



Full wwPDB EM Validation Report ⓘ

Nov 28, 2023 – 06:21 PM JST

PDB ID : 8WEA
EMDB ID : EMD-37476
Title : Human L-type voltage-gated calcium channel Cav1.2 (Class II) in the presence of pinaverium at 3.2 Angstrom resolution
Authors : Gao, S.; Yao, X.; Fan, X.; Yan, N.
Deposited on : 2023-09-17
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:

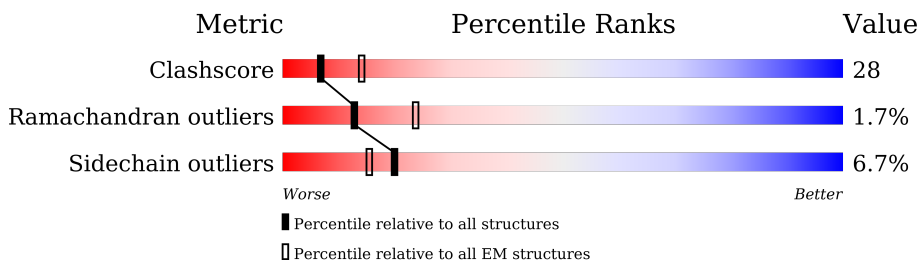
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 $\leq 5\%$. 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	2201	
2	D	1103	
3	B	3	
4	C	2	
4	F	2	
4	G	2	
5	E	4	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 17188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1206	9335	6116	1541	1617	61	0	0

- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	948	7570	4803	1269	1467	31	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



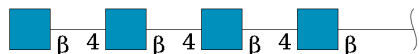
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0

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

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

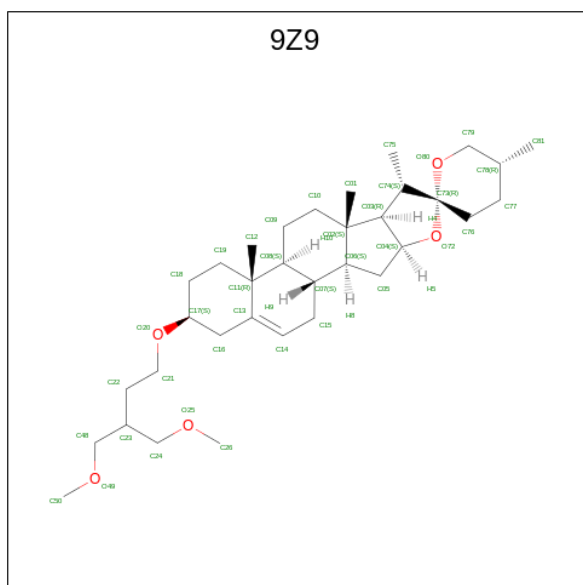


Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
5	E	4	56	32	4	20	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

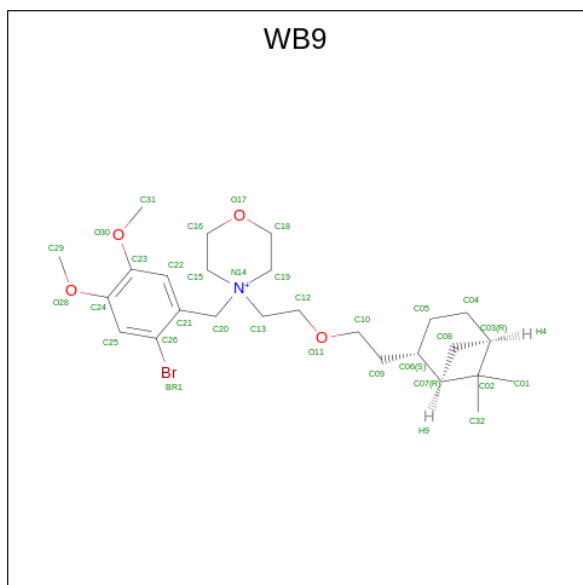
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spir ost-5-en (three-letter code: 9Z9) (formula: C₃₄H₅₆O₅) (labeled as "Ligand of Interest" by depositor).



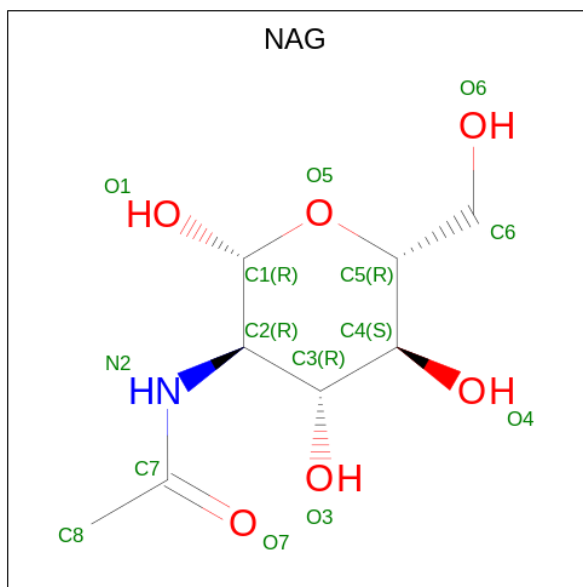
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			39	34	5	

- Molecule 8 is 4-[(2-bromanyl-4,5-dimethoxy-phenyl)methyl]-4-[2-[2-[(1 {R},2 {S},5 {R})-6,6-dimethyl-2-bicyclo[3.1.1]heptanyl]ethoxy]ethyl]morpholin-4-ium (three-letter code: WB9) (formula: C₂₆H₄₁BrNO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
8	A	1	Total	Br	C	N	O	0
			32	1	26	1	4	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

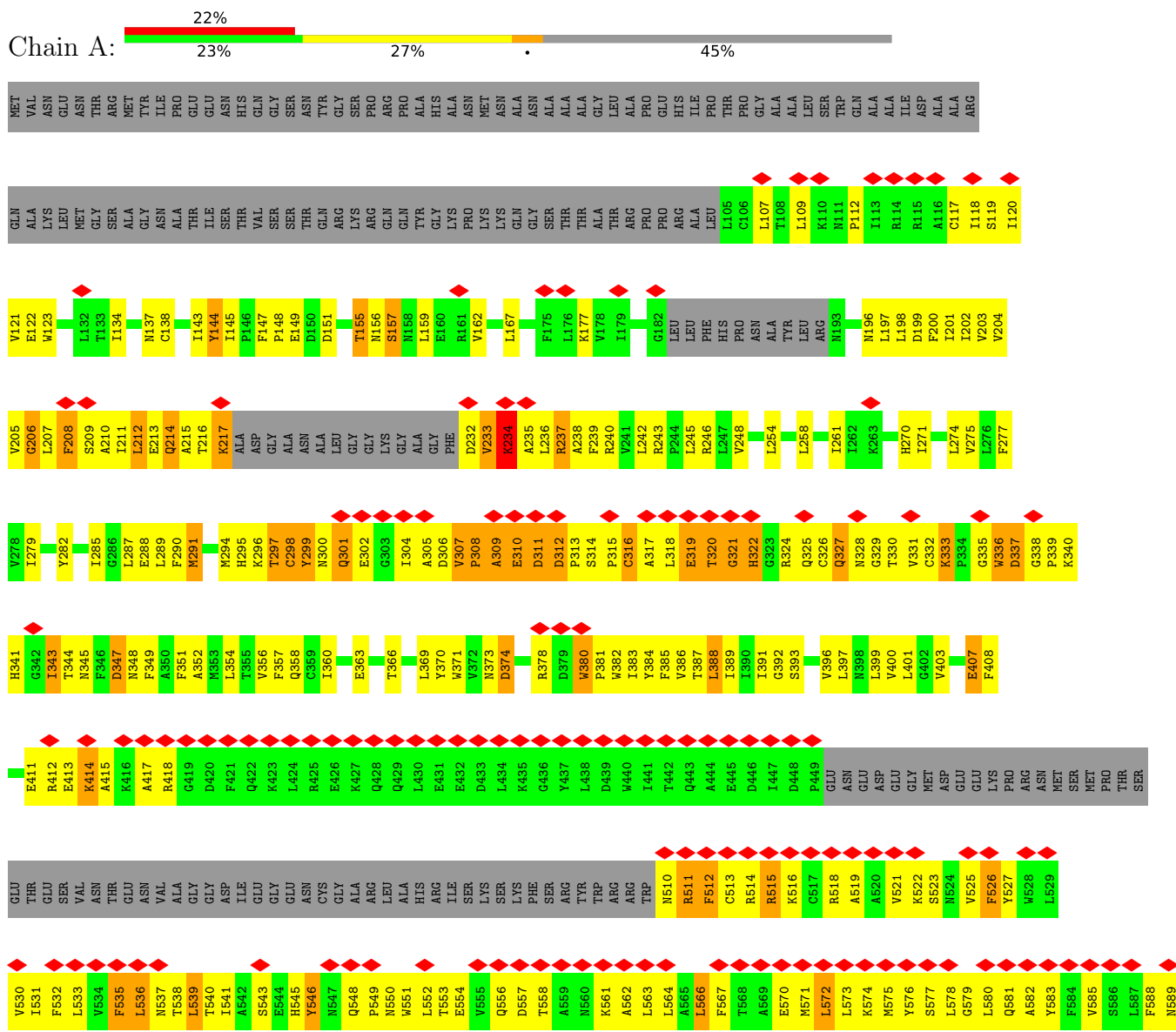


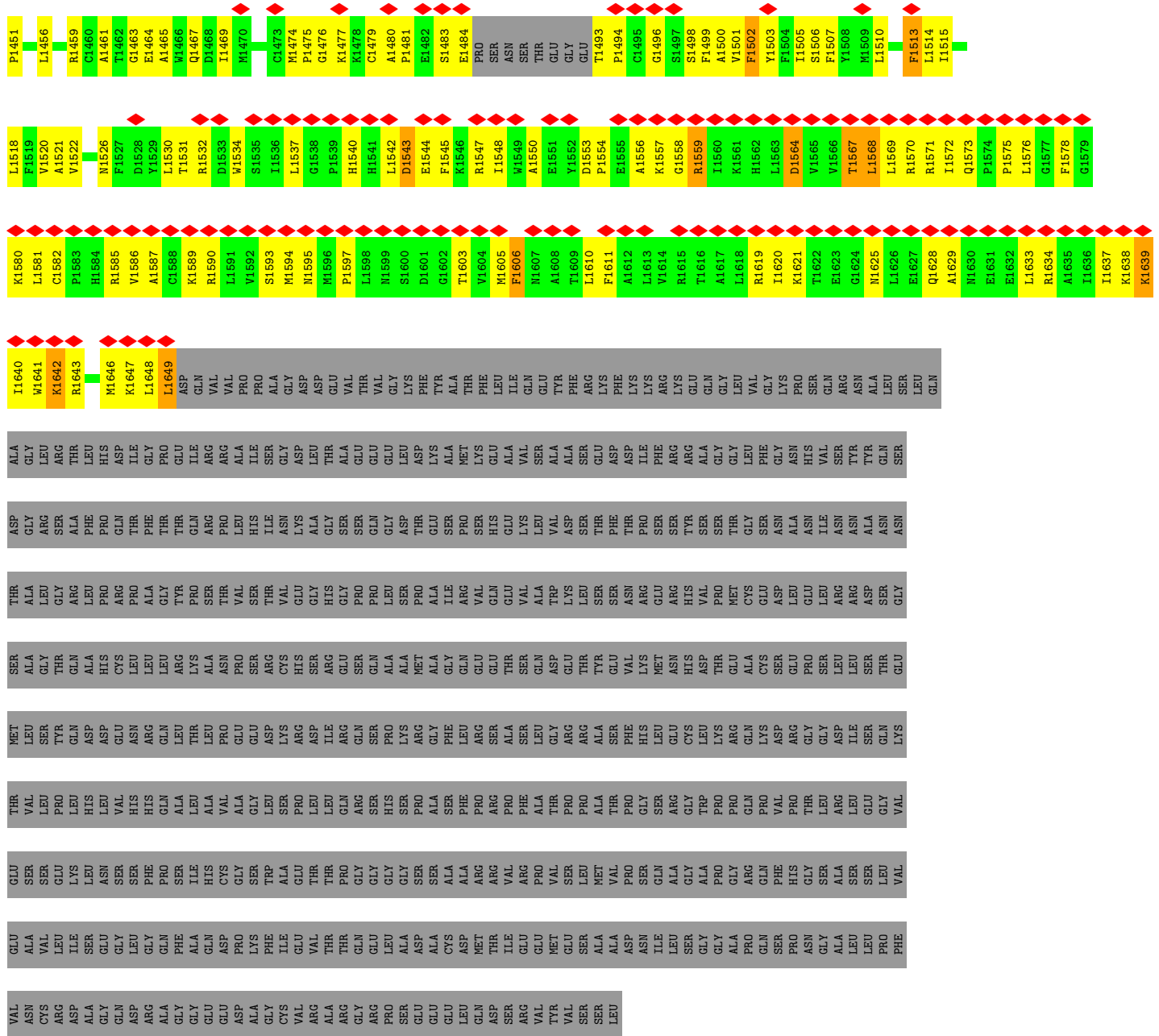
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots i

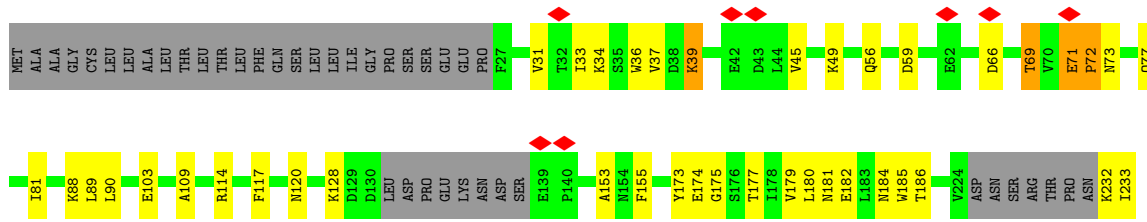
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

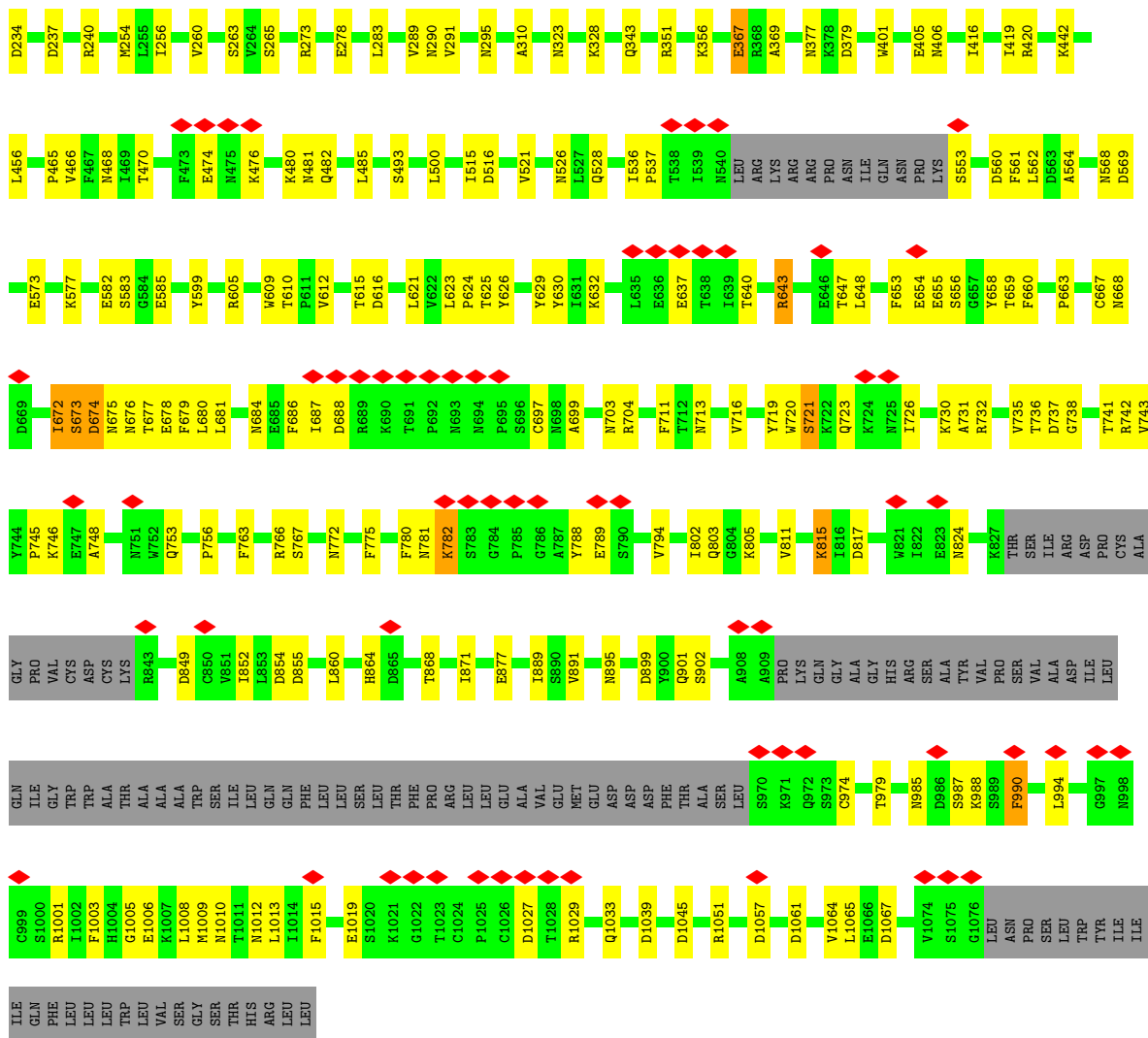
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1C





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





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299035	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.106	Depositor
Minimum map value	-2.750	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, WB9, 9Z9, CA

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	0.50	0/9535	0.61	0/12941
2	D	0.26	0/7728	0.49	0/10477
All	All	0.41	0/17263	0.56	0/23418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9335	0	9194	766	0
2	D	7570	0	7371	170	0
3	B	42	0	37	4	0
4	C	28	0	25	0	0
4	F	28	0	25	1	0
4	G	28	0	25	1	0
5	E	56	0	49	4	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	39	0	0	0	0
8	A	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	28	0	26	2	0
All	All	17188	0	16752	934	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 28.

