



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 10:45 PM EST

PDB ID : 6WI1  
EMDB ID : EMD-21682  
Title : GluN1b-GluN2B NMDA receptor in active conformation stabilized by inter-GluN1b-GluN2B subunit cross-linking  
Authors : Chou, T.; Tajima, N.; Furukawa, H.  
Deposited on : 2020-04-08  
Resolution : 3.62 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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) : 2.31.2

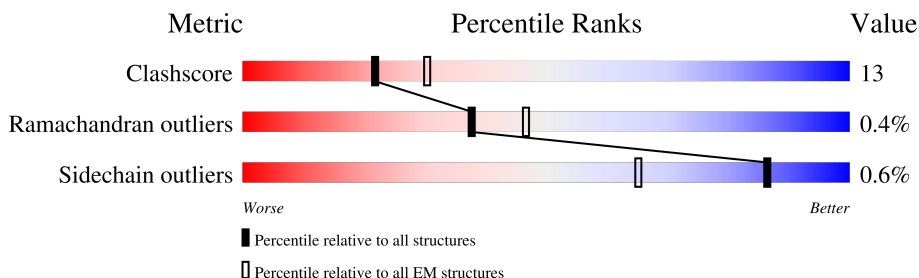
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.62 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	
1	C	868	
2	B	883	
2	D	883	
3	E	2	
3	F	2	
3	G	2	
3	H	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	NAG	E	2	X	-	-	-
3	NAG	G	2	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23366 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 Ionotropic glutamate receptor , NMDA receptor GluN1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	806	Total	C	N	O	S	0	0
			5910	3771	1008	1100	31		
1	C	806	Total	C	N	O	S	0	0
			5910	3771	1008	1100	31		

- Molecule 2 is a protein called Ionotropic glutamate receptor , NMDA receptor GluN2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	785	Total	C	N	O	S	0	0
			5661	3635	912	1080	34		
2	D	785	Total	C	N	O	S	0	0
			5661	3635	912	1080	34		

- Molecule 3 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		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

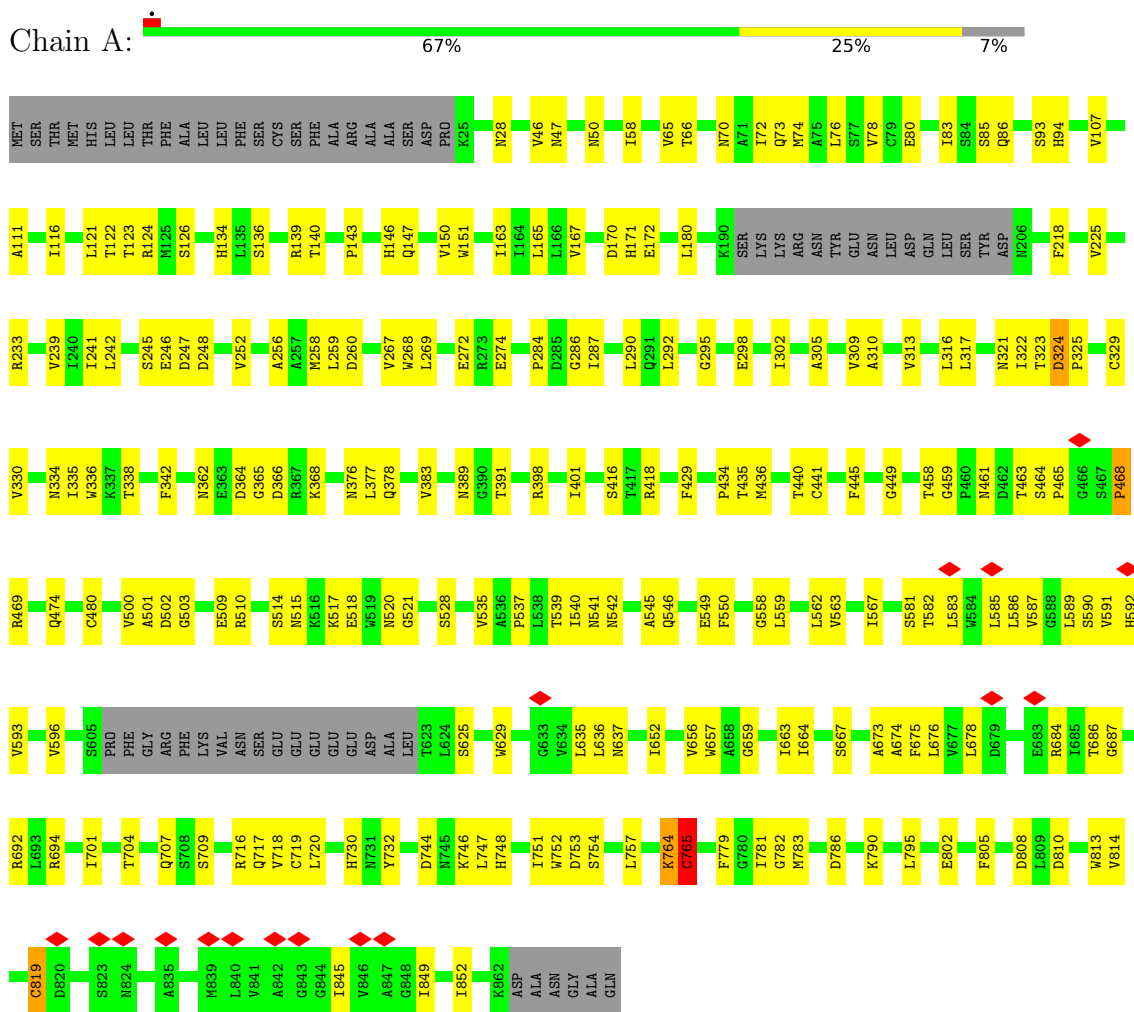


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total	C	N	O	0
			28	16	2	10	
4	A	1	Total	C	N	O	0
			28	16	2	10	
4	B	1	Total	C	N	O	0
			28	16	2	10	
4	B	1	Total	C	N	O	0
			28	16	2	10	
4	C	1	Total	C	N	O	0
			28	16	2	10	
4	C	1	Total	C	N	O	0
			28	16	2	10	
4	D	1	Total	C	N	O	0
			28	16	2	10	
4	D	1	Total	C	N	O	0
			28	16	2	10	

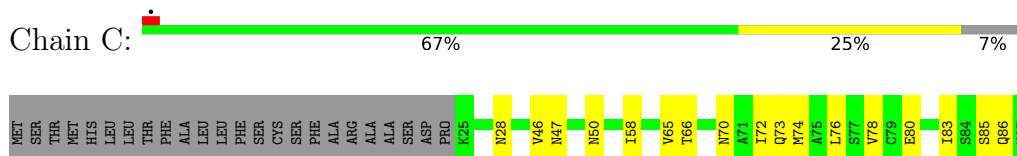
### 3 Residue-property plots [i](#)

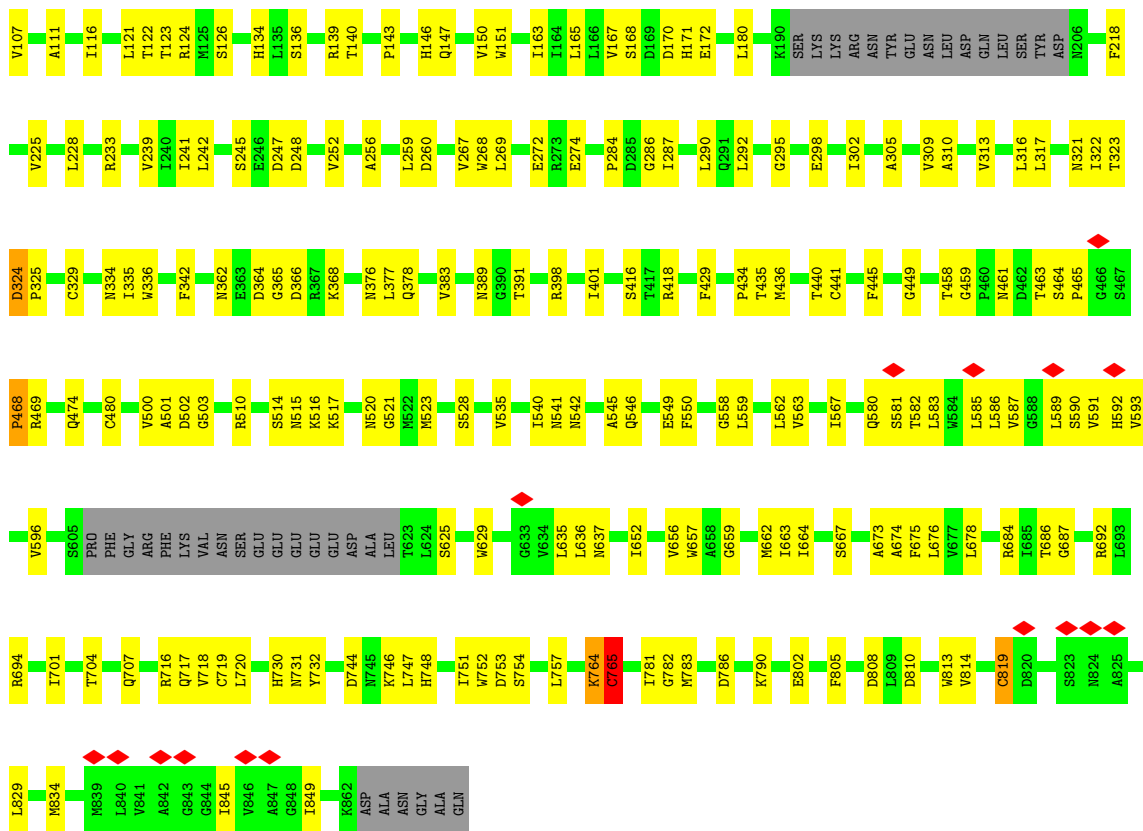
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ionotropic glutamate receptor , NMDA receptor GluN1b

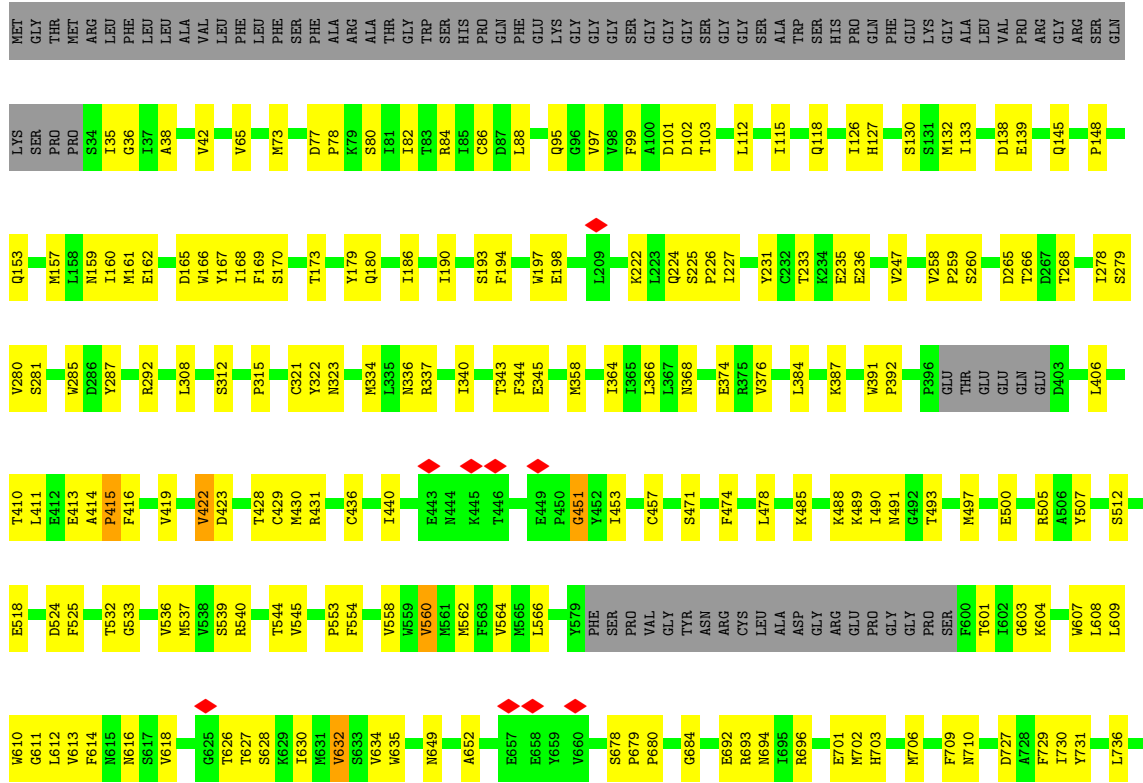


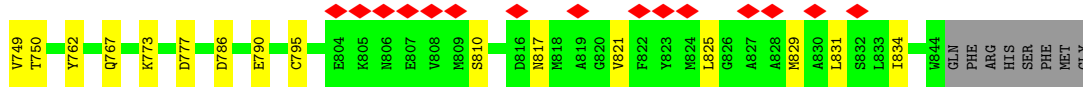
- Molecule 1: Ionotropic glutamate receptor , NMDA receptor GluN1b



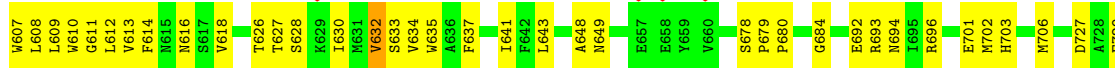
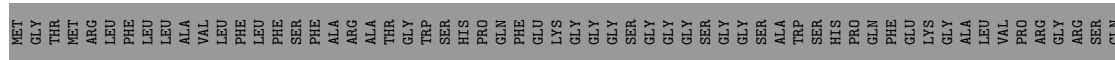


