLN
1	A	753	HIS
1	B	23	ASN
1	B	118	ASN
1	B	193	GLN
1	B	245	GLN
1	B	260	GLN
1	B	338	HIS
1	B	465	HIS
1	B	492	ASN
1	B	734	GLN

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 (i)

8 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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	1.62	3 (21%)	17,19,21	2.30	4 (23%)
2	NAG	C	2	2	14,14,15	1.80	4 (28%)	17,19,21	1.56	6 (35%)
2	NAG	D	1	1,2	14,14,15	1.70	3 (21%)	17,19,21	1.27	3 (17%)
2	NAG	D	2	2	14,14,15	1.80	4 (28%)	17,19,21	1.23	2 (11%)
2	NAG	E	1	1,2	14,14,15	1.84	4 (28%)	17,19,21	1.70	5 (29%)
2	NAG	E	2	2	14,14,15	1.76	4 (28%)	17,19,21	1.21	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.72	3 (21%)	17,19,21	1.20	2 (11%)
2	NAG	F	2	2	14,14,15	1.72	3 (21%)	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	3.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C7-N2	3.29	1.45	1.34
2	D	2	NAG	O5-C1	3.26	1.48	1.43
2	C	2	NAG	C7-N2	3.25	1.45	1.34
2	D	2	NAG	C7-N2	3.24	1.45	1.34
2	C	1	NAG	C7-N2	3.23	1.45	1.34
2	E	2	NAG	C7-N2	3.23	1.45	1.34
2	F	2	NAG	C7-N2	3.21	1.45	1.34
2	E	1	NAG	C7-N2	3.19	1.45	1.34
2	D	1	NAG	C7-N2	3.18	1.45	1.34
2	E	2	NAG	O5-C1	3.07	1.48	1.43
2	C	2	NAG	O5-C1	3.04	1.48	1.43
2	D	1	NAG	O5-C1	3.03	1.48	1.43
2	F	1	NAG	O5-C1	3.02	1.48	1.43
2	F	2	NAG	O5-C1	2.96	1.48	1.43
2	C	2	NAG	O5-C5	2.54	1.48	1.43
2	E	1	NAG	O5-C5	2.45	1.48	1.43
2	C	1	NAG	O5-C1	2.42	1.47	1.43
2	D	2	NAG	O5-C5	2.34	1.48	1.43
2	E	2	NAG	O5-C5	2.33	1.48	1.43
2	C	2	NAG	C3-C2	-2.28	1.47	1.52
2	F	2	NAG	O5-C5	2.28	1.48	1.43
2	E	1	NAG	C3-C2	-2.28	1.47	1.52
2	C	1	NAG	O5-C5	2.18	1.47	1.43
2	D	2	NAG	C3-C2	-2.14	1.48	1.52
2	D	1	NAG	O5-C5	2.12	1.47	1.43
2	E	2	NAG	C3-C2	-2.04	1.48	1.52
2	F	1	NAG	O7-C7	-2.00	1.18	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C3-C4-C5	5.22	119.55	110.24
2	C	1	NAG	C1-O5-C5	-4.77	105.73	112.19
2	E	1	NAG	C1-O5-C5	3.43	116.84	112.19
2	C	1	NAG	C4-C3-C2	3.25	115.78	111.02
2	C	2	NAG	C2-N2-C7	-3.16	118.41	122.90
2	D	2	NAG	C2-N2-C7	-3.08	118.52	122.90
2	F	2	NAG	C2-N2-C7	-2.88	118.80	122.90
2	D	1	NAG	C2-N2-C7	-2.78	118.94	122.90
2	F	1	NAG	C8-C7-N2	2.56	120.43	116.10
2	F	2	NAG	C8-C7-N2	2.53	120.39	116.10
2	E	2	NAG	C2-N2-C7	-2.52	119.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C2-N2-C7	-2.52	119.32	122.90
2	C	2	NAG	C6-C5-C4	-2.48	107.19	113.00
2	C	2	NAG	C8-C7-N2	2.43	120.21	116.10
2	D	1	NAG	C8-C7-N2	2.42	120.19	116.10
2	D	2	NAG	C8-C7-N2	2.40	120.16	116.10
2	E	2	NAG	C8-C7-N2	2.36	120.10	116.10
2	C	2	NAG	C1-O5-C5	2.35	115.37	112.19
2	E	1	NAG	C3-C4-C5	2.24	114.24	110.24
2	C	1	NAG	C8-C7-N2	2.24	119.89	116.10
2	E	1	NAG	C8-C7-N2	2.21	119.84	116.10
2	C	2	NAG	O5-C5-C4	2.09	115.92	110.83
2	E	1	NAG	O5-C1-C2	2.08	114.58	111.29
2	D	1	NAG	C6-C5-C4	-2.06	108.17	113.00
2	E	1	NAG	C1-C2-N2	-2.04	107.00	110.49
2	C	2	NAG	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