All (934) 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:511:ARG:CZ	1:A:512:PHE:CE1	1.97	1.46
1:A:511:ARG:NH2	1:A:512:PHE:HE1	1.00	1.44
1:A:511:ARG:NH2	1:A:512:PHE:CE1	1.93	1.36
1:A:511:ARG:CZ	1:A:512:PHE:HE1	1.32	1.28
1:A:282:TYR:CD2	1:A:384:TYR:HE1	1.55	1.25
1:A:282:TYR:HD2	1:A:384:TYR:CE1	1.61	1.18
1:A:1214:LEU:HD11	1:A:1643:ARG:HG2	1.42	1.00
1:A:511:ARG:NE	1:A:512:PHE:CE1	2.33	0.97
2:D:72:PRO:HA	2:D:629:TYR:HA	1.46	0.97
1:A:282:TYR:CD2	1:A:384:TYR:CE1	2.44	0.94
1:A:201:ILE:O	1:A:205:VAL:HG23	1.68	0.94
1:A:363:GLU:HG3	1:A:708:TRP:HE1	1.32	0.92
1:A:1260:HIS:HD2	1:A:1263:GLN:HB3	1.34	0.91
1:A:1597:PRO:HB3	1:A:1646:MET:HG2	1.53	0.91
1:A:1567:THR:HA	1:A:1570:ARG:HB2	1.52	0.90
1:A:537:ASN:HB2	1:A:563:LEU:HD12	1.53	0.90
1:A:200:PHE:O	1:A:203:VAL:HG12	1.72	0.89
1:A:538:THR:HG23	1:A:627:ILE:HG13	1.55	0.88
1:A:201:ILE:O	1:A:204:VAL:CG1	2.20	0.88
1:A:921:ASP:HB2	1:A:929:ARG:HD3	1.53	0.88
1:A:511:ARG:H	1:A:511:ARG:HD3	1.39	0.87
1:A:620:ARG:HA	1:A:623:ARG:HD3	1.59	0.85
1:A:592:ASP:HA	1:A:625:LEU:HD21	1.59	0.85
1:A:969:ILE:HG22	1:A:970:LEU:HD13	1.61	0.83
1:A:512:PHE:HA	1:A:515:ARG:HD2	1.59	0.83
1:A:408:PHE:CE1	1:A:749:LEU:HB3	2.14	0.82
1:A:1374:THR:HG23	1:A:1377:ARG:HH21	1.46	0.81
1:A:1313:GLY:O	1:A:1316:ILE:HG12	1.81	0.81
1:A:204:VAL:HG13	1:A:205:VAL:H	1.45	0.80
1:A:634:TRP:HA	1:A:637:LEU:HB3	1.62	0.80
1:A:624:LEU:HA	1:A:627:ILE:HD13	1.64	0.80
1:A:1260:HIS:CD2	1:A:1263:GLN:HB3	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ASN:HD21	3:B:1:NAG:H62	1.46	0.79
1:A:1377:ARG:HG3	1:A:1380:ARG:HH12	1.47	0.79
1:A:713:TYR:HA	1:A:716:ILE:HG12	1.63	0.79
1:A:201:ILE:O	1:A:204:VAL:HG13	1.82	0.78
1:A:543:SER:HB3	1:A:552:LEU:HD11	1.65	0.78
1:A:279:ILE:HD11	1:A:360:ILE:HD13	1.64	0.78
1:A:299:TYR:HB2	1:A:333:LYS:HG3	1.64	0.78
1:A:511:ARG:NE	1:A:512:PHE:CD1	2.52	0.77
1:A:702:ILE:HG23	1:A:708:TRP:HB2	1.67	0.77
1:A:254:LEU:HD13	1:A:656:LEU:HD22	1.67	0.77
1:A:563:LEU:HA	1:A:566:LEU:HD22	1.65	0.77
1:A:511:ARG:HH21	1:A:512:PHE:HE1	1.29	0.77
1:A:298:CYS:O	1:A:308:PRO:HD2	1.84	0.76
1:A:316:CYS:SG	1:A:317:ALA:N	2.58	0.76
1:A:1031:ARG:C	1:A:1033:LYS:H	1.85	0.76
1:A:369:LEU:HD23	1:A:369:LEU:O	1.86	0.75
1:A:1573:GLN:HG3	1:A:1575:PRO:HG2	1.68	0.75
1:A:204:VAL:HG13	1:A:205:VAL:N	2.01	0.75
1:A:201:ILE:HA	1:A:204:VAL:CG1	2.17	0.74
1:A:701:GLN:HG3	1:A:706:GLU:HB2	1.69	0.74
1:A:382:TRP:CH2	1:A:383:ILE:HG12	2.22	0.74
1:A:702:ILE:HA	1:A:708:TRP:HB3	1.70	0.74
1:A:1585:ARG:HG2	1:A:1586:VAL:H	1.52	0.74
1:A:287:LEU:O	1:A:291:MET:CG	2.35	0.74
1:A:201:ILE:O	1:A:204:VAL:HG12	1.87	0.73
1:A:1611:PHE:HD1	1:A:1649:LEU:HA	1.51	0.73
1:A:541:ILE:HD12	1:A:627:ILE:HD11	1.67	0.73
1:A:382:TRP:CE3	1:A:383:ILE:HA	2.24	0.73
1:A:1634:ARG:HB2	1:A:1640:ILE:HG13	1.71	0.72
2:D:716:VAL:HA	2:D:720:TRP:HB2	1.69	0.72
1:A:408:PHE:HB3	1:A:753:VAL:HG21	1.71	0.72
1:A:901:ILE:O	1:A:905:LEU:HB2	1.90	0.72
2:D:39:LYS:NZ	2:D:824:ASN:O	2.22	0.72
1:A:354:LEU:HD23	1:A:354:LEU:O	1.90	0.71
1:A:624:LEU:O	1:A:627:ILE:HB	1.88	0.71
1:A:595:VAL:HB	1:A:625:LEU:HD23	1.71	0.71
1:A:1085:THR:HB	1:A:1088:GLU:HG3	1.70	0.71
1:A:1312:ILE:O	1:A:1316:ILE:HG23	1.90	0.71
1:A:407:GLU:HA	1:A:407:GLU:OE1	1.91	0.71
1:A:888:ARG:HG3	1:A:889:PHE:H	1.54	0.71
1:A:1548:ILE:HG23	1:A:1570:ARG:HH21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:860:LEU:HD12	2:D:1013:LEU:HD21	1.72	0.70
1:A:366:THR:HG21	1:A:1459:ARG:HG3	1.73	0.70
1:A:289:LEU:HD12	1:A:289:LEU:N	2.06	0.70
1:A:927:SER:O	1:A:928:PHE:C	2.29	0.69
1:A:270:HIS:NE2	1:A:1393:GLY:HA3	2.07	0.69
1:A:1436:ASN:O	1:A:1439:THR:HG22	1.90	0.69
1:A:211:ILE:O	1:A:214:GLN:HB3	1.94	0.68
1:A:906:ILE:HA	1:A:909:PHE:CD2	2.29	0.68
2:D:528:GLN:O	2:D:901:GLN:NE2	2.27	0.68
1:A:201:ILE:C	1:A:204:VAL:HG12	2.14	0.68
1:A:336:TRP:CH2	1:A:339:PRO:HA	2.29	0.67
1:A:200:PHE:O	1:A:203:VAL:CG1	2.40	0.67
1:A:201:ILE:HA	1:A:204:VAL:HG12	1.76	0.67
1:A:294:MET:CE	1:A:345:ASN:HA	2.24	0.67
1:A:960:PHE:O	1:A:963:ILE:HB	1.95	0.67
1:A:1407:ALA:C	1:A:1409:PRO:HD3	2.14	0.67
1:A:1568:LEU:HD13	1:A:1569:LEU:HG	1.77	0.67
1:A:1611:PHE:CD1	1:A:1649:LEU:HA	2.29	0.66
1:A:382:TRP:CZ3	1:A:383:ILE:HG12	2.30	0.66
1:A:1569:LEU:HD22	1:A:1572:ILE:HD13	1.77	0.66
1:A:1647:LYS:HG3	1:A:1648:LEU:H	1.60	0.66
2:D:109:ALA:HA	2:D:470:THR:HG22	1.78	0.66
1:A:1205:ASN:O	1:A:1208:GLN:HG2	1.95	0.66
1:A:391:ILE:HG12	1:A:391:ILE:O	1.96	0.66
1:A:203:VAL:HG13	1:A:204:VAL:N	2.09	0.66
1:A:1568:LEU:HD12	1:A:1569:LEU:H	1.61	0.66
1:A:965:THR:O	1:A:968:ILE:HB	1.96	0.66
1:A:968:ILE:HA	1:A:971:LYS:HB2	1.78	0.66
1:A:1567:THR:HA	1:A:1570:ARG:CB	2.23	0.66
1:A:143:ILE:O	1:A:144:TYR:C	2.32	0.65
1:A:345:ASN:OD1	1:A:351:PHE:HD2	1.78	0.65
1:A:1053:VAL:O	1:A:1057:THR:HG23	1.96	0.65
1:A:1215:LYS:HA	1:A:1643:ARG:HH22	1.61	0.65
1:A:511:ARG:HD3	1:A:511:ARG:N	2.12	0.65
1:A:515:ARG:HG2	1:A:516:LYS:N	2.10	0.65
1:A:1122:LEU:HD22	1:A:1122:LEU:H	1.62	0.65
1:A:1284:VAL:O	1:A:1287:ILE:HG13	1.97	0.65
1:A:756:LEU:HD21	1:A:1179:ASN:HA	1.79	0.65
1:A:961:THR:HA	1:A:964:PHE:CD2	2.32	0.65
1:A:107:LEU:HG	1:A:109:LEU:H	1.63	0.64
1:A:204:VAL:HG13	1:A:205:VAL:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:HB	1:A:237:ARG:HB2	1.79	0.64
1:A:399:LEU:O	1:A:403:VAL:HG23	1.96	0.64
1:A:545:HIS:CD2	1:A:552:LEU:HD22	2.33	0.64
1:A:1429:VAL:HG13	1:A:1430:PHE:H	1.62	0.64
1:A:1186:ILE:O	1:A:1189:PHE:N	2.30	0.64
1:A:1191:GLU:O	1:A:1192:GLN:C	2.36	0.64
1:A:1302:PRO:O	1:A:1305:VAL:HG12	1.98	0.64
1:A:213:GLU:HA	1:A:216:THR:CG2	2.28	0.64
1:A:414:LYS:C	1:A:414:LYS:HD2	2.18	0.64
1:A:603:THR:O	1:A:606:VAL:HG22	1.97	0.64
1:A:1083:LYS:HD2	1:A:1088:GLU:HB3	1.79	0.64
2:D:802:ILE:HG22	2:D:803:GLN:OE1	1.97	0.64
1:A:354:LEU:HD23	1:A:354:LEU:C	2.17	0.64
1:A:1060:GLN:HE22	1:A:1169:TYR:HD1	1.46	0.64
1:A:287:LEU:O	1:A:291:MET:HG2	1.98	0.64
1:A:593:CYS:O	1:A:596:VAL:HG12	1.98	0.63
2:D:177:THR:HG22	2:D:181:ASN:ND2	2.12	0.63
1:A:201:ILE:CA	1:A:204:VAL:HG12	2.27	0.63
2:D:583:SER:HB2	2:D:610:THR:HG22	1.80	0.63
1:A:1250:LEU:O	1:A:1254:ILE:HG13	1.97	0.63
1:A:606:VAL:O	1:A:607:GLU:C	2.37	0.63
1:A:955:ASN:O	1:A:959:VAL:HG13	1.99	0.62
1:A:1422:TYR:CE2	1:A:1507:PHE:HB2	2.34	0.62
2:D:647:THR:HB	2:D:713:ASN:HD22	1.64	0.62
1:A:370:TYR:CD1	1:A:1444:ASN:HB3	2.34	0.62
1:A:275:VAL:HG22	1:A:396:VAL:HG11	1.81	0.62
1:A:1403:LYS:HA	1:A:1406:GLN:HE22	1.64	0.62
2:D:174:GLU:HA	2:D:179:VAL:HG11	1.80	0.62
1:A:1319:ILE:O	1:A:1322:GLU:HG2	2.00	0.62
1:A:673:PHE:HB3	1:A:677:PHE:CE1	2.35	0.62
1:A:702:ILE:HA	1:A:708:TRP:CB	2.29	0.62
2:D:71:GLU:HB3	2:D:630:TYR:CE1	2.35	0.62
1:A:539:LEU:HG	1:A:540:THR:N	2.15	0.61
1:A:1288:LEU:O	1:A:1291:ILE:HG22	2.00	0.61
1:A:309:ALA:O	1:A:310:GLU:C	2.38	0.61
1:A:748:PHE:O	1:A:749:LEU:C	2.39	0.61
1:A:965:THR:O	1:A:968:ILE:N	2.32	0.61
2:D:640:THR:HA	2:D:643:ARG:HE	1.64	0.61
1:A:625:LEU:HA	1:A:628:PHE:CZ	2.35	0.61
1:A:1501:VAL:O	1:A:1505:ILE:HG22	1.99	0.61
2:D:648:LEU:HD12	2:D:680:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1001:ARG:HE	2:D:1019:GLU:HB2	1.65	0.61
1:A:518:ARG:HA	1:A:577:SER:OG	2.00	0.61
1:A:134:ILE:HD11	1:A:246:ARG:HD3	1.80	0.61
2:D:673:SER:H	2:D:679:PHE:HD2	1.47	0.61
1:A:308:PRO:O	1:A:310:GLU:N	2.33	0.61
2:D:568:ASN:OD1	2:D:569:ASP:N	2.32	0.61
1:A:378:ARG:HB2	1:A:378:ARG:CZ	2.31	0.61
1:A:583:TYR:HE2	1:A:593:CYS:SG	2.23	0.61
1:A:1476:GLY:O	1:A:1493:THR:HB	2.00	0.61
1:A:370:TYR:CE1	1:A:1444:ASN:HB3	2.36	0.61
1:A:233:VAL:O	1:A:234:LYS:C	2.38	0.60
1:A:1377:ARG:HG3	1:A:1380:ARG:NH1	2.15	0.60
1:A:387:THR:O	1:A:391:ILE:HG22	2.01	0.60
1:A:588:PHE:HZ	1:A:629:LYS:HA	1.66	0.60
1:A:1310:ILE:CD1	1:A:1383:ARG:HG3	2.31	0.60
1:A:206:GLY:O	1:A:207:LEU:C	2.38	0.60
1:A:894:HIS:HA	1:A:897:VAL:HG22	1.82	0.60
1:A:681:GLU:HB2	1:A:685:ARG:HH22	1.67	0.60
2:D:31:VAL:HA	2:D:34:LYS:HE2	1.83	0.60
1:A:412:ARG:NH2	1:A:758:ASP:N	2.49	0.60
1:A:512:PHE:O	1:A:516:LYS:HD3	2.01	0.60
1:A:707:ASP:O	1:A:711:VAL:HG23	2.02	0.60
2:D:1009:MET:SD	2:D:1009:MET:N	2.75	0.60
1:A:550:ASN:HA	1:A:553:THR:OG1	2.02	0.60
1:A:617:SER:HB3	1:A:1069:GLN:HG3	1.84	0.60
1:A:1089:CYS:SG	1:A:1109:ARG:HB3	2.42	0.60
2:D:730:LYS:HE2	2:D:817:ASP:HB3	1.84	0.60
1:A:199:ASP:OD2	1:A:246:ARG:NH2	2.35	0.60
1:A:1310:ILE:HD13	1:A:1383:ARG:HG3	1.84	0.60
1:A:1594:MET:HB2	1:A:1648:LEU:HD22	1.83	0.60
1:A:917:LEU:HD23	1:A:917:LEU:H	1.66	0.60
1:A:137:ASN:HD22	1:A:243:ARG:HD2	1.65	0.59
1:A:340:LYS:HE2	1:A:371:TRP:HH2	1.67	0.59
1:A:523:SER:HB3	1:A:525:VAL:HG12	1.84	0.59
1:A:1422:TYR:HE2	1:A:1507:PHE:CA	2.15	0.59
1:A:373:ASN:ND2	1:A:378:ARG:HG3	2.17	0.59
1:A:701:GLN:CG	1:A:706:GLU:HB2	2.31	0.59
1:A:1031:ARG:C	1:A:1033:LYS:N	2.51	0.59
1:A:1459:ARG:HD3	1:A:1469:ILE:HD11	1.84	0.59
1:A:302:GLU:HG2	1:A:329:GLY:O	2.03	0.59
1:A:920:GLU:O	1:A:922:PRO:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1568:LEU:HD12	1:A:1569:LEU:N	2.18	0.59
2:D:260:VAL:HG23	2:D:295:ASN:HB3	1.84	0.59
1:A:901:ILE:HA	1:A:905:LEU:HG	1.83	0.59
1:A:1075:LEU:HB2	1:A:1113:ASN:HD21	1.68	0.59
2:D:585:GLU:N	2:D:585:GLU:OE2	2.36	0.59
2:D:780:PHE:HE1	9:D:1203:NAG:H4	1.67	0.59
1:A:204:VAL:O	1:A:208:PHE:HB2	2.03	0.59
1:A:307:VAL:HG21	1:A:313:PRO:HB3	1.83	0.59
1:A:924:GLN:HE22	1:A:927:SER:N	2.01	0.59
1:A:956:ALA:O	1:A:959:VAL:HG22	2.03	0.59
1:A:1639:LYS:HD2	1:A:1640:ILE:N	2.18	0.59
2:D:659:THR:OG1	2:D:742:ARG:NH1	2.36	0.59
1:A:155:THR:O	1:A:159:LEU:HD12	2.03	0.59
1:A:1422:TYR:HE2	1:A:1507:PHE:HA	1.66	0.58
1:A:290:PHE:HE2	1:A:384:TYR:CD2	2.21	0.58
1:A:1316:ILE:HD11	1:A:1376:PHE:CD1	2.38	0.58
1:A:1403:LYS:HD2	1:A:1406:GLN:HE22	1.67	0.58
1:A:1449:THR:O	1:A:1450:PHE:C	2.41	0.58
1:A:961:THR:O	1:A:965:THR:HG23	2.02	0.58
1:A:1537:LEU:HD11	1:A:1576:LEU:HG	1.84	0.58
1:A:673:PHE:HB3	1:A:677:PHE:HE1	1.67	0.58
1:A:1211:GLU:HG3	1:A:1637:ILE:HD11	1.84	0.58
2:D:526:ASN:ND2	2:D:564:ALA:O	2.35	0.58
1:A:536:LEU:O	1:A:539:LEU:HB3	2.02	0.58
1:A:591:PHE:CE1	1:A:625:LEU:HD13	2.38	0.58
2:D:599:TYR:OH	2:D:854:ASP:OD2	2.20	0.58
2:D:240:ARG:NH2	2:D:278:GLU:O	2.36	0.58
1:A:533:LEU:HD13	1:A:536:LEU:HD23	1.84	0.58
2:D:537:PRO:HD3	2:D:974:CYS:HB3	1.84	0.58
1:A:1118:PHE:HZ	1:A:1166:PHE:CZ	2.22	0.57
1:A:385:PHE:O	1:A:386:VAL:C	2.41	0.57
1:A:1224:PRO:HG2	1:A:1230:TYR:HD1	1.69	0.57
2:D:889:ILE:HG23	2:D:891:VAL:HG13	1.86	0.57
1:A:324:ARG:HB2	1:A:374:ASP:OD1	2.03	0.57
1:A:712:MET:HA	1:A:733:PHE:CD2	2.40	0.57
1:A:1532:ARG:HD2	1:A:1534:TRP:CE3	2.39	0.57
1:A:1296:LYS:H	1:A:1296:LYS:HD2	1.69	0.57
1:A:285:ILE:O	1:A:289:LEU:HD13	2.04	0.57
1:A:378:ARG:HB3	1:A:378:ARG:NH1	2.19	0.57
1:A:1168:ILE:O	1:A:1169:TYR:C	2.43	0.57
2:D:788:TYR:OH	2:D:868:THR:O	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:NAG:H62	5:E:3:NAG:H61	1.86	0.57
2:D:90:LEU:HD12	2:D:615:THR:HG21	1.85	0.57
1:A:591:PHE:CE1	1:A:625:LEU:HB2	2.40	0.56
1:A:670:MET:HE1	1:A:692:PHE:HB2	1.87	0.56
1:A:1597:PRO:HA	1:A:1647:LYS:HB3	1.86	0.56
1:A:382:TRP:CE3	1:A:383:ILE:N	2.73	0.56
1:A:1063:PHE:O	1:A:1066:ILE:HB	2.05	0.56
1:A:1559:ARG:NH1	1:A:1605:MET:SD	2.76	0.56
1:A:313:PRO:HB2	1:A:336:TRP:CE2	2.40	0.56
1:A:340:LYS:O	1:A:341:HIS:HB2	2.05	0.56
1:A:363:GLU:HG3	1:A:708:TRP:NE1	2.14	0.56
1:A:581:GLN:O	1:A:585:VAL:HG23	2.05	0.56
1:A:1439:THR:HG23	1:A:1441:ILE:H	1.69	0.56
1:A:1611:PHE:CD1	1:A:1649:LEU:HD12	2.40	0.56
1:A:270:HIS:CD2	1:A:1393:GLY:HA3	2.40	0.56
1:A:274:LEU:HD13	1:A:1398:LEU:HD11	1.87	0.56
1:A:382:TRP:CE3	1:A:383:ILE:CA	2.88	0.56
1:A:1640:ILE:HG12	1:A:1640:ILE:O	2.06	0.56
1:A:927:SER:O	1:A:929:ARG:N	2.38	0.56
1:A:1155:ILE:HG22	1:A:1156:TYR:HD2	1.69	0.56
2:D:672:ILE:HA	2:D:679:PHE:HE2	1.70	0.56
1:A:415:ALA:O	1:A:418:ARG:HB2	2.05	0.56
1:A:905:LEU:HB3	1:A:909:PHE:CZ	2.41	0.56
1:A:602:GLU:O	1:A:606:VAL:HG13	2.06	0.56
2:D:1027:ASP:OD1	2:D:1027:ASP:N	2.38	0.56
2:D:743:VAL:HG12	2:D:745:PRO:HD2	1.88	0.56
2:D:753:GLN:OE1	2:D:753:GLN:N	2.39	0.56
2:D:803:GLN:HG2	2:D:805:LYS:HD2	1.87	0.56
1:A:343:ILE:HD12	1:A:713:TYR:CD1	2.41	0.56
1:A:710:SER:HA	1:A:713:TYR:CD2	2.40	0.56
1:A:1401:PHE:CZ	1:A:1530:LEU:HD21	2.41	0.56
1:A:271:ILE:HD11	1:A:1397:LEU:HD13	1.86	0.56
1:A:892:GLN:O	1:A:896:ILE:HG13	2.06	0.56
1:A:1160:VAL:O	1:A:1163:SER:HB3	2.06	0.56
1:A:1034:GLY:HA3	8:A:2303:WB9:C29	2.36	0.55
2:D:625:THR:HG22	2:D:626:TYR:H	1.71	0.55
1:A:1061:PHE:HA	1:A:1125:MET:SD	2.46	0.55
2:D:128:LYS:NZ	2:D:234:ASP:OD2	2.39	0.55
1:A:620:ARG:HG2	1:A:623:ARG:NH1	2.22	0.55
2:D:577:LYS:HE3	2:D:609:TRP:HZ2	1.71	0.55
1:A:201:ILE:HA	1:A:204:VAL:HG11	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:HE1	1:A:335:GLY:HA3	1.72	0.55
1:A:588:PHE:CZ	1:A:629:LYS:HA	2.41	0.55
2:D:621:LEU:HD21	2:D:623:LEU:HD22	1.88	0.55
1:A:1308:PHE:HD2	1:A:1309:LEU:HD12	1.72	0.55
1:A:308:PRO:O	1:A:309:ALA:C	2.44	0.55
1:A:910:ILE:HA	1:A:913:SER:HB3	1.88	0.55
2:D:775:PHE:CE1	2:D:794:VAL:HG13	2.41	0.55
1:A:909:PHE:O	1:A:913:SER:HB2	2.07	0.55
1:A:382:TRP:CZ3	1:A:383:ILE:HA	2.41	0.55
1:A:537:ASN:HB2	1:A:563:LEU:CD1	2.34	0.55
1:A:570:GLU:O	1:A:573:LEU:HG	2.06	0.55
2:D:120:ASN:OD1	3:B:1:NAG:H61	2.06	0.55
1:A:387:THR:O	1:A:388:LEU:C	2.44	0.55
1:A:412:ARG:HH12	1:A:757:ALA:HB3	1.71	0.55
2:D:775:PHE:H	2:D:1012:ASN:ND2	2.04	0.55
1:A:564:LEU:HD11	1:A:599:GLY:HA3	1.89	0.54
2:D:673:SER:N	2:D:679:PHE:HD2	2.05	0.54
1:A:205:VAL:HG11	1:A:239:PHE:CD2	2.42	0.54
1:A:213:GLU:HA	1:A:216:THR:HG23	1.88	0.54
1:A:339:PRO:HG3	1:A:344:THR:O	2.07	0.54
1:A:540:THR:HA	1:A:556:GLN:NE2	2.21	0.54
1:A:1399:TRP:CH2	1:A:1403:LYS:HG2	2.42	0.54
1:A:344:THR:HG21	1:A:371:TRP:HZ3	1.71	0.54
1:A:672:LEU:HD21	1:A:729:VAL:HG22	1.88	0.54
1:A:1116:PHE:CD1	1:A:1127:ALA:HB1	2.42	0.54
1:A:1232:VAL:HG21	1:A:1291:ILE:O	2.08	0.54
1:A:1559:ARG:CG	1:A:1603:THR:HA	2.38	0.54
1:A:378:ARG:CZ	1:A:378:ARG:CB	2.86	0.54
1:A:724:PHE:HB3	1:A:725:PRO:HD3	1.87	0.54
1:A:1220:ARG:HB3	1:A:1556:ALA:N	2.23	0.54
1:A:1479:CYS:SG	1:A:1494:PRO:HD2	2.48	0.54
1:A:1573:GLN:HG3	1:A:1575:PRO:CG	2.36	0.54
1:A:167:LEU:HD21	1:A:243:ARG:HH22	1.71	0.54