• Molecule 2: Ionotropic glutamate receptor , NMDA receptor GluN2B

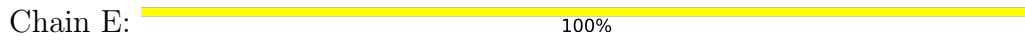




• Molecule 2: Ionotropic glutamate receptor , NMDA receptor GluN2B



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



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





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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	155641	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 ( $e^-/\text{\AA}^2$ )	64.5	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	17.319	Depositor
Minimum map value	-6.912	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.873	Depositor
Recommended contour level	2.77	Depositor
Map size ( $\text{\AA}$ )	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.37, 1.37, 1.37	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

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	0.37	0/6037	0.51	3/8242 (0.0%)
1	C	0.37	0/6037	0.51	3/8242 (0.0%)
2	B	0.39	0/5776	0.52	0/7897
2	D	0.39	0/5776	0.52	0/7897
All	All	0.38	0/23626	0.51	6/32278 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
2	B	0	2
2	D	0	2
All	All	0	10

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	765	CYS	CA-CB-SG	7.03	126.66	114.00
1	A	765	CYS	CA-CB-SG	7.03	126.64	114.00
1	C	819	CYS	CA-CB-SG	5.40	123.73	114.00
1	A	819	CYS	CA-CB-SG	5.40	123.71	114.00
1	A	786	ASP	C-N-CA	-5.10	108.94	121.70
1	C	786	ASP	C-N-CA	-5.10	108.94	121.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ASP	Peptide
1	A	567	ILE	Peptide
1	A	764	LYS	Peptide
2	B	165	ASP	Peptide
2	B	474	PHE	Peptide
1	C	324	ASP	Peptide
1	C	567	ILE	Peptide
1	C	764	LYS	Peptide
2	D	165	ASP	Peptide
2	D	474	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5910	0	5583	144	0
1	C	5910	0	5583	149	0
2	B	5661	0	5230	151	0
2	D	5661	0	5230	161	0
3	E	28	0	25	1	0
3	F	28	0	25	1	0
3	G	28	0	25	1	0
3	H	28	0	25	1	0
4	A	28	0	26	0	0
4	B	28	0	26	2	0
4	C	28	0	26	0	0
4	D	28	0	26	1	0
All	All	23366	0	21830	583	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 13.