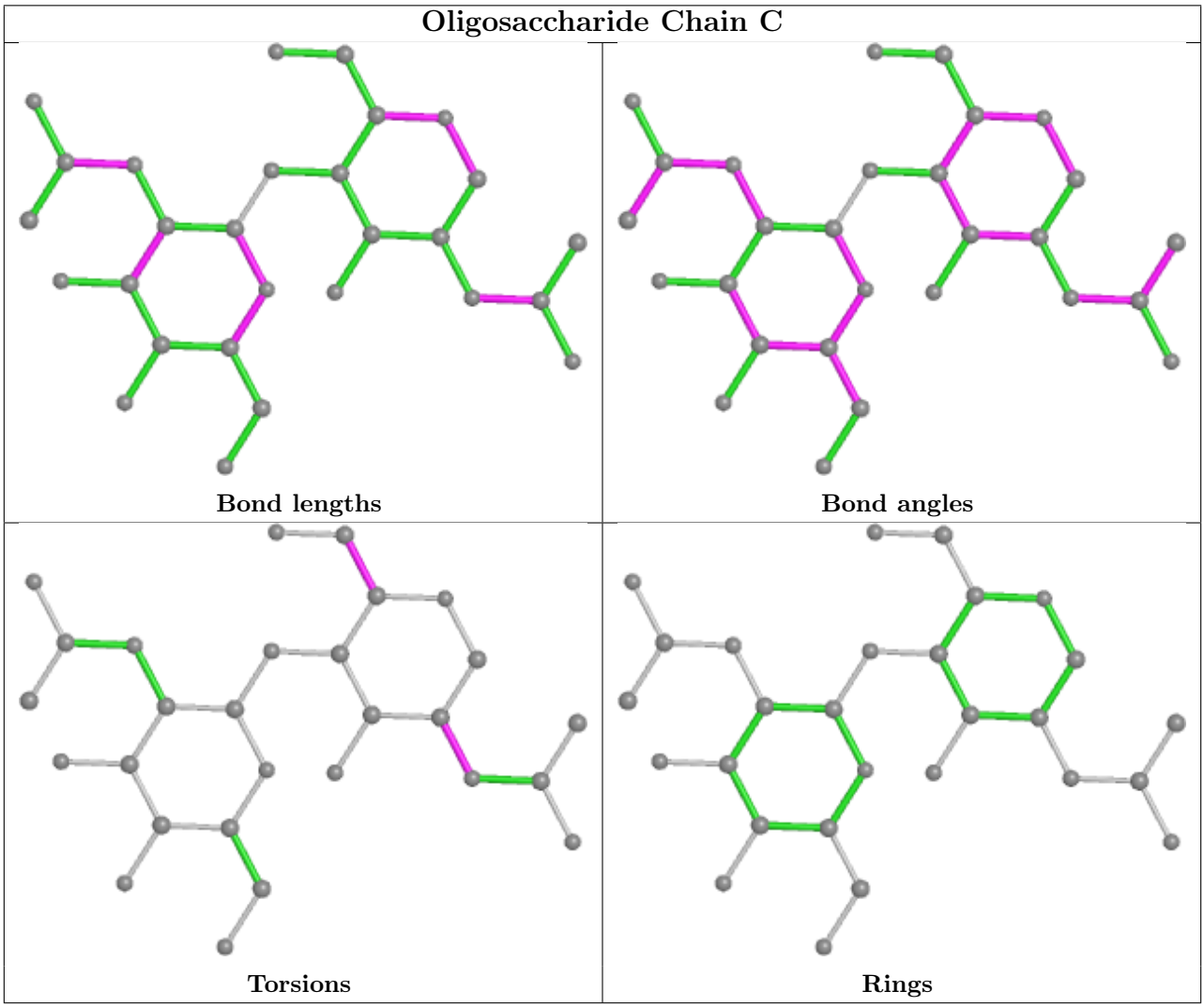
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

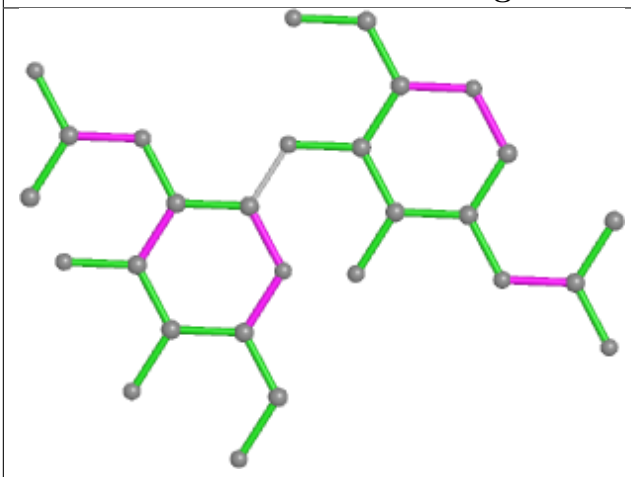
4 monomers are involved in 5 short contacts:

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

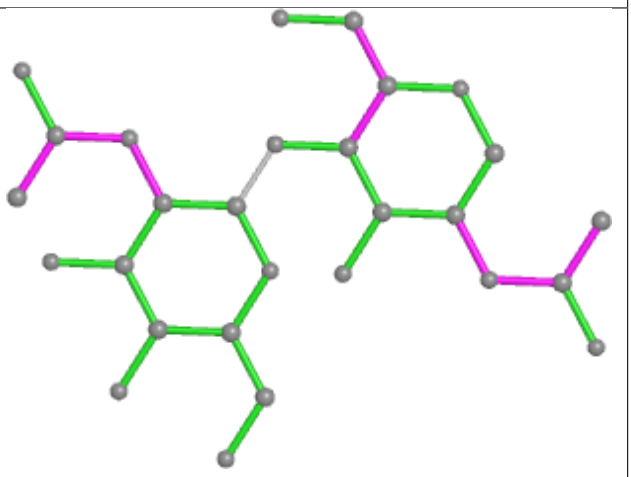
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