1:A:311:ASP:O	1:A:312:ASP:C	2.43	0.54
1:A:1170:ILE:O	1:A:1171:ILE:C	2.46	0.54
2:D:237:ASP:OD2	2:D:420:ARG:NH1	2.40	0.54
2:D:994:LEU:HB2	2:D:1003:PHE:HE2	1.72	0.54
1:A:964:PHE:O	1:A:967:GLU:HB2	2.07	0.54
2:D:254:MET:HE3	2:D:283:LEU:HD21	1.89	0.54
2:D:599:TYR:HD2	2:D:766:ARG:HH21	1.56	0.53
1:A:408:PHE:HE1	1:A:749:LEU:HB3	1.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:TYR:CZ	1:A:1107:GLN:HB2	2.42	0.53
1:A:313:PRO:HB2	1:A:336:TRP:CZ2	2.43	0.53
1:A:637:LEU:O	1:A:640:LEU:HG	2.08	0.53
1:A:972:MET:O	1:A:973:THR:C	2.45	0.53
1:A:1233:TRP:HA	1:A:1292:ALA:HB1	1.90	0.53
1:A:1233:TRP:O	1:A:1234:TYR:C	2.45	0.53
2:D:474:GLU:OE1	2:D:474:GLU:N	2.41	0.53
2:D:647:THR:HB	2:D:713:ASN:ND2	2.23	0.53
2:D:735:VAL:HB	2:D:811:VAL:HG12	1.89	0.53
1:A:177:LYS:NZ	1:A:196:ASN:HD21	2.07	0.53
1:A:662:ILE:HD13	1:A:700:PHE:CE1	2.44	0.53
1:A:718:ALA:O	1:A:719:TYR:C	2.46	0.53
1:A:928:PHE:O	1:A:952:ILE:HG13	2.08	0.53
1:A:663:ILE:HG23	1:A:692:PHE:HZ	1.74	0.53
1:A:1078:CYS:HB2	1:A:1111:TRP:CE3	2.43	0.53
1:A:1282:PHE:O	1:A:1285:GLU:HG3	2.07	0.53
1:A:282:TYR:CE2	1:A:384:TYR:CE1	2.97	0.53
1:A:408:PHE:HE1	1:A:750:ALA:N	2.07	0.53
1:A:540:THR:HA	1:A:556:GLN:HE22	1.72	0.53
1:A:713:TYR:HA	1:A:716:ILE:CG1	2.37	0.53
1:A:1545:PHE:CD1	1:A:1610:LEU:HD13	2.43	0.53
1:A:602:GLU:HB3	1:A:619:LEU:HD23	1.91	0.53
1:A:673:PHE:HE2	1:A:729:VAL:HG13	1.74	0.53
1:A:730:CYS:C	1:A:732:TYR:N	2.59	0.53
1:A:296:LYS:HD3	1:A:318:LEU:HD21	1.90	0.53
1:A:1121:VAL:O	1:A:1125:MET:HG2	2.09	0.53
1:A:336:TRP:O	1:A:337:ASP:C	2.47	0.52
1:A:1164:ILE:HA	1:A:1167:ILE:HD12	1.90	0.52
1:A:1174:ALA:O	1:A:1175:PHE:C	2.47	0.52
1:A:369:LEU:HD23	1:A:369:LEU:C	2.30	0.52
1:A:734:ILE:O	1:A:737:PHE:N	2.41	0.52
1:A:1597:PRO:HA	1:A:1647:LYS:CB	2.39	0.52
1:A:306:ASP:O	1:A:307:VAL:C	2.47	0.52
1:A:1120:ASN:O	1:A:1121:VAL:C	2.48	0.52
1:A:1316:ILE:O	1:A:1320:LEU:HD13	2.09	0.52
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.91	0.52
1:A:248:VAL:HG23	1:A:660:LEU:HD23	1.90	0.52
1:A:327:GLN:HG2	1:A:328:ASN:CG	2.30	0.52
1:A:370:TYR:CE1	1:A:1444:ASN:CB	2.92	0.52
1:A:1164:ILE:O	1:A:1168:ILE:HG12	2.10	0.52
1:A:654:LEU:HD22	1:A:747:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ALA:O	1:A:754:ASP:N	2.43	0.52
1:A:661:PHE:CZ	1:A:736:LEU:HD12	2.45	0.52
1:A:1513:PHE:O	1:A:1514:LEU:C	2.45	0.52
2:D:656:SER:OG	2:D:713:ASN:ND2	2.42	0.52
2:D:789:GLU:N	2:D:789:GLU:OE1	2.42	0.52
1:A:335:GLY:O	1:A:336:TRP:C	2.48	0.52
1:A:514:ARG:O	1:A:518:ARG:HD3	2.09	0.52
1:A:928:PHE:CE1	1:A:952:ILE:HG12	2.45	0.52
1:A:1399:TRP:CZ3	1:A:1403:LYS:HG2	2.45	0.52
1:A:1526:ASN:O	1:A:1530:LEU:HD23	2.10	0.52
1:A:370:TYR:CD1	1:A:1444:ASN:CB	2.92	0.52
1:A:1320:LEU:O	1:A:1323:THR:OG1	2.27	0.52
2:D:577:LYS:NZ	2:D:582:GLU:OE1	2.43	0.52
1:A:730:CYS:C	1:A:732:TYR:H	2.14	0.52
1:A:748:PHE:O	1:A:751:ILE:N	2.43	0.52
1:A:751:ILE:O	1:A:755:ASN:HB3	2.09	0.52
2:D:852:ILE:HB	2:D:1013:LEU:HD22	1.90	0.52
1:A:378:ARG:NH1	1:A:378:ARG:CB	2.73	0.51
1:A:704:THR:OG1	1:A:706:GLU:HG2	2.10	0.51
1:A:1581:LEU:HD21	1:A:1585:ARG:HD3	1.92	0.51
2:D:1006:GLU:O	2:D:1015:PHE:N	2.29	0.51
1:A:298:CYS:SG	1:A:330:THR:HB	2.50	0.51
1:A:356:VAL:O	1:A:360:ILE:HG23	2.10	0.51
1:A:408:PHE:CB	1:A:753:VAL:HG21	2.40	0.51
1:A:634:TRP:O	1:A:635:ASN:C	2.49	0.51
1:A:755:ASN:O	1:A:756:LEU:C	2.47	0.51
1:A:928:PHE:CD1	1:A:952:ILE:HG12	2.45	0.51
1:A:1212:TYR:OH	1:A:1543:ASP:HA	2.10	0.51
1:A:314:SER:O	1:A:315:PRO:C	2.46	0.51
1:A:1087:ALA:HA	1:A:1090:LYS:NZ	2.25	0.51
1:A:1212:TYR:CE2	1:A:1542:LEU:HB3	2.46	0.51
1:A:1590:ARG:HA	1:A:1593:SER:HB3	1.92	0.51
2:D:290:ASN:ND2	2:D:343:GLN:OE1	2.44	0.51
2:D:673:SER:OG	2:D:678:GLU:HG3	2.10	0.51
1:A:340:LYS:HE2	1:A:371:TRP:CH2	2.46	0.51
1:A:1116:PHE:HD1	1:A:1127:ALA:HB1	1.74	0.51
1:A:1434:ALA:HA	1:A:1480:ALA:HB2	1.92	0.51
2:D:780:PHE:CE1	9:D:1203:NAG:H4	2.46	0.51
1:A:966:LEU:O	1:A:970:LEU:HD22	2.10	0.51
1:A:546:TYR:CE2	1:A:1073:GLY:HA2	2.45	0.51
1:A:1122:LEU:O	1:A:1125:MET:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:GLY:O	1:A:580:LEU:C	2.48	0.51
1:A:925:HIS:NE2	1:A:1484:GLU:HB3	2.26	0.51
1:A:287:LEU:C	1:A:287:LEU:HD12	2.30	0.51
1:A:336:TRP:CE2	1:A:338:GLY:O	2.64	0.51
1:A:749:LEU:O	1:A:750:ALA:C	2.49	0.51
1:A:1163:SER:O	1:A:1167:ILE:HG13	2.11	0.51
1:A:1586:VAL:O	1:A:1587:ALA:C	2.49	0.51
2:D:616:ASP:OD1	2:D:616:ASP:N	2.44	0.51
1:A:203:VAL:CG1	1:A:204:VAL:N	2.72	0.51
1:A:285:ILE:O	1:A:289:LEU:CD1	2.58	0.51
1:A:300:ASN:OD1	1:A:331:VAL:HB	2.10	0.51
1:A:1550:ALA:HA	1:A:1553:ASP:HB3	1.92	0.51
1:A:1647:LYS:HG3	1:A:1648:LEU:HD12	1.93	0.51
1:A:532:PHE:HD1	1:A:533:LEU:HD22	1.75	0.51
1:A:118:ILE:HG13	1:A:119:SER:H	1.77	0.50
1:A:623:ARG:HB3	1:A:626:ARG:CZ	2.41	0.50
1:A:1573:GLN:CG	1:A:1575:PRO:HG2	2.39	0.50
2:D:485:LEU:HD22	5:E:1:NAG:H82	1.91	0.50
1:A:897:VAL:HA	1:A:902:PHE:CB	2.41	0.50
1:A:1474:MET:HB3	1:A:1475:PRO:HD2	1.93	0.50
1:A:730:CYS:O	1:A:732:TYR:N	2.44	0.50
1:A:1499:PHE:CE1	1:A:1503:TYR:HB2	2.46	0.50
1:A:672:LEU:HD23	1:A:719:TYR:CE1	2.47	0.50
1:A:897:VAL:HA	1:A:902:PHE:HB2	1.93	0.50
2:D:704:ARG:HH21	2:D:737:ASP:HB3	1.75	0.50
1:A:356:VAL:HG13	1:A:388:LEU:HD21	1.94	0.50
1:A:752:ALA:HA	1:A:756:LEU:HD22	1.93	0.50
1:A:1278:PHE:O	1:A:1282:PHE:HD2	1.94	0.50
1:A:1405:PHE:CG	1:A:1408:LEU:HD21	2.46	0.50
1:A:210:ALA:O	1:A:214:GLN:N	2.44	0.50
1:A:357:PHE:C	1:A:357:PHE:CD2	2.84	0.50
1:A:899:ASP:O	1:A:900:THR:C	2.50	0.50
1:A:1159:ARG:HH12	1:A:1160:VAL:HG22	1.77	0.50
1:A:1432:LYS:O	1:A:1433:ILE:C	2.48	0.50
1:A:343:ILE:HD12	1:A:716:ILE:HD11	1.92	0.50
1:A:1247:VAL:O	1:A:1251:LEU:HD13	2.12	0.50
2:D:637:GLU:HG2	2:D:640:THR:HG23	1.93	0.50
1:A:289:LEU:N	1:A:289:LEU:CD1	2.73	0.49
1:A:1185:VAL:O	1:A:1187:VAL:N	2.45	0.49
1:A:351:PHE:CD1	1:A:351:PHE:N	2.81	0.49
1:A:510:ASN:N	1:A:513:CYS:HG	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:O	1:A:540:THR:C	2.49	0.49
1:A:681:GLU:C	1:A:683:GLN:N	2.63	0.49
1:A:725:PRO:HA	1:A:728:LEU:HD23	1.93	0.49
1:A:1078:CYS:HB2	1:A:1111:TRP:HE3	1.77	0.49
2:D:672:ILE:HA	2:D:679:PHE:CE2	2.46	0.49
1:A:208:PHE:O	1:A:209:SER:C	2.49	0.49
1:A:591:PHE:CD1	1:A:625:LEU:HD13	2.47	0.49
1:A:661:PHE:HZ	1:A:736:LEU:HD12	1.77	0.49
1:A:900:THR:HG23	1:A:904:ASN:HB2	1.93	0.49
1:A:1420:PHE:O	1:A:1424:VAL:HG22	2.12	0.49
2:D:612:VAL:HG21	2:D:615:THR:HG23	1.94	0.49
1:A:201:ILE:HG13	1:A:202:ILE:N	2.27	0.49
1:A:238:ALA:HA	1:A:671:GLN:HG2	1.93	0.49
1:A:567:PHE:O	1:A:571:MET:HG2	2.12	0.49
1:A:1159:ARG:NH2	1:A:1160:VAL:HA	2.27	0.49
1:A:1169:TYR:CG	1:A:1170:ILE:N	2.81	0.49
2:D:37:VAL:HG21	2:D:1006:GLU:HG2	1.95	0.49
1:A:159:LEU:HA	1:A:162:VAL:HG22	1.93	0.49
1:A:414:LYS:O	1:A:417:ALA:HB3	2.13	0.49
1:A:966:LEU:C	1:A:968:ILE:H	2.14	0.49
1:A:1097:LYS:HB2	1:A:1105:ILE:HD11	1.93	0.49
1:A:211:ILE:HA	1:A:214:GLN:HB3	1.94	0.49
1:A:418:ARG:HE	1:A:418:ARG:HA	1.78	0.49
1:A:601:LEU:O	1:A:604:ILE:HG22	2.13	0.49
1:A:604:ILE:O	1:A:607:GLU:HB2	2.13	0.49
1:A:1075:LEU:HB3	1:A:1114:SER:OG	2.12	0.49
1:A:1502:PHE:CD1	1:A:1502:PHE:C	2.86	0.49
2:D:442:LYS:NZ	2:D:465:PRO:O	2.46	0.49
2:D:775:PHE:HE1	2:D:794:VAL:HG13	1.77	0.49
1:A:155:THR:O	1:A:159:LEU:N	2.46	0.49
1:A:1422:TYR:HE2	1:A:1507:PHE:CB	2.26	0.49
2:D:69:THR:HG23	2:D:632:LYS:HB3	1.94	0.49
2:D:994:LEU:HB3	2:D:1001:ARG:HB2	1.95	0.49
1:A:349:PHE:C	1:A:349:PHE:CD2	2.85	0.49
1:A:397:LEU:HD12	1:A:397:LEU:O	2.12	0.49
1:A:548:GLN:CB	1:A:552:LEU:HD23	2.43	0.49
1:A:623:ARG:HE	1:A:626:ARG:NH2	2.11	0.49
1:A:121:VAL:HG12	1:A:122:GLU:HG3	1.95	0.48
1:A:261:ILE:HG12	1:A:746:ASN:HD22	1.77	0.48
1:A:349:PHE:O	1:A:352:ALA:HB3	2.13	0.48
2:D:775:PHE:H	2:D:1012:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:N	1:A:351:PHE:HD1	2.10	0.48
1:A:1306:PHE:CZ	1:A:1310:ILE:HD11	2.48	0.48
2:D:621:LEU:HD11	2:D:623:LEU:HD13	1.94	0.48
1:A:599:GLY:O	1:A:602:GLU:HG2	2.12	0.48
1:A:1218:PRO:HD3	1:A:1606:PHE:CE1	2.47	0.48
1:A:1445:ASN:ND2	1:A:1459:ARG:HH11	2.11	0.48
1:A:1499:PHE:HE1	1:A:1503:TYR:HD2	1.61	0.48
1:A:1557:LYS:HG3	1:A:1558:GLY:H	1.77	0.48
1:A:924:GLN:CD	1:A:927:SER:HB3	2.34	0.48
1:A:1502:PHE:HD1	1:A:1502:PHE:O	1.96	0.48
1:A:408:PHE:HB3	1:A:753:VAL:CG2	2.42	0.48
1:A:1569:LEU:HD11	1:A:1587:ALA:HB1	1.94	0.48
2:D:660:PHE:HB2	2:D:741:THR:HB	1.95	0.48
2:D:766:ARG:NH2	2:D:855:ASP:OD2	2.46	0.48
1:A:1450:PHE:N	1:A:1451:PRO:HD2	2.28	0.48
1:A:151:ASP:OD2	2:D:263:SER:HB3	2.14	0.48
1:A:248:VAL:HG23	1:A:660:LEU:CD2	2.42	0.48
1:A:1290:LEU:HD21	1:A:1298:TYR:CD2	2.48	0.48
2:D:680:LEU:O	2:D:684:ASN:ND2	2.32	0.48
1:A:318:LEU:C	1:A:320:THR:H	2.16	0.48
1:A:511:ARG:CZ	1:A:512:PHE:CZ	2.81	0.48
1:A:1405:PHE:CD2	1:A:1408:LEU:HD21	2.49	0.48
1:A:1421:ILE:O	1:A:1425:ILE:HG12	2.13	0.48
1:A:1620:ILE:O	1:A:1621:LYS:HD3	2.14	0.48
1:A:892:GLN:HA	1:A:895:ARG:HD2	1.95	0.48
2:D:256:ILE:HB	2:D:291:VAL:HG22	1.96	0.48
1:A:1185:VAL:O	1:A:1186:ILE:C	2.51	0.48
2:D:468:ASN:HB3	2:D:481:ASN:HA	1.96	0.48
2:D:763:PHE:O	2:D:767:SER:OG	2.25	0.48
1:A:673:PHE:CE2	1:A:729:VAL:HG13	2.48	0.47
1:A:928:PHE:O	1:A:929:ARG:C	2.51	0.47
1:A:1573:GLN:HG3	1:A:1575:PRO:CD	2.44	0.47
2:D:103:GLU:N	2:D:103:GLU:OE1	2.46	0.47
2:D:377:ASN:HD21	2:D:406:ASN:HD22	1.62	0.47
1:A:200:PHE:C	1:A:203:VAL:HG12	2.34	0.47
1:A:515:ARG:HG2	1:A:516:LYS:HD2	1.95	0.47
1:A:527:TYR:O	1:A:531:ILE:HD13	2.14	0.47
1:A:908:PHE:O	1:A:912:LEU:HD23	2.14	0.47
2:D:71:GLU:N	2:D:630:TYR:O	2.45	0.47
2:D:560:ASP:OD1	2:D:561:PHE:N	2.48	0.47
1:A:1501:VAL:HG13	1:A:1502:PHE:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:GLU:CG	1:A:685:ARG:HH12	2.28	0.47
1:A:1159:ARG:O	1:A:1160:VAL:C	2.52	0.47
2:D:745:PRO:HG2	2:D:748:ALA:HB3	1.96	0.47
1:A:599:GLY:O	1:A:603:THR:HG23	2.15	0.47
1:A:757:ALA:O	1:A:758:ASP:C	2.53	0.47
1:A:1408:LEU:HD23	1:A:1522:VAL:HG22	1.96	0.47
2:D:416:ILE:HA	2:D:419:ILE:HD12	1.97	0.47
1:A:117:CYS:HA	1:A:120:ILE:HB	1.96	0.47
1:A:271:ILE:O	1:A:275:VAL:HG23	2.14	0.47
1:A:626:ARG:O	1:A:627:ILE:C	2.51	0.47
1:A:681:GLU:HB2	1:A:685:ARG:NH2	2.28	0.47
1:A:1379:PHE:O	1:A:1380:ARG:C	2.53	0.47
1:A:147:PHE:HD1	1:A:148:PRO:HD2	1.80	0.47
1:A:387:THR:HG22	1:A:391:ILE:CG2	2.44	0.47
1:A:397:LEU:O	1:A:400:VAL:CG2	2.63	0.47
1:A:511:ARG:HG2	1:A:512:PHE:N	2.29	0.47
1:A:527:TYR:O	1:A:530:VAL:HG22	2.15	0.47
1:A:545:HIS:CE1	1:A:548:GLN:HA	2.50	0.47
1:A:897:VAL:CG1	1:A:970:LEU:HD12	2.45	0.47
1:A:1030:ASN:O	1:A:1033:LYS:N	2.48	0.47
1:A:1286:MET:CE	1:A:1308:PHE:HA	2.44	0.47
2:D:781:ASN:C	2:D:782:LYS:HG3	2.35	0.47
1:A:612:SER:O	1:A:616:ILE:HG13	2.15	0.47
1:A:666:SER:HB2	1:A:692:PHE:CE2	2.50	0.47
1:A:1254:ILE:HG22	1:A:1254:ILE:O	2.14	0.47
1:A:1480:ALA:HB1	1:A:1481:PRO:HD2	1.96	0.47
1:A:1625:ASN:HA	1:A:1628:GLN:HB3	1.97	0.47
1:A:214:GLN:HG3	1:A:215:ALA:N	2.29	0.47
1:A:519:ALA:O	1:A:523:SER:N	2.43	0.47
1:A:711:VAL:HG12	1:A:733:PHE:CE1	2.50	0.47
2:D:668:ASN:OD1	2:D:668:ASN:N	2.48	0.47
1:A:924:GLN:NE2	1:A:927:SER:HB3	2.29	0.47
1:A:956:ALA:HA	1:A:959:VAL:HG22	1.97	0.47
1:A:971:LYS:HA	1:A:971:LYS:HD2	1.58	0.47
1:A:1447:PHE:CZ	1:A:1456:LEU:HD22	2.50	0.47
1:A:1585:ARG:CG	1:A:1586:VAL:H	2.24	0.47
1:A:1629:ALA:O	1:A:1633:LEU:HG	2.15	0.47
1:A:1648:LEU:H	1:A:1648:LEU:HD12	1.80	0.47
2:D:562:LEU:HD12	2:D:1051:ARG:HE	1.79	0.47
1:A:930:ASN:O	1:A:931:HIS:C	2.54	0.46
1:A:1378:LEU:O	1:A:1379:PHE:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1513:PHE:O	1:A:1515:ILE:N	2.48	0.46
1:A:1559:ARG:HG3	1:A:1603:THR:HA	1.96	0.46
2:D:731:ALA:HB3	2:D:815:LYS:HB2	1.97	0.46
1:A:261:ILE:HG12	1:A:746:ASN:ND2	2.29	0.46
1:A:532:PHE:CD2	1:A:535:PHE:HE2	2.34	0.46
1:A:546:TYR:HA	1:A:1072:LYS:HD2	1.97	0.46
1:A:665:PHE:CD2	1:A:736:LEU:HD13	2.50	0.46
2:D:699:ALA:O	2:D:703:ASN:HB2	2.15	0.46
1:A:291:MET:SD	1:A:291:MET:C	2.94	0.46
1:A:522:LYS:HA	1:A:522:LYS:HE2	1.97	0.46
1:A:548:GLN:HG3	1:A:553:THR:HG22	1.97	0.46
1:A:681:GLU:C	1:A:683:GLN:H	2.18	0.46
1:A:1544:GLU:HA	1:A:1547:ARG:NE	2.31	0.46
2:D:673:SER:OG	2:D:679:PHE:HB2	2.15	0.46
2:D:1039:ASP:N	2:D:1039:ASP:OD1	2.49	0.46
1:A:369:LEU:HG	1:A:385:PHE:CD2	2.51	0.46
1:A:412:ARG:HH22	1:A:757:ALA:CB	2.28	0.46
1:A:1403:LYS:HA	1:A:1406:GLN:NE2	2.30	0.46
2:D:232:LYS:HG3	2:D:233:ILE:HG12	1.98	0.46
2:D:677:THR:O	2:D:681:LEU:HG	2.16	0.46
1:A:712:MET:HA	1:A:733:PHE:CE2	2.51	0.46
1:A:1215:LYS:CA	1:A:1643:ARG:HH22	2.27	0.46
1:A:1286:MET:HE2	1:A:1308:PHE:HA	1.97	0.46
1:A:1414:LEU:HD23	1:A:1414:LEU:HA	1.83	0.46
2:D:232:LYS:HA	2:D:232:LYS:HD3	1.69	0.46
1:A:254:LEU:HD23	1:A:254:LEU:H	1.81	0.46
1:A:378:ARG:HB3	1:A:378:ARG:HH11	1.80	0.46
1:A:666:SER:OG	1:A:696:LEU:HD23	2.16	0.46
2:D:49:LYS:HB3	2:D:49:LYS:HE2	1.70	0.46
2:D:868:THR:O	2:D:871:ILE:HG12	2.14	0.46
1:A:200:PHE:O	1:A:204:VAL:HG12	2.16	0.46
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.81	0.46
1:A:548:GLN:HB2	1:A:552:LEU:HD23	1.96	0.46
1:A:1230:TYR:HD2	1:A:1231:LYS:HD2	1.80	0.46
2:D:71:GLU:O	2:D:630:TYR:N	2.47	0.46
2:D:73:ASN:HD21	2:D:630:TYR:HB3	1.81	0.46
2:D:89:LEU:HD22	2:D:500:LEU:HD11	1.98	0.46
1:A:1559:ARG:HG2	1:A:1603:THR:HA	1.96	0.46
1:A:1564:ASP:HA	1:A:1567:THR:HG23	1.97	0.46
1:A:699:VAL:O	1:A:703:LEU:HG	2.15	0.46
1:A:1570:ARG:HD2	1:A:1571:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:VAL:HG11	2:D:1006:GLU:HG2	1.98	0.46
1:A:532:PHE:CE2	1:A:535:PHE:HE2	2.33	0.45
1:A:1211:GLU:OE2	1:A:1638:LYS:HB2	2.16	0.45
1:A:1408:LEU:HD22	1:A:1518:LEU:HD11	1.98	0.45
1:A:1475:PRO:HA	1:A:1496:GLY:O	2.17	0.45
2:D:730:LYS:HE2	2:D:817:ASP:CB	2.47	0.45
1:A:1097:LYS:HE3	1:A:1105:ILE:CD1	2.47	0.45
1:A:1240:TYR:O	1:A:1243:TYR:HB2	2.16	0.45
2:D:177:THR:HG22	2:D:181:ASN:HD22	1.81	0.45
2:D:736:THR:HG23	2:D:738:GLY:H	1.81	0.45
1:A:155:THR:HG22	1:A:159:LEU:CD1	2.45	0.45
1:A:207:LEU:O	1:A:211:ILE:HG12	2.17	0.45
1:A:1502:PHE:CD1	1:A:1502:PHE:O	2.69	0.45
1:A:1573:GLN:HG3	1:A:1575:PRO:HD2	1.98	0.45
1:A:1578:PHE:CD2	1:A:1581:LEU:HD22	2.51	0.45
1:A:120:ILE:HA	1:A:123:TRP:CE2	2.52	0.45
1:A:237:ARG:HD2	1:A:240:ARG:NE	2.32	0.45
1:A:545:HIS:O	1:A:548:GLN:HB3	2.15	0.45