All (583) 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)
2:D:169:PHE:HB3	2:D:225:SER:HB2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PHE:HB3	2:B:225:SER:HB2	1.53	0.89
2:D:440:ILE:HG22	2:D:451:GLY:HA3	1.62	0.82
1:C:324:ASP:O	1:C:336:TRP:NE1	2.13	0.82
2:B:440:ILE:HG22	2:B:451:GLY:HA3	1.61	0.81
1:A:324:ASP:O	1:A:336:TRP:NE1	2.13	0.81
1:A:286:GLY:H	1:A:377:LEU:HB3	1.50	0.77
1:A:86:GLN:HB3	1:A:325:PRO:HG2	1.68	0.75
2:D:537:MET:HA	2:D:749:VAL:HA	1.69	0.75
1:C:86:GLN:HB3	1:C:325:PRO:HG2	1.68	0.74
1:C:286:GLY:H	1:C:377:LEU:HB3	1.50	0.74
2:D:101:ASP:OD1	2:D:102:ASP:N	2.19	0.74
2:B:77:ASP:OD1	2:B:80:SER:N	2.15	0.74
2:D:77:ASP:OD1	2:D:80:SER:N	2.15	0.73
2:B:537:MET:HA	2:B:749:VAL:HA	1.69	0.73
1:A:378:GLN:HE22	1:A:401:ILE:HG13	1.55	0.72
2:D:308:LEU:O	2:D:312:SER:N	2.16	0.72
2:B:101:ASP:OD1	2:B:102:ASP:N	2.19	0.72
1:C:378:GLN:HE22	1:C:401:ILE:HG13	1.55	0.71
2:B:130:SER:O	2:B:145:GLN:NE2	2.23	0.71
2:B:308:LEU:HD21	2:B:315:PRO:HD3	1.73	0.71
2:D:130:SER:O	2:D:145:GLN:NE2	2.23	0.70
1:A:591:VAL:HG12	1:A:657:TRP:HZ2	1.56	0.70
1:A:143:PRO:HD2	1:A:146:HIS:CD2	2.27	0.70
2:D:544:THR:HG22	2:D:545:VAL:H	1.57	0.70
2:B:308:LEU:O	2:B:312:SER:N	2.16	0.69
1:C:591:VAL:HG12	1:C:657:TRP:HZ2	1.56	0.69
2:B:544:THR:HG22	2:B:545:VAL:H	1.57	0.69
2:B:414:ALA:O	2:B:416:PHE:N	2.25	0.69
1:C:143:PRO:HD2	1:C:146:HIS:CD2	2.27	0.69
2:B:162:GLU:HB3	2:B:197:TRP:CH2	2.28	0.69
2:B:436:CYS:HB3	2:B:478:LEU:HD23	1.76	0.68
2:D:308:LEU:HD21	2:D:315:PRO:HD3	1.73	0.68
2:D:414:ALA:O	2:D:416:PHE:N	2.25	0.68
2:D:162:GLU:HB3	2:D:197:TRP:CH2	2.28	0.68
1:A:70:ASN:OD1	1:A:73:GLN:N	2.20	0.68
1:C:70:ASN:OD1	1:C:73:GLN:N	2.20	0.68
1:A:753:ASP:OD1	1:A:754:SER:N	2.26	0.68
1:C:744:ASP:HB3	1:C:746:LYS:HE2	1.76	0.68
2:B:627:THR:HA	2:B:630:ILE:HD12	1.76	0.67
2:B:167:TYR:HB2	2:B:169:PHE:CE2	2.30	0.67
2:D:627:THR:HA	2:D:630:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:N	1:A:274:GLU:OE1	2.28	0.67
1:A:744:ASP:HB3	1:A:746:LYS:HE2	1.76	0.66
2:D:436:CYS:HB3	2:D:478:LEU:HD23	1.76	0.66
2:D:167:TYR:HB2	2:D:169:PHE:CE2	2.30	0.66
1:A:46:VAL:O	1:A:50:ASN:ND2	2.29	0.66
1:C:46:VAL:O	1:C:50:ASN:ND2	2.29	0.66
1:C:274:GLU:OE1	1:C:274:GLU:N	2.28	0.66
2:D:222:LYS:HA	2:D:224:GLN:HE22	1.61	0.66
2:D:413:GLU:HG3	2:D:414:ALA:H	1.60	0.66
1:A:802:GLU:OE1	2:D:694:ASN:ND2	2.26	0.65
2:B:222:LYS:HA	2:B:224:GLN:HE22	1.61	0.65
2:B:632:VAL:HA	2:B:635:TRP:HB2	1.78	0.65
2:B:413:GLU:HG3	2:B:414:ALA:H	1.61	0.64
2:D:632:VAL:HA	2:D:635:TRP:HB2	1.78	0.64
1:C:225:VAL:HG11	1:C:252:VAL:HG12	1.79	0.64
1:A:225:VAL:HG11	1:A:252:VAL:HG12	1.79	0.63
2:D:279:SER:OG	2:D:280:VAL:N	2.31	0.63
1:C:753:ASP:OD1	1:C:754:SER:N	2.26	0.63
2:D:278:ILE:HD11	2:D:391:TRP:CH2	2.33	0.63
2:B:279:SER:OG	2:B:280:VAL:N	2.31	0.63
1:C:686:THR:HG22	1:C:687:GLY:H	1.63	0.63
1:A:163:ILE:HD11	1:A:241:ILE:HG13	1.80	0.63
1:A:686:THR:HG22	1:A:687:GLY:H	1.63	0.63
2:D:162:GLU:HB3	2:D:197:TRP:HH2	1.64	0.62
2:B:278:ILE:HD11	2:B:391:TRP:CH2	2.33	0.62
2:B:190:ILE:HD12	2:B:197:TRP:HB3	1.82	0.62
2:D:422:VAL:HG23	2:D:423:ASP:H	1.64	0.62
1:C:376:ASN:OD1	1:C:377:LEU:N	2.32	0.62
2:D:536:VAL:O	2:D:750:THR:N	2.31	0.62
1:A:376:ASN:OD1	1:A:377:LEU:N	2.32	0.62
1:C:163:ILE:HD11	1:C:241:ILE:HG13	1.80	0.61
2:B:160:ILE:HD11	2:B:364:ILE:HG12	1.83	0.61
2:B:536:VAL:O	2:B:750:THR:N	2.31	0.61
1:A:78:VAL:HG21	1:A:107:VAL:HG12	1.82	0.61
2:D:430:MET:SD	2:D:431:ARG:N	2.74	0.61
1:A:242:LEU:HD11	1:A:252:VAL:HG21	1.83	0.60
2:B:430:MET:SD	2:B:431:ARG:N	2.74	0.60
2:D:190:ILE:HD12	2:D:197:TRP:HB3	1.82	0.60
2:D:524:ASP:OD1	2:D:525:PHE:N	2.31	0.60
2:B:162:GLU:HB3	2:B:197:TRP:HH2	1.64	0.60
2:B:422:VAL:HG23	2:B:423:ASP:H	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD11	1:C:252:VAL:HG21	1.83	0.60
2:D:553:PRO:O	2:D:649:ASN:ND2	2.35	0.60
2:B:553:PRO:O	2:B:649:ASN:ND2	2.35	0.60
1:C:83:ILE:HG23	1:C:329:CYS:HB3	1.83	0.60
2:B:368:ASN:ND2	2:B:374:GLU:OE2	2.34	0.60
1:A:362:ASN:OD1	1:A:366:ASP:N	2.33	0.60
2:D:368:ASN:ND2	2:D:374:GLU:OE2	2.34	0.60
2:D:160:ILE:HD11	2:D:364:ILE:HG12	1.83	0.60
2:D:609:LEU:HA	2:D:612:LEU:HD12	1.82	0.60
2:B:266:THR:HG22	2:B:268:THR:H	1.67	0.60
2:B:609:LEU:HA	2:B:612:LEU:HD12	1.83	0.60
1:C:78:VAL:HG21	1:C:107:VAL:HG12	1.82	0.59
1:A:256:ALA:O	1:A:260:ASP:N	2.35	0.59
2:D:410:THR:OG1	2:D:411:LEU:N	2.35	0.59
1:A:83:ILE:HG23	1:A:329:CYS:HB3	1.83	0.59
2:D:601:THR:O	2:D:604:LYS:N	2.33	0.59
1:A:245:SER:OG	1:A:247:ASP:OD1	2.20	0.59
1:A:716:ARG:NH2	2:D:786:ASP:OD1	2.35	0.59
1:C:73:GLN:HA	1:C:76:LEU:HD12	1.84	0.59
1:C:245:SER:OG	1:C:247:ASP:OD1	2.20	0.59
1:A:93:SER:OG	1:A:94:HIS:N	2.34	0.59
2:B:410:THR:OG1	2:B:411:LEU:N	2.35	0.59
1:C:65:VAL:HG12	1:C:66:THR:H	1.68	0.59
2:B:169:PHE:CB	2:B:225:SER:HB2	2.32	0.59
1:C:416:SER:OG	1:C:418:ARG:O	2.21	0.59
1:A:70:ASN:ND2	2:B:322:TYR:O	2.36	0.58
1:C:256:ALA:O	1:C:260:ASP:N	2.35	0.58
1:A:65:VAL:HG12	1:A:66:THR:H	1.68	0.58
2:D:702:MET:O	2:D:706:MET:HB2	2.03	0.58
2:D:266:THR:HG22	2:D:268:THR:H	1.67	0.58
2:B:702:MET:O	2:B:706:MET:HB2	2.03	0.58
1:C:93:SER:OG	1:C:94:HIS:N	2.34	0.58
1:A:73:GLN:HA	1:A:76:LEU:HD12	1.84	0.58
1:A:416:SER:OG	1:A:418:ARG:O	2.21	0.58
2:D:287:TYR:HD2	2:D:292:ARG:HE	1.51	0.58
2:B:287:TYR:HD2	2:B:292:ARG:HE	1.51	0.58
1:C:94:HIS:N	1:C:122:THR:OG1	2.37	0.58
2:D:138:ASP:OD1	2:D:139:GLU:N	2.34	0.58
2:D:562:MET:O	2:D:566:LEU:HG	2.04	0.57
1:C:362:ASN:OD1	1:C:366:ASP:N	2.33	0.57
2:B:138:ASP:OD1	2:B:139:GLU:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:MET:O	2:B:566:LEU:HG	2.04	0.57
2:B:626:THR:HG23	2:B:628:SER:H	1.69	0.57
1:A:94:HIS:N	1:A:122:THR:OG1	2.37	0.57
1:A:502:ASP:N	1:A:502:ASP:OD1	2.36	0.57
1:A:591:VAL:HG11	1:A:635:LEU:HD22	1.87	0.57
1:C:591:VAL:HG11	1:C:635:LEU:HD22	1.87	0.56
1:A:86:GLN:NE2	1:A:325:PRO:O	2.39	0.56
1:A:562:LEU:HB2	1:A:757:LEU:HD21	1.87	0.56
1:A:583:LEU:HD13	1:A:586:LEU:HD21	1.87	0.56
1:C:502:ASP:OD1	1:C:502:ASP:N	2.36	0.56
2:D:38:ALA:HB3	2:D:97:VAL:HG23	1.86	0.56
2:D:626:THR:HG23	2:D:628:SER:H	1.69	0.56
1:A:673:ALA:HA	1:A:676:LEU:HD12	1.87	0.56
1:C:126:SER:N	1:C:172:GLU:OE2	2.28	0.56
1:C:86:GLN:NE2	1:C:325:PRO:O	2.38	0.56
1:C:673:ALA:HA	1:C:676:LEU:HD12	1.88	0.56
2:D:169:PHE:CB	2:D:225:SER:HB2	2.32	0.56
1:A:74:MET:O	1:A:78:VAL:HG23	2.06	0.55
2:B:38:ALA:HB3	2:B:97:VAL:HG23	1.86	0.55
1:C:70:ASN:ND2	2:D:323:ASN:HA	2.21	0.55
1:C:583:LEU:HD13	1:C:586:LEU:HD21	1.87	0.55
1:A:362:ASN:HA	1:A:368:LYS:HD3	1.88	0.55
2:B:601:THR:O	2:B:604:LYS:N	2.33	0.55
1:C:322:ILE:HG23	1:C:323:THR:H	1.71	0.55
2:B:166:TRP:HH2	2:B:428:THR:HG1	1.55	0.55
1:A:72:ILE:HD11	2:B:118:GLN:HB3	1.88	0.55
1:A:435:THR:HA	1:A:441:CYS:HB3	1.89	0.55
1:A:591:VAL:HG12	1:A:657:TRP:CZ2	2.40	0.55
1:C:362:ASN:HA	1:C:368:LYS:HD3	1.87	0.55
2:D:321:CYS:O	2:D:323:ASN:N	2.40	0.55
1:A:28:ASN:ND2	1:A:85:SER:OG	2.40	0.55
1:C:562:LEU:HB2	1:C:757:LEU:HD21	1.87	0.55
1:C:652:ILE:O	1:C:656:VAL:HG23	2.07	0.55
1:A:652:ILE:O	1:A:656:VAL:HG23	2.07	0.54
2:B:524:ASP:OD1	2:B:525:PHE:N	2.31	0.54
1:C:591:VAL:HG12	1:C:657:TRP:CZ2	2.40	0.54
2:B:321:CYS:O	2:B:323:ASN:N	2.40	0.54
1:C:74:MET:O	1:C:78:VAL:HG23	2.06	0.54
2:B:773:LYS:NZ	2:B:777:ASP:OD2	2.40	0.54
1:C:28:ASN:ND2	1:C:85:SER:OG	2.40	0.54
1:A:445:PHE:HB3	1:A:449:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:PHE:HB3	1:C:449:GLY:HA2	1.89	0.54
2:D:610:TRP:HA	2:D:613:VAL:HG12	1.90	0.54
1:A:322:ILE:HG23	1:A:323:THR:H	1.71	0.54
1:C:151:TRP:CD1	1:C:269:LEU:HD13	2.43	0.54
1:C:245:SER:OG	1:C:248:ASP:OD2	2.24	0.54
1:A:659:GLY:O	1:A:663:ILE:HG12	2.08	0.53
1:C:659:GLY:O	1:C:663:ILE:HG12	2.08	0.53
2:D:166:TRP:HH2	2:D:428:THR:HG1	1.55	0.53
2:D:727:ASP:OD1	2:D:727:ASP:N	2.41	0.53
2:D:773:LYS:NZ	2:D:777:ASP:OD2	2.40	0.53
2:B:727:ASP:OD1	2:B:727:ASP:N	2.41	0.53
1:C:435:THR:HA	1:C:441:CYS:HB3	1.89	0.53
2:B:278:ILE:HD11	2:B:391:TRP:CZ2	2.44	0.53
2:B:500:GLU:OE2	2:B:505:ARG:NH1	2.40	0.53
1:A:151:TRP:CD1	1:A:269:LEU:HD13	2.44	0.53
1:A:233:ARG:HH22	1:A:259:LEU:HD22	1.73	0.53
1:A:468:PRO:O	1:A:469:ARG:HG2	2.09	0.53
1:C:233:ARG:HH22	1:C:259:LEU:HD22	1.73	0.53
2:D:278:ILE:HD11	2:D:391:TRP:CZ2	2.44	0.53
2:B:610:TRP:HA	2:B:613:VAL:HG12	1.90	0.52
1:C:468:PRO:O	1:C:469:ARG:HG2	2.09	0.52
1:A:58:ILE:HD13	1:A:317:LEU:HD11	1.91	0.52
1:A:121:LEU:HA	1:A:140:THR:HG22	1.91	0.52
1:A:535:VAL:HG22	1:A:781:ILE:HD12	1.92	0.52
1:C:70:ASN:HD22	2:D:323:ASN:HA	1.74	0.52
1:C:70:ASN:ND2	2:D:322:TYR:O	2.43	0.52
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.92	0.52
2:D:260:SER:HB2	2:D:280:VAL:O	2.10	0.52
2:D:260:SER:HB2	2:D:281:SER:HA	1.92	0.52
2:D:608:LEU:O	2:D:612:LEU:HG	2.09	0.52
2:B:260:SER:HB2	2:B:280:VAL:O	2.10	0.52
2:B:608:LEU:O	2:B:612:LEU:HG	2.09	0.52
1:C:58:ILE:HD13	1:C:317:LEU:HD11	1.91	0.52
2:B:260:SER:HB2	2:B:281:SER:HA	1.92	0.51
2:B:821:VAL:O	2:B:825:LEU:HG	2.10	0.51
1:A:165:LEU:HD22	1:A:180:LEU:HD23	1.91	0.51
1:A:239:VAL:HA	1:A:267:VAL:O	2.11	0.51
2:D:173:THR:HG1	2:D:179:TYR:HE1	1.58	0.51
2:D:507:TYR:HA	2:D:767:GLN:HG3	1.92	0.51
1:C:535:VAL:HG22	1:C:781:ILE:HD12	1.92	0.51
2:D:821:VAL:O	2:D:825:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ILE:HD12	1:A:730:HIS:CD2	2.46	0.51
2:B:173:THR:HG1	2:B:179:TYR:HE1	1.58	0.51
1:C:239:VAL:HA	1:C:267:VAL:O	2.11	0.51
1:A:247:ASP:OD1	1:A:248:ASP:N	2.44	0.51
2:B:507:TYR:HA	2:B:767:GLN:HG3	1.92	0.51
1:C:121:LEU:HA	1:C:140:THR:HG22	1.91	0.51
1:C:701:ILE:HD12	1:C:730:HIS:CD2	2.46	0.51
1:C:752:TRP:CG	1:C:753:ASP:N	2.79	0.51
2:D:500:GLU:OE2	2:D:505:ARG:NH1	2.40	0.51
1:C:247:ASP:OD1	1:C:248:ASP:N	2.44	0.51
1:A:124:ARG:NH1	1:A:272:GLU:OE2	2.44	0.50
2:D:167:TYR:HB2	2:D:169:PHE:CZ	2.46	0.50
1:A:752:TRP:CG	1:A:753:ASP:N	2.79	0.50
1:A:298:GLU:O	1:A:302:ILE:HG12	2.12	0.50
2:B:612:LEU:HD13	2:B:635:TRP:HB3	1.93	0.50
1:A:540:ILE:HG23	1:A:550:PHE:CD2	2.46	0.50
1:C:124:ARG:NH1	1:C:272:GLU:OE2	2.44	0.50
1:C:305:ALA:O	1:C:309:VAL:HG23	2.11	0.50
2:D:222:LYS:HA	2:D:224:GLN:NE2	2.26	0.50
1:A:305:ALA:O	1:A:309:VAL:HG23	2.11	0.50
2:B:490:ILE:N	2:B:493:THR:O	2.44	0.50
1:C:298:GLU:O	1:C:302:ILE:HG12	2.12	0.50
1:C:540:ILE:HG23	1:C:550:PHE:CD2	2.46	0.50
2:D:153:GLN:HE22	2:D:260:SER:HB3	1.77	0.50
2:B:167:TYR:HB2	2:B:169:PHE:CZ	2.47	0.50
2:B:786:ASP:OD1	1:C:716:ARG:NH2	2.45	0.50
2:B:222:LYS:HA	2:B:224:GLN:NE2	2.26	0.49
2:B:518:GLU:OE1	2:B:693:ARG:NE	2.38	0.49
2:B:169:PHE:O	2:B:170:SER:OG	2.26	0.49
1:C:58:ILE:HG21	1:C:317:LEU:HD13	1.95	0.49
1:A:330:VAL:HA	2:B:77:ASP:OD2	2.12	0.49
1:A:436:MET:N	1:A:440:THR:O	2.44	0.49
2:B:153:GLN:HE22	2:B:260:SER:HB3	1.77	0.49
2:B:554:PHE:HA	1:C:829:LEU:HB3	1.94	0.49
2:D:817:ASN:O	2:D:821:VAL:HG23	2.12	0.49
2:B:42:VAL:HG13	2:B:73:MET:HB3	1.94	0.49
1:C:436:MET:N	1:C:440:THR:O	2.44	0.49
1:C:520:ASN:OD1	1:C:521:GLY:N	2.45	0.49
2:D:612:LEU:HD13	2:D:635:TRP:HB3	1.94	0.49
2:B:440:ILE:HG22	2:B:451:GLY:CA	2.40	0.49
2:B:817:ASN:O	2:B:821:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ILE:O	2:D:127:HIS:HB2	2.13	0.49
2:D:132:MET:H	2:D:145:GLN:NE2	2.11	0.48
2:B:344:PHE:CD2	2:B:345:GLU:HB2	2.48	0.48
1:C:674:ALA:O	1:C:678:LEU:HG	2.14	0.48
2:D:423:ASP:HB2	2:D:429:CYS:HA	1.95	0.48
2:D:614:PHE:HB2	2:D:616:ASN:HD22	1.78	0.48
1:A:70:ASN:ND2	2:B:323:ASN:HA	2.28	0.48
1:A:520:ASN:OD1	1:A:521:GLY:N	2.45	0.48
2:B:159:ASN:O	2:B:162:GLU:HG3	2.14	0.48
2:D:42:VAL:HG13	2:D:73:MET:HB3	1.94	0.48
1:A:510:ARG:HA	1:A:517:LYS:HA	1.96	0.48
2:B:701:GLU:N	2:B:701:GLU:OE1	2.46	0.48
2:D:258:VAL:HG23	2:D:279:SER:HB2	1.96	0.48
2:B:419:VAL:HG12	2:B:457:CYS:SG	2.53	0.48
2:B:423:ASP:HB2	2:B:429:CYS:HA	1.95	0.48
2:B:614:PHE:HB2	2:B:616:ASN:HD22	1.78	0.48
2:D:159:ASN:O	2:D:162:GLU:HG3	2.14	0.48
2:D:692:GLU:OE2	2:D:703:HIS:NE2	2.47	0.48
3:G:1:NAG:O6	3:G:2:NAG:N2	2.46	0.48
1:A:635:LEU:HG	1:A:636:LEU:HD22	1.95	0.48
2:B:652:ALA:HB2	1:C:676:LEU:HD13	1.95	0.48
2:B:126:ILE:O	2:B:127:HIS:HB2	2.14	0.48
2:D:35:ILE:HG13	2:D:65:VAL:HG23	1.96	0.48
2:B:132:MET:H	2:B:145:GLN:NE2	2.11	0.48
2:B:258:VAL:HG23	2:B:279:SER:HB2	1.96	0.48
2:B:692:GLU:OE2	2:B:703:HIS:NE2	2.47	0.48
1:C:268:TRP:HZ2	1:C:284:PRO:HG3	1.79	0.48
2:B:42:VAL:HB	2:B:101:ASP:OD2	2.14	0.47
2:B:696:ARG:HB2	2:B:703:HIS:CD2	2.49	0.47
1:A:592:HIS:O	1:A:596:VAL:HG23	2.14	0.47
2:D:344:PHE:CD2	2:D:345:GLU:HB2	2.48	0.47
1:A:58:ILE:HG21	1:A:317:LEU:HD13	1.95	0.47
1:A:674:ALA:O	1:A:678:LEU:HG	2.14	0.47
2:B:169:PHE:CE2	2:B:226:PRO:HG2	2.48	0.47
1:C:732:TYR:HE2	1:C:747:LEU:HD22	1.79	0.47
2:D:82:ILE:HD13	2:D:115:ILE:HD11	1.96	0.47
2:D:419:VAL:HG12	2:D:457:CYS:SG	2.53	0.47
2:B:102:ASP:N	2:B:102:ASP:OD1	2.45	0.47
2:D:265:ASP:OD1	2:D:265:ASP:N	2.45	0.47
2:B:82:ILE:HD13	2:B:115:ILE:HD11	1.96	0.47
2:D:169:PHE:CE2	2:D:226:PRO:HG2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASN:OD1	1:A:365:GLY:N	2.48	0.47
2:B:825:LEU:O	2:B:829:MET:HG3	2.15	0.47
1:C:704:THR:HG22	1:C:751:ILE:O	2.15	0.47
2:D:696:ARG:HB2	2:D:703:HIS:CD2	2.49	0.47
1:A:126:SER:N	1:A:172:GLU:OE2	2.28	0.47
1:A:732:TYR:HE2	1:A:747:LEU:HD22	1.79	0.47
1:C:65:VAL:HG12	1:C:66:THR:N	2.29	0.47
