Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 06:00 PM EST

PDB ID	:	6CNA
EMDB ID	:	EMD-7529
Title	:	GluN1-GluN2B NMDA receptors with exon 5
Authors	:	Furukawa, H.; Grant, T.; Grigorieff, N.
Deposited on	:	2018-03-07
Resolution	:	4.60 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 (i) 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 (i)) were used in the production of this report:

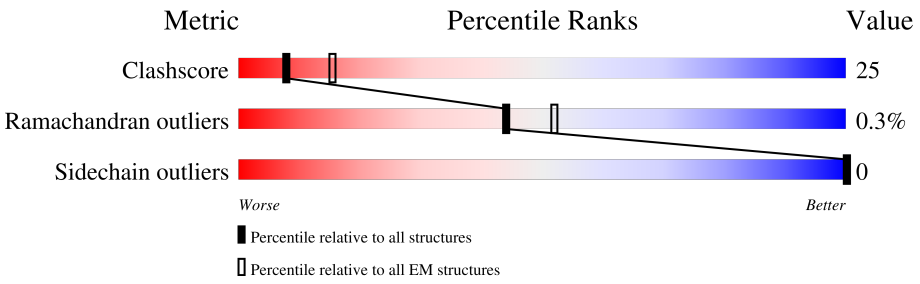
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	838	9% 60% 35% 5%
1	C	838	9% 61% 34% 5%
2	B	812	10% 60% 36% .
2	D	812	10% 60% 36% .
3	E	2	50% 100%
3	F	2	50% 50%
3	G	2	50% 50%
3	H	2	50% 100%

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50%
3	J	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21426 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	795	5381	3385	946	1026	24	1	0
1	C	795	5381	3385	946	1026	24	1	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	conflict	UNP P35439
A	260	ASP	ASN	conflict	UNP P35439
A	371	GLN	ASN	conflict	UNP P35439
A	492	GLN	ASN	conflict	UNP P35439
A	512	GLN	ASN	conflict	UNP P35439
A	792	GLN	ASN	conflict	UNP P35439
A	831	CYS	PHE	conflict	UNP P35439
A	840	ILE	LEU	conflict	UNP P35439
A	860	SER	-	expression tag	UNP P35439
A	861	ARG	-	expression tag	UNP P35439
A	862	ALA	-	expression tag	UNP P35439
C	61	GLN	ASN	conflict	UNP P35439
C	260	ASP	ASN	conflict	UNP P35439
C	371	GLN	ASN	conflict	UNP P35439
C	492	GLN	ASN	conflict	UNP P35439
C	512	GLN	ASN	conflict	UNP P35439
C	792	GLN	ASN	conflict	UNP P35439
C	831	CYS	PHE	conflict	UNP P35439
C	840	ILE	LEU	conflict	UNP P35439
C	860	SER	-	expression tag	UNP P35439
C	861	ARG	-	expression tag	UNP P35439
C	862	ALA	-	expression tag	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	785	5178	3284	859	1007	28	0	0
2	D	785	5178	3284	859	1007	28	0	0

There are 12 discrepancies between the modelled and reference sequences:

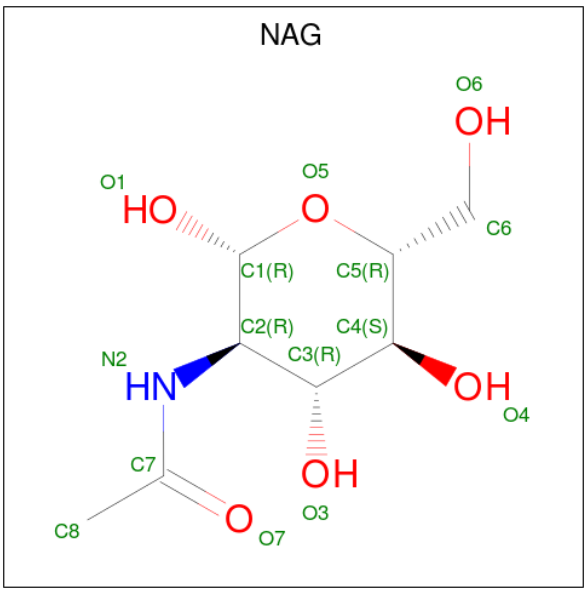
Chain	Residue	Modelled	Actual	Comment	Reference
B	214	CYS	SER	conflict	UNP Q00960
B	348	ASP	ASN	conflict	UNP Q00960
B	557	CYS	ASP	conflict	UNP Q00960
B	838	SER	CYS	conflict	UNP Q00960
B	844	LYS	-	expression tag	UNP Q00960
B	845	SER	-	expression tag	UNP Q00960
D	214	CYS	SER	conflict	UNP Q00960
D	348	ASP	ASN	conflict	UNP Q00960
D	557	CYS	ASP	conflict	UNP Q00960
D	838	SER	CYS	conflict	UNP Q00960
D	844	LYS	-	expression tag	UNP Q00960
D	845	SER	-	expression tag	UNP Q00960

- 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	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