1:A:546:TYR:CE2	1:A:1073:GLY:CA	3.00	0.45
1:A:625:LEU:HA	1:A:628:PHE:CE2	2.51	0.45
1:A:1225:LYS:HE2	1:A:1225:LYS:HB3	1.77	0.45
2:D:377:ASN:HD21	2:D:406:ASN:ND2	2.15	0.45
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.16	0.45
1:A:663:ILE:HG23	1:A:692:PHE:CZ	2.50	0.45
1:A:670:MET:O	1:A:674:GLY:HA3	2.16	0.45
1:A:1218:PRO:HG2	1:A:1557:LYS:O	2.15	0.45
1:A:1413:LEU:O	1:A:1416:VAL:HG22	2.16	0.45
2:D:667:CYS:HA	2:D:697:CYS:HB2	1.99	0.45
2:D:716:VAL:O	2:D:721:SER:N	2.50	0.45
1:A:261:ILE:HD12	1:A:657:LEU:HD23	1.98	0.45
1:A:592:ASP:HA	1:A:625:LEU:CD2	2.38	0.45
1:A:713:TYR:CA	1:A:716:ILE:HG12	2.42	0.45
1:A:750:ALA:O	1:A:751:ILE:C	2.54	0.45
2:D:663:PRO:HD3	2:D:756:PRO:HB2	1.99	0.45
1:A:366:THR:O	1:A:370:TYR:CD2	2.70	0.45
1:A:659:PHE:O	1:A:663:ILE:HG12	2.16	0.45
1:A:701:GLN:NE2	1:A:707:ASP:HB2	2.31	0.45
2:D:77:GLN:O	2:D:81:ILE:HG12	2.17	0.45
1:A:1311:VAL:O	1:A:1315:ILE:HG13	2.17	0.45
1:A:1312:ILE:HG13	1:A:1313:GLY:N	2.31	0.45
2:D:849:ASP:OD1	2:D:864:HIS:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:CYS:H	1:A:120:ILE:HG13	1.82	0.45
1:A:354:LEU:C	1:A:354:LEU:CD2	2.84	0.45
1:A:912:LEU:HA	1:A:915:ILE:HG12	1.98	0.45
2:D:573:GLU:N	2:D:573:GLU:OE2	2.49	0.45
2:D:979:THR:O	2:D:1033:GLN:NE2	2.42	0.45
1:A:1264:SER:O	1:A:1267:PHE:N	2.49	0.44
2:D:88:LYS:HB3	2:D:88:LYS:HE3	1.72	0.44
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.82	0.44
1:A:1432:LYS:HD2	1:A:1483:SER:OG	2.17	0.44
1:A:578:LEU:HD22	1:A:583:TYR:HD1	1.81	0.44
1:A:625:LEU:O	1:A:626:ARG:C	2.53	0.44
1:A:1096:TYR:HA	1:A:1103:HIS:O	2.17	0.44
1:A:1310:ILE:HG21	1:A:1383:ARG:HG3	1.99	0.44
1:A:1568:LEU:CD1	1:A:1569:LEU:HG	2.47	0.44
2:D:994:LEU:HB2	2:D:1003:PHE:CE2	2.52	0.44
1:A:204:VAL:CG1	1:A:205:VAL:H	2.22	0.44
1:A:418:ARG:HA	1:A:418:ARG:NE	2.33	0.44
1:A:658:LEU:O	1:A:662:ILE:HG13	2.17	0.44
1:A:1277:LEU:O	1:A:1281:LEU:HG	2.17	0.44
2:D:772:ASN:HB2	2:D:1010:ASN:O	2.17	0.44
2:D:994:LEU:N	2:D:1001:ARG:O	2.45	0.44
1:A:1430:PHE:CZ	1:A:1500:ALA:HA	2.53	0.44
2:D:114:ARG:HH12	2:D:117:PHE:HE1	1.65	0.44
2:D:515:ILE:HG22	2:D:521:VAL:HG12	2.00	0.44
2:D:605:ARG:HD3	2:D:624:PRO:HB3	2.00	0.44
2:D:1061:ASP:N	2:D:1061:ASP:OD1	2.51	0.44
1:A:347:ASP:O	1:A:348:ASN:HB3	2.18	0.44
1:A:369:LEU:C	1:A:369:LEU:CD2	2.85	0.44
1:A:523:SER:CB	1:A:525:VAL:HG12	2.47	0.44
1:A:901:ILE:HG23	1:A:902:PHE:H	1.83	0.44
2:D:351:ARG:HH22	2:D:356:LYS:HD3	1.82	0.44
2:D:480:LYS:HD2	5:E:1:NAG:H2	1.99	0.44
2:D:1057:ASP:OD1	2:D:1057:ASP:N	2.39	0.44
1:A:201:ILE:CA	1:A:204:VAL:CG1	2.88	0.44
1:A:624:LEU:HD23	1:A:1062:MET:HG3	1.99	0.44
1:A:955:ASN:O	1:A:958:TYR:HB3	2.17	0.44
1:A:1214:LEU:O	1:A:1215:LYS:C	2.56	0.44
1:A:1265:CYS:O	1:A:1266:LEU:C	2.53	0.44
1:A:1502:PHE:CE1	1:A:1506:SER:HB3	2.53	0.44
1:A:1586:VAL:O	1:A:1589:LYS:N	2.51	0.44
2:D:59:ASP:OD2	2:D:59:ASP:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1064:VAL:HG23	2:D:1065:LEU:HD13	1.99	0.44
1:A:212:LEU:O	1:A:216:THR:HG23	2.18	0.44
1:A:213:GLU:HA	1:A:216:THR:OG1	2.18	0.44
1:A:327:GLN:HG2	1:A:328:ASN:N	2.33	0.44
1:A:382:TRP:CE3	1:A:382:TRP:C	2.91	0.44
1:A:557:ASP:CG	1:A:561:LYS:HE3	2.38	0.44
1:A:1118:PHE:HD1	1:A:1124:ALA:HB2	1.83	0.44
1:A:1210:VAL:HG13	1:A:1611:PHE:CE2	2.53	0.44
1:A:1220:ARG:HB3	1:A:1556:ALA:CA	2.48	0.44
1:A:1585:ARG:HG2	1:A:1586:VAL:N	2.27	0.44
1:A:1638:LYS:HG3	1:A:1638:LYS:O	2.17	0.44
1:A:297:THR:O	1:A:299:TYR:N	2.51	0.44
1:A:582:ALA:O	1:A:585:VAL:HB	2.18	0.44
1:A:1548:ILE:HD11	1:A:1571:ARG:HD2	2.00	0.44
1:A:1642:LYS:HD2	1:A:1643:ARG:N	2.33	0.44
2:D:990:PHE:O	2:D:1005:GLY:N	2.51	0.44
1:A:290:PHE:CE2	1:A:384:TYR:CD2	3.05	0.43
1:A:521:VAL:HG23	1:A:574:LYS:HE3	1.99	0.43
1:A:1390:ARG:O	1:A:1395:ARG:NH1	2.51	0.43
2:D:988:LYS:H	2:D:988:LYS:HG2	1.67	0.43
1:A:290:PHE:CE2	1:A:384:TYR:HD2	2.35	0.43
1:A:412:ARG:NH1	1:A:757:ALA:HB3	2.33	0.43
1:A:1264:SER:O	1:A:1267:PHE:HB3	2.18	0.43
1:A:1422:TYR:HE2	1:A:1507:PHE:HB2	1.78	0.43
2:D:686:PHE:HD2	2:D:687:ILE:HD13	1.82	0.43
2:D:985:ASN:ND2	2:D:987:SER:OG	2.52	0.43
1:A:366:THR:CG2	1:A:1459:ARG:HG3	2.46	0.43
1:A:414:LYS:C	1:A:414:LYS:CD	2.86	0.43
1:A:573:LEU:HD12	1:A:574:LYS:N	2.33	0.43
1:A:580:LEU:HG	1:A:581:GLN:N	2.34	0.43
1:A:596:VAL:O	1:A:600:ILE:HG13	2.18	0.43
1:A:651:ILE:O	1:A:655:LEU:HG	2.17	0.43
1:A:1093:TYR:CE1	1:A:1107:GLN:HB2	2.54	0.43
1:A:1161:GLU:H	1:A:1161:GLU:HG3	1.54	0.43
1:A:1502:PHE:CD1	1:A:1506:SER:HB3	2.53	0.43
1:A:1625:ASN:HB3	1:A:1628:GLN:OE1	2.17	0.43
2:D:615:THR:OG1	2:D:616:ASP:N	2.51	0.43
1:A:318:LEU:O	1:A:320:THR:N	2.51	0.43
1:A:1117:ASP:O	1:A:1123:ALA:HB3	2.17	0.43
1:A:1499:PHE:CE1	1:A:1503:TYR:HD2	2.37	0.43
2:D:658:TYR:N	2:D:743:VAL:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ALA:O	1:A:753:VAL:C	2.57	0.43
1:A:968:ILE:C	1:A:971:LYS:H	2.21	0.43
1:A:1461:ALA:C	1:A:1463:GLY:H	2.22	0.43
1:A:1530:LEU:HA	1:A:1530:LEU:HD13	1.74	0.43
2:D:175:GLY:HA2	2:D:180:LEU:HD11	2.00	0.43
2:D:736:THR:HG23	2:D:738:GLY:N	2.33	0.43
1:A:412:ARG:HH2	1:A:757:ALA:HB1	1.83	0.43
1:A:521:VAL:HG21	1:A:578:LEU:HD11	2.00	0.43
2:D:720:TRP:CZ2	2:D:732:ARG:HB3	2.53	0.43
1:A:149:GLU:HG2	2:D:328:LYS:HB2	2.01	0.43
1:A:370:TYR:HE1	1:A:1444:ASN:O	2.01	0.43
1:A:537:ASN:O	1:A:538:THR:C	2.57	0.43
1:A:968:ILE:HD12	1:A:971:LYS:HB2	2.01	0.43
1:A:1467:GLN:CD	1:A:1467:GLN:H	2.21	0.43
1:A:1520:VAL:HG13	1:A:1521:ALA:N	2.34	0.43
1:A:234:LYS:O	1:A:235:ALA:C	2.55	0.43
1:A:654:LEU:HD13	1:A:747:VAL:HA	2.01	0.43
1:A:959:VAL:HG23	1:A:960:PHE:CD1	2.53	0.43
1:A:1078:CYS:SG	1:A:1079:SER:N	2.92	0.43
1:A:1118:PHE:HZ	1:A:1166:PHE:HZ	1.63	0.43
1:A:1553:ASP:OD1	1:A:1557:LYS:HB3	2.19	0.43
1:A:148:PRO:HB3	2:D:265:SER:OG	2.18	0.43
1:A:301:GLN:O	1:A:302:GLU:C	2.55	0.43
1:A:339:PRO:HG2	1:A:340:LYS:H	1.83	0.43
1:A:397:LEU:O	1:A:400:VAL:HG22	2.19	0.43
1:A:548:GLN:HG3	1:A:553:THR:CG2	2.49	0.43
1:A:1265:CYS:HA	1:A:1268:LYS:NZ	2.34	0.43
1:A:1382:MET:O	1:A:1385:VAL:HG12	2.19	0.43
2:D:37:VAL:HG13	2:D:1008:LEU:HD13	2.01	0.43
1:A:204:VAL:CG1	1:A:205:VAL:N	2.71	0.43
1:A:1303:TRP:CZ2	1:A:1389:SER:HB3	2.54	0.43
1:A:1585:ARG:HE	1:A:1587:ALA:H	1.67	0.43
1:A:618:VAL:O	1:A:622:VAL:HG23	2.19	0.42
1:A:900:THR:O	1:A:901:ILE:C	2.57	0.42
1:A:967:GLU:OE2	1:A:970:LEU:HD23	2.18	0.42
1:A:1234:TYR:O	1:A:1238:SER:N	2.52	0.42
2:D:182:GLU:O	2:D:186:THR:OG1	2.21	0.42
2:D:674:ASP:O	2:D:676:ASN:N	2.51	0.42
1:A:400:VAL:HG23	1:A:401:LEU:HD13	2.00	0.42
1:A:620:ARG:HD2	1:A:1069:GLN:NE2	2.33	0.42
1:A:1532:ARG:HD2	1:A:1534:TRP:CZ3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:536:ILE:H	2:D:536:ILE:HG12	1.64	0.42
1:A:287:LEU:HD12	1:A:288:GLU:N	2.35	0.42
1:A:373:ASN:OD1	1:A:381:PRO:HB2	2.18	0.42
1:A:615:GLY:O	1:A:619:LEU:HD13	2.19	0.42
1:A:889:PHE:CE1	1:A:890:ARG:HG3	2.55	0.42
1:A:965:THR:OG1	1:A:966:LEU:N	2.52	0.42
1:A:1219:LEU:HD12	1:A:1220:ARG:H	1.83	0.42
1:A:1429:VAL:HG13	1:A:1430:PHE:N	2.30	0.42
1:A:1429:VAL:HG22	1:A:1430:PHE:CD1	2.54	0.42
1:A:1501:VAL:HG13	1:A:1502:PHE:N	2.35	0.42
2:D:56:GLN:HG3	2:D:719:TYR:CE2	2.54	0.42
2:D:688:ASP:OD1	2:D:688:ASP:N	2.36	0.42
1:A:626:ARG:O	1:A:629:LYS:N	2.48	0.42
1:A:686:ARG:O	1:A:694:GLN:NE2	2.53	0.42
1:A:705:GLY:HA2	1:A:708:TRP:CD1	2.54	0.42
1:A:928:PHE:O	1:A:931:HIS:HB3	2.20	0.42
2:D:289:VAL:HG12	2:D:310:ALA:HB2	2.01	0.42
2:D:723:GLN:HB2	2:D:726:ILE:HD11	2.01	0.42
1:A:299:TYR:CB	1:A:333:LYS:HG3	2.41	0.42
1:A:616:ILE:O	1:A:620:ARG:HG3	2.20	0.42
1:A:691:ASN:OD1	1:A:694:GLN:HB2	2.19	0.42
1:A:701:GLN:O	1:A:705:GLY:N	2.52	0.42
1:A:1068:VAL:HG13	1:A:1069:GLN:N	2.34	0.42
1:A:1078:CYS:HA	1:A:1110:SER:O	2.19	0.42
1:A:1315:ILE:O	1:A:1319:ILE:HG12	2.20	0.42
1:A:274:LEU:CD1	1:A:1398:LEU:HD21	2.49	0.42
1:A:290:PHE:HE2	1:A:384:TYR:CE2	2.38	0.42
1:A:546:TYR:CA	1:A:1072:LYS:HD2	2.50	0.42
1:A:562:ALA:O	1:A:566:LEU:HD13	2.20	0.42
1:A:889:PHE:CZ	1:A:890:ARG:HG3	2.54	0.42
2:D:185:TRP:HA	3:B:1:NAG:H82	2.01	0.42
4:F:1:NAG:H61	4:F:2:NAG:N2	2.34	0.42
1:A:120:ILE:HA	1:A:123:TRP:NE1	2.34	0.42
1:A:300:ASN:OD1	1:A:331:VAL:N	2.53	0.42
1:A:554:GLU:O	1:A:558:THR:HG23	2.19	0.42
2:D:153:ALA:O	2:D:155:PHE:N	2.52	0.42
2:D:155:PHE:HA	2:D:456:LEU:HD11	2.02	0.42
2:D:895:ASN:OD1	4:G:1:NAG:H2	2.20	0.42
1:A:411:GLU:O	1:A:414:LYS:HG3	2.19	0.42
1:A:1423:ALA:O	1:A:1424:VAL:C	2.54	0.42
2:D:36:TRP:O	2:D:39:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:VAL:O	2:D:49:LYS:N	2.50	0.42
1:A:287:LEU:O	1:A:291:MET:HG3	2.16	0.42
1:A:321:GLY:C	1:A:322:HIS:CG	2.93	0.42
1:A:602:GLU:OE1	1:A:623:ARG:HD2	2.19	0.42
1:A:749:LEU:O	1:A:752:ALA:N	2.53	0.42
1:A:1087:ALA:HA	1:A:1090:LYS:HZ2	1.84	0.42
1:A:1224:PRO:HB2	1:A:1230:TYR:HB2	2.01	0.42
2:D:34:LYS:HA	2:D:37:VAL:HB	2.02	0.42
2:D:77:GLN:OE1	2:D:77:GLN:HA	2.19	0.42
1:A:205:VAL:O	1:A:208:PHE:HB3	2.20	0.42
1:A:624:LEU:HG	1:A:627:ILE:HG12	2.02	0.42
1:A:625:LEU:HG	1:A:626:ARG:N	2.34	0.42
1:A:1211:GLU:HG3	1:A:1637:ILE:CD1	2.50	0.42
2:D:367:GLU:OE1	2:D:369:ALA:N	2.53	0.42
1:A:336:TRP:CD2	1:A:338:GLY:O	2.73	0.41
1:A:1310:ILE:HD12	1:A:1383:ARG:HG3	2.00	0.41
1:A:1480:ALA:O	1:A:1483:SER:HB3	2.20	0.41
2:D:401:TRP:CZ2	2:D:405:GLU:HG3	2.55	0.41
2:D:482:GLN:HE22	2:D:1067:ASP:HB2	1.84	0.41
5:E:3:NAG:H4	5:E:4:NAG:H2	1.49	0.41
1:A:348:ASN:OD1	1:A:349:PHE:N	2.50	0.41
1:A:662:ILE:HD13	1:A:700:PHE:CZ	2.54	0.41
1:A:1595:ASN:O	1:A:1648:LEU:HD13	2.20	0.41
2:D:466:VAL:HG23	2:D:485:LEU:HB2	2.02	0.41
2:D:672:ILE:H	2:D:672:ILE:HG13	1.48	0.41
1:A:233:VAL:O	1:A:235:ALA:N	2.53	0.41
1:A:233:VAL:O	1:A:236:LEU:N	2.53	0.41
1:A:387:THR:HG22	1:A:391:ILE:HG21	2.02	0.41
1:A:550:ASN:O	1:A:551:TRP:C	2.57	0.41
2:D:852:ILE:HG23	2:D:1015:PHE:HD1	1.85	0.41
1:A:258:LEU:HD12	1:A:258:LEU:O	2.19	0.41
1:A:380:TRP:H	1:A:381:PRO:HD3	1.86	0.41
1:A:908:PHE:O	1:A:909:PHE:C	2.58	0.41
1:A:1422:TYR:CE2	1:A:1507:PHE:HA	2.52	0.41
1:A:1498:SER:C	1:A:1500:ALA:N	2.71	0.41
1:A:148:PRO:HB3	2:D:265:SER:HG	1.85	0.41
1:A:297:THR:O	1:A:298:CYS:C	2.59	0.41
1:A:888:ARG:HG3	1:A:889:PHE:HD2	1.85	0.41
1:A:900:THR:O	1:A:903:THR:N	2.53	0.41
1:A:921:ASP:O	1:A:930:ASN:ND2	2.53	0.41
1:A:1030:ASN:C	1:A:1032:ALA:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:LYS:O	2:D:173:TYR:CG	2.74	0.41
1:A:1403:LYS:HA	1:A:1403:LYS:HD2	1.66	0.41
1:A:1506:SER:O	1:A:1510:LEU:HD13	2.20	0.41
1:A:1557:LYS:HA	1:A:1557:LYS:HD3	1.81	0.41
2:D:817:ASP:N	2:D:817:ASP:OD1	2.46	0.41
1:A:209:SER:HA	1:A:212:LEU:HD22	2.02	0.41
1:A:279:ILE:HD13	1:A:279:ILE:HA	1.83	0.41
1:A:549:PRO:O	1:A:553:THR:HG23	2.20	0.41
1:A:1063:PHE:CZ	1:A:1168:ILE:HB	2.55	0.41
1:A:1216:ALA:C	1:A:1217:ARG:HD2	2.41	0.41
1:A:1403:LYS:HD2	1:A:1406:GLN:NE2	2.34	0.41
1:A:1459:ARG:CG	1:A:1464:GLU:HB2	2.51	0.41
1:A:1499:PHE:HE2	1:A:1502:PHE:CD2	2.39	0.41
2:D:654:GLU:HA	2:D:746:LYS:HE3	2.03	0.41
1:A:147:PHE:HD1	1:A:148:PRO:CD	2.34	0.41
1:A:572:LEU:O	1:A:575:MET:HB2	2.20	0.41
1:A:676:LYS:O	1:A:718:ALA:HB1	2.21	0.41
1:A:1052:ILE:O	1:A:1053:VAL:C	2.58	0.41
1:A:1178:MET:O	1:A:1179:ASN:C	2.59	0.41
1:A:1224:PRO:HG2	1:A:1230:TYR:CD1	2.54	0.41
1:A:298:CYS:SG	1:A:330:THR:CB	3.08	0.41
1:A:318:LEU:HD23	1:A:332:CYS:HB3	2.02	0.41
1:A:699:VAL:HG13	1:A:736:LEU:HD21	2.02	0.41
1:A:748:PHE:O	1:A:750:ALA:N	2.54	0.41
1:A:888:ARG:HG3	1:A:889:PHE:N	2.30	0.41
1:A:1118:PHE:HD1	1:A:1124:ALA:CB	2.34	0.41
1:A:1155:ILE:HD13	1:A:1155:ILE:HA	1.89	0.41
1:A:1239:THR:HG23	1:A:1240:TYR:N	2.36	0.41
2:D:184:ASN:O	3:B:1:NAG:H82	2.21	0.41
1:A:213:GLU:O	1:A:217:LYS:HD3	2.21	0.41
1:A:525:VAL:HG13	1:A:526:PHE:N	2.36	0.41
1:A:617:SER:HA	1:A:1069:GLN:HE21	1.86	0.41
1:A:966:LEU:C	1:A:968:ILE:N	2.74	0.41
1:A:1474:MET:O	1:A:1477:LYS:HD3	2.21	0.41
1:A:1570:ARG:HD2	1:A:1570:ARG:C	2.41	0.41
2:D:482:GLN:NE2	2:D:1067:ASP:HB2	2.36	0.41
1:A:242:LEU:HA	1:A:245:LEU:HD23	2.03	0.40
1:A:702:ILE:HD11	1:A:711:VAL:HG11	2.03	0.40
1:A:728:LEU:HA	1:A:731:ILE:HG23	2.03	0.40
1:A:1117:ASP:OD1	1:A:1117:ASP:N	2.54	0.40
1:A:1168:ILE:C	1:A:1170:ILE:N	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:PRO:HD2	1:A:1410:TYR:H	1.85	0.40
1:A:1581:LEU:HD23	1:A:1582:CYS:O	2.22	0.40
2:D:33:ILE:O	2:D:37:VAL:N	2.48	0.40
1:A:313:PRO:HG2	1:A:336:TRP:HE1	1.86	0.40
1:A:332:CYS:C	1:A:333:LYS:HG2	2.41	0.40
1:A:537:ASN:HD21	1:A:626:ARG:HH21	1.70	0.40
1:A:963:ILE:O	1:A:966:LEU:HB3	2.21	0.40
1:A:1215:LYS:H	1:A:1643:ARG:HH12	1.68	0.40
1:A:1224:PRO:HG3	1:A:1233:TRP:CG	2.56	0.40
1:A:1456:LEU:HD23	1:A:1456:LEU:C	2.42	0.40
1:A:1465:ALA:HA	1:A:1467:GLN:OE1	2.20	0.40
1:A:1589:LYS:HD2	1:A:1589:LYS:HA	1.88	0.40
1:A:1647:LYS:HD3	1:A:1647:LYS:HA	1.83	0.40
2:D:66:ASP:OD1	2:D:66:ASP:N	2.52	0.40
1:A:199:ASP:OD1	1:A:246:ARG:NE	2.54	0.40
1:A:277:PHE:CD2	1:A:1388:LEU:HG	2.56	0.40
1:A:295:HIS:NE2	1:A:347:ASP:OD2	2.54	0.40
1:A:370:TYR:HD1	1:A:1444:ASN:HB3	1.83	0.40
1:A:380:TRP:N	1:A:381:PRO:HD3	2.35	0.40
1:A:387:THR:O	1:A:389:ILE:N	2.55	0.40
1:A:510:ASN:HB2	1:A:512:PHE:CZ	2.57	0.40
1:A:514:ARG:NH2	1:A:576:TYR:HB3	2.37	0.40
1:A:556:GLN:NE2	1:A:556:GLN:HA	2.35	0.40
1:A:893:CYS:O	1:A:897:VAL:HG22	2.21	0.40
1:A:924:GLN:CD	1:A:927:SER:H	2.25	0.40
1:A:1155:ILE:O	1:A:1159:ARG:HB3	2.21	0.40
1:A:1215:LYS:HE3	1:A:1215:LYS:HB3	1.89	0.40
1:A:1235:VAL:O	1:A:1238:SER:N	2.51	0.40
2:D:128:LYS:H	2:D:128:LYS:HG2	1.67	0.40
1:A:156:ASN:O	1:A:157:SER:C	2.60	0.40
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.93	0.40
1:A:392:GLY:O	1:A:396:VAL:HB	2.22	0.40
1:A:393:SER:O	1:A:397:LEU:CB	2.69	0.40
1:A:546:TYR:N	1:A:1072:LYS:HD2	2.36	0.40
1:A:1085:THR:HG22	1:A:1087:ALA:H	1.87	0.40
1:A:1382:MET:O	1:A:1383:ARG:C	2.60	0.40
1:A:1066:ILE:O	1:A:1070:LEU:HG	2.22	0.40
1:A:1236:VAL:HG23	1:A:1237:ASN:OD1	2.21	0.40
1:A:1498:SER:O	1:A:1500:ALA:N	2.54	0.40
1:A:1540:HIS:HA	1:A:1543:ASP:OD1	2.21	0.40
2:D:899:ASP:OD1	2:D:902:SER:HB3	2.22	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	1180/2201 (54%)	998 (85%)	148 (12%)	34 (3%)	4	28
2	D	936/1103 (85%)	883 (94%)	51 (5%)	2 (0%)	47	79
All	All	2116/3304 (64%)	1881 (89%)	199 (9%)	36 (2%)	13	42