1:C:694:ARG:NH2	2:D:795:CYS:HA	2.30	0.47
1:C:510:ARG:HA	1:C:517:LYS:HA	1.96	0.47
1:C:592:HIS:O	1:C:596:VAL:HG23	2.14	0.47
2:B:678:SER:O	2:B:680:PRO:HD2	2.15	0.47
2:D:231:TYR:HD1	2:D:259:PRO:HG3	1.80	0.47
2:D:334:MET:SD	2:D:334:MET:N	2.88	0.47
2:B:193:SER:OG	2:B:194:PHE:N	2.48	0.47
2:D:490:ILE:N	2:D:493:THR:O	2.44	0.47
2:B:35:ILE:HG13	2:B:65:VAL:HG23	1.96	0.46
2:D:102:ASP:N	2:D:102:ASP:OD1	2.45	0.46
1:A:625:SER:O	1:A:629:TRP:HD1	1.98	0.46
2:B:334:MET:SD	2:B:334:MET:N	2.88	0.46
2:B:518:GLU:CD	2:B:693:ARG:HE	2.18	0.46
2:D:42:VAL:HB	2:D:101:ASP:OD2	2.14	0.46
2:D:193:SER:OG	2:D:194:PHE:N	2.48	0.46
2:D:678:SER:O	2:D:680:PRO:HD2	2.15	0.46
1:A:268:TRP:HZ2	1:A:284:PRO:HG3	1.79	0.46
1:A:514:SER:OG	1:A:515:ASN:N	2.47	0.46
2:B:287:TYR:CE2	2:B:292:ARG:HG2	2.51	0.46
2:B:411:LEU:HD23	2:B:497:MET:SD	2.55	0.46
1:C:362:ASN:OD1	1:C:365:GLY:N	2.48	0.46
1:C:635:LEU:HG	1:C:636:LEU:HD22	1.95	0.46
1:C:684:ARG:O	1:C:692:ARG:NH2	2.49	0.46
1:A:65:VAL:HG12	1:A:66:THR:N	2.29	0.46
1:A:586:LEU:O	1:A:589:LEU:HG	2.15	0.46
1:A:704:THR:HG22	1:A:751:ILE:O	2.15	0.46
2:B:166:TRP:HH2	2:B:428:THR:OG1	1.98	0.46
2:B:235:GLU:H	2:B:235:GLU:CD	2.18	0.46
1:C:586:LEU:O	1:C:589:LEU:HG	2.15	0.46
1:C:625:SER:O	1:C:629:TRP:HD1	1.98	0.46
2:B:684:GLY:HA3	2:B:729:PHE:CD1	2.51	0.46
1:A:684:ARG:O	1:A:692:ARG:NH2	2.49	0.46
2:D:169:PHE:O	2:D:170:SER:OG	2.26	0.46
2:D:411:LEU:HD23	2:D:497:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:VAL:O	1:C:591:VAL:HG13	2.16	0.46
2:D:440:ILE:HG22	2:D:451:GLY:CA	2.40	0.46
2:D:825:LEU:O	2:D:829:MET:HG3	2.15	0.46
1:A:461:ASN:C	1:A:463:THR:H	2.19	0.46
1:A:718:VAL:HG13	1:A:719:CYS:H	1.81	0.46
2:D:166:TRP:HH2	2:D:428:THR:OG1	1.98	0.46
1:C:718:VAL:HG13	1:C:719:CYS:H	1.81	0.46
2:D:78:PRO:O	2:D:82:ILE:HG12	2.16	0.46
1:A:123:THR:O	1:A:139:ARG:NH2	2.46	0.45
1:A:321:ASN:C	1:A:323:THR:HG23	2.37	0.45
1:A:810:ASP:OD1	1:A:814:VAL:HB	2.16	0.45
1:C:167:VAL:O	1:C:218:PHE:HB3	2.16	0.45
1:C:514:SER:OG	1:C:515:ASN:N	2.47	0.45
1:C:652:ILE:HG12	2:D:607:TRP:CH2	2.51	0.45
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.51	0.45
2:B:558:VAL:HG13	1:C:834:MET:SD	2.55	0.45
2:D:491:ASN:N	4:D:903:NAG:O7	2.50	0.45
2:D:518:GLU:OE1	2:D:693:ARG:NE	2.38	0.45
1:A:245:SER:OG	1:A:248:ASP:OD2	2.24	0.45
2:B:491:ASN:N	4:B:903:NAG:O7	2.50	0.45
1:C:637:ASN:O	1:C:637:ASN:ND2	2.49	0.45
2:D:414:ALA:HB1	2:D:415:PRO:CD	2.47	0.45
2:D:701:GLU:OE1	2:D:701:GLU:N	2.46	0.45
3:E:1:NAG:O6	3:E:2:NAG:N2	2.46	0.45
1:C:810:ASP:OD1	1:C:814:VAL:HB	2.16	0.45
2:D:488:LYS:NZ	2:D:489:LYS:O	2.49	0.45
2:D:684:GLY:HA3	2:D:729:PHE:CD1	2.51	0.45
1:A:637:ASN:O	1:A:637:ASN:ND2	2.49	0.45
1:C:292:LEU:HD23	1:C:295:GLY:H	1.81	0.45
2:B:231:TYR:HD1	2:B:259:PRO:HG3	1.80	0.45
1:C:461:ASN:C	1:C:463:THR:H	2.19	0.45
1:C:549:GLU:HG2	1:C:790:LYS:HG3	1.99	0.45
2:D:630:ILE:O	2:D:633:SER:OG	2.26	0.45
1:A:167:VAL:O	1:A:218:PHE:HB3	2.16	0.45
2:B:179:TYR:HD2	2:B:180:GLN:CD	2.20	0.45
2:B:488:LYS:NZ	2:B:489:LYS:O	2.49	0.45
1:A:72:ILE:H	1:A:72:ILE:HD12	1.82	0.45
1:C:72:ILE:HD12	1:C:72:ILE:H	1.82	0.45
2:B:78:PRO:O	2:B:82:ILE:HG12	2.16	0.45
1:C:284:PRO:O	1:C:287:ILE:HG23	2.17	0.45
2:D:539:SER:OG	2:D:540:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD23	1:A:295:GLY:H	1.81	0.45
1:A:549:GLU:HG2	1:A:790:LYS:HG3	1.99	0.45
2:B:247:VAL:HG12	2:B:247:VAL:O	2.17	0.45
1:C:321:ASN:C	1:C:323:THR:HG23	2.37	0.45
1:C:541:ASN:OD1	1:C:541:ASN:N	2.50	0.44
2:D:553:PRO:HB3	2:D:649:ASN:HB3	1.98	0.44
1:A:284:PRO:O	1:A:287:ILE:HG23	2.17	0.44
1:C:47:ASN:HA	1:C:50:ASN:HD22	1.82	0.44
1:A:47:ASN:HA	1:A:50:ASN:HD22	1.82	0.44
1:A:334:ASN:OD1	1:A:335:ILE:N	2.46	0.44
2:B:391:TRP:CD2	2:B:392:PRO:HD2	2.53	0.44
1:C:383:VAL:HG21	1:C:398:ARG:HH22	1.82	0.44
1:C:383:VAL:HG21	1:C:398:ARG:NH2	2.33	0.44
2:D:247:VAL:HG12	2:D:247:VAL:O	2.17	0.44
1:A:83:ILE:HG22	1:A:329:CYS:H	1.82	0.44
1:A:694:ARG:NH2	2:B:795:CYS:HA	2.31	0.44
2:B:566:LEU:HD22	2:B:635:TRP:CH2	2.52	0.44
2:D:235:GLU:H	2:D:235:GLU:CD	2.18	0.44
1:A:587:VAL:O	1:A:591:VAL:HG13	2.16	0.44
2:B:198:GLU:N	2:B:198:GLU:OE1	2.51	0.44
2:B:344:PHE:CE2	2:B:345:GLU:HB2	2.52	0.44
2:B:536:VAL:HG22	2:B:730:ILE:HG12	1.99	0.44
2:B:694:ASN:ND2	1:C:802:GLU:OE1	2.45	0.44
2:B:343:THR:HB	3:F:1:NAG:H82	1.99	0.44
2:B:553:PRO:HB3	2:B:649:ASN:HB3	1.98	0.44
2:D:391:TRP:CD2	2:D:392:PRO:HD2	2.52	0.44
2:D:566:LEU:HD22	2:D:635:TRP:CH2	2.52	0.44
1:A:563:VAL:HG23	1:A:748:HIS:O	2.18	0.44
2:D:84:ARG:O	2:D:88:LEU:HG	2.18	0.44
2:D:179:TYR:HD2	2:D:180:GLN:CD	2.20	0.44
2:B:84:ARG:O	2:B:88:LEU:HG	2.18	0.44
2:B:99:PHE:CD2	2:B:112:LEU:HD21	2.53	0.44
2:B:414:ALA:HB1	2:B:415:PRO:CD	2.47	0.44
1:C:558:GLY:O	1:C:559:LEU:HD23	2.18	0.44
2:D:36:GLY:HA3	2:D:95:GLN:H	1.83	0.44
2:D:157:MET:O	2:D:161:MET:HG3	2.18	0.44
2:D:344:PHE:CE2	2:D:345:GLU:HB2	2.52	0.44
2:D:518:GLU:CD	2:D:693:ARG:HE	2.18	0.44
2:B:790:GLU:OE1	2:B:790:GLU:N	2.51	0.44
1:C:147:GLN:HE22	1:C:272:GLU:N	2.16	0.44
1:C:542:ASN:HA	1:C:545:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:PHE:CD2	2:D:112:LEU:HD21	2.53	0.44
1:A:676:LEU:HD11	2:D:648:ALA:HB1	2.00	0.43
2:B:265:ASP:OD1	2:B:265:ASP:N	2.45	0.43
2:B:536:VAL:HA	2:B:729:PHE:O	2.18	0.43
1:C:316:LEU:HD22	1:C:342:PHE:CD1	2.53	0.43
1:C:582:THR:HG23	1:C:583:LEU:H	1.83	0.43
1:A:316:LEU:HD22	1:A:342:PHE:CD1	2.53	0.43
2:B:36:GLY:HA3	2:B:95:GLN:H	1.83	0.43
2:B:731:TYR:HB3	2:B:736:LEU:HD11	2.01	0.43
2:D:198:GLU:OE1	2:D:198:GLU:N	2.51	0.43
2:B:133:ILE:HD13	2:B:148:PRO:O	2.18	0.43
1:A:170:ASP:OD1	1:A:171:HIS:N	2.52	0.43
1:A:539:THR:OG1	1:A:709:SER:OG	2.32	0.43
1:C:83:ILE:HG22	1:C:329:CYS:H	1.82	0.43
1:A:389:ASN:O	1:A:391:THR:N	2.52	0.43
1:A:540:ILE:HD12	1:A:550:PHE:CD2	2.53	0.43
1:A:541:ASN:OD1	1:A:541:ASN:N	2.50	0.43
1:A:562:LEU:HB2	1:A:757:LEU:HD11	2.01	0.43
2:B:336:ASN:OD1	2:B:337:ARG:N	2.52	0.43
2:B:406:LEU:HD22	2:B:507:TYR:CD2	2.54	0.43
1:C:464:SER:N	1:C:465:PRO:HD2	2.34	0.43
1:A:383:VAL:HG21	1:A:398:ARG:HH22	1.82	0.43
1:A:464:SER:N	1:A:465:PRO:HD2	2.34	0.43
1:A:542:ASN:HA	1:A:545:ALA:HB3	1.99	0.43
2:B:285:TRP:CD1	2:B:285:TRP:N	2.87	0.43
2:B:539:SER:OG	2:B:540:ARG:N	2.50	0.43
2:D:336:ASN:OD1	2:D:337:ARG:N	2.52	0.43
1:A:383:VAL:HG21	1:A:398:ARG:NH2	2.33	0.43
1:A:582:THR:HG23	1:A:583:LEU:H	1.83	0.43
1:C:170:ASP:OD1	1:C:171:HIS:N	2.52	0.43
1:C:325:PRO:HA	1:C:336:TRP:CE2	2.54	0.43
2:D:265:ASP:O	2:D:266:THR:OG1	2.36	0.43
2:D:536:VAL:HA	2:D:729:PHE:O	2.18	0.43
1:C:123:THR:O	1:C:139:ARG:NH2	2.45	0.43
1:C:458:THR:OG1	1:C:459:GLY:N	2.52	0.43
1:C:540:ILE:HD12	1:C:550:PHE:CD2	2.53	0.43
1:C:662:MET:HE2	2:D:643:LEU:HD11	2.01	0.43
1:C:523:MET:HE3	1:C:523:MET:HB3	1.98	0.43
2:D:260:SER:O	2:D:260:SER:OG	2.32	0.43
2:D:343:THR:HB	3:H:1:NAG:H82	1.99	0.43
2:D:790:GLU:OE1	2:D:790:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:HE22	1:A:272:GLU:N	2.16	0.43
1:A:310:ALA:HA	1:A:313:VAL:HG12	2.01	0.43
1:A:558:GLY:O	1:A:559:LEU:HD23	2.18	0.43
2:B:102:ASP:O	2:B:103:THR:OG1	2.30	0.43
2:B:157:MET:O	2:B:161:MET:HG3	2.18	0.43
2:D:536:VAL:HG22	2:D:730:ILE:HG12	1.99	0.43
1:C:590:SER:HA	1:C:593:VAL:HG22	2.00	0.42
2:D:133:ILE:HD13	2:D:148:PRO:O	2.18	0.42
2:B:358:MET:H	2:B:358:MET:HG2	1.57	0.42
1:C:310:ALA:HA	1:C:313:VAL:HG12	2.01	0.42
1:C:562:LEU:HB2	1:C:757:LEU:HD11	2.01	0.42
2:D:336:ASN:O	2:D:340:ILE:HG12	2.19	0.42
1:A:590:SER:HA	1:A:593:VAL:HG22	2.00	0.42
2:B:560:VAL:O	2:B:564:VAL:HG22	2.20	0.42
2:B:611:GLY:HA3	2:B:618:VAL:HG21	2.01	0.42
1:C:765:CYS:HB3	1:C:819:CYS:HB2	1.87	0.42
2:D:406:LEU:HD22	2:D:507:TYR:CD2	2.54	0.42
2:D:731:TYR:HB3	2:D:736:LEU:HD11	2.01	0.42
1:A:795:LEU:HD12	2:D:517:GLU:HG3	2.01	0.42
2:B:336:ASN:O	2:B:340:ILE:HG12	2.19	0.42
2:B:558:VAL:HG13	1:C:834:MET:HE3	2.02	0.42
1:C:717:GLN:HG2	1:C:720:LEU:HD12	2.02	0.42
1:C:782:GLY:O	1:C:783:MET:HG3	2.19	0.42
1:A:782:GLY:O	1:A:783:MET:HG3	2.19	0.42
1:A:845:ILE:O	1:A:849:ILE:HG12	2.19	0.42
2:B:169:PHE:HB2	2:B:227:ILE:O	2.20	0.42
1:C:150:VAL:HG21	1:C:290:LEU:HD13	2.01	0.42
2:D:233:THR:OG1	2:D:236:GLU:HG3	2.20	0.42
1:A:150:VAL:HG21	1:A:290:LEU:HD13	2.02	0.42
1:C:389:ASN:O	1:C:391:THR:N	2.52	0.42
1:C:563:VAL:HG23	1:C:748:HIS:O	2.18	0.42
2:D:285:TRP:CD1	2:D:285:TRP:N	2.87	0.42
2:B:411:LEU:HD22	2:B:485:LYS:O	2.20	0.42
1:C:581:SER:O	1:C:585:LEU:HB2	2.20	0.42
1:A:325:PRO:HA	1:A:336:TRP:CE2	2.54	0.42
1:A:500:VAL:HG13	1:A:503:GLY:H	1.85	0.42
1:A:509:GLU:O	1:A:518:GLU:N	2.41	0.42
1:A:717:GLN:HG2	1:A:720:LEU:HD12	2.02	0.42
1:A:765:CYS:HB3	1:A:819:CYS:HB2	1.87	0.42
1:C:362:ASN:HD21	1:C:364:ASP:HB2	1.85	0.42
1:C:580:GLN:O	1:C:581:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:VAL:HG22	1:C:168:SER:H	1.85	0.42
1:C:434:PRO:HA	1:C:474:GLN:HE22	1.85	0.42
1:C:516:LYS:HA	2:D:192:ASN:ND2	2.34	0.42
1:C:664:ILE:O	1:C:667:SER:OG	2.28	0.42
1:C:704:THR:N	1:C:731:ASN:OD1	2.47	0.42
2:B:387:LYS:NZ	2:B:392:PRO:HG3	2.35	0.41
1:C:520:ASN:HD22	1:C:707:GLN:HG2	1.85	0.41
2:D:268:THR:O	2:D:268:THR:OG1	2.33	0.41
2:D:566:LEU:HB3	2:D:609:LEU:HD21	2.02	0.41
2:D:611:GLY:HA3	2:D:618:VAL:HG21	2.01	0.41
1:A:429:PHE:HB3	1:A:480:CYS:SG	2.60	0.41
2:B:603:GLY:O	2:B:607:TRP:HE3	2.03	0.41
1:C:845:ILE:O	1:C:849:ILE:HG12	2.19	0.41
2:D:168:ILE:HG13	2:D:190:ILE:HD11	2.02	0.41
1:A:134:HIS:O	1:A:136:SER:N	2.53	0.41
1:A:434:PRO:HA	1:A:474:GLN:HE22	1.85	0.41
2:B:168:ILE:HG13	2:B:190:ILE:HD11	2.02	0.41
1:C:111:ALA:HB1	1:C:116:ILE:HB	2.03	0.41
1:C:134:HIS:O	1:C:136:SER:N	2.53	0.41
1:C:500:VAL:HG13	1:C:503:GLY:H	1.85	0.41
1:C:718:VAL:HG13	1:C:719:CYS:N	2.35	0.41
2:D:159:ASN:HB3	2:D:384:LEU:HD11	2.01	0.41
2:D:366:LEU:HD23	2:D:376:VAL:HG21	2.02	0.41
1:A:500:VAL:HG22	1:A:501:ALA:H	1.85	0.41
2:B:233:THR:OG1	2:B:236:GLU:HG3	2.20	0.41
2:B:451:GLY:O	2:B:453:ILE:HG12	2.21	0.41
1:C:500:VAL:HG22	1:C:501:ALA:H	1.85	0.41
2:D:169:PHE:HB2	2:D:227:ILE:O	2.20	0.41
1:A:458:THR:OG1	1:A:459:GLY:N	2.52	0.41
2:B:566:LEU:HB3	2:B:609:LEU:HD21	2.02	0.41
2:D:387:LYS:NZ	2:D:392:PRO:HG3	2.35	0.41
2:D:569:VAL:HA	2:D:572:VAL:HG12	2.03	0.41
2:D:603:GLY:O	2:D:607:TRP:HE3	2.03	0.41
1:A:111:ALA:HB1	1:A:116:ILE:HB	2.02	0.41
1:A:537:PRO:HB3	1:A:779:PHE:CZ	2.56	0.41
1:A:581:SER:O	1:A:585:LEU:HB2	2.20	0.41
1:A:718:VAL:HG13	1:A:719:CYS:N	2.35	0.41
2:D:158:LEU:HD23	2:D:158:LEU:HA	1.79	0.41
2:D:451:GLY:O	2:D:453:ILE:HG12	2.21	0.41
1:A:542:ASN:O	1:A:546:GLN:HG2	2.21	0.41
2:B:159:ASN:HB3	2:B:384:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:LEU:HA	2:B:834:ILE:HG12	2.03	0.41
1:C:80:GLU:OE1	1:C:83:ILE:HD11	2.21	0.41
1:C:675:PHE:HD1	1:C:678:LEU:HD12	1.86	0.41
1:A:675:PHE:HD1	1:A:678:LEU:HD12	1.86	0.41
1:A:852:ILE:HB	2:D:627:THR:HG21	2.03	0.41
2:D:411:LEU:HD22	2:D:485:LYS:O	2.20	0.41
2:D:560:VAL:O	2:D:564:VAL:HG22	2.20	0.41
1:A:147:GLN:HE22	1:A:272:GLU:H	1.69	0.41
1:A:258:MET:HE3	1:A:258:MET:HB3	1.98	0.41
1:A:805:PHE:HA	1:A:808:ASP:OD2	2.21	0.41
2:B:491:ASN:ND2	4:B:903:NAG:O7	2.54	0.41
2:B:532:THR:OG1	2:B:533:GLY:N	2.54	0.41
1:C:80:GLU:HA	1:C:83:ILE:HG12	2.03	0.41
1:C:228:LEU:HD12	1:C:228:LEU:HA	1.93	0.41
1:C:542:ASN:O	1:C:546:GLN:HG2	2.21	0.41
2:D:112:LEU:HB3	2:D:123:ILE:HD11	2.03	0.41
2:D:186:ILE:O	2:D:190:ILE:HG12	2.21	0.41
2:D:532:THR:OG1	2:D:533:GLY:N	2.54	0.41
1:A:520:ASN:HD22	1:A:707:GLN:HG2	1.85	0.41
1:A:664:ILE:O	1:A:667:SER:OG	2.28	0.41
2:B:186:ILE:O	2:B:190:ILE:HG12	2.21	0.41
1:C:429:PHE:HB3	1:C:480:CYS:SG	2.60	0.41
2:B:366:LEU:HD23	2:B:376:VAL:HG21	2.02	0.40
2:B:630:ILE:O	2:B:634:VAL:HG23	2.20	0.40
2:D:478:LEU:HA	2:D:478:LEU:HD12	1.84	0.40
2:D:512:SER:HA	2:D:762:TYR:CE2	2.56	0.40
2:D:831:LEU:O	2:D:834:ILE:HG12	2.21	0.40
1:A:80:GLU:OE1	1:A:83:ILE:HD11	2.21	0.40
1:A:246:GLU:HG2	1:A:247:ASP:N	2.37	0.40
2:B:126:ILE:CD1	2:B:292:ARG:HB3	2.51	0.40
2:D:85:ILE:HD11	2:D:115:ILE:HD13	2.03	0.40
1:A:336:TRP:NE1	1:A:338:THR:HG22	2.37	0.40
1:A:362:ASN:HD21	1:A:364:ASP:HB2	1.85	0.40
2:B:153:GLN:NE2	2:B:260:SER:HB3	2.36	0.40
1:C:334:ASN:OD1	1:C:335:ILE:N	2.46	0.40
1:C:732:TYR:CE2	1:C:747:LEU:HD22	2.57	0.40
2:D:605:ALA:O	2:D:608:LEU:HG	2.21	0.40
2:D:831:LEU:HA	2:D:834:ILE:HG12	2.03	0.40
2:B:709:PHE:HD1	2:B:710:ASN:O	2.05	0.40
2:D:153:GLN:NE2	2:D:260:SER:HB3	2.36	0.40
2:D:637:PHE:O	2:D:641:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASP:O	2:B:266:THR:OG1	2.36	0.40
2:B:512:SER:HA	2:B:762:TYR:CE2	2.56	0.40
1:C:88:TYR:CE1	1:C:325:PRO:HG3	2.57	0.40
1:C:515:ASN:C	2:D:192:ASN:HD21	2.24	0.40
1:C:805:PHE:HA	1:C:808:ASP:OD2	2.21	0.40
2:D:126:ILE:CD1	2:D:292:ARG:HB3	2.51	0.40
2:D:353:GLU:OE2	2:D:353:GLU:N	2.53	0.40
2:D:630:ILE:O	2:D:634:VAL:HG23	2.20	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	800/868 (92%)	691 (86%)	106 (13%)	3 (0%)	34	71
1	C	800/868 (92%)	692 (86%)	105 (13%)	3 (0%)	34	71
2	B	779/883 (88%)	652 (84%)	123 (16%)	4 (0%)	29	67
2	D	779/883 (88%)	652 (84%)	123 (16%)	4 (0%)	29	67
All	All	3158/3502 (90%)	2687 (85%)	457 (14%)	14 (0%)	38	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	CYS
1	C	765	CYS
1	A	764	LYS
1	C	764	LYS
2	B	415	PRO
2	D	415	PRO
1	A	468	PRO