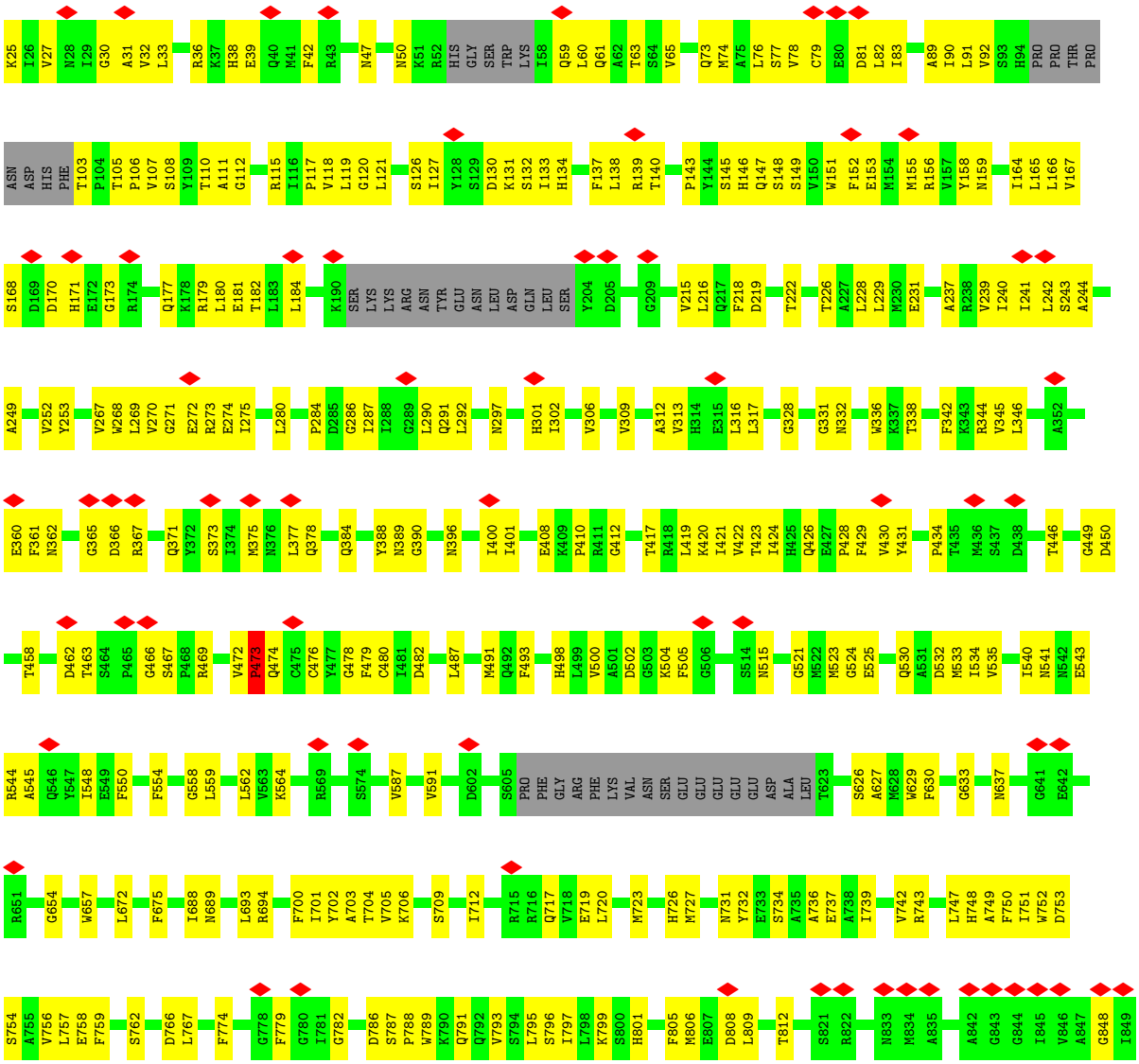
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	42	24	3	15	0
			Total	C	N	O	
4	A	1	42	24	3	15	0
			Total	C	N	O	
4	A	1	42	24	3	15	0
			Total	C	N	O	
4	B	1	28	16	2	10	0
			Total	C	N	O	
4	B	1	28	16	2	10	0
			Total	C	N	O	
4	C	1	42	24	3	15	0
			Total	C	N	O	
4	C	1	42	24	3	15	0
			Total	C	N	O	
4	C	1	42	24	3	15	0
			Total	C	N	O	
4	D	1	28	16	2	10	0
			Total	C	N	O	
4	D	1	28	16	2	10	0

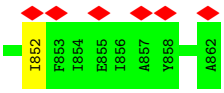
3 Residue-property plots (i)

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: Glutamate receptor ionotropic, NMDA 1

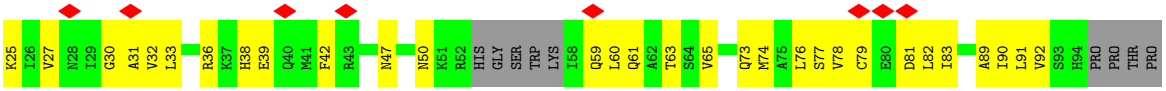
Chain A: 9% 60% 35% 5%

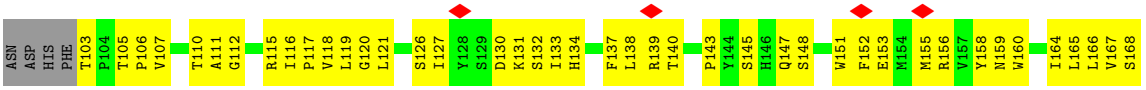


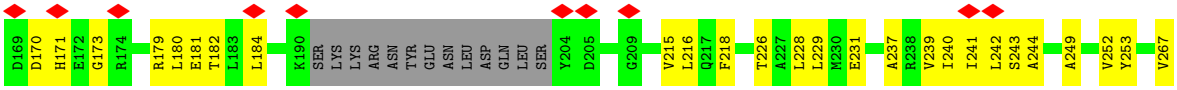


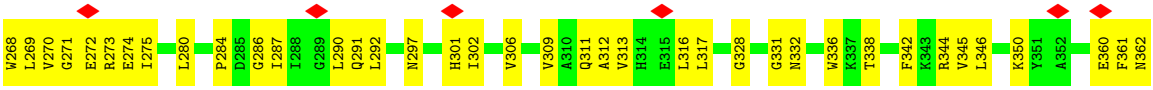
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

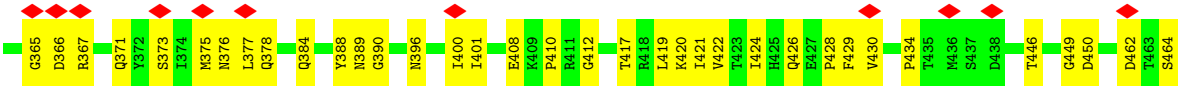
Chain C:

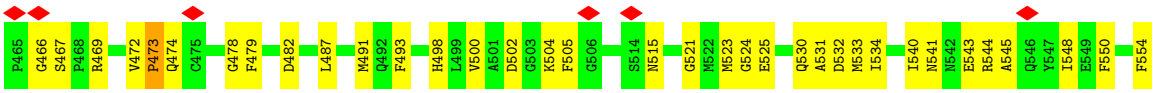


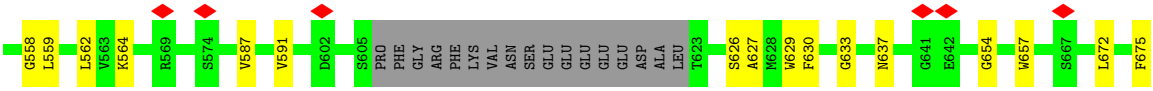


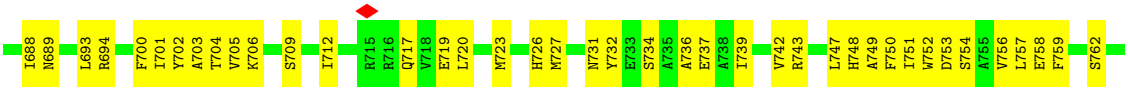


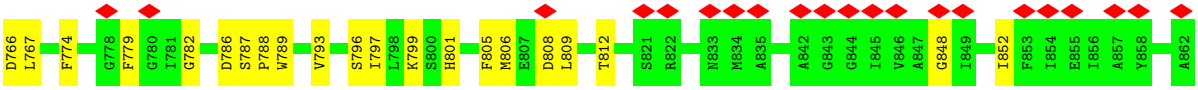






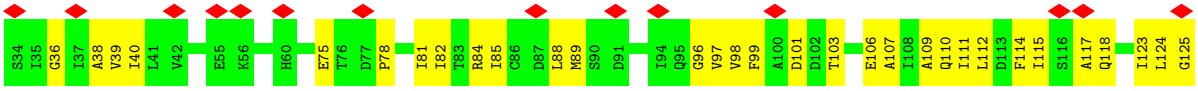


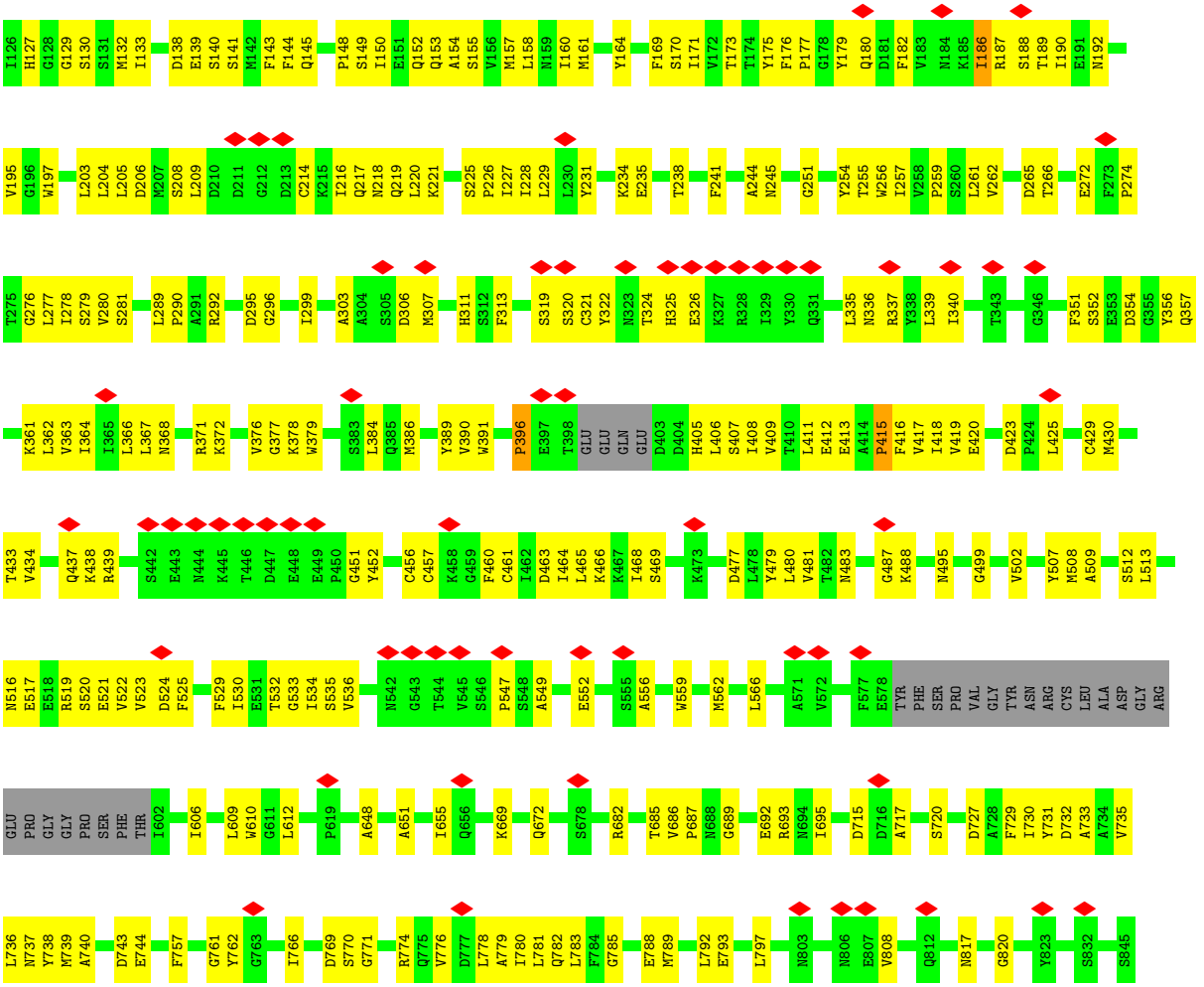




- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

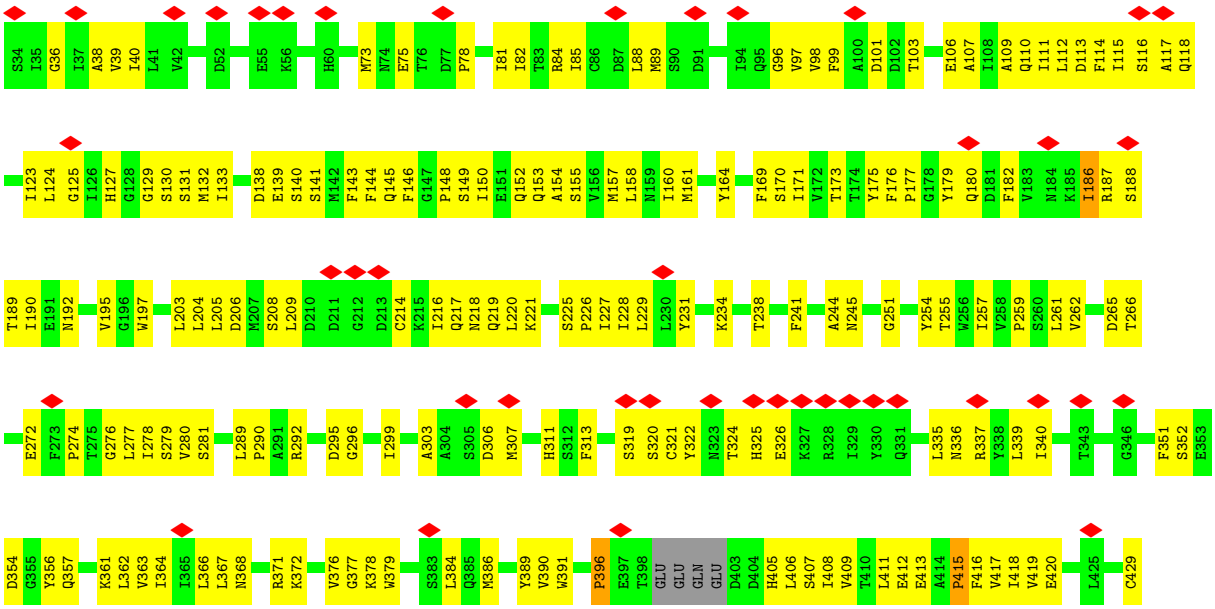
Chain B:

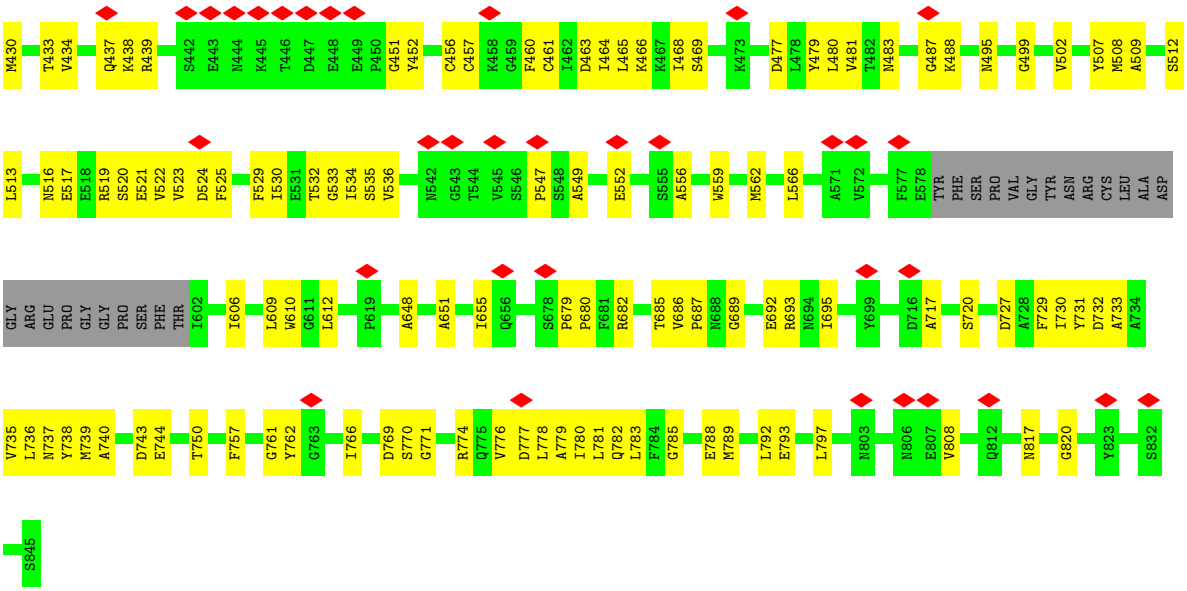




- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

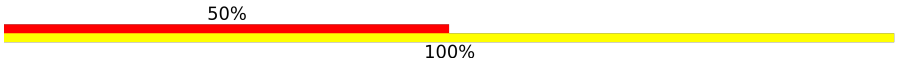
Chain D:





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

Chain E:



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

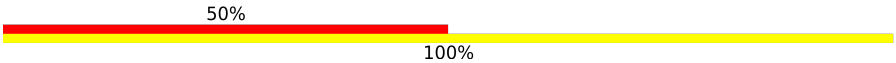
Chain F:

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

Chain G:

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

Chain H:



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

Chain I:

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

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73790	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	96	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	40.923	Depositor
Minimum map value	-29.179	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.443	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	0/5485	0.59	5/7535 (0.1%)
1	C	0.41	1/5485 (0.0%)	0.55	2/7535 (0.0%)
2	B	0.39	0/5272	0.53	1/7260 (0.0%)
2	D	0.39	0/5272	0.53	1/7260 (0.0%)
All	All	0.39	1/21514 (0.0%)	0.55	9/29590 (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	1
1	C	0	1
2	B	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	472	VAL	C-N	13.15	1.59	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	VAL	C-N-CD	12.69	155.05	128.40
1	A	473	PRO	O-C-N	-10.69	105.59	122.70
1	A	472	VAL	O-C-N	9.49	139.13	121.10
1	C	472	VAL	C-N-CD	8.75	146.78	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	VAL	C-N-CA	-7.21	91.74	122.00
1	A	472	VAL	CA-C-N	-6.21	99.72	117.10
2	D	396	PRO	N-CA-CB	6.05	110.57	103.30
2	B	396	PRO	N-CA-CB	6.02	110.53	103.30
1	C	473	PRO	C-N-CA	-5.02	109.15	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	473	PRO	Mainchain
2	B	415	PRO	Peptide
1	C	473	PRO	Mainchain
2	D	415	PRO	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	5381	0	4492	243	0
1	C	5381	0	4492	236	0
2	B	5178	0	4192	258	0
2	D	5178	0	4192	258	0
3	E	28	0	25	3	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	3	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	42	0	39	0	0
4	D	28	0	26	0	0
All	All	21426	0	17648	985	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 25.