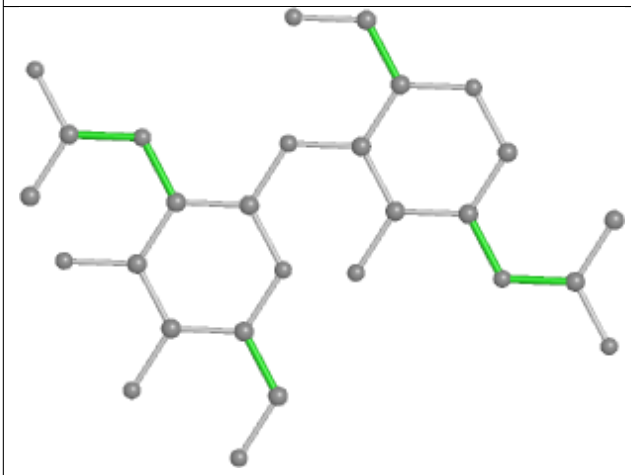
Oligosaccharide Chain D



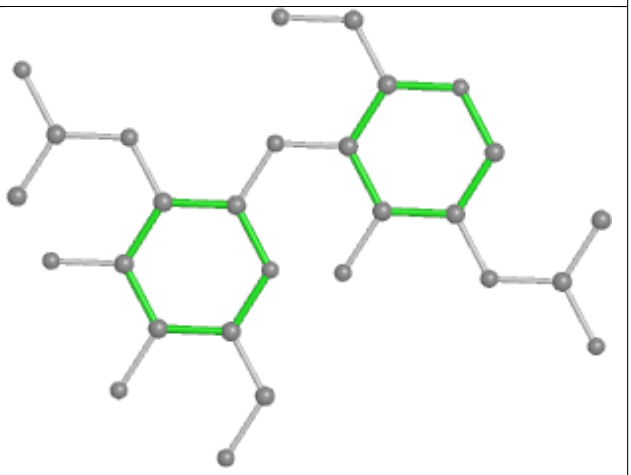
Bond lengths



Bond angles

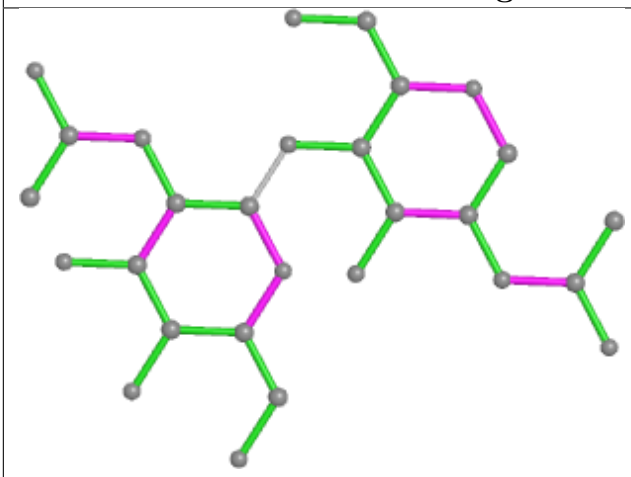


Torsions

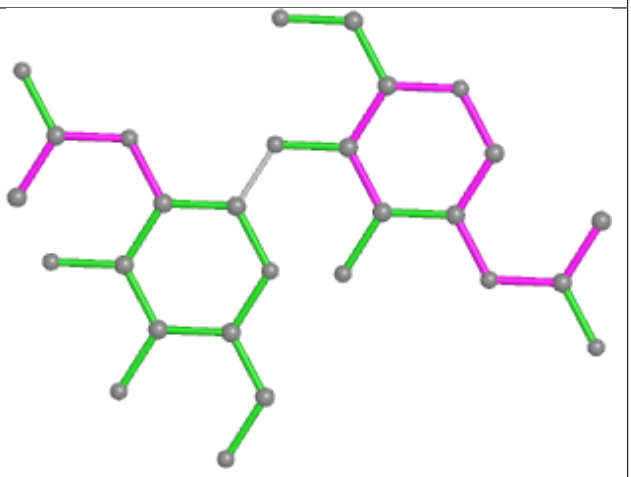


Rings

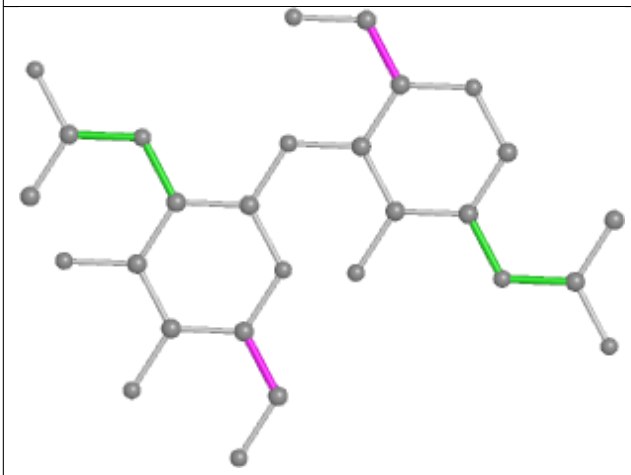
Oligosaccharide Chain E



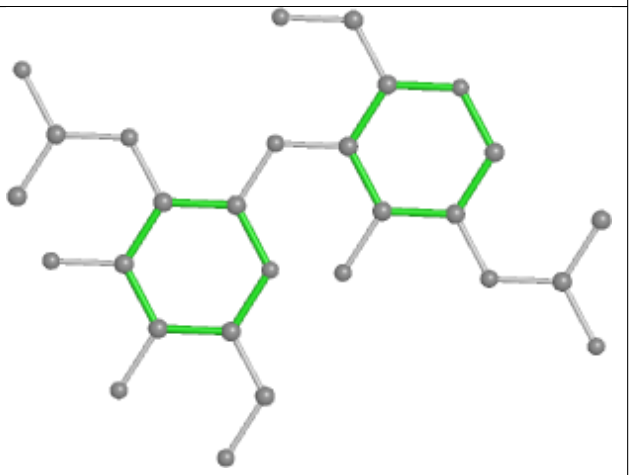
Bond lengths



Bond angles

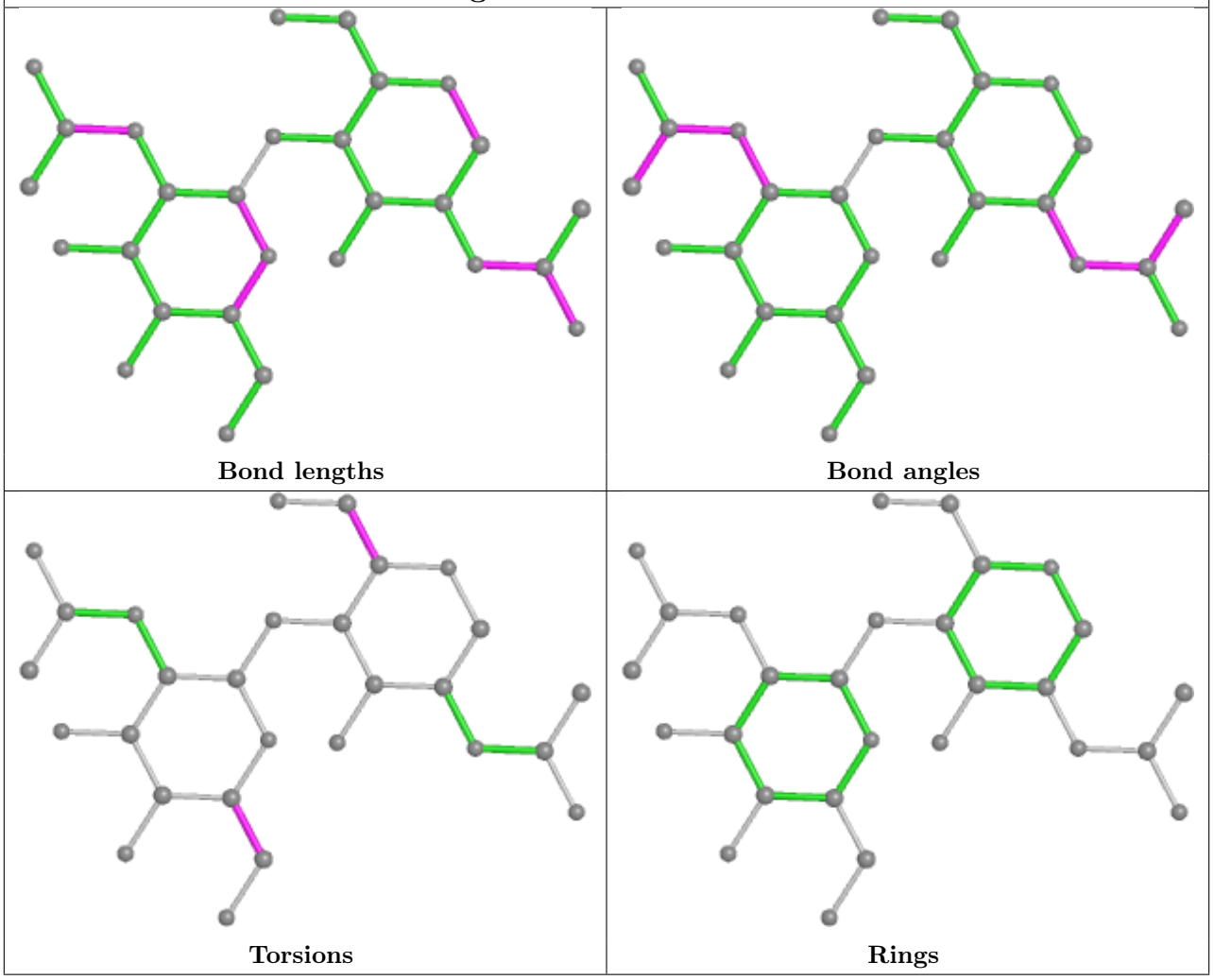


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1106	1	14,14,15	1.75	3 (21%)	17,19,21	1.40	4 (23%)
5	NAG	B	1107	1	14,14,15	1.80	4 (28%)	17,19,21	1.18	2 (11%)
5	NAG	A	1105	1	14,14,15	1.76	3 (21%)	17,19,21	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	TRP	A	1108	-	14,16,16	1.15	1 (7%)	16,22,22	0.84	0
5	NAG	A	1107	1	14,14,15	1.77	3 (21%)	17,19,21	1.04	0
5	NAG	B	1105	1	14,14,15	1.80	4 (28%)	17,19,21	1.09	1 (5%)
6	TRP	B	1108	-	14,16,16	1.14	1 (7%)	16,22,22	0.85	0
5	NAG	A	1106	1	14,14,15	1.84	3 (21%)	17,19,21	1.31	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1106	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1107	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1105	1	-	2/6/23/26	0/1/1/1
6	TRP	A	1108	-	-	2/7/8/8	0/2/2/2
5	NAG	A	1107	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1105	1	-	2/6/23/26	0/1/1/1
6	TRP	B	1108	-	-	1/7/8/8	0/2/2/2
5	NAG	A	1106	1	-	0/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	NAG	O5-C1	3.50	1.49	1.43
5	A	1107	NAG	C7-N2	3.32	1.45	1.34
5	B	1105	NAG	C7-N2	3.32	1.45	1.34
5	B	1106	NAG	C7-N2	3.31	1.45	1.34
5	B	1107	NAG	C7-N2	3.29	1.45	1.34
5	A	1105	NAG	O5-C1	3.26	1.48	1.43
5	A	1106	NAG	C7-N2	3.23	1.45	1.34
5	A	1105	NAG	C7-N2	3.21	1.45	1.34
5	A	1107	NAG	O5-C1	3.12	1.48	1.43
5	B	1105	NAG	O5-C1	3.08	1.48	1.43