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Mol	Chain	Res	Type
1	C	468	PRO
2	D	679	PRO
2	B	679	PRO
2	B	422	VAL
2	B	451	GLY
2	D	422	VAL
2	D	451	GLY

### 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	589/748 (79%)	587 (100%)	2 (0%)	92	97
1	C	589/748 (79%)	587 (100%)	2 (0%)	92	97
2	B	558/762 (73%)	553 (99%)	5 (1%)	78	89
2	D	558/762 (73%)	553 (99%)	5 (1%)	78	89
All	All	2294/3020 (76%)	2280 (99%)	14 (1%)	86	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	SER
1	A	813	TRP
2	B	86	CYS
2	B	471	SER
2	B	560	VAL
2	B	632	VAL
2	B	810	SER
1	C	528	SER
1	C	813	TRP
2	D	86	CYS
2	D	471	SER
2	D	560	VAL
2	D	632	VAL
2	D	810	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	50	ASN
1	A	134	HIS
1	A	147	GLN
1	A	217	GLN
1	A	311	GLN
1	A	314	HIS
1	A	392	HIS
1	A	426	GLN
1	A	726	HIS
1	A	730	HIS
2	B	616	ASN
2	B	649	ASN
2	B	782	GLN
1	C	28	ASN
1	C	50	ASN
1	C	134	HIS
1	C	147	GLN
1	C	217	GLN
1	C	311	GLN
1	C	314	HIS
1	C	392	HIS
1	C	426	GLN
1	C	726	HIS
1	C	730	HIS
2	D	616	ASN
2	D	649	ASN
2	D	782	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

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
3	NAG	E	1	2,3	14,14,15	0.53	0	17,19,21	0.68	0
3	NAG	E	2	3	14,14,15	0.17	0	17,19,21	0.53	0
3	NAG	F	1	2,3	14,14,15	0.27	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	G	1	2,3	14,14,15	0.53	0	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	0.16	0	17,19,21	0.54	0
3	NAG	H	1	2,3	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.44	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	E	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1
3	G	2	NAG	C1

All (14) torsion outliers are listed below:

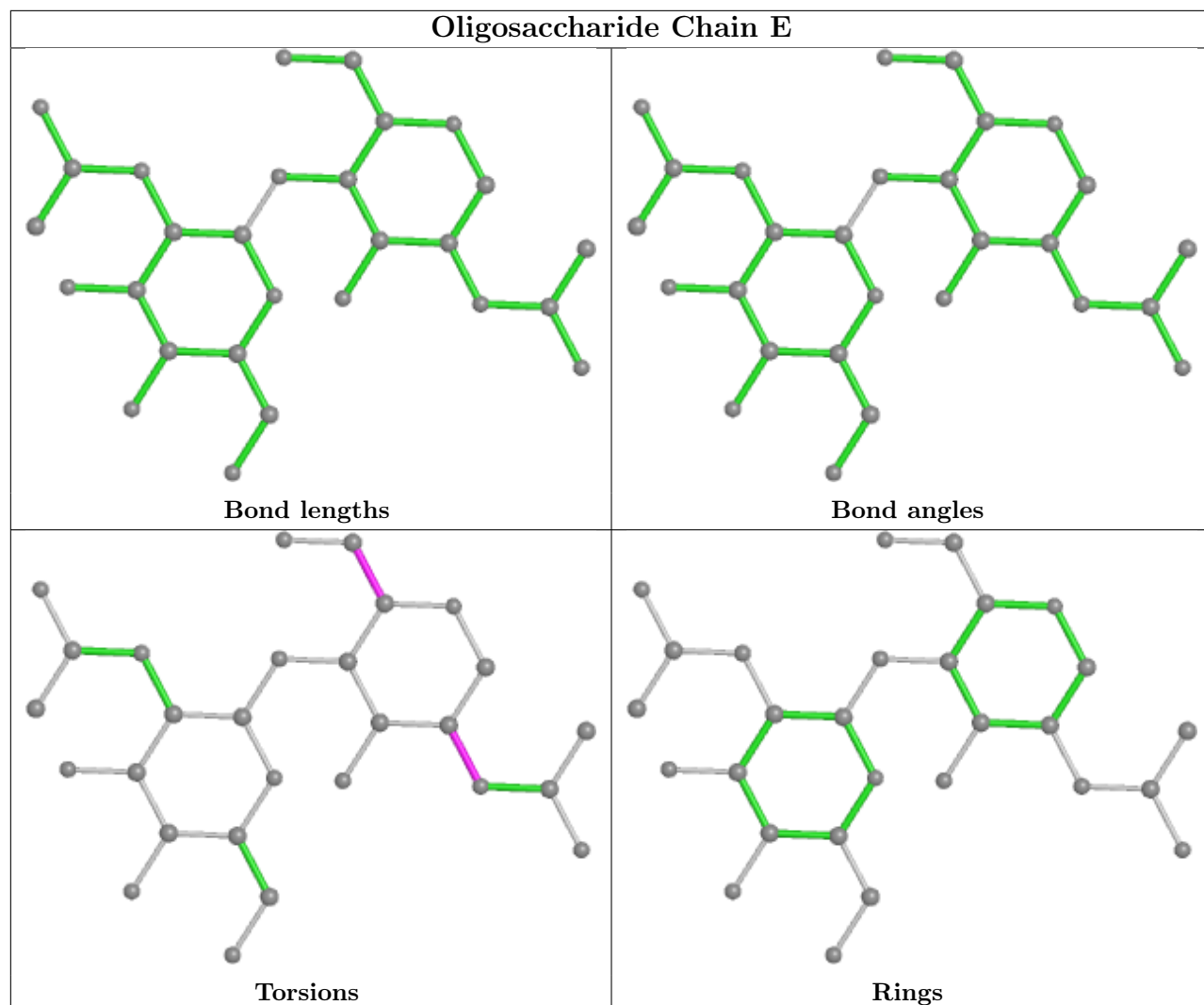
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7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

There are no ring outliers.