All (985) 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:C:164:ILE:HB	1:C:240:ILE:HA	1.41	1.00
1:A:164:ILE:HB	1:A:240:ILE:HA	1.40	0.99
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.50	0.93
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.50	0.92
1:A:562:LEU:HD11	1:A:767:LEU:HB3	1.52	0.91
1:C:562:LEU:HD11	1:C:767:LEU:HB3	1.52	0.90
2:B:606:ILE:O	2:B:610:TRP:HB3	1.74	0.88
2:D:606:ILE:O	2:D:610:TRP:HB3	1.74	0.88
1:A:720:LEU:O	1:A:723:MET:N	2.08	0.86
1:C:720:LEU:O	1:C:723:MET:N	2.08	0.86
2:B:351:PHE:HA	2:B:357:GLN:HA	1.59	0.84
2:B:366:LEU:HB3	2:B:376:VAL:HG11	1.59	0.84
1:C:328:GLY:O	1:C:332:ASN:ND2	2.11	0.84
2:D:241:PHE:O	2:D:245:ASN:HB2	1.78	0.84
2:B:241:PHE:O	2:B:245:ASN:HB2	1.78	0.83
1:C:216:LEU:HB3	1:C:228:LEU:HD23	1.61	0.83
1:A:328:GLY:O	1:A:332:ASN:ND2	2.11	0.82
2:D:97:VAL:HB	2:D:123:ILE:HG12	1.59	0.82
2:D:366:LEU:HB3	2:D:376:VAL:HG11	1.59	0.82
2:B:97:VAL:HB	2:B:123:ILE:HG12	1.59	0.82
2:D:351:PHE:HA	2:D:357:GLN:HA	1.59	0.82
2:D:420:GLU:H	2:D:456:CYS:HB2	1.45	0.82
2:B:420:GLU:H	2:B:456:CYS:HB2	1.45	0.81
1:A:216:LEU:HB3	1:A:228:LEU:HD23	1.61	0.80
1:C:426:GLN:HG3	1:C:428:PRO:HD2	1.61	0.80
1:C:78:VAL:O	1:C:82:LEU:HB2	1.81	0.80
2:B:363:VAL:HA	2:B:378:LYS:HA	1.64	0.80
1:A:78:VAL:O	1:A:82:LEU:HB2	1.81	0.79
1:A:426:GLN:HG3	1:A:428:PRO:HD2	1.61	0.79
2:D:363:VAL:HA	2:D:378:LYS:HA	1.64	0.79
1:C:558:GLY:O	1:C:754:SER:N	2.16	0.79
2:D:133:ILE:HG12	2:D:150:ILE:HD11	1.65	0.79
2:D:362:LEU:HD12	2:D:379:TRP:CD1	2.19	0.78
1:A:558:GLY:O	1:A:754:SER:N	2.16	0.78
2:B:522:VAL:HG23	2:B:523:VAL:HG13	1.65	0.78
2:D:512:SER:HB2	2:D:762:TYR:CZ	2.19	0.78
2:D:127:HIS:O	2:D:130:SER:OG	2.02	0.77
2:B:362:LEU:HD12	2:B:379:TRP:CD1	2.19	0.77
2:B:38:ALA:O	2:B:98:VAL:N	2.14	0.77
2:D:148:PRO:HB2	2:D:153:GLN:HG2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HA	2:B:98:VAL:HB	1.67	0.77
2:B:133:ILE:HG12	2:B:150:ILE:HD11	1.65	0.77
2:D:39:VAL:HA	2:D:98:VAL:HB	1.67	0.76
2:B:127:HIS:O	2:B:130:SER:OG	2.02	0.76
2:B:512:SER:HB2	2:B:762:TYR:CZ	2.19	0.76
1:C:426:GLN:H	1:C:430:VAL:HB	1.51	0.76
2:D:522:VAL:HG23	2:D:523:VAL:HG13	1.65	0.76
2:D:109:ALA:HB2	2:D:130:SER:HA	1.68	0.76
2:B:148:PRO:HB2	2:B:153:GLN:HG2	1.66	0.75
2:B:109:ALA:HB2	2:B:130:SER:HA	1.68	0.75
1:A:426:GLN:H	1:A:430:VAL:HB	1.51	0.75
2:B:149:SER:O	2:B:153:GLN:N	2.18	0.75
1:A:758:GLU:O	1:A:762:SER:OG	2.05	0.75
1:A:151:TRP:HB3	1:A:269:LEU:HD21	1.68	0.75
2:B:280:VAL:HG22	2:B:364:ILE:HA	1.69	0.75
2:D:280:VAL:HG22	2:D:364:ILE:HA	1.69	0.74
2:D:130:SER:O	2:D:145:GLN:NE2	2.20	0.74
2:D:149:SER:O	2:D:153:GLN:N	2.19	0.74
1:A:704:THR:HB	1:A:751:ILE:HB	1.69	0.73
2:B:130:SER:O	2:B:145:GLN:NE2	2.20	0.73
1:A:155:MET:O	1:A:159:ASN:N	2.21	0.73
1:A:38:HIS:O	1:A:42:PHE:HB2	1.89	0.73
2:D:148:PRO:O	2:D:153:GLN:NE2	2.22	0.73
1:C:297:ASN:O	1:C:301:HIS:ND1	2.22	0.73
1:C:848:GLY:O	1:C:852:ILE:CB	2.37	0.73
2:D:38:ALA:O	2:D:98:VAL:N	2.14	0.73
1:C:155:MET:O	1:C:159:ASN:N	2.21	0.72
1:C:758:GLU:O	1:C:762:SER:OG	2.05	0.72
2:D:138:ASP:OD2	2:D:140:SER:OG	2.06	0.72
1:C:151:TRP:HB3	1:C:269:LEU:HD21	1.68	0.72
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.72	0.72
2:B:362:LEU:HD12	2:B:379:TRP:HD1	1.55	0.72
2:D:367:LEU:HD11	2:D:371:ARG:HA	1.72	0.72
1:C:704:THR:HB	1:C:751:ILE:HB	1.69	0.72
1:A:297:ASN:O	1:A:301:HIS:ND1	2.22	0.72
1:A:727:MET:O	1:A:731:ASN:ND2	2.23	0.72
1:C:38:HIS:O	1:C:42:PHE:HB2	1.89	0.72
1:A:848:GLY:O	1:A:852:ILE:CB	2.37	0.71
2:D:516:ASN:OD1	2:D:519:ARG:N	2.23	0.71
2:B:138:ASP:OD2	2:B:140:SER:OG	2.06	0.71
2:B:516:ASN:OD1	2:B:519:ARG:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:727:MET:O	1:C:731:ASN:ND2	2.23	0.71
2:B:408:ILE:HG23	2:B:509:ALA:HA	1.73	0.71
1:A:239:VAL:HA	1:A:267:VAL:HB	1.72	0.71