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	A	304	ILE
1	A	309	ALA
1	A	752	ALA
1	A	929	ARG
1	A	931	HIS
1	A	975	TYR
1	A	1186	ILE
2	D	72	PRO
1	A	206	GLY
1	A	305	ALA
1	A	336	TRP
1	A	753	VAL
1	A	928	PHE
1	A	144	TYR
1	A	208	PHE
1	A	234	LYS
1	A	321	GLY
1	A	322	HIS
1	A	974	ALA
1	A	1033	LYS
1	A	308	PRO

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Mol	Chain	Res	Type
1	A	319	GLU
1	A	748	PHE
1	A	903	THR
1	A	971	LYS
1	A	1170	ILE
1	A	1554	PRO
2	D	675	ASN
1	A	388	LEU
1	A	1409	PRO
1	A	310	GLU
1	A	1025	PRO
1	A	1171	ILE
1	A	952	ILE
1	A	380	TRP

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	961/1896 (51%)	863 (90%)	98 (10%)	7 29
2	D	837/971 (86%)	814 (97%)	23 (3%)	44 75
All	All	1798/2867 (63%)	1677 (93%)	121 (7%)	20 50

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	CYS
1	A	145	ILE
1	A	155	THR
1	A	157	SER
1	A	212	LEU
1	A	214	GLN
1	A	217	LYS
1	A	232	ASP
1	A	233	VAL

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Mol	Chain	Res	Type
1	A	234	LYS
1	A	237	ARG
1	A	291	MET
1	A	297	THR
1	A	298	CYS
1	A	299	TYR
1	A	301	GLN
1	A	307	VAL
1	A	311	ASP
1	A	312	ASP
1	A	316	CYS
1	A	319	GLU
1	A	320	THR
1	A	325	GLN
1	A	326	CYS
1	A	327	GLN
1	A	333	LYS
1	A	337	ASP
1	A	343	ILE
1	A	347	ASP
1	A	358	GLN
1	A	374	ASP
1	A	407	GLU
1	A	414	LYS
1	A	511	ARG
1	A	512	PHE
1	A	515	ARG
1	A	526	PHE
1	A	535	PHE
1	A	536	LEU
1	A	539	LEU
1	A	546	TYR
1	A	566	LEU
1	A	572	LEU
1	A	589	ASN
1	A	592	ASP
1	A	621	CYS
1	A	625	LEU
1	A	626	ARG
1	A	694	GLN
1	A	732	TYR
1	A	749	LEU

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Mol	Chain	Res	Type
1	A	751	ILE
1	A	753	VAL
1	A	901	ILE
1	A	903	THR
1	A	917	LEU
1	A	955	ASN
1	A	957	ASP
1	A	962	SER
1	A	966	LEU
1	A	967	GLU
1	A	968	ILE
1	A	969	ILE
1	A	970	LEU
1	A	971	LYS
1	A	972	MET
1	A	1112	GLU
1	A	1113	ASN
1	A	1117	ASP
1	A	1159	ARG
1	A	1161	GLU
1	A	1221	ARG
1	A	1225	LYS
1	A	1248	LEU
1	A	1252	ASN
1	A	1260	HIS
1	A	1275	ASN
1	A	1405	PHE
1	A	1408	LEU
1	A	1411	VAL
1	A	1422	TYR
1	A	1424	VAL
1	A	1443	ARG
1	A	1502	PHE
1	A	1513	PHE
1	A	1531	THR
1	A	1543	ASP
1	A	1559	ARG
1	A	1564	ASP
1	A	1567	THR
1	A	1568	LEU
1	A	1580	LYS
1	A	1606	PHE

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Mol	Chain	Res	Type
1	A	1619	ARG
1	A	1639	LYS
1	A	1641	TRP
1	A	1642	LYS
1	A	1649	LEU
2	D	39	LYS
2	D	69	THR
2	D	71	GLU
2	D	367	GLU
2	D	379	ASP
2	D	476	LYS
2	D	493	SER
2	D	516	ASP
2	D	553	SER
2	D	643	ARG
2	D	653	PHE
2	D	655	GLU
2	D	672	ILE
2	D	673	SER
2	D	674	ASP
2	D	711	PHE
2	D	721	SER
2	D	782	LYS
2	D	815	LYS
2	D	877	GLU
2	D	990	PHE
2	D	1029	ARG
2	D	1045	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	196	ASN
1	A	270	HIS
1	A	327	GLN
1	A	556	GLN
1	A	560	ASN
1	A	589	ASN
1	A	1069	GLN
1	A	1113	ASN
1	A	1157	ASN

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Mol	Chain	Res	Type
1	A	1229	GLN
1	A	1252	ASN
1	A	1259	GLN
1	A	1260	HIS
1	A	1272	ASN
1	A	1304	ASN
1	A	1445	ASN
2	D	73	ASN
2	D	181	ASN
2	D	406	ASN
2	D	713	ASN
2	D	717	GLN
2	D	985	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

13 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	$\# Z > 2$
3	NAG	B	1	2,3	14,14,15	0.88	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	B	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	B	3	3	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	C	1	2,4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	C	2	4	14,14,15	0.57	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1	2,5	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	E	2	5	14,14,15	0.71	0	17,19,21	1.96	7 (41%)
5	NAG	E	3	5	14,14,15	0.69	0	17,19,21	1.43	3 (17%)
5	NAG	E	4	5	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
4	NAG	F	1	2,4	14,14,15	0.47	0	17,19,21	0.52	0
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	G	1	2,4	14,14,15	0.48	0	17,19,21	0.39	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.41	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
3	NAG	B	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	B	3	3	-	2/6/23/26	0/1/1/1
4	NAG	C	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	3	5	-	6/6/23/26	0/1/1/1
5	NAG	E	4	5	-	5/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	O5-C1	3.03	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	4.72	118.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	C2-N2-C7	-3.85	117.41	122.90
5	E	3	NAG	O4-C4-C3	-3.42	102.43	110.35
5	E	2	NAG	C1-C2-N2	-3.22	104.98	110.49
5	E	2	NAG	O5-C1-C2	3.07	116.14	111.29
5	E	2	NAG	O3-C3-C2	-2.77	103.73	109.47
5	E	3	NAG	C1-O5-C5	2.46	115.53	112.19
5	E	4	NAG	C4-C3-C2	2.35	114.47	111.02
5	E	2	NAG	O5-C5-C4	-2.34	105.12	110.83
5	E	2	NAG	O4-C4-C3	2.32	115.70	110.35
5	E	3	NAG	C1-C2-N2	-2.16	106.79	110.49
5	E	2	NAG	C3-C4-C5	-2.16	106.39	110.24

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	NAG	C3-C2-N2-C7
5	E	3	NAG	C8-C7-N2-C2
5	E	3	NAG	O7-C7-N2-C2
5	E	4	NAG	C8-C7-N2-C2
5	E	4	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
5	E	4	NAG	C1-C2-N2-C7
5	E	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
3	B	3	NAG	C8-C7-N2-C2
3	B	3	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C4-C5-C6-O6
5	E	4	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

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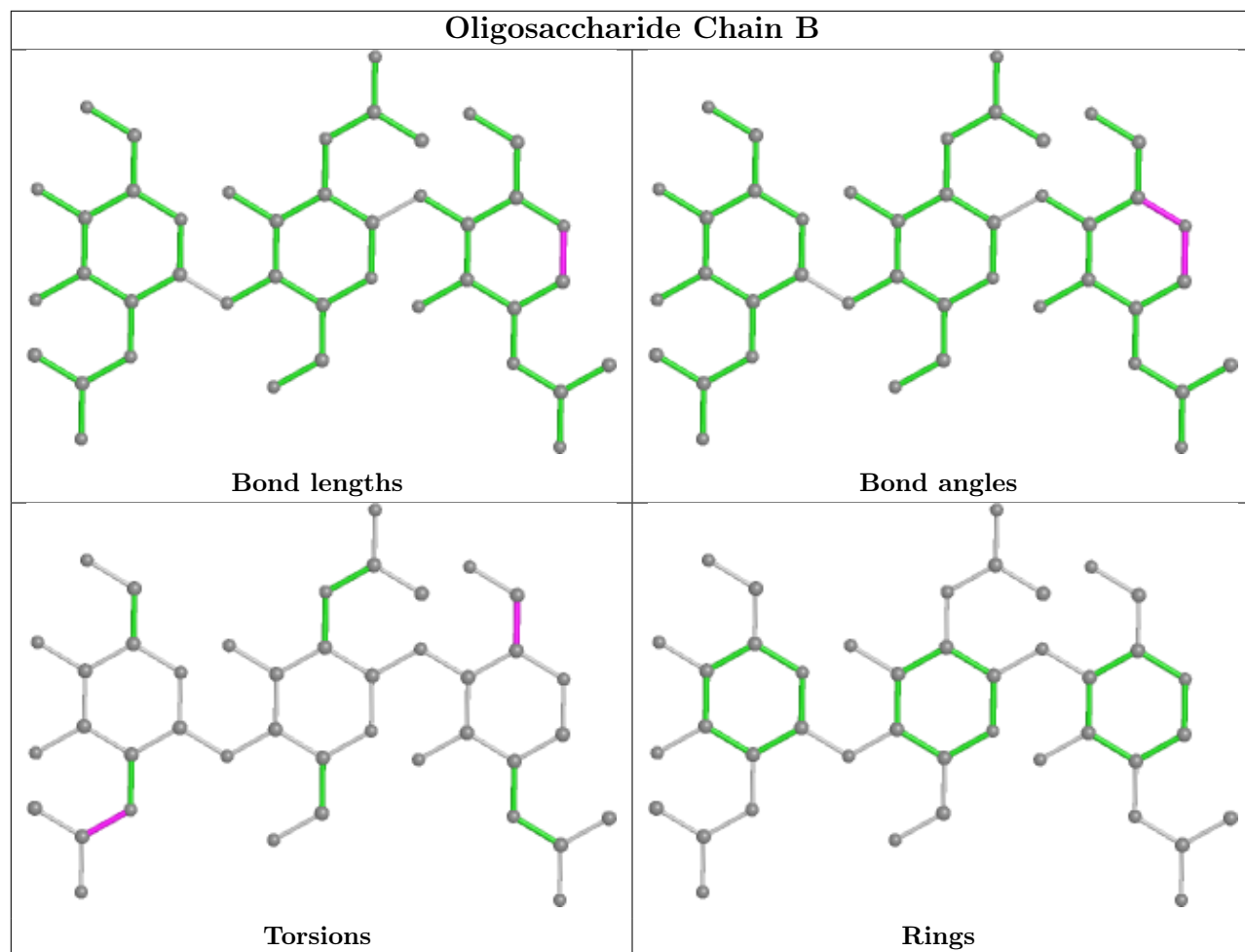
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C4-C5-C6-O6
5	E	4	NAG	C4-C5-C6-O6
5	E	3	NAG	C1-C2-N2-C7
4	C	1	NAG	C3-C2-N2-C7
4	C	2	NAG	C3-C2-N2-C7
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C1-C2-N2-C7

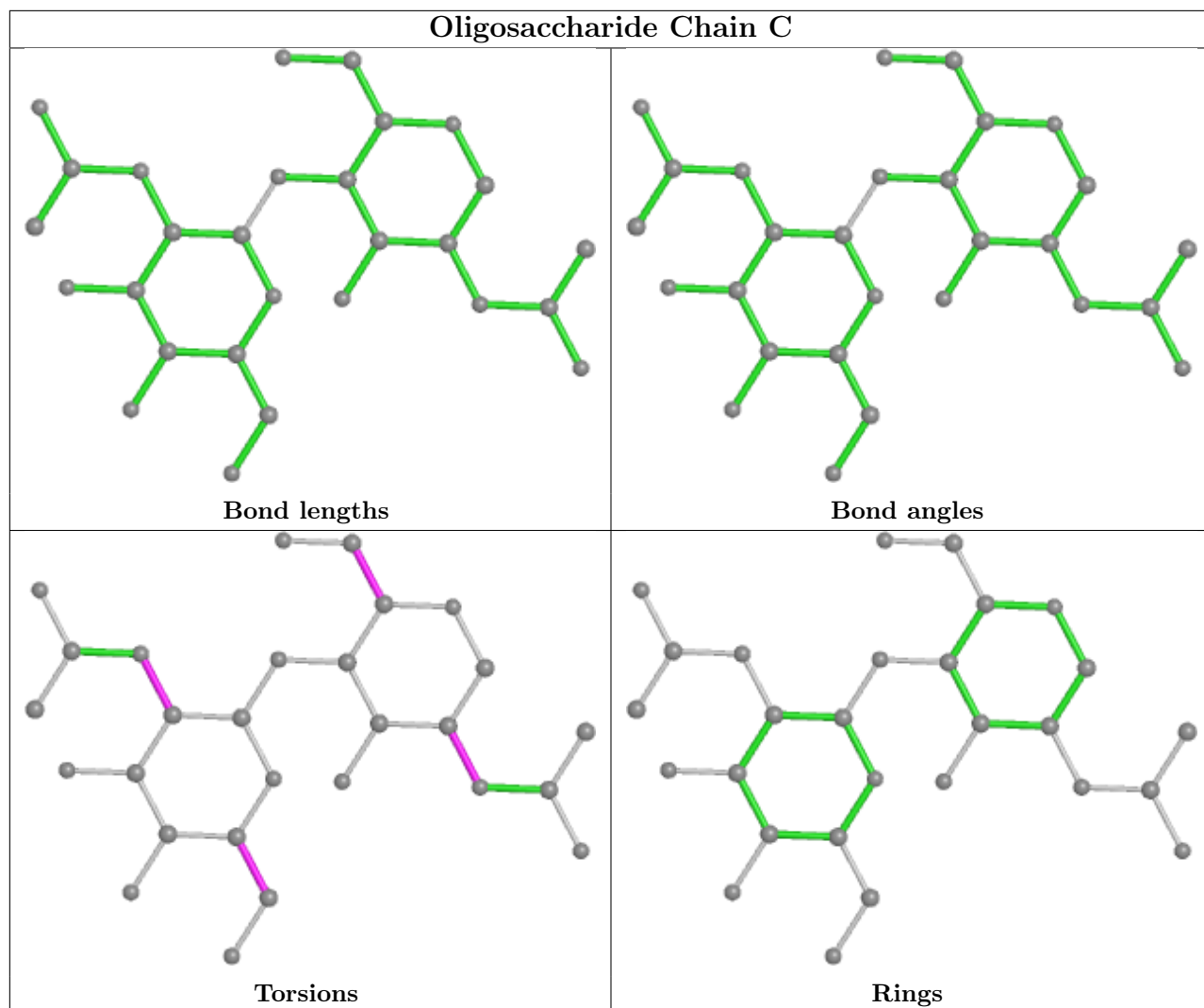
There are no ring outliers.