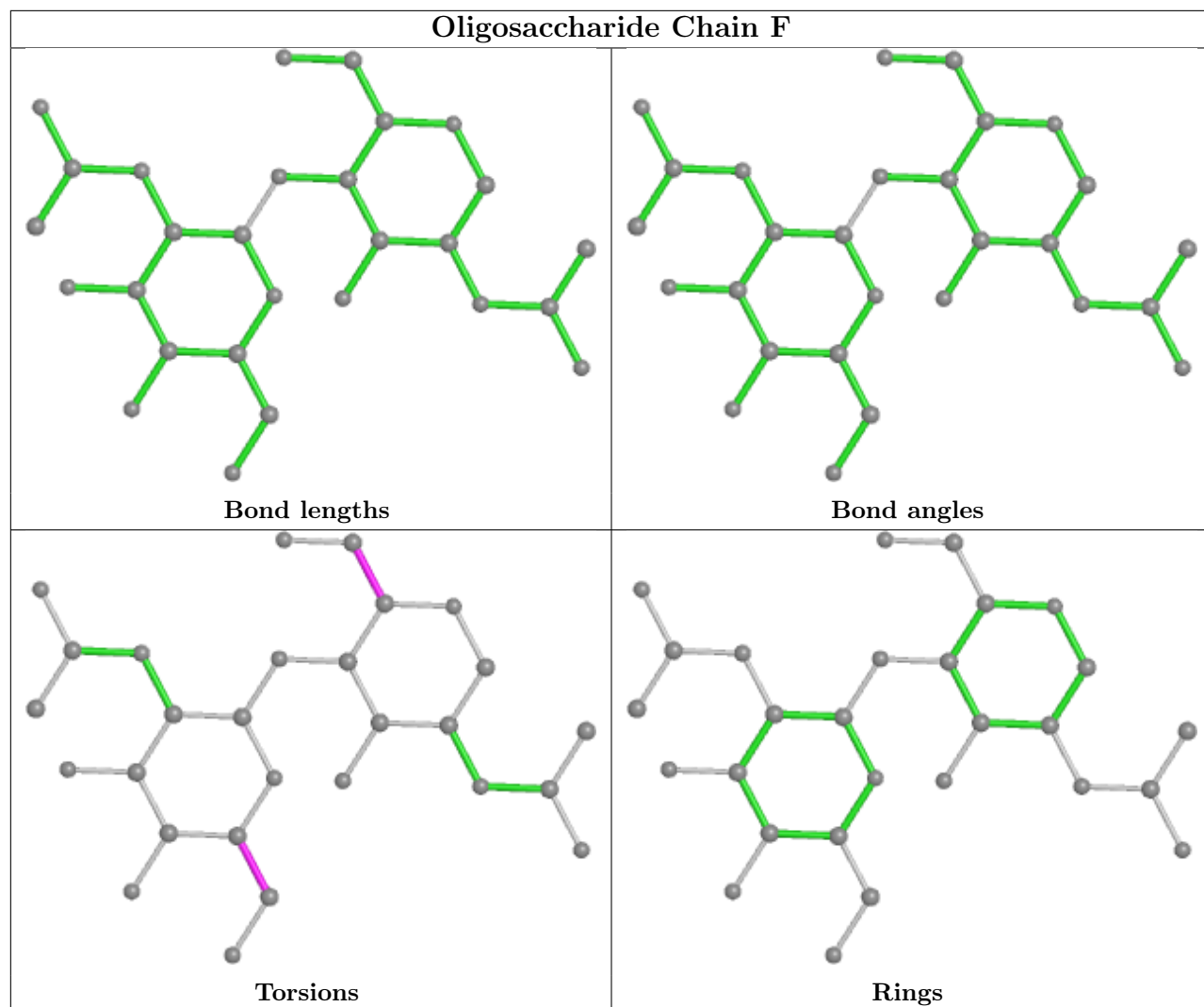
6 monomers are involved in 4 short contacts:

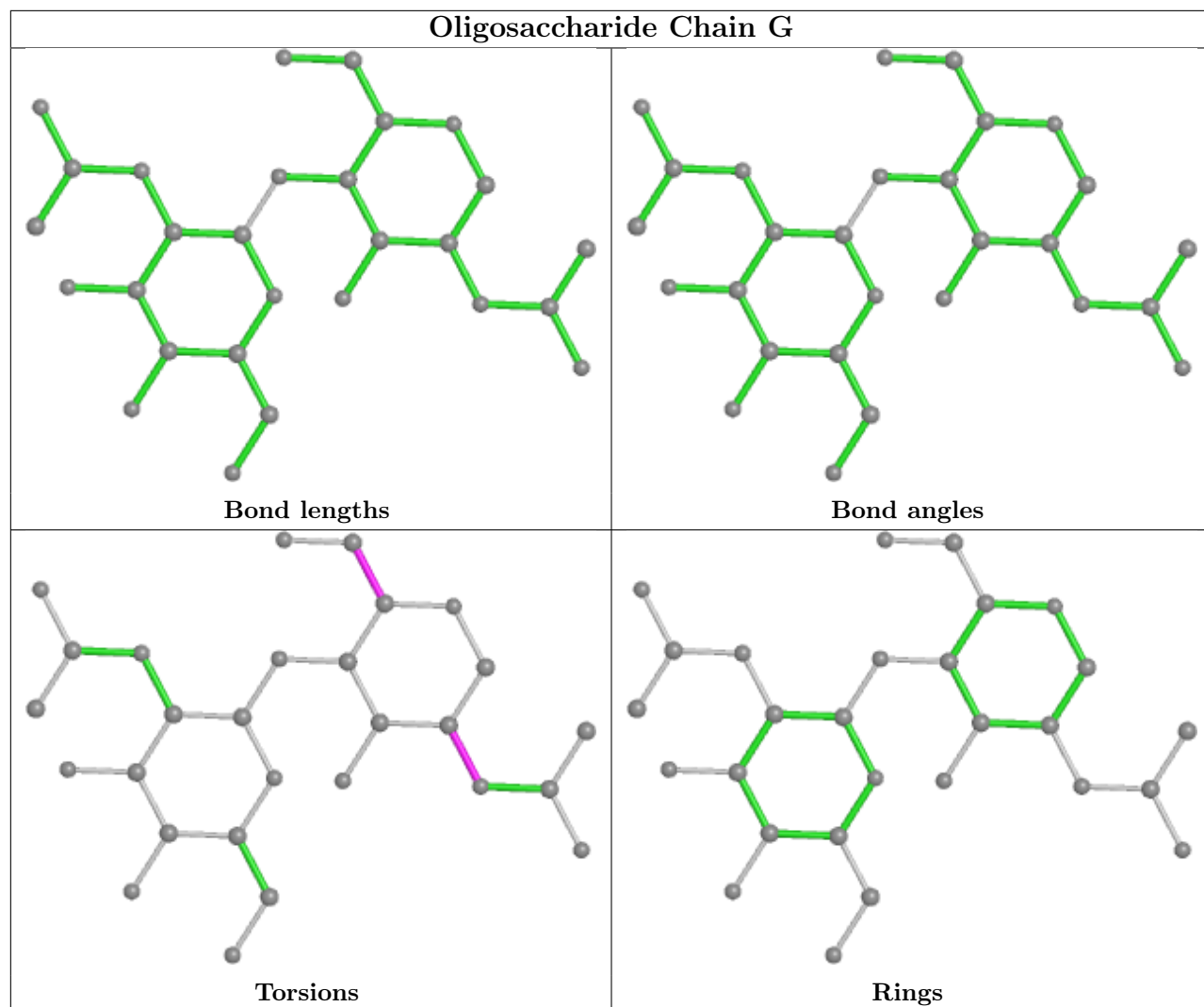
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	E	1	NAG	1	0
3	G	1	NAG	1	0
3	H	1	NAG	1	0
3	F	1	NAG	1	0
3	E	2	NAG	1	0

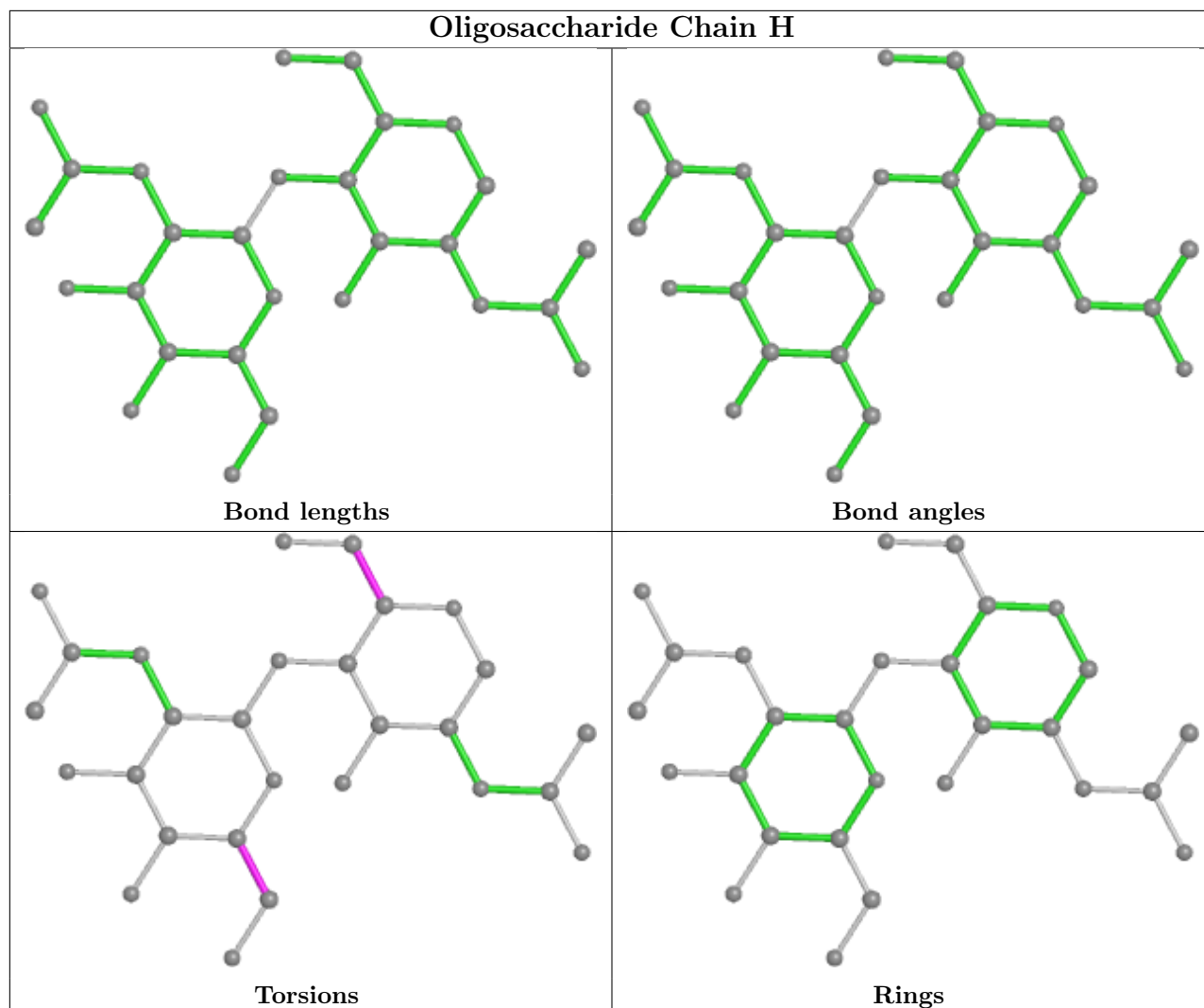
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	D	903	2	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	A	902	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	A	901	1	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	B	904	2	14,14,15	0.27	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	903	2	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	C	902	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	C	901	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	D	904	2	14,14,15	0.27	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	A	902	1	-	2/6/23/26	0/1/1/1
4	NAG	A	901	1	-	2/6/23/26	0/1/1/1
4	NAG	B	904	2	-	3/6/23/26	0/1/1/1
4	NAG	B	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	902	1	-	2/6/23/26	0/1/1/1
4	NAG	C	901	1	-	2/6/23/26	0/1/1/1
4	NAG	D	904	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NAG	O5-C5-C6-O6
4	C	902	NAG	O5-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	A	901	NAG	O5-C5-C6-O6
4	C	901	NAG	O5-C5-C6-O6
4	A	902	NAG	C4-C5-C6-O6
4	C	902	NAG	C4-C5-C6-O6
4	A	901	NAG	C4-C5-C6-O6
4	C	901	NAG	C4-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	D	903	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	903	NAG	O5-C5-C6-O6
4	B	904	NAG	C3-C2-N2-C7
4	D	904	NAG	C3-C2-N2-C7
4	B	903	NAG	C4-C5-C6-O6
4	D	903	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	903	NAG	1	0
4	B	903	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

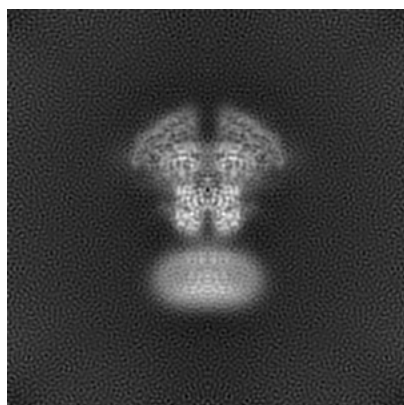
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21682. These allow visual inspection of the internal detail of the map and identification of artifacts.