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.72	0.71
2:B:148:PRO:O	2:B:153:GLN:NE2	2.22	0.71
2:D:362:LEU:HD12	2:D:379:TRP:HD1	1.55	0.71
2:B:367:LEU:HD11	2:B:371:ARG:HA	1.72	0.70
1:A:362:ASN:H	1:A:366:ASP:H	1.39	0.70
1:C:362:ASN:OD1	1:C:366:ASP:N	2.25	0.70
2:D:408:ILE:HG23	2:D:509:ALA:HA	1.73	0.70
2:D:736:LEU:O	2:D:740:ALA:HB2	1.92	0.70
1:C:239:VAL:HA	1:C:267:VAL:HB	1.72	0.70
1:A:362:ASN:OD1	1:A:366:ASP:N	2.25	0.70
1:C:78:VAL:O	1:C:83:ILE:N	2.20	0.70
1:A:130:ASP:OD1	1:A:131:LYS:N	2.25	0.69
2:B:736:LEU:O	2:B:740:ALA:HB2	1.92	0.69
2:D:203:LEU:HD13	2:D:219:GLN:HB3	1.74	0.69
1:C:424:ILE:HG21	1:C:505:PHE:HE1	1.57	0.69
1:A:424:ILE:HG21	1:A:505:PHE:HE1	1.57	0.69
1:C:717:GLN:NE2	1:C:719:GLU:OE2	2.26	0.69
1:C:31:ALA:HA	1:C:91:LEU:H	1.57	0.69
1:C:77:SER:O	1:C:81:ASP:HB2	1.93	0.69
2:B:368:ASN:ND2	2:B:372:LYS:O	2.26	0.68
1:A:78:VAL:O	1:A:83:ILE:N	2.20	0.68
2:B:407:SER:HB3	2:B:507:TYR:H	1.59	0.68
1:C:130:ASP:OD1	1:C:131:LYS:N	2.25	0.68
2:D:407:SER:HB3	2:D:507:TYR:H	1.59	0.68
1:A:31:ALA:HA	1:A:91:LEU:H	1.57	0.68
2:B:203:LEU:HD13	2:B:219:GLN:HB3	1.74	0.68
1:C:362:ASN:H	1:C:366:ASP:H	1.39	0.68
1:A:130:ASP:OD2	1:A:132:SER:OG	2.11	0.68
2:D:487:GLY:O	2:D:519:ARG:NH2	2.27	0.68
2:B:487:GLY:O	2:B:519:ARG:NH2	2.27	0.68
1:C:130:ASP:OD2	1:C:132:SER:OG	2.11	0.68
1:A:361:PHE:HB3	1:A:365:GLY:HA2	1.75	0.68
2:D:466:LYS:O	2:D:469:SER:OG	2.09	0.68
2:B:780:ILE:HA	2:B:783:LEU:HD13	1.76	0.68
2:D:368:ASN:ND2	2:D:372:LYS:O	2.26	0.68
1:A:77:SER:O	1:A:81:ASP:HB2	1.93	0.68
1:A:717:GLN:NE2	1:A:719:GLU:OE2	2.26	0.67
1:A:274:GLU:N	1:A:274:GLU:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ALA:O	1:C:316:LEU:HB3	1.95	0.67
1:A:92:VAL:H	1:A:120:GLY:HA2	1.59	0.67
2:B:36:GLY:O	2:B:96:GLY:N	2.28	0.67
1:C:274:GLU:OE1	1:C:274:GLU:N	2.27	0.67
1:A:371:GLN:NE2	1:A:389:ASN:OD1	2.28	0.67
1:C:361:PHE:HB3	1:C:365:GLY:HA2	1.75	0.67
1:A:216:LEU:HD13	1:A:228:LEU:HB3	1.77	0.67
2:D:780:ILE:HA	2:D:783:LEU:HD13	1.76	0.67
1:A:27:VAL:O	1:A:61:GLN:N	2.27	0.67
2:D:187:ARG:HA	2:D:190:ILE:HD12	1.77	0.66
2:B:466:LYS:O	2:B:469:SER:OG	2.09	0.66
1:C:27:VAL:O	1:C:61:GLN:N	2.27	0.66
1:A:312:ALA:O	1:A:316:LEU:HB3	1.94	0.66
2:D:437:GLN:H	2:D:479:TYR:HA	1.61	0.66
1:A:543:GLU:OE1	1:A:543:GLU:N	2.27	0.66
2:B:437:GLN:H	2:B:479:TYR:HA	1.61	0.66
1:A:739:ILE:O	1:A:743:ARG:HB2	1.95	0.66
2:B:225:SER:HB2	2:B:228:ILE:HG13	1.77	0.66
1:C:216:LEU:HD13	1:C:228:LEU:HB3	1.77	0.66
1:C:543:GLU:OE1	1:C:543:GLU:N	2.27	0.66
1:C:371:GLN:NE2	1:C:389:ASN:OD1	2.28	0.66
2:D:36:GLY:O	2:D:96:GLY:N	2.28	0.66
1:C:739:ILE:O	1:C:743:ARG:HB2	1.95	0.65
2:D:225:SER:HB2	2:D:228:ILE:HG13	1.78	0.65
1:A:170:ASP:OD1	1:A:173:GLY:N	2.20	0.65
2:B:274:PRO:HD2	2:B:277:LEU:HD22	1.78	0.65
1:C:92:VAL:H	1:C:120:GLY:HA2	1.59	0.65
2:D:778:LEU:HA	2:D:781:LEU:HD12	1.79	0.65
1:A:388:TYR:OH	1:A:390:GLY:O	2.14	0.65
2:D:354:ASP:HB2	2:D:356:TYR:HE1	1.62	0.65
2:B:187:ARG:HA	2:B:190:ILE:HD12	1.77	0.65
2:B:778:LEU:HA	2:B:781:LEU:HD12	1.79	0.65
2:D:368:ASN:OD1	2:D:371:ARG:N	2.30	0.65
2:D:106:GLU:OE1	2:D:106:GLU:N	2.24	0.65
2:B:408:ILE:HA	2:B:508:MET:O	1.97	0.65
1:A:389:ASN:HB3	3:E:1:NAG:HN2	1.62	0.64
2:B:368:ASN:OD1	2:B:371:ARG:N	2.30	0.64
1:C:389:ASN:HB3	3:H:1:NAG:HN2	1.62	0.64
2:B:354:ASP:HB2	2:B:356:TYR:HE1	1.61	0.64
1:A:139:ARG:NH2	1:A:366:ASP:OD2	2.31	0.64
1:A:467:SER:O	1:A:469[A]:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:ILE:HA	2:D:508:MET:O	1.97	0.64
2:D:415:PRO:HB3	2:D:738:TYR:CE2	2.33	0.64
1:A:139:ARG:NH2	1:A:143:PRO:HD3	2.13	0.63
2:B:106:GLU:OE1	2:B:106:GLU:N	2.24	0.63
1:C:139:ARG:NH2	1:C:366:ASP:OD2	2.31	0.63
1:A:111:ALA:O	1:A:115:ARG:N	2.31	0.63
1:A:801:HIS:CE1	1:A:806:MET:HG3	2.33	0.63