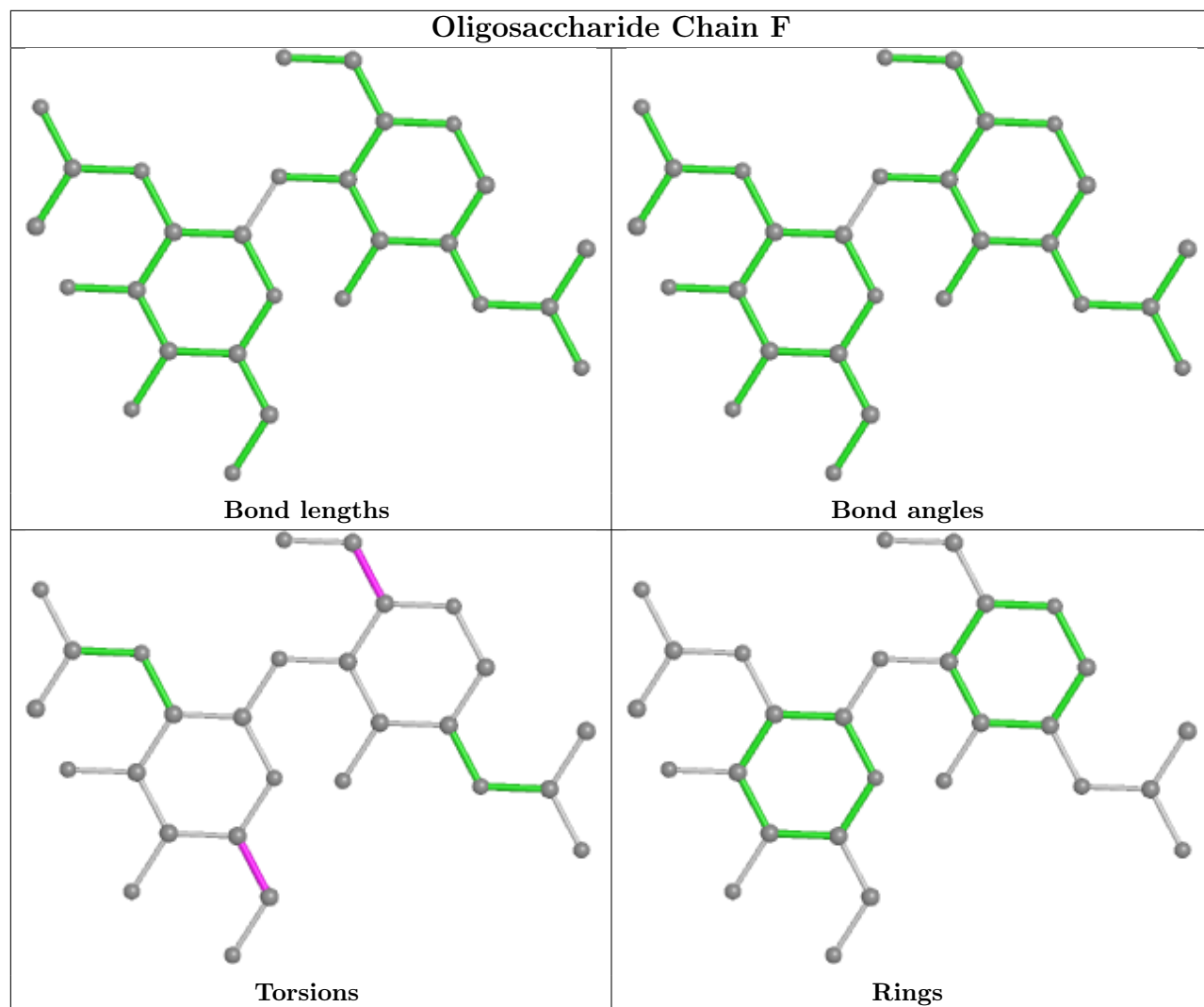
8 monomers are involved in 10 short contacts:

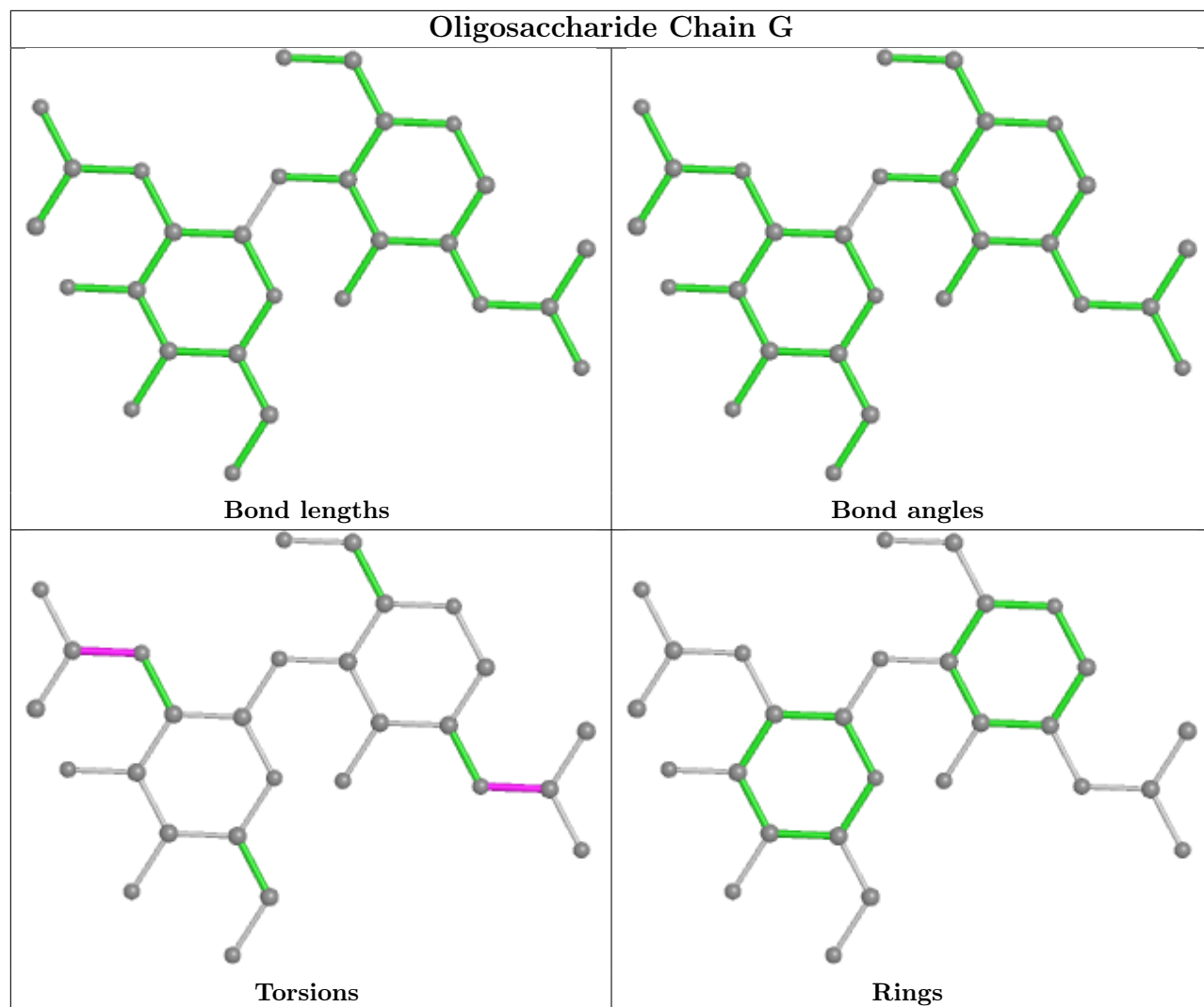
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	1	0
5	E	3	NAG	2	0
5	E	1	NAG	2	0
4	F	1	NAG	1	0
5	E	4	NAG	1	0
4	F	2	NAG	1	0
3	B	1	NAG	4	0
4	G	1	NAG	1	0

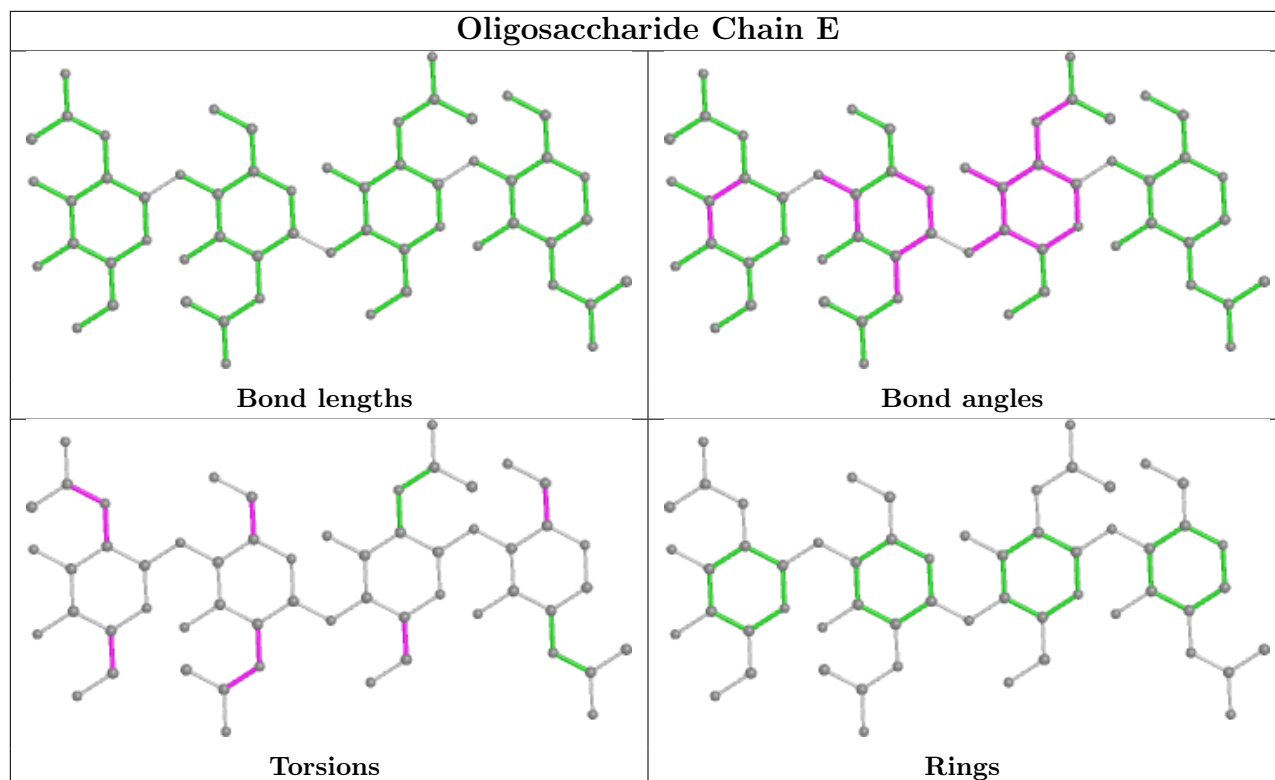
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
9	NAG	D	1203	2	14,14,15	1.14	1 (7%)	17,19,21	1.19	1 (5%)
7	9Z9	A	2302	-	44,44,44	1.69	11 (25%)	66,68,68	1.57	14 (21%)
9	NAG	D	1202	2	14,14,15	0.44	0	17,19,21	0.40	0
8	WB9	A	2303	-	35,35,35	1.54	7 (20%)	48,51,51	6.99	21 (43%)

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
9	NAG	D	1203	2	-	1/6/23/26	0/1/1/1
7	9Z9	A	2302	-	-	5/12/100/100	0/6/6/6
9	NAG	D	1202	2	-	4/6/23/26	0/1/1/1
8	WB9	A	2303	-	-	15/18/53/53	0/5/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2302	9Z9	C11-C08	-3.90	1.49	1.56
9	D	1203	NAG	O5-C1	3.86	1.49	1.43
7	A	2302	9Z9	C11-C13	-3.80	1.45	1.52
7	A	2302	9Z9	O80-C79	-3.77	1.38	1.43
7	A	2302	9Z9	C09-C08	-3.58	1.47	1.53
8	A	2303	WB9	C05-C06	3.48	1.61	1.53
8	A	2303	WB9	C15-N14	-3.28	1.42	1.51
8	A	2303	WB9	C05-C04	3.24	1.61	1.52
8	A	2303	WB9	C19-N14	-2.89	1.43	1.51
7	A	2302	9Z9	C10-C02	-2.84	1.49	1.54
7	A	2302	9Z9	C01-C02	-2.56	1.49	1.54
7	A	2302	9Z9	C10-C09	-2.53	1.48	1.53
8	A	2303	WB9	C20-C21	2.50	1.56	1.51
7	A	2302	9Z9	C02-C03	-2.49	1.51	1.56
8	A	2303	WB9	O30-C23	2.49	1.41	1.37
7	A	2302	9Z9	O80-C73	-2.46	1.38	1.42
7	A	2302	9Z9	C19-C11	-2.28	1.49	1.54
7	A	2302	9Z9	C16-C17	2.27	1.57	1.52
8	A	2303	WB9	O28-C24	2.20	1.40	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2303	WB9	C02-C07-C06	-25.98	67.13	113.91
8	A	2303	WB9	C04-C03-C02	-22.51	66.33	111.51
8	A	2303	WB9	C08-C03-C04	19.70	134.76	108.69
8	A	2303	WB9	C08-C07-C06	15.88	135.21	107.66
8	A	2303	WB9	C32-C02-C01	-14.72	74.81	108.67
8	A	2303	WB9	C01-C02-C03	-8.39	78.74	115.33
8	A	2303	WB9	C32-C02-C07	-6.82	79.82	115.70
8	A	2303	WB9	C04-C05-C06	-6.60	97.39	112.24
8	A	2303	WB9	C29-O28-C24	-5.35	109.45	117.53
9	D	1203	NAG	C1-O5-C5	4.71	118.58	112.19
8	A	2303	WB9	C31-O30-C23	-4.49	110.76	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2302	9Z9	O80-C73-C76	4.12	114.60	110.77
7	A	2302	9Z9	C17-C16-C13	3.83	117.47	111.52
7	A	2302	9Z9	C09-C10-C02	-3.52	106.75	112.78
8	A	2303	WB9	C32-C02-C03	3.49	130.53	115.33
8	A	2303	WB9	C07-C08-C03	3.17	90.46	86.20
7	A	2302	9Z9	C09-C08-C07	-2.99	107.44	111.75
8	A	2303	WB9	C12-C13-N14	-2.86	111.57	116.95
8	A	2303	WB9	O28-C24-C23	2.76	119.25	115.41
8	A	2303	WB9	C01-C02-C07	2.75	130.16	115.70
8	A	2303	WB9	O30-C23-C24	2.72	119.19	115.41
7	A	2302	9Z9	C09-C08-C11	-2.68	109.54	113.08
7	A	2302	9Z9	C08-C07-C06	-2.54	105.69	109.09
7	A	2302	9Z9	O80-C73-O72	-2.53	102.72	109.78
7	A	2302	9Z9	C05-C06-C02	-2.50	100.58	103.91
7	A	2302	9Z9	C18-C17-C16	2.46	114.65	110.99
8	A	2303	WB9	C22-C21-C26	2.37	119.30	116.51
7	A	2302	9Z9	C10-C09-C08	-2.35	109.04	113.11
7	A	2302	9Z9	C16-C13-C11	2.34	119.53	116.42
8	A	2303	WB9	C16-C15-N14	-2.34	107.41	111.89
8	A	2303	WB9	O28-C24-C25	-2.24	120.26	124.12
7	A	2302	9Z9	C77-C78-C79	2.23	111.65	108.56
8	A	2303	WB9	C10-C09-C06	-2.12	109.25	113.17
7	A	2302	9Z9	C10-C02-C03	-2.12	112.07	115.46
8	A	2303	WB9	O30-C23-C22	-2.09	120.53	124.12
7	A	2302	9Z9	C48-C23-C24	-2.03	107.75	111.00

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2302	9Z9	C24-C23-C48-O49
8	A	2303	WB9	C05-C06-C09-C10
8	A	2303	WB9	C07-C06-C09-C10
8	A	2303	WB9	O11-C12-C13-N14
8	A	2303	WB9	C12-C13-N14-C15
8	A	2303	WB9	C12-C13-N14-C19
8	A	2303	WB9	C21-C20-N14-C13
8	A	2303	WB9	C21-C20-N14-C15
8	A	2303	WB9	C21-C20-N14-C19
8	A	2303	WB9	C13-C12-O11-C10
8	A	2303	WB9	C25-C24-O28-C29
9	D	1202	NAG	C4-C5-C6-O6

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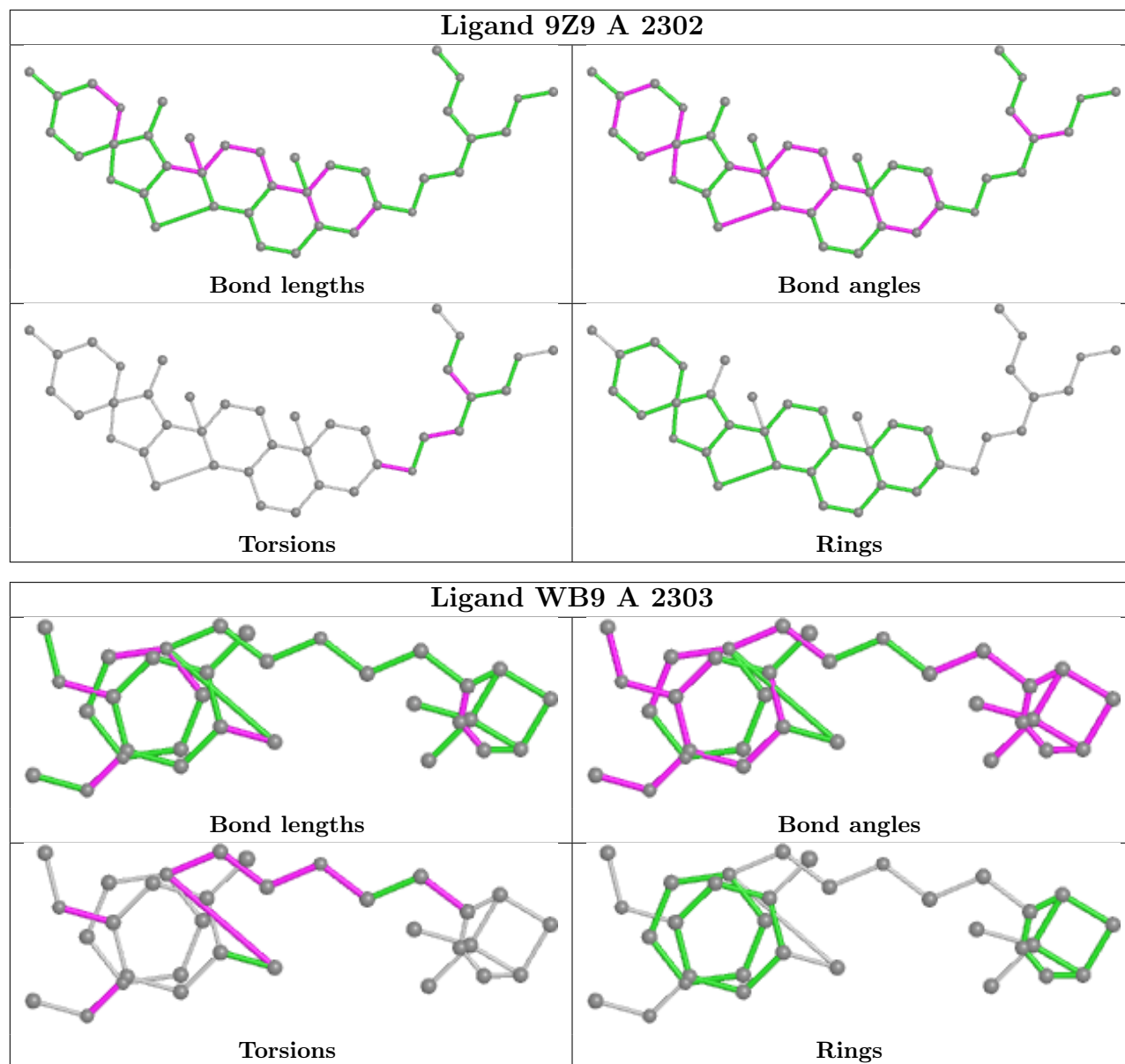
Mol	Chain	Res	Type	Atoms
9	D	1202	NAG	C8-C7-N2-C2
9	D	1202	NAG	O7-C7-N2-C2
7	A	2302	9Z9	C22-C23-C48-O49
8	A	2303	WB9	C22-C23-O30-C31
8	A	2303	WB9	C23-C24-O28-C29
9	D	1202	NAG	O5-C5-C6-O6
8	A	2303	WB9	C24-C23-O30-C31
9	D	1203	NAG	O5-C5-C6-O6
7	A	2302	9Z9	O20-C21-C22-C23
7	A	2302	9Z9	C18-C17-O20-C21
8	A	2303	WB9	C12-C13-N14-C20
7	A	2302	9Z9	C16-C17-O20-C21
8	A	2303	WB9	C09-C10-O11-C12

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1203	NAG	2	0
8	A	2303	WB9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

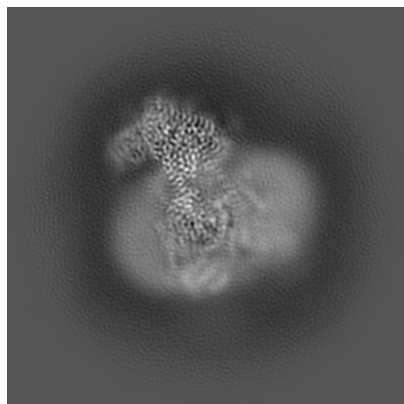
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37476. These allow visual inspection of the internal detail of the map and identification of artifacts.