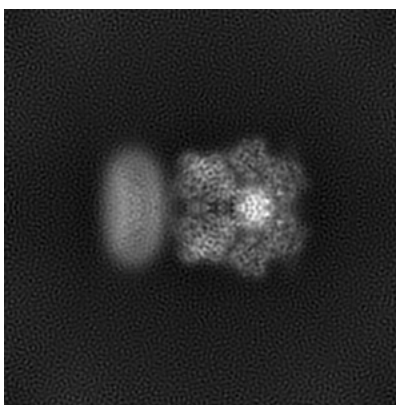
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

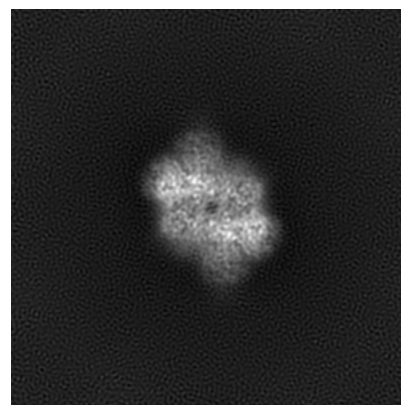
#### 6.1.1 Primary map



X



Y

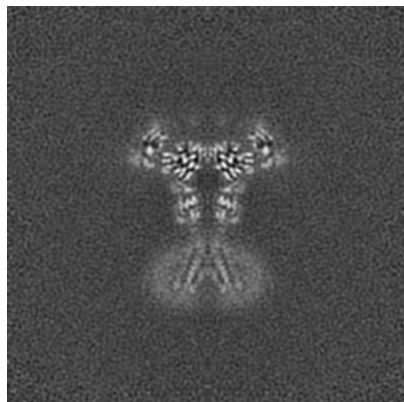


Z

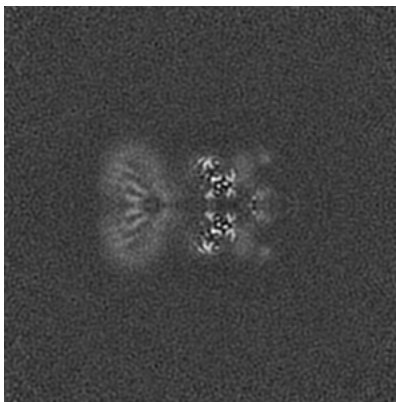
The images above show the map projected in three orthogonal directions.

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

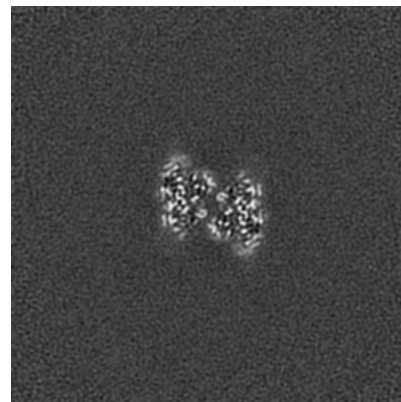
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

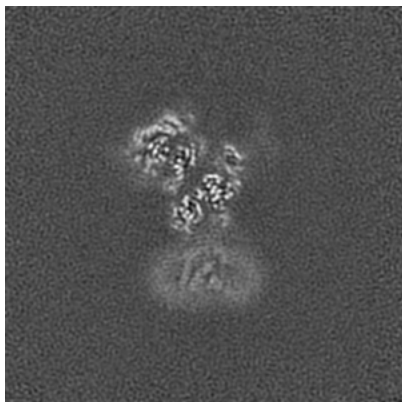


Z Index: 128

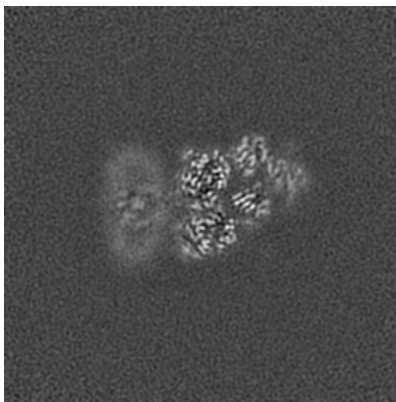
The images above show central slices of the map in three orthogonal directions.

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

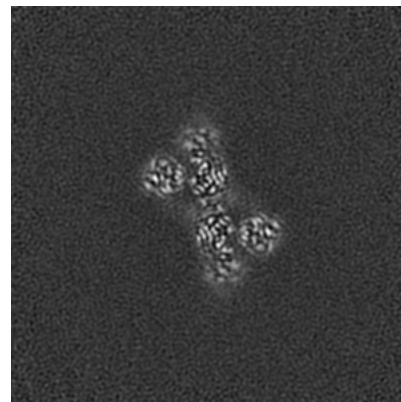
### 6.3.1 Primary map



X Index: 137



Y Index: 118



Z Index: 159

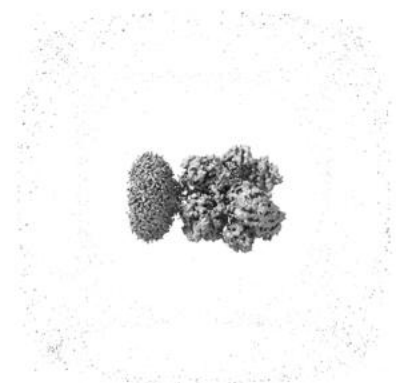
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

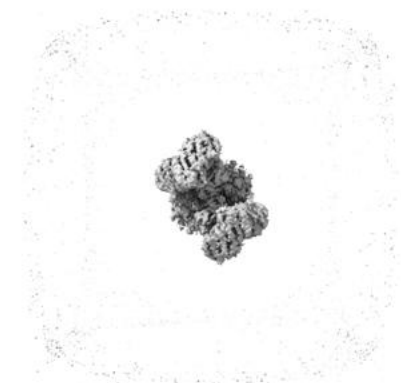
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

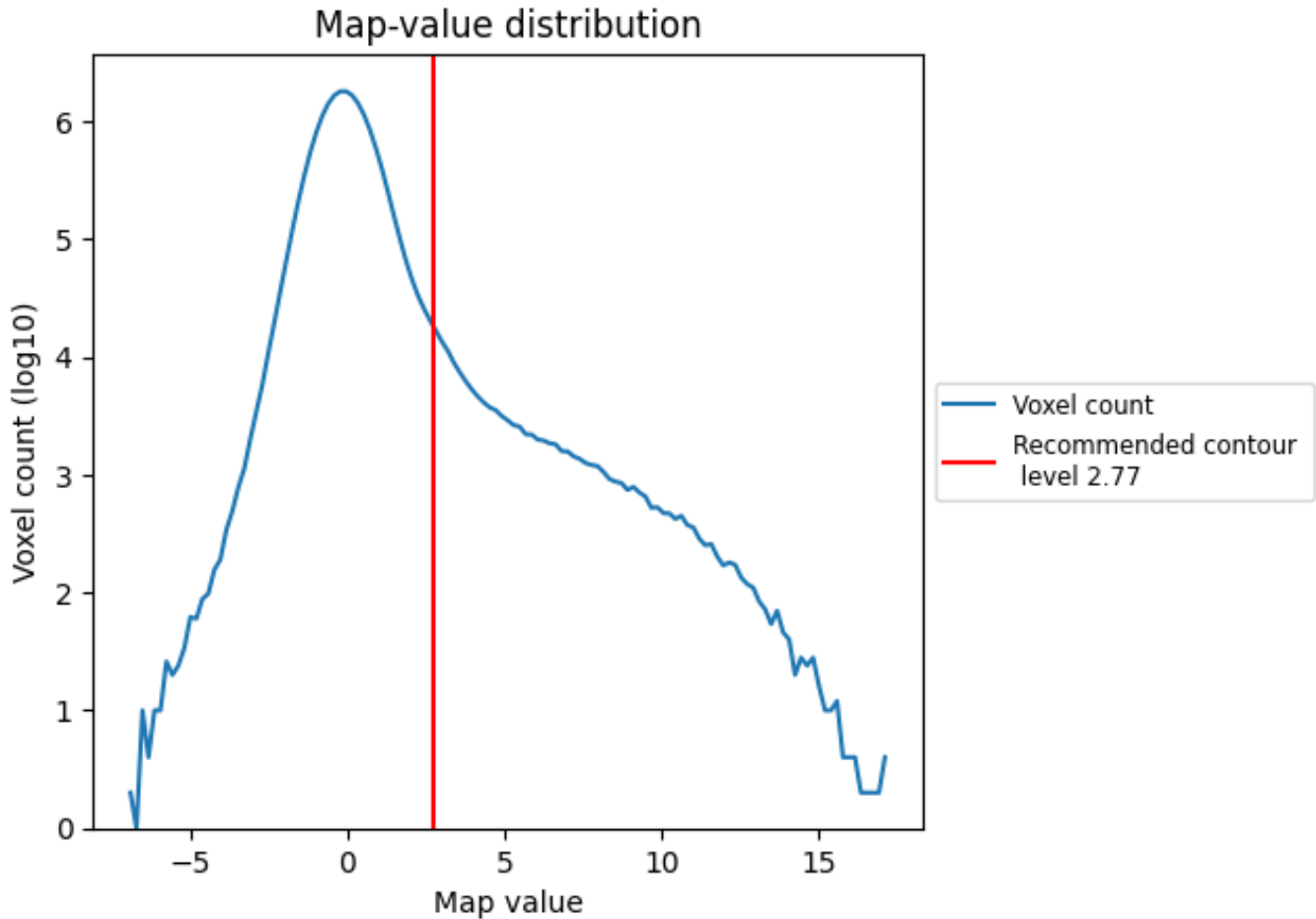
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

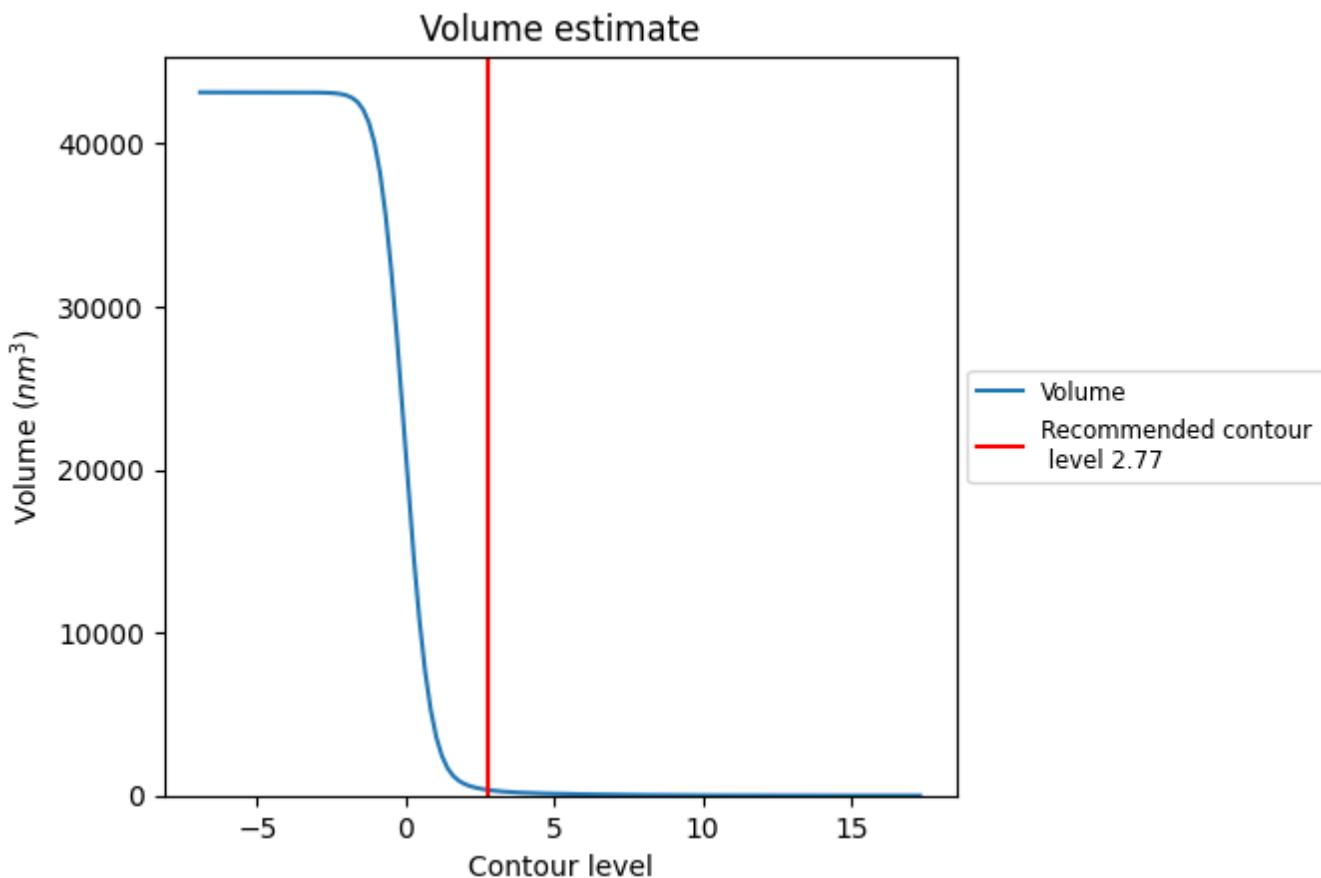
This section contains the results of statistical analysis of the map.