1:C:181:GLU:HA	1:C:184:LEU:HB2	1.81	0.63
1:C:801:HIS:CE1	1:C:806:MET:HG3	2.33	0.63
1:A:428:PRO:HG3	1:A:756:VAL:HG22	1.81	0.63
1:A:750:PHE:CZ	1:A:752:TRP:HB2	2.34	0.63
2:B:415:PRO:HB3	2:B:738:TYR:CE2	2.33	0.63
2:B:552:GLU:O	2:B:556:ALA:N	2.32	0.63
1:C:467:SER:O	1:C:469[A]:ARG:NH1	2.31	0.63
2:D:274:PRO:HD2	2:D:277:LEU:HD22	1.79	0.63
1:C:111:ALA:O	1:C:115:ARG:N	2.31	0.63
2:D:552:GLU:O	2:D:556:ALA:N	2.31	0.63
2:D:689:GLY:O	2:D:693:ARG:N	2.27	0.63
1:A:117:PRO:HG2	1:A:342:PHE:HD2	1.64	0.62
2:B:354:ASP:HB2	2:B:356:TYR:CE1	2.34	0.62
1:A:181:GLU:HA	1:A:184:LEU:HB2	1.81	0.62
2:D:171:ILE:HG12	2:D:229:LEU:HB2	1.79	0.62
2:B:171:ILE:HG12	2:B:229:LEU:HB2	1.79	0.62
1:C:139:ARG:NH2	1:C:143:PRO:HD3	2.13	0.62
2:D:220:LEU:HD13	2:D:244:ALA:HB2	1.81	0.62
2:B:220:LEU:HD13	2:B:244:ALA:HB2	1.81	0.62
1:C:143:PRO:HG2	1:C:145:SER:OG	2.00	0.62
1:C:428:PRO:HG3	1:C:756:VAL:HG22	1.81	0.62
2:D:82:ILE:HG12	2:D:115:ILE:HD11	1.82	0.62
2:D:354:ASP:HB2	2:D:356:TYR:CE1	2.34	0.62
2:B:389:TYR:HD2	2:B:390:VAL:HG23	1.65	0.62
1:C:750:PHE:CZ	1:C:752:TRP:HB2	2.34	0.61
1:C:117:PRO:HG2	1:C:342:PHE:HD2	1.64	0.61
1:C:523:MET:SD	1:C:544:ARG:NE	2.74	0.61
2:D:241:PHE:O	2:D:245:ASN:CB	2.47	0.61
1:C:313:VAL:HG13	1:C:317:LEU:HD12	1.82	0.61
2:D:389:TYR:HD2	2:D:390:VAL:HG23	1.65	0.61
1:A:523:MET:SD	1:A:544:ARG:NE	2.74	0.61
1:A:143:PRO:HG2	1:A:145:SER:OG	2.00	0.61
1:A:313:VAL:HG13	1:A:317:LEU:HD12	1.82	0.60
2:B:82:ILE:HG12	2:B:115:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:TYR:O	2:B:325:HIS:ND1	2.32	0.60
2:D:149:SER:C	2:D:153:GLN:HG3	2.22	0.60
1:A:627:ALA:O	1:A:630:PHE:N	2.34	0.60
1:C:170:ASP:OD1	1:C:173:GLY:N	2.20	0.60
1:C:388:TYR:OH	1:C:390:GLY:O	2.14	0.60
1:C:627:ALA:O	1:C:630:PHE:N	2.34	0.60
2:D:205:LEU:HD22	2:D:216:ILE:HG23	1.83	0.60
1:A:805:PHE:O	1:A:809:LEU:HG	2.01	0.60
2:B:149:SER:C	2:B:153:GLN:HG3	2.22	0.60
2:B:439:ARG:HA	2:B:451:GLY:O	2.02	0.60
1:A:30:GLY:N	1:A:89:ALA:O	2.23	0.60
2:B:689:GLY:O	2:B:693:ARG:N	2.27	0.60
1:A:633:GLY:O	1:A:637:ASN:N	2.34	0.60
1:C:73:GLN:HA	1:C:76:LEU:HD12	1.83	0.60
2:B:513:LEU:HD21	2:B:525:PHE:HE1	1.67	0.59
1:C:119:LEU:HD11	1:C:138:LEU:HB2	1.83	0.59
2:D:780:ILE:HG12	2:D:783:LEU:HD22	1.84	0.59
1:C:139:ARG:HH21	1:C:366:ASP:CG	2.04	0.59
2:D:439:ARG:HA	2:D:451:GLY:O	2.02	0.59
1:A:73:GLN:HA	1:A:76:LEU:HD12	1.83	0.59
1:A:139:ARG:HH21	1:A:366:ASP:CG	2.04	0.59
2:B:241:PHE:O	2:B:245:ASN:CB	2.47	0.59
1:C:226:THR:HA	1:C:229:LEU:HD12	1.84	0.59
1:A:362:ASN:OD1	1:A:365:GLY:N	2.36	0.59
1:A:119:LEU:HD11	1:A:138:LEU:HB2	1.82	0.59
1:A:709:SER:HA	1:A:712:ILE:HD12	1.84	0.59
2:B:205:LEU:HD22	2:B:216:ILE:HG23	1.83	0.59
1:A:719:GLU:HG3	1:A:720:LEU:HD12	1.84	0.59
1:C:805:PHE:O	1:C:809:LEU:HG	2.01	0.59
2:D:133:ILE:HG22	2:D:261:LEU:HD21	1.85	0.59
1:C:633:GLY:O	1:C:637:ASN:N	2.34	0.59
2:D:409:VAL:HG22	2:D:481:VAL:HB	1.84	0.59
2:D:409:VAL:HB	2:D:479:TYR:CZ	2.38	0.59
1:A:226:THR:HA	1:A:229:LEU:HD12	1.84	0.59
2:B:150:ILE:HA	2:B:153:GLN:OE1	2.03	0.59
2:B:780:ILE:HG12	2:B:783:LEU:HD22	1.83	0.59
1:C:362:ASN:OD1	1:C:365:GLY:N	2.36	0.59
1:C:709:SER:HA	1:C:712:ILE:HD12	1.84	0.59
2:B:109:ALA:HA	2:B:112:LEU:HD12	1.85	0.58
2:D:513:LEU:HD21	2:D:525:PHE:HE1	1.67	0.58
1:A:525:GLU:HB3	1:A:530:GLN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASP:OD1	2:B:266:THR:N	2.36	0.58
2:B:138:ASP:OD1	2:B:139:GLU:N	2.37	0.58
2:D:265:ASP:OD1	2:D:266:THR:N	2.36	0.58
2:D:692:GLU:O	2:D:695:ILE:N	2.36	0.58
1:A:487:LEU:O	1:A:491:MET:N	2.35	0.58
1:C:164:ILE:O	1:C:241:ILE:N	2.36	0.58
1:C:719:GLU:HG3	1:C:720:LEU:HD12	1.84	0.58
2:D:150:ILE:HA	2:D:153:GLN:OE1	2.03	0.58
1:C:79:CYS:HA	1:C:83:ILE:HB	1.86	0.58
2:D:729:PHE:CE2	2:D:731:TYR:HB2	2.39	0.58
2:D:322:TYR:O	2:D:325:HIS:ND1	2.32	0.58