5	B	1107	NAG	O5-C1	3.04	1.48	1.43
5	B	1106	NAG	O5-C1	3.02	1.48	1.43
5	B	1107	NAG	O5-C5	2.55	1.48	1.43
5	B	1105	NAG	O5-C5	2.49	1.48	1.43
5	A	1106	NAG	O5-C5	2.45	1.48	1.43
5	B	1106	NAG	O5-C5	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	NAG	O5-C5	2.22	1.47	1.43
5	A	1105	NAG	O5-C5	2.19	1.47	1.43
6	A	1108	TRP	CD1-NE1	-2.16	1.32	1.36
6	B	1108	TRP	CD1-NE1	-2.10	1.32	1.36
5	B	1105	NAG	C3-C2	-2.09	1.48	1.52
5	B	1107	NAG	C3-C2	-2.07	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1106	NAG	C2-N2-C7	-2.93	118.73	122.90
5	B	1106	NAG	C3-C4-C5	2.85	115.33	110.24
5	A	1106	NAG	C8-C7-N2	2.43	120.21	116.10
5	A	1105	NAG	C8-C7-N2	2.35	120.08	116.10
5	B	1107	NAG	C6-C5-C4	-2.26	107.72	113.00
5	B	1106	NAG	C8-C7-N2	2.25	119.91	116.10
5	B	1107	NAG	C3-C4-C5	2.23	114.22	110.24
5	B	1105	NAG	C6-C5-C4	-2.16	107.95	113.00
5	B	1106	NAG	C2-N2-C7	-2.03	120.02	122.90
5	B	1106	NAG	C4-C3-C2	2.00	113.96	111.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1107	NAG	O5-C5-C6-O6
5	B	1106	NAG	O5-C5-C6-O6
5	A	1105	NAG	O5-C5-C6-O6
5	A	1107	NAG	C4-C5-C6-O6
5	B	1106	NAG	C4-C5-C6-O6
5	A	1105	NAG	C4-C5-C6-O6
5	B	1106	NAG	C1-C2-N2-C7
6	A	1108	TRP	C-CA-CB-CG
6	B	1108	TRP	CA-CB-CG-CD1
6	A	1108	TRP	N-CA-CB-CG
5	B	1105	NAG	C1-C2-N2-C7
5	B	1107	NAG	C1-C2-N2-C7
5	A	1107	NAG	C1-C2-N2-C7
5	A	1107	NAG	C3-C2-N2-C7
5	B	1105	NAG	C3-C2-N2-C7
5	B	1106	NAG	C3-C2-N2-C7
5	B	1107	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1108	TRP	1	0
6	B	1108	TRP	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.

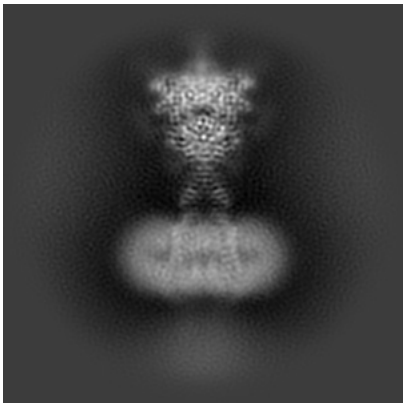
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30645. These allow visual inspection of the internal detail of the map and identification of artifacts.