### 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.

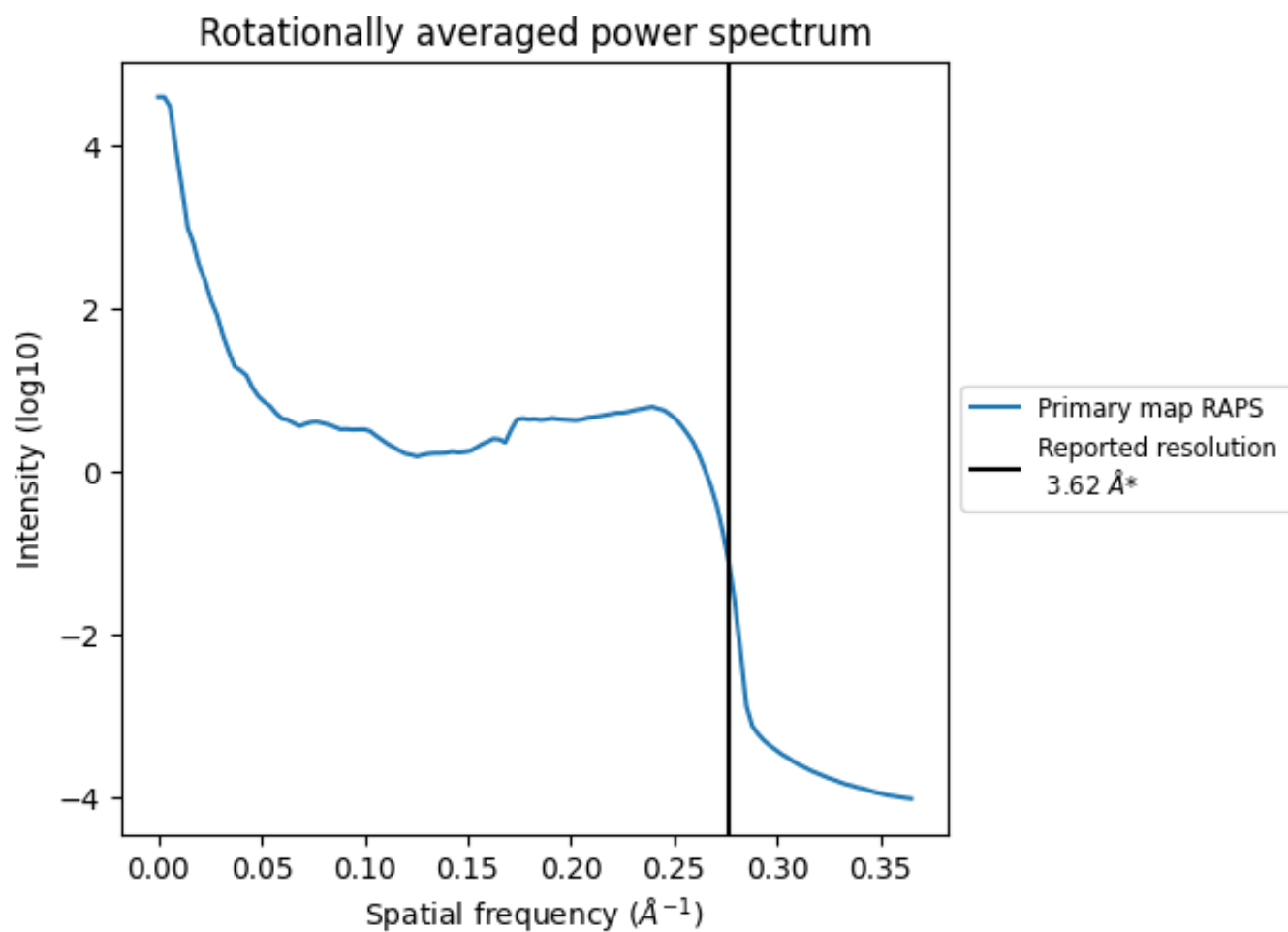
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350  $\text{nm}^3$ ; this corresponds to an approximate mass of 316 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  $0.276 \text{\AA}^{-1}$

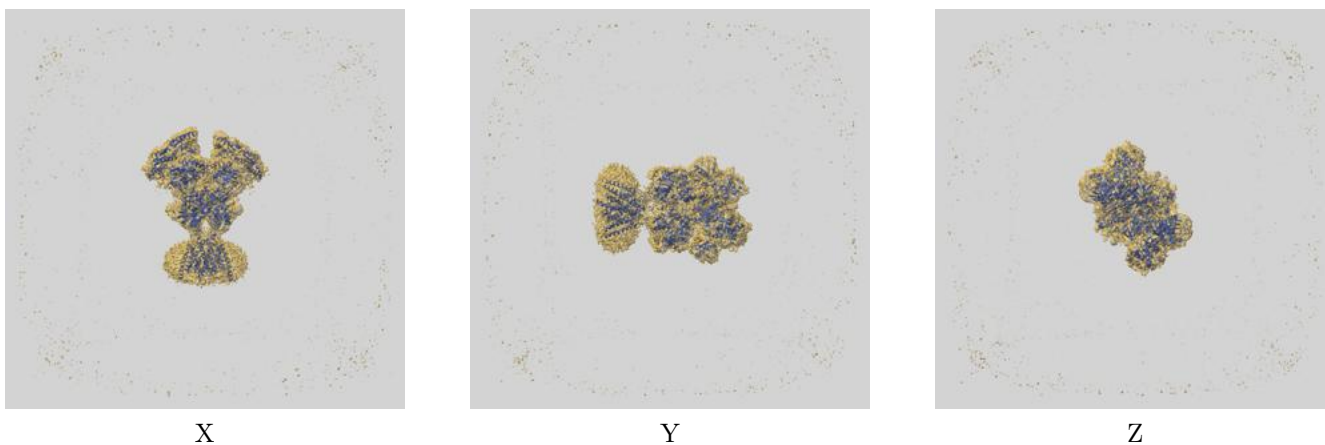
## 8 Fourier-Shell correlation

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

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

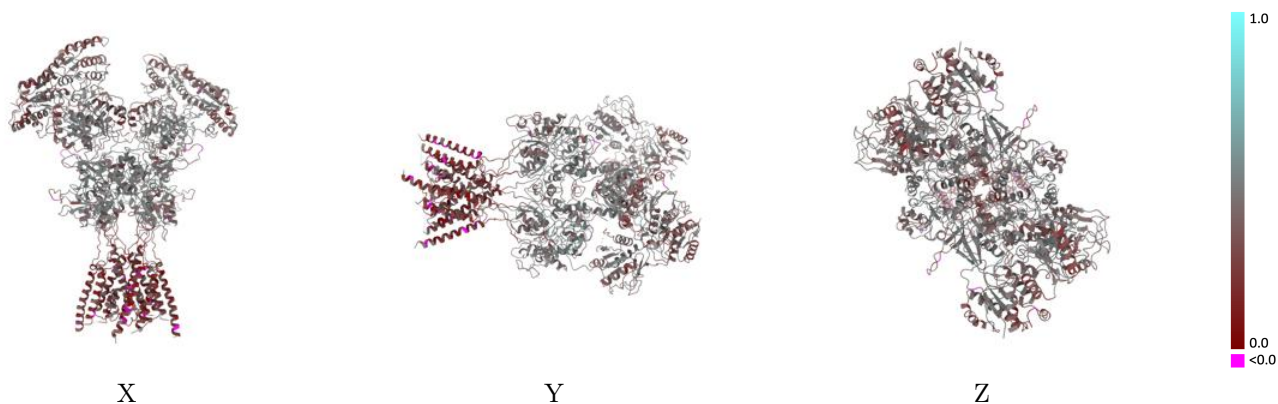
This section contains information regarding the fit between EMDB map EMD-21682 and PDB model 6WI1. Per-residue inclusion information can be found in section 3 on page 6.

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



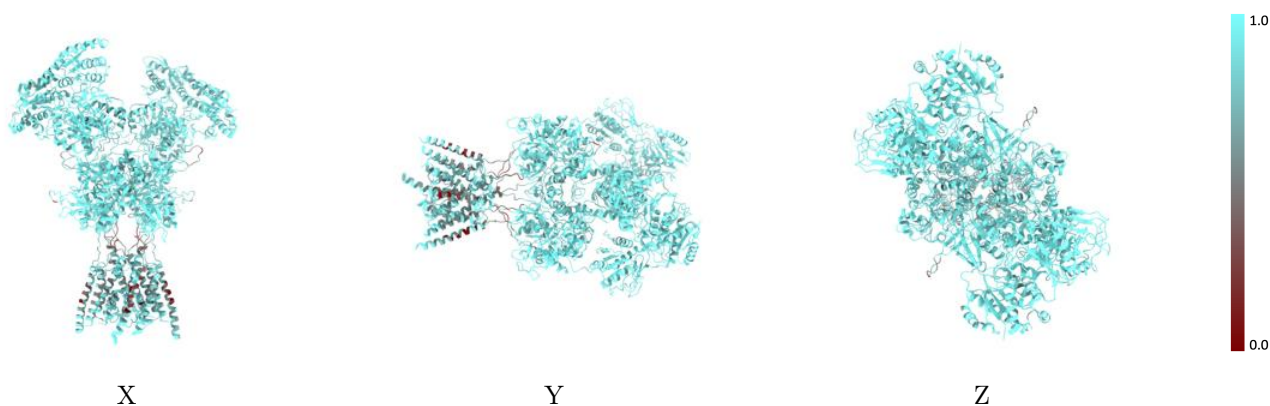
The images above show the 3D surface view of the map at the recommended contour level 2.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



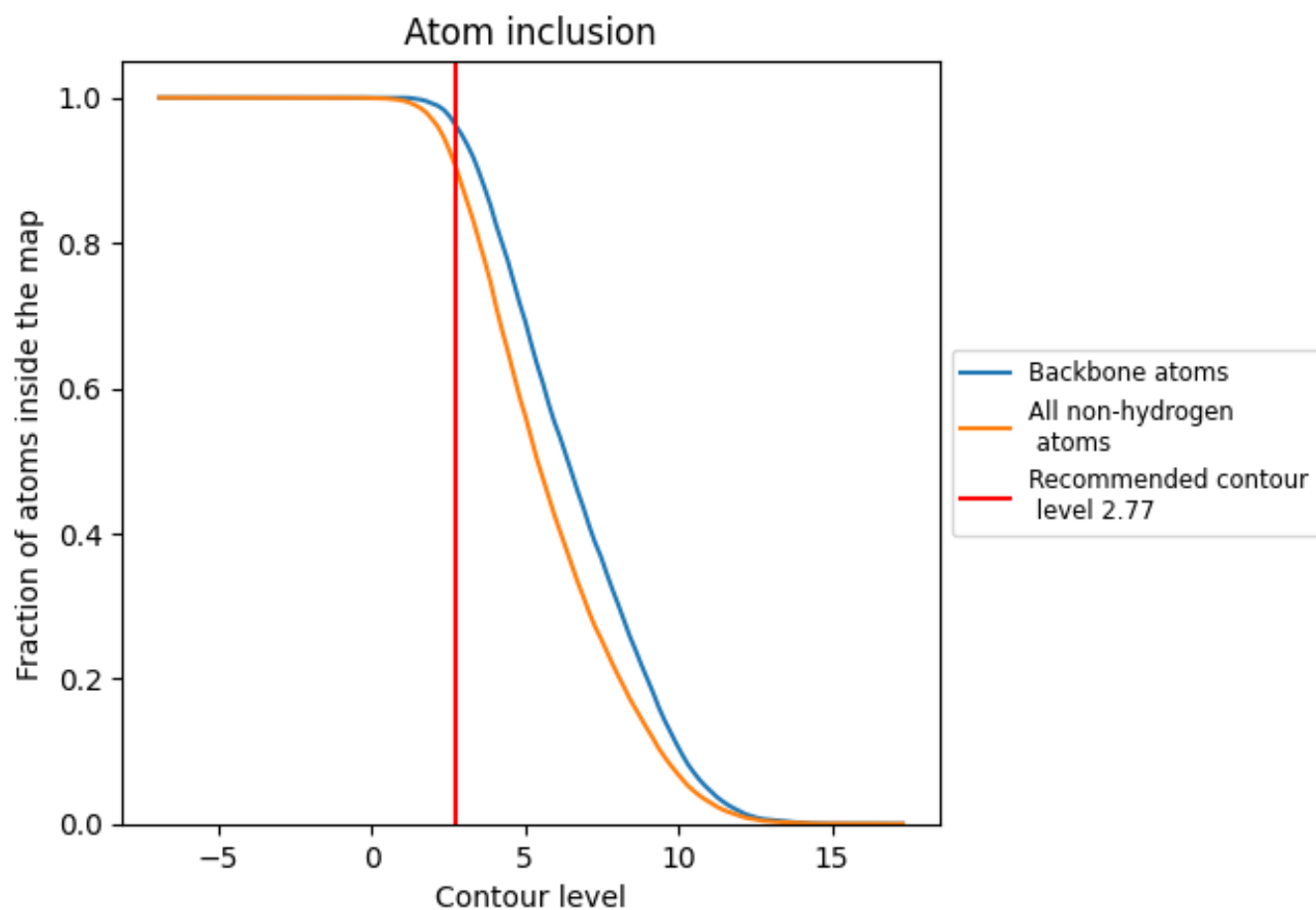
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.77).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (2.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9018	 0.4040
A	 0.9140	 0.4100
B	 0.8893	 0.3980
C	 0.9125	 0.4090
D	 0.8913	 0.3980
E	 0.8571	 0.4610
F	 0.8929	 0.4030
G	 0.8214	 0.4300
H	 0.8929	 0.4040