2:D:736:LEU:O	2:D:740:ALA:CB	2.51	0.58
2:B:409:VAL:HG22	2:B:481:VAL:HB	1.84	0.58
2:B:736:LEU:O	2:B:740:ALA:CB	2.51	0.58
1:C:420:LYS:O	1:C:533:MET:N	2.36	0.58
1:C:720:LEU:HG	1:C:723:MET:SD	2.44	0.58
2:B:692:GLU:O	2:B:695:ILE:N	2.36	0.58
1:A:79:CYS:HA	1:A:83:ILE:HB	1.86	0.57
1:A:127:ILE:HG13	1:A:134:HIS:NE2	2.19	0.57
1:A:720:LEU:HG	1:A:723:MET:SD	2.44	0.57
1:C:487:LEU:O	1:C:491:MET:N	2.35	0.57
1:C:525:GLU:HB3	1:C:530:GLN:HB2	1.85	0.57
2:B:409:VAL:HB	2:B:479:TYR:CZ	2.38	0.57
1:C:82:LEU:HD13	1:C:90:ILE:HD13	1.86	0.57
2:B:729:PHE:CE2	2:B:731:TYR:HB2	2.39	0.57
2:D:138:ASP:OD1	2:D:139:GLU:N	2.37	0.57
2:D:685:THR:HA	2:D:729:PHE:CE1	2.39	0.57
2:B:274:PRO:HG2	2:B:277:LEU:HB2	1.87	0.57
1:A:544:ARG:O	1:A:548:ILE:N	2.33	0.57
2:B:133:ILE:HG22	2:B:261:LEU:HD21	1.85	0.57
2:B:488:LYS:N	2:B:495:ASN:OD1	2.37	0.57
2:D:155:SER:HA	2:D:158:LEU:HD12	1.86	0.57
1:C:127:ILE:HG13	1:C:134:HIS:NE2	2.19	0.57
1:C:275:ILE:O	1:C:280:LEU:HB2	2.05	0.57
2:B:218:ASN:OD1	2:D:218:ASN:ND2	2.38	0.57
2:D:516:ASN:HD21	2:D:519:ARG:HG3	1.69	0.57
1:A:286:GLY:H	1:A:377:LEU:HD23	1.70	0.57
2:B:516:ASN:HD21	2:B:519:ARG:HG3	1.69	0.57
2:B:155:SER:HA	2:B:158:LEU:HD12	1.86	0.57
2:B:685:THR:HA	2:B:729:PHE:CE1	2.39	0.57
2:D:109:ALA:HA	2:D:112:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:296:GLY:HA2	2:D:299:ILE:HD12	1.87	0.57
1:A:82:LEU:HD13	1:A:90:ILE:HD13	1.86	0.56
2:B:143:PHE:CE2	2:B:145:GLN:HG3	2.40	0.56
2:B:157:MET:HA	2:B:160:ILE:HD12	1.86	0.56
1:C:286:GLY:H	1:C:377:LEU:HD23	1.69	0.56
2:B:38:ALA:H	2:B:97:VAL:HA	1.71	0.56
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.40	0.56
2:D:99:PHE:O	2:D:125:GLY:HA2	2.05	0.56
2:D:157:MET:HA	2:D:160:ILE:HD12	1.86	0.56
2:D:176:PHE:CD1	2:D:177:PRO:HD2	2.40	0.56
1:C:25:LYS:O	1:C:59:GLN:N	2.34	0.56
1:C:500:VAL:HG13	1:C:502:ASP:O	2.06	0.56
2:D:274:PRO:HG2	2:D:277:LEU:HB2	1.87	0.56
1:C:30:GLY:N	1:C:89:ALA:O	2.23	0.56
1:C:801:HIS:ND1	1:C:806:MET:HG3	2.21	0.56
2:B:158:LEU:HD13	2:B:189:THR:HG21	1.87	0.56
2:D:182:PHE:O	2:D:186:ILE:HG12	2.06	0.56
2:B:99:PHE:O	2:B:125:GLY:HA2	2.05	0.56
2:B:409:VAL:HG23	2:B:479:TYR:O	2.05	0.56
1:C:544:ARG:O	1:C:548:ILE:N	2.33	0.56
2:D:409:VAL:HG23	2:D:479:TYR:O	2.05	0.56
1:A:801:HIS:ND1	1:A:806:MET:HG3	2.21	0.56
2:B:412:GLU:HA	2:B:417:VAL:HB	1.88	0.56
1:A:420:LYS:O	1:A:533:MET:N	2.36	0.55
2:B:534:ILE:N	2:B:757:PHE:O	2.39	0.55
1:C:291:GLN:HB2	1:C:373:SER:HB2	1.88	0.55
2:D:776:VAL:O	2:D:779:ALA:HB3	2.06	0.55
2:D:412:GLU:HA	2:D:417:VAL:HB	1.88	0.55
2:D:529:PHE:CD2	2:D:530:ILE:HG12	2.42	0.55
1:A:25:LYS:O	1:A:59:GLN:N	2.34	0.55
1:A:275:ILE:O	1:A:280:LEU:HB2	2.05	0.55
1:C:554:PHE:N	1:C:779:PHE:O	2.29	0.55
1:C:809:LEU:O	1:C:812:THR:OG1	2.22	0.55
1:A:750:PHE:CE2	1:A:752:TRP:HB2	2.41	0.55
2:D:158:LEU:HD13	2:D:189:THR:HG21	1.87	0.55
1:A:500:VAL:HG13	1:A:502:ASP:O	2.06	0.55
2:B:182:PHE:O	2:B:186:ILE:HG12	2.06	0.55
2:B:218:ASN:ND2	2:D:218:ASN:OD1	2.38	0.55
2:B:296:GLY:HA2	2:B:299:ILE:HD12	1.87	0.55
1:C:750:PHE:CE2	1:C:752:TRP:HB2	2.41	0.55
2:D:517:GLU:O	2:D:520:SER:OG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:PHE:CE2	2:D:145:GLN:HG3	2.40	0.55
2:B:188:SER:O	2:B:192:ASN:ND2	2.40	0.55
2:B:817:ASN:O	2:B:820:GLY:N	2.40	0.55
1:A:153:GLU:OE1	1:A:156:ARG:NH1	2.40	0.55
1:A:219:ASP:O	1:A:222:THR:OG1	2.20	0.55
1:A:521:GLY:O	1:A:524:GLY:N	2.40	0.55
2:B:529:PHE:CD2	2:B:530:ILE:HG12	2.42	0.55
1:C:693:LEU:HG	1:C:702:TYR:CE1	2.42	0.55
2:D:226:PRO:O	2:D:254:TYR:HA	2.07	0.55
1:A:153:GLU:OE1	1:A:156:ARG:HD3	2.07	0.55
2:B:413:GLU:O	2:B:416:PHE:N	2.39	0.55
2:D:188:SER:O	2:D:192:ASN:ND2	2.40	0.55
2:D:488:LYS:N	2:D:495:ASN:OD1	2.37	0.55
2:B:251:GLY:O	2:B:254:TYR:HB2	2.07	0.54
1:C:74:MET:O	1:C:78:VAL:HG23	2.07	0.54
2:D:164:TYR:CE