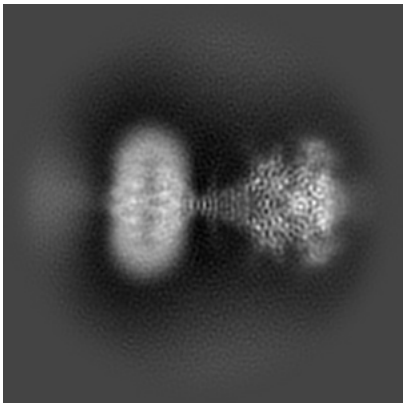
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

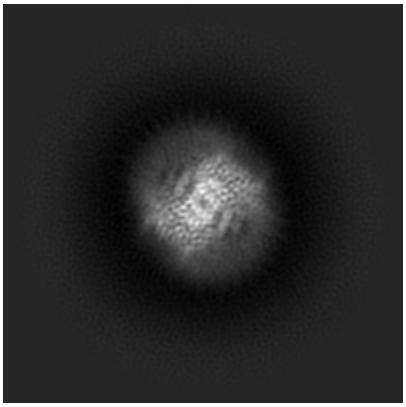
6.1.1 Primary map



X



Y

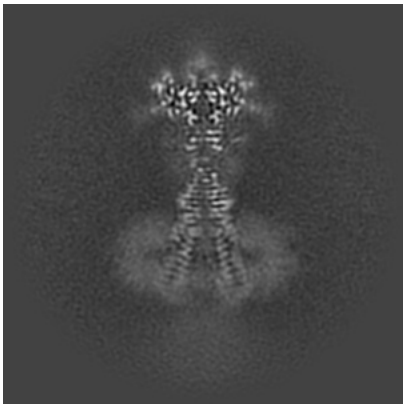


Z

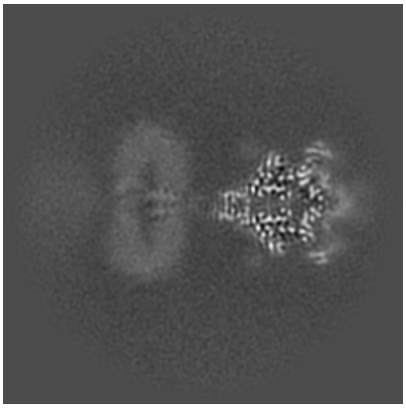
The images above show the map projected in three orthogonal directions.

6.2 Central slices

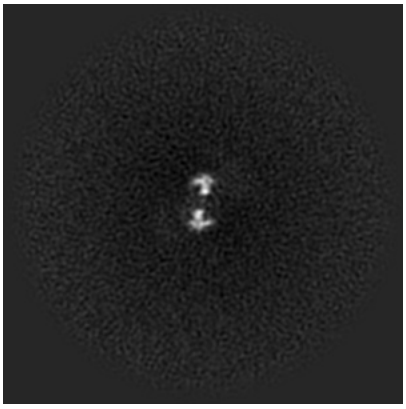
6.2.1 Primary map



X Index: 140



Y Index: 140

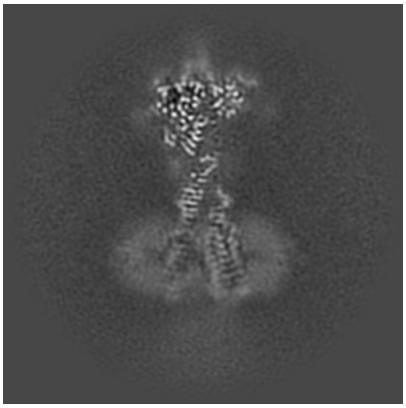


Z Index: 140

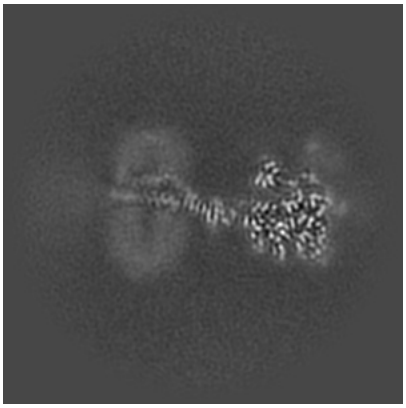
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

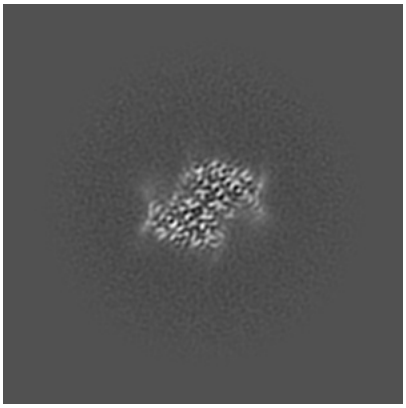
6.3.1 Primary map



X Index: 136



Y Index: 131



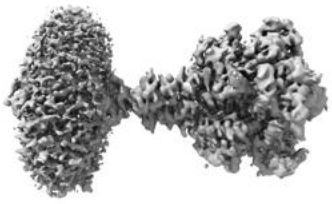
Z Index: 216

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

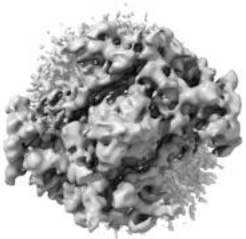
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