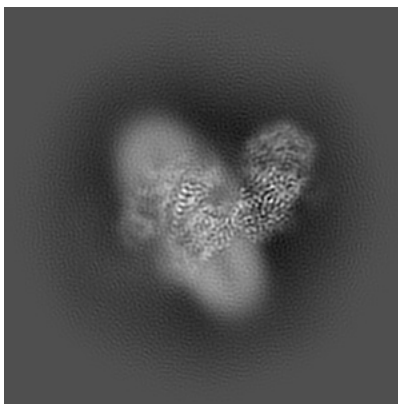
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

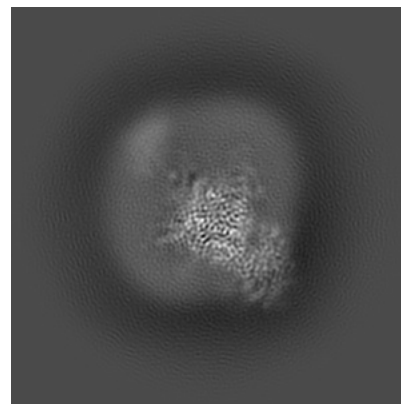
6.1.1 Primary map



X

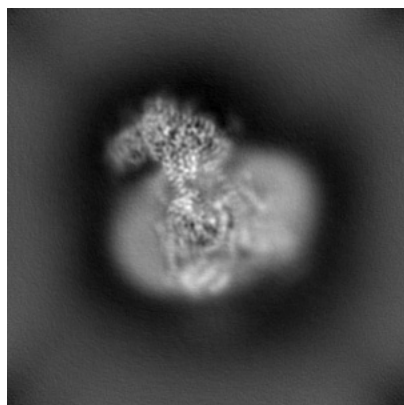


Y

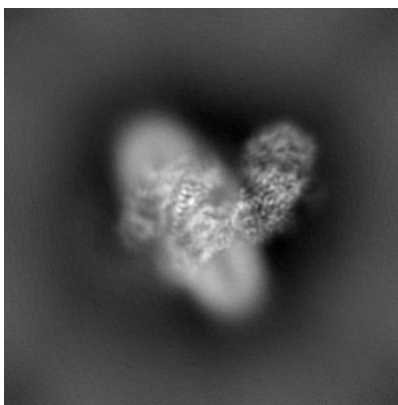


Z

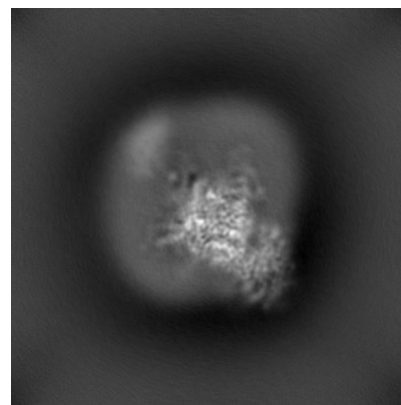
6.1.2 Raw map



X



Y

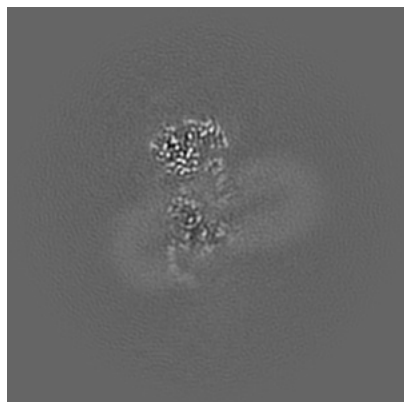


Z

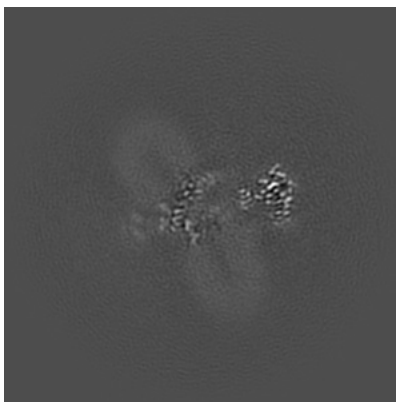
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

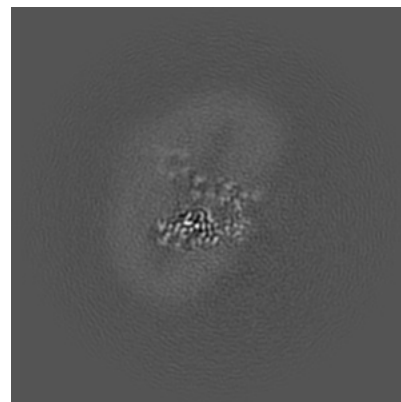
6.2.1 Primary map



X Index: 140

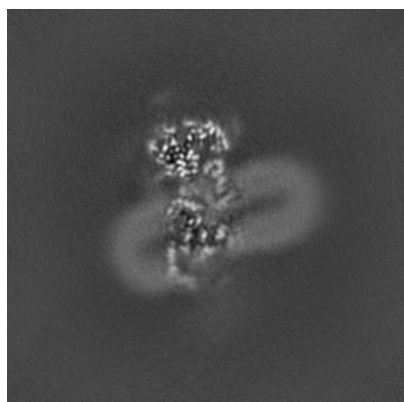


Y Index: 140

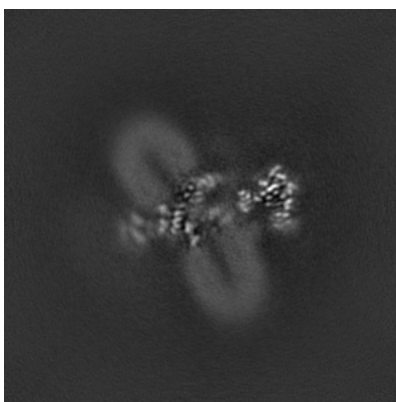


Z Index: 140

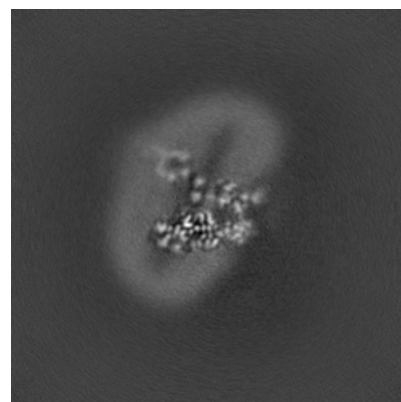
6.2.2 Raw map



X Index: 140



Y Index: 140

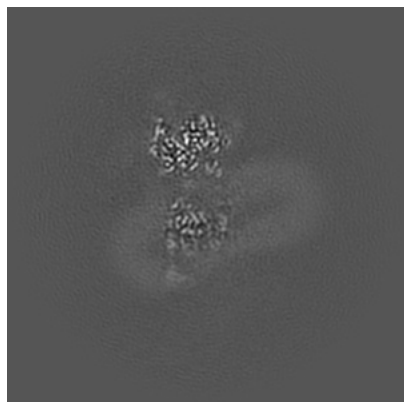


Z Index: 140

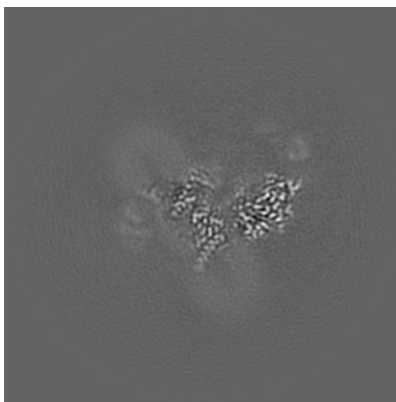
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

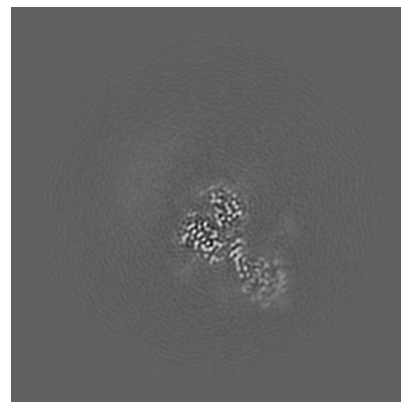
6.3.1 Primary map



X Index: 143

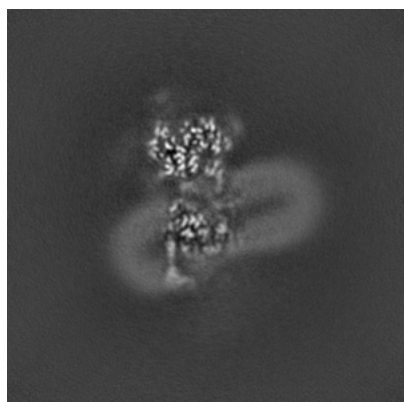


Y Index: 127

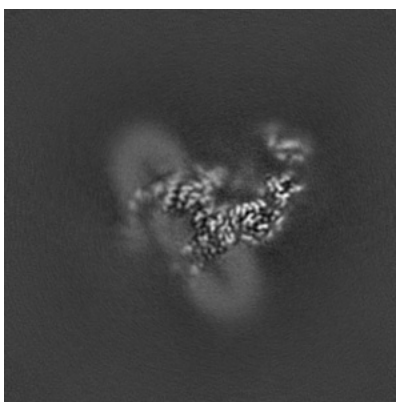


Z Index: 182

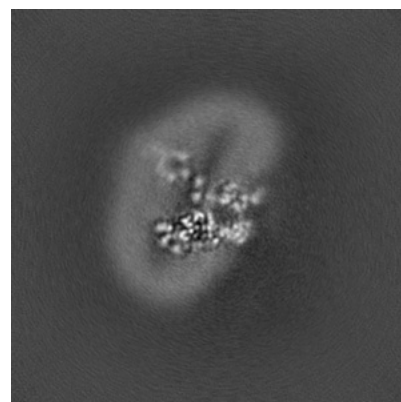
6.3.2 Raw map



X Index: 142



Y Index: 122

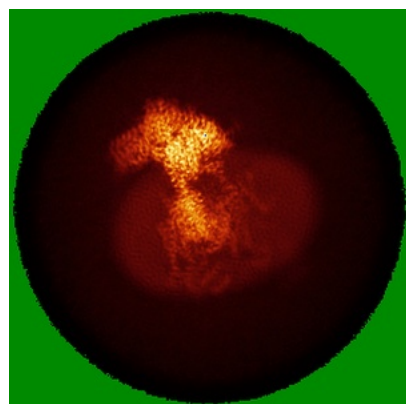


Z Index: 141

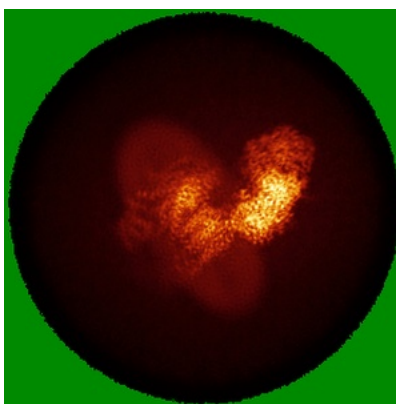
The images above show the largest variance slices of the map in three orthogonal directions.

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

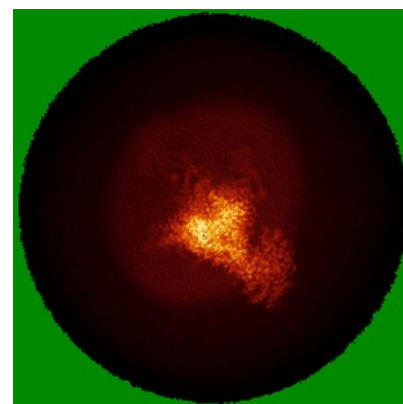
6.4.1 Primary map



X

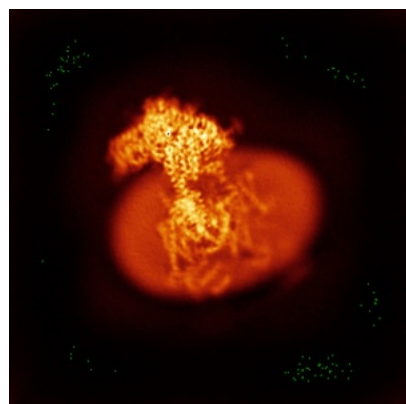


Y

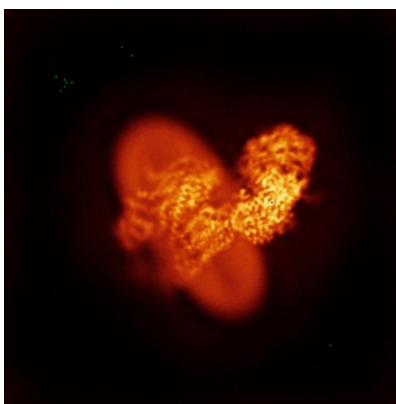


Z

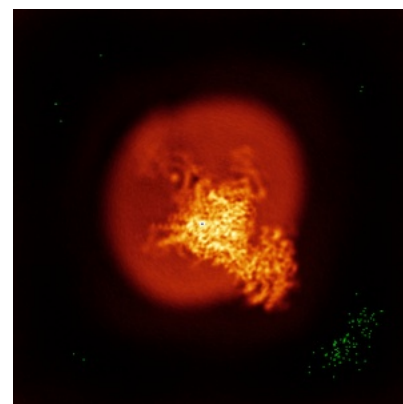
6.4.2 Raw map



X



Y

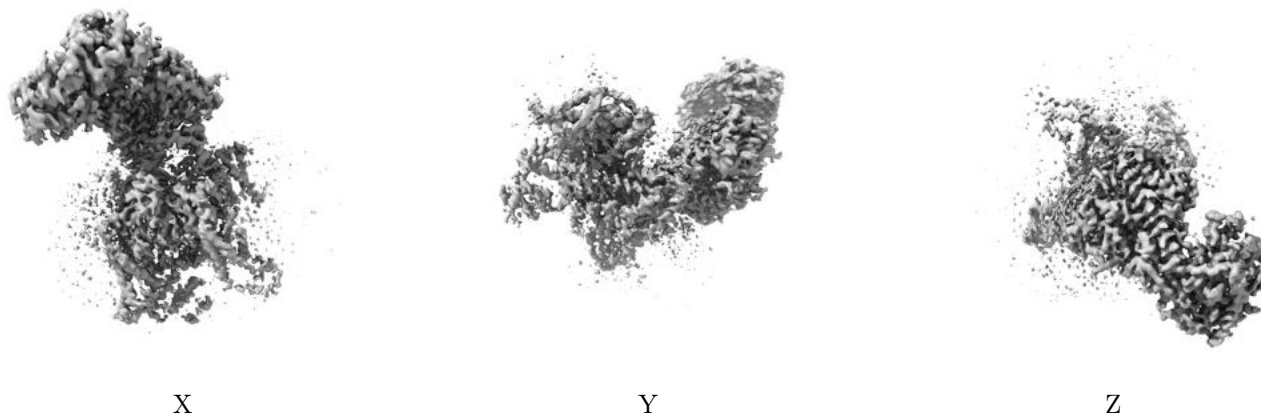


Z

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.

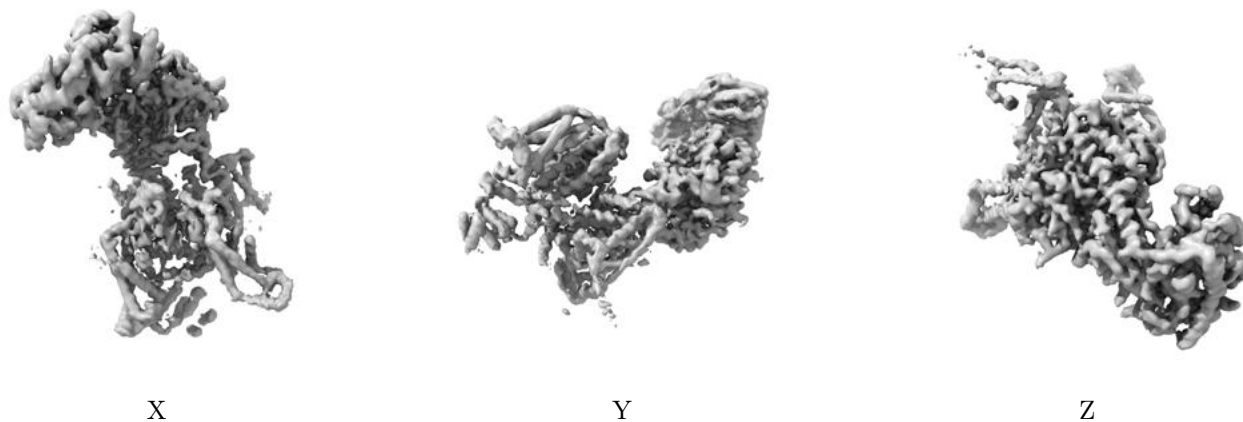
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

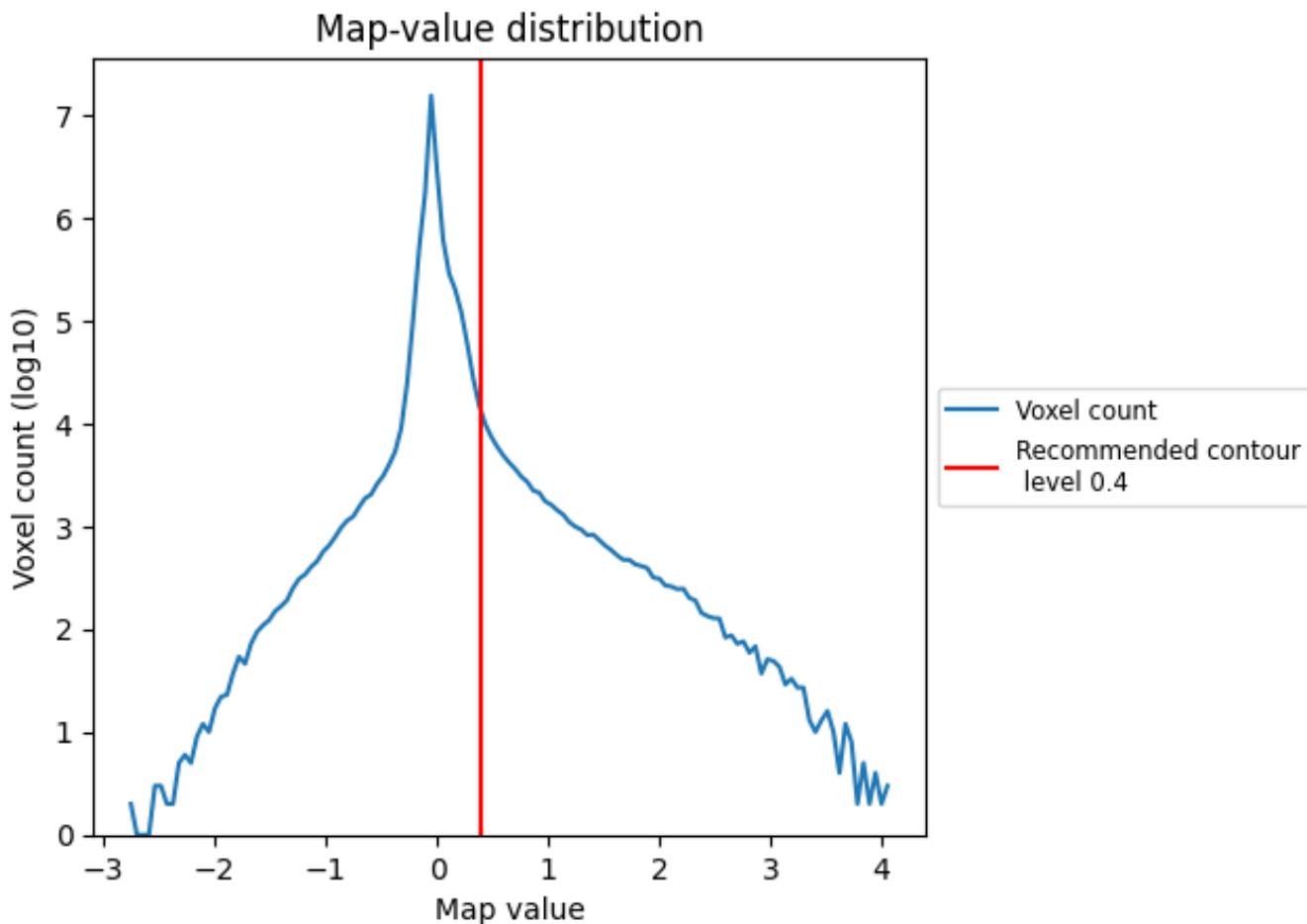
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