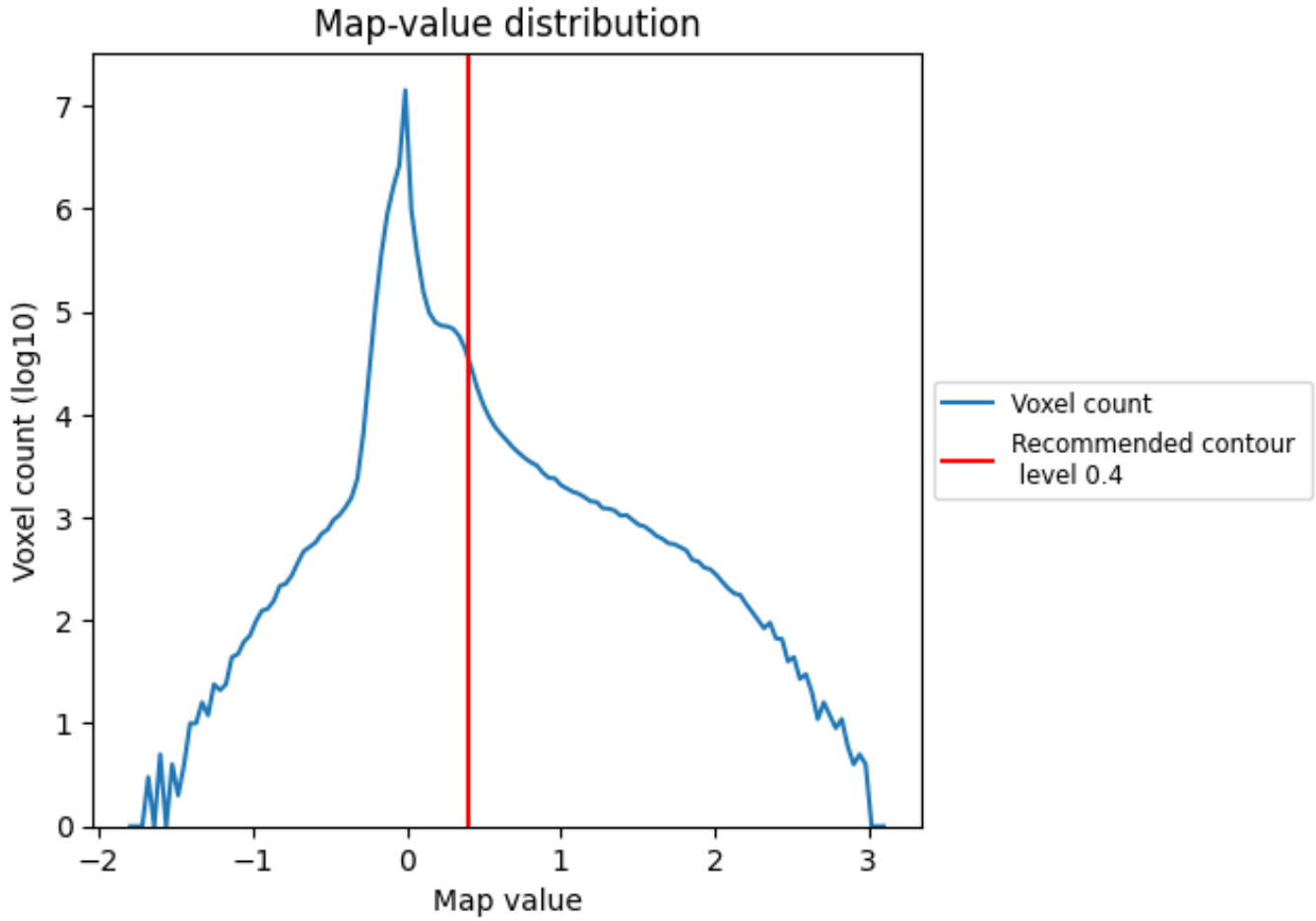
6.5 Mask visualisation (i)

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

7 Map analysis

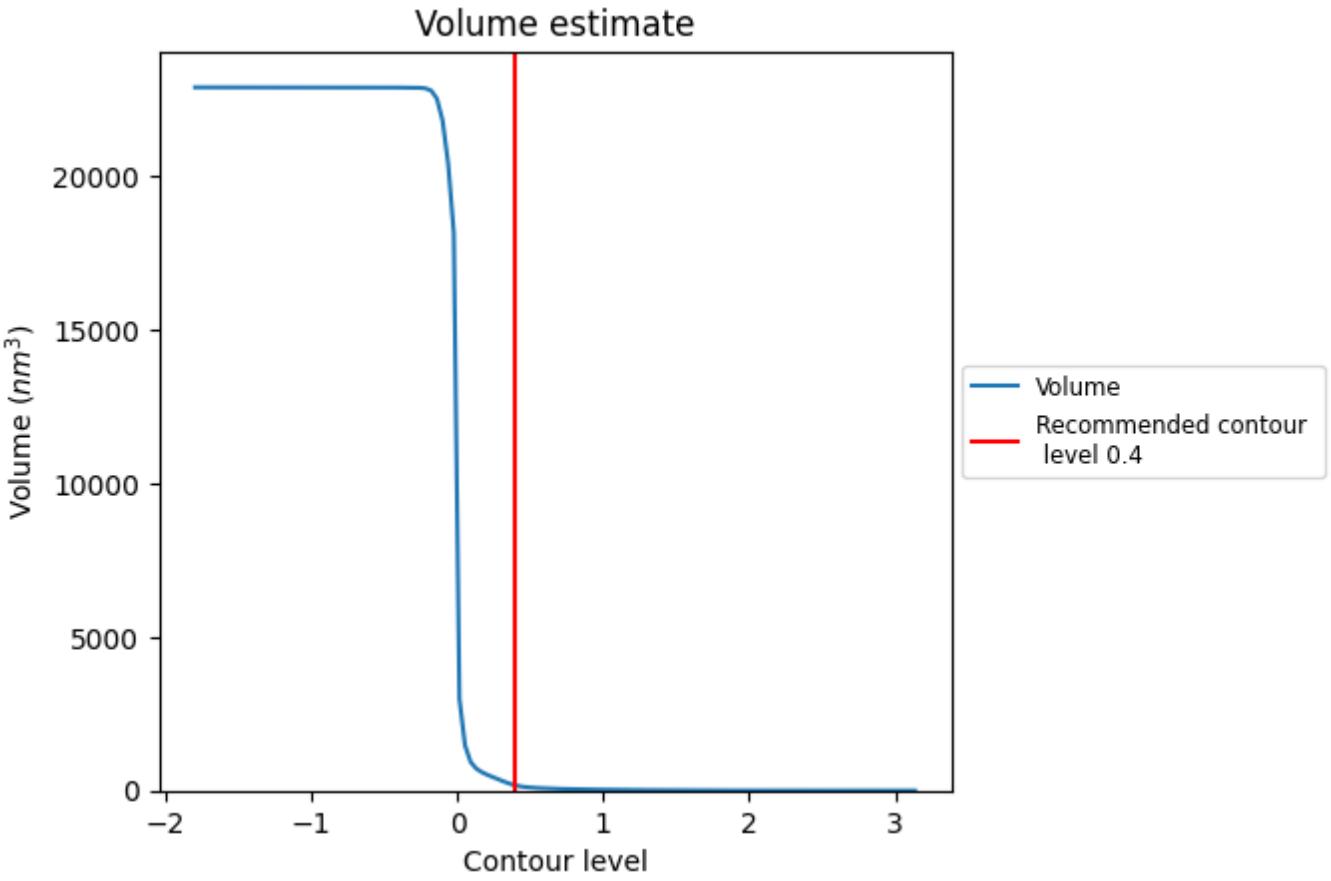
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

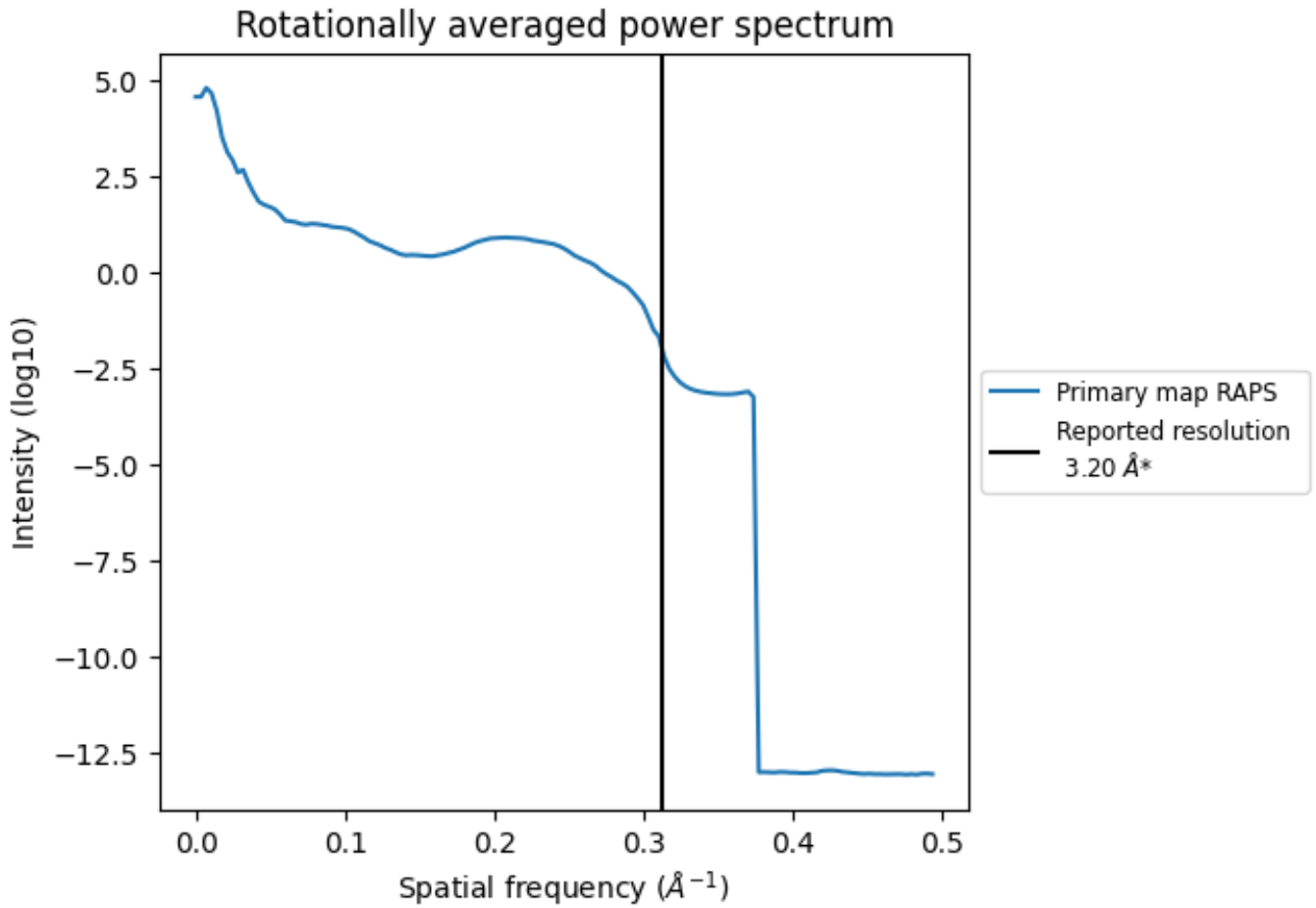
7.2 Volume estimate



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 153 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

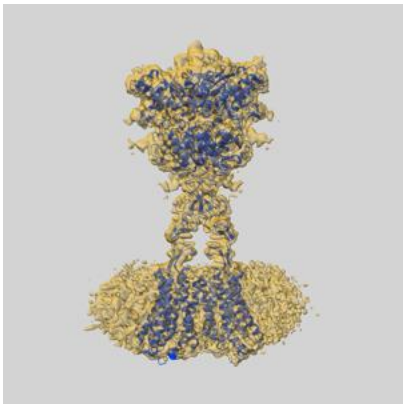
8 Fourier-Shell correlation

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

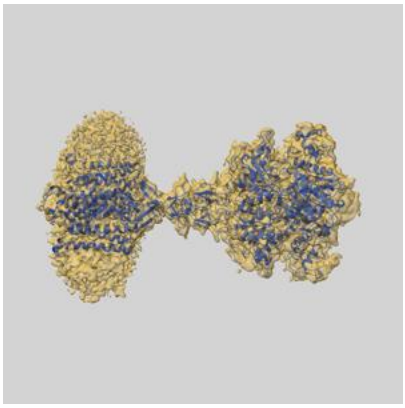
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30645 and PDB model 7DD6. Per-residue inclusion information can be found in section 3 on page 6.

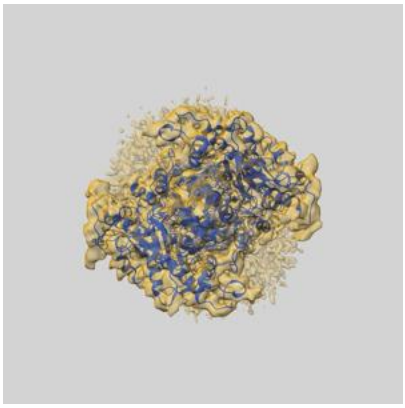
9.1 Map-model overlay



X



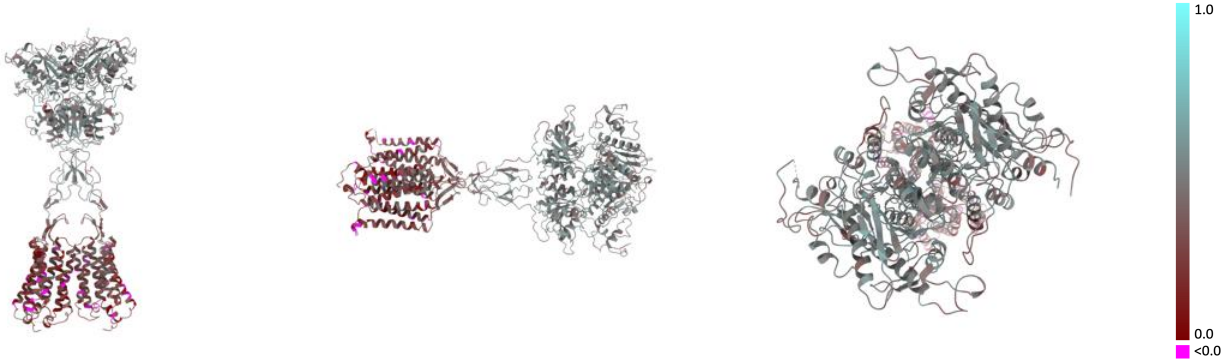
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