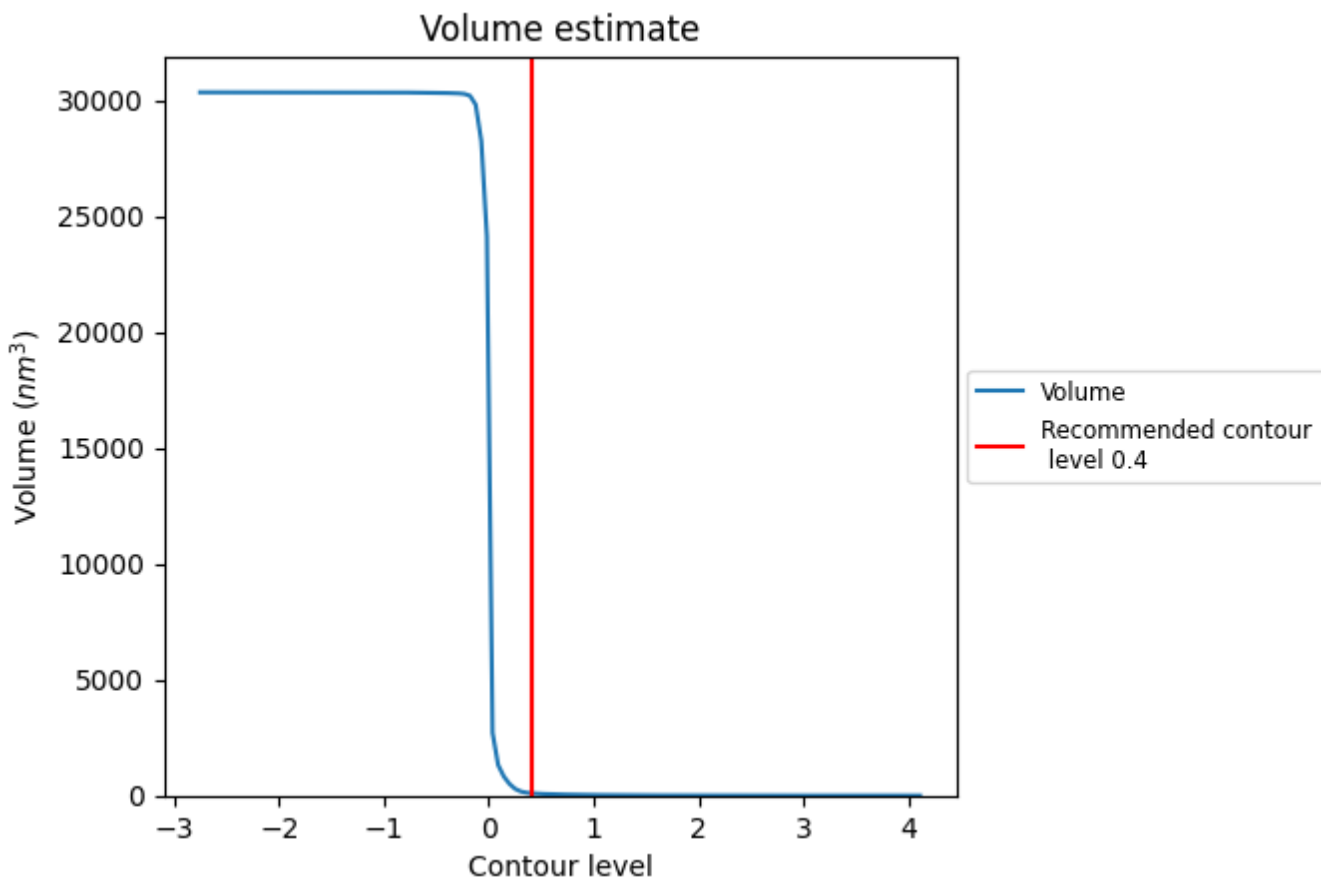
This section contains the results of statistical analysis of the map.

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.

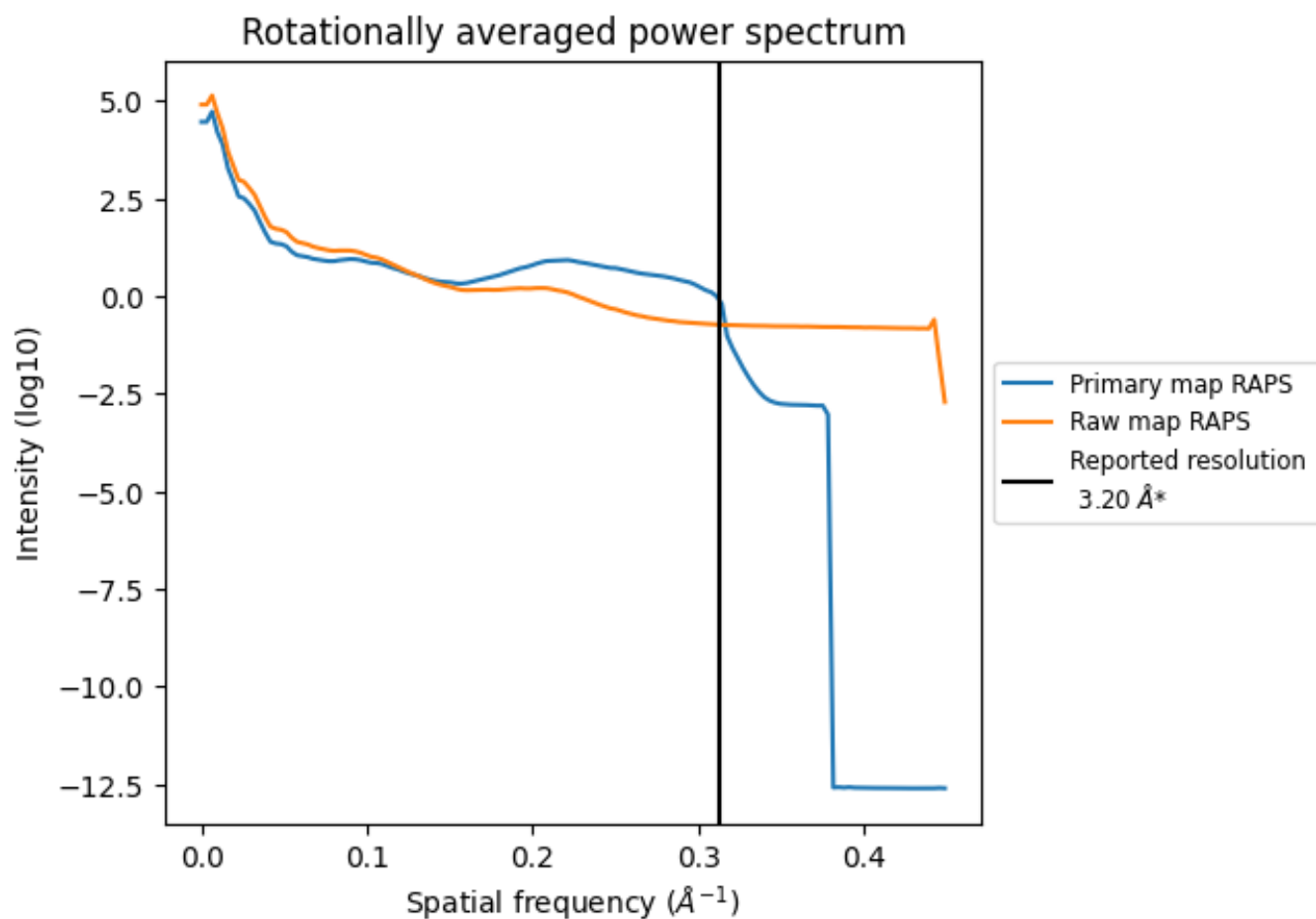
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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](#)

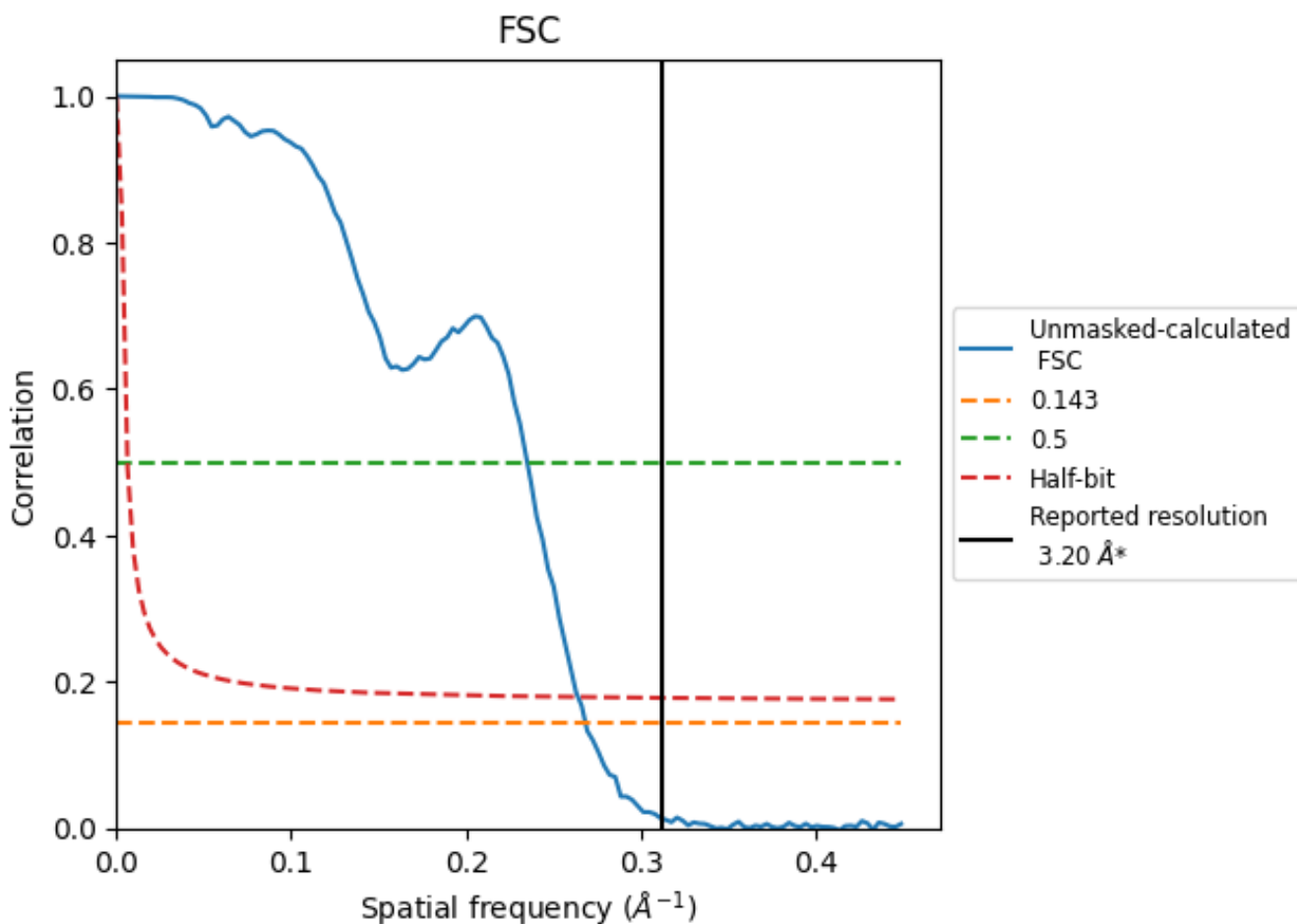


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

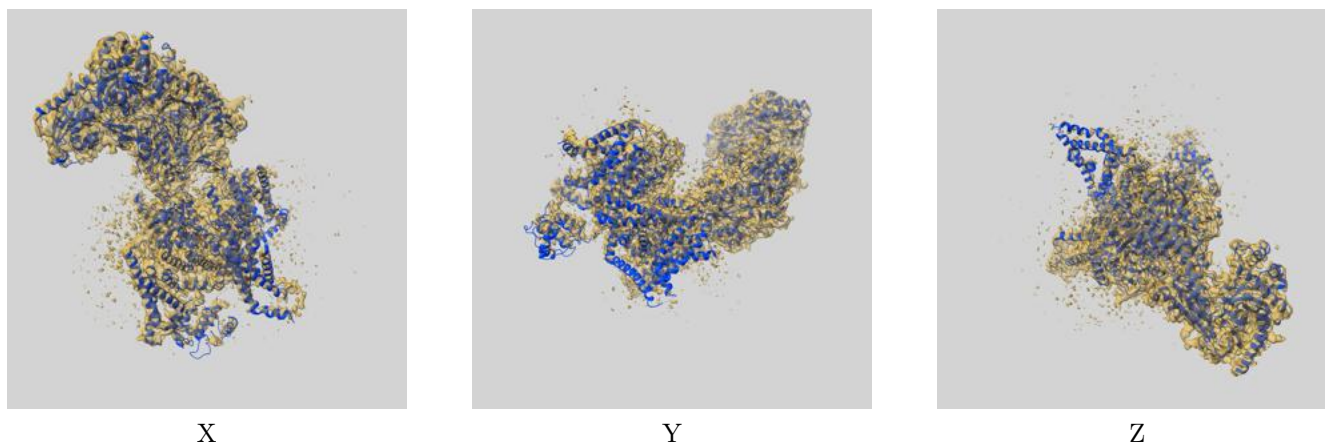
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.26	3.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.73 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

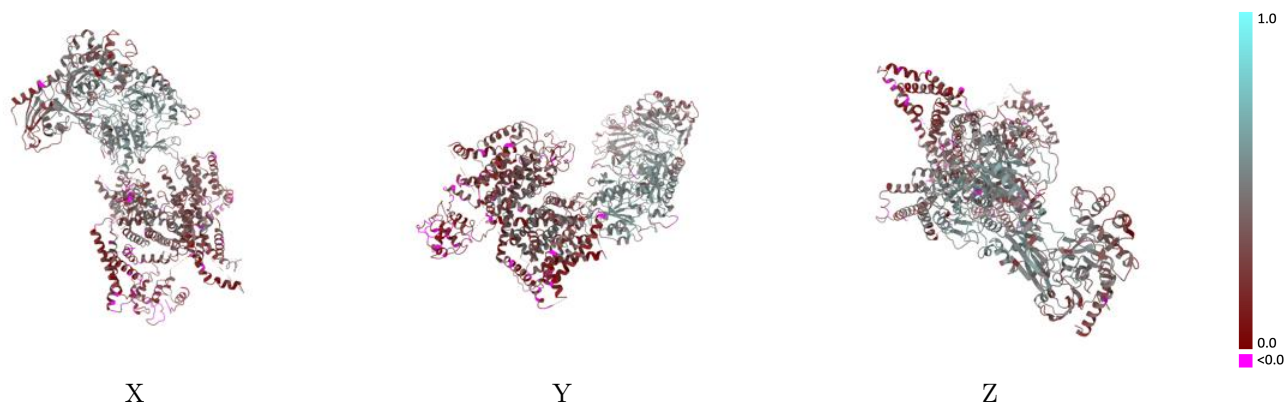
This section contains information regarding the fit between EMDB map EMD-37476 and PDB model 8WEA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



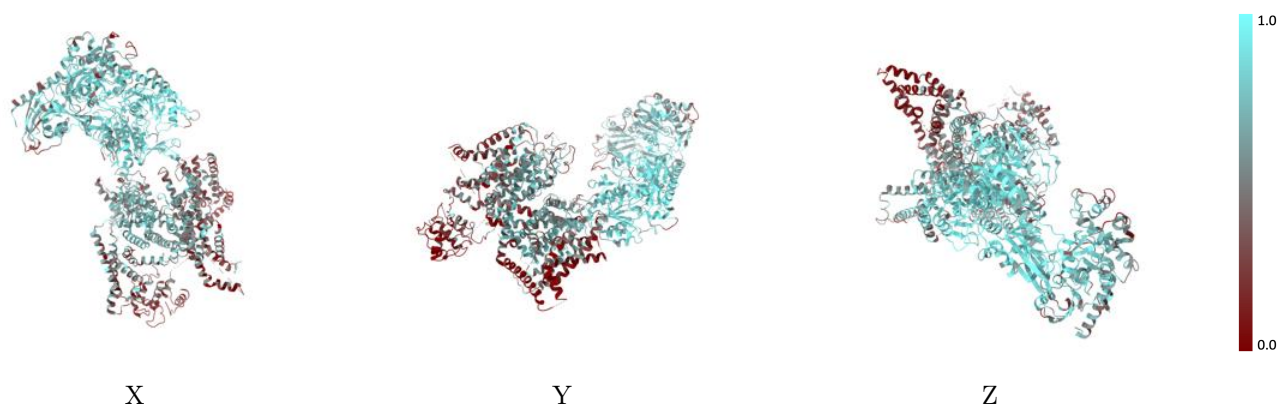
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



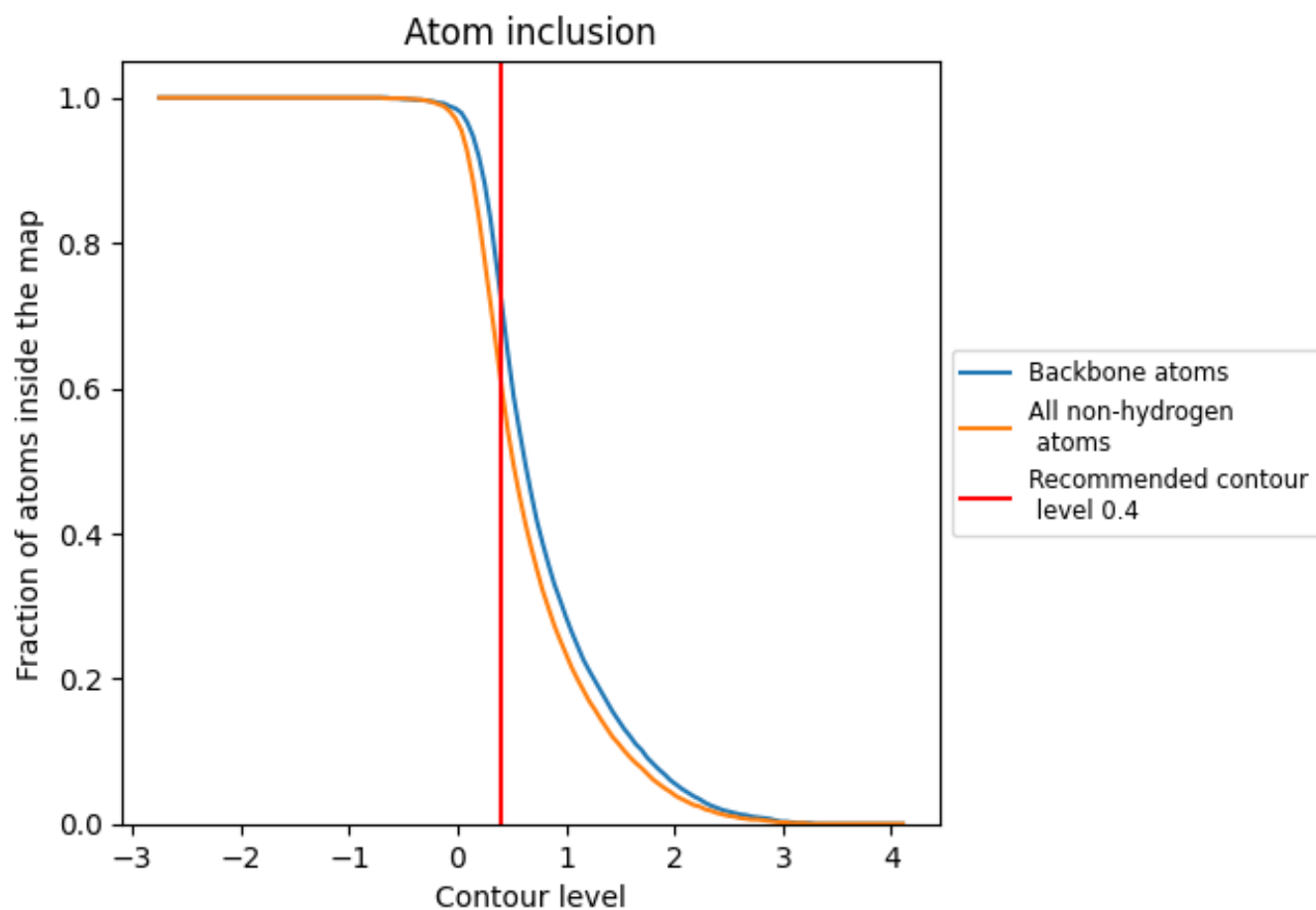
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

















9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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	 0.6080	 0.3490
A	 0.4720	 0.2600
B	 0.4290	 0.3350
C	 0.2860	 0.3440
D	 0.7790	 0.4590
E	 0.7860	 0.5040
F	 0.3210	 0.2010
G	 0.5360	 0.3500