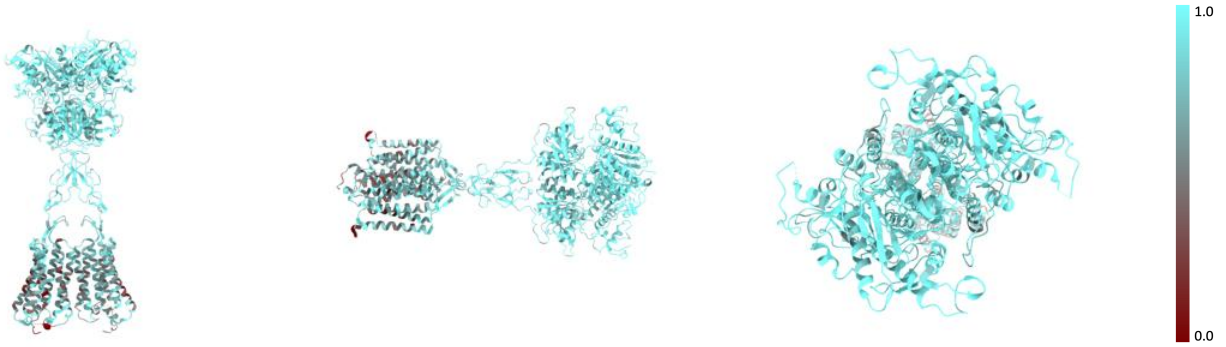
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

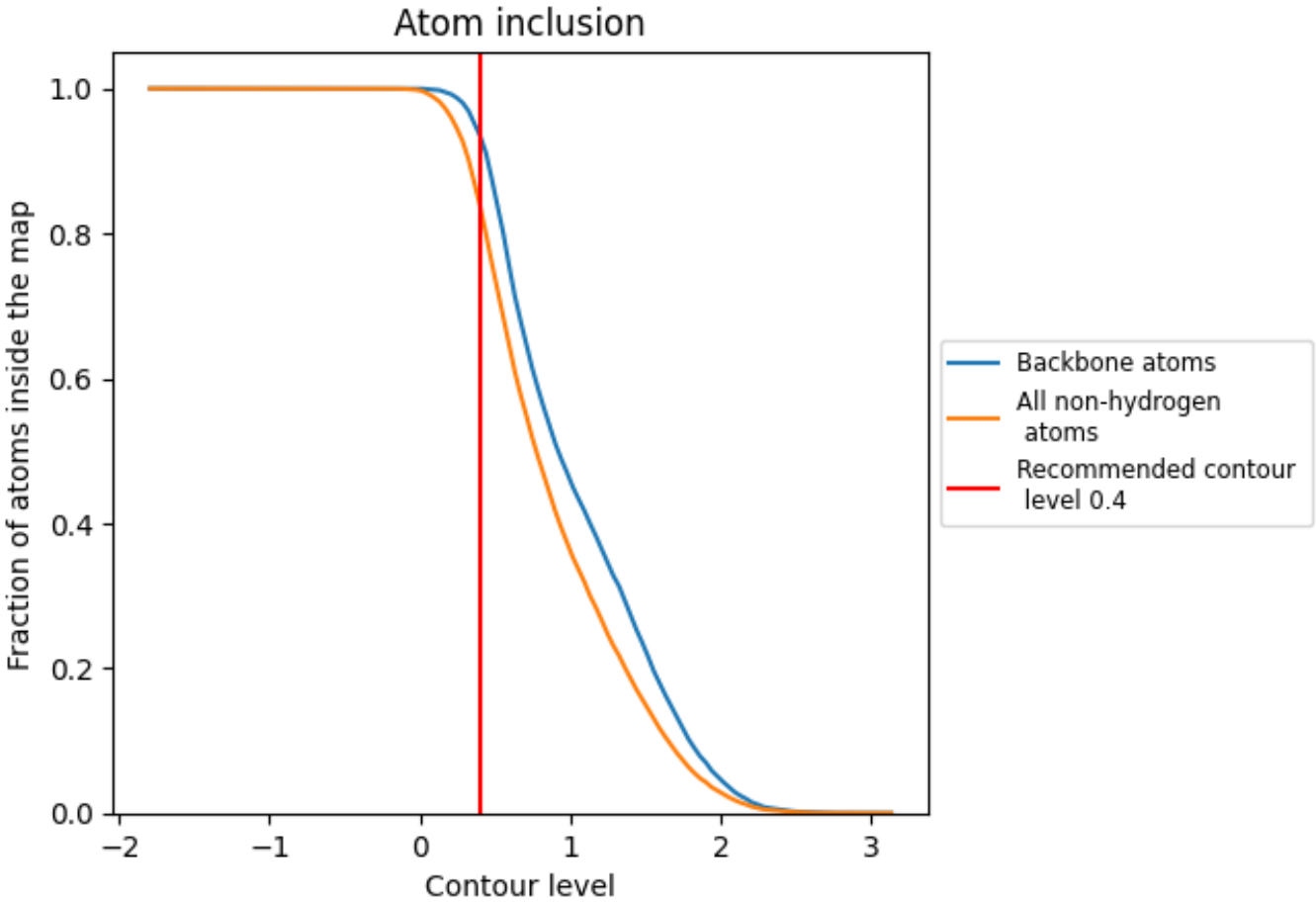
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8391	0.4100
A	0.8433	0.4100
B	0.8338	0.4080
C	0.8929	0.4190
D	0.9643	0.5370
E	0.8214	0.4240
F	0.9286	0.4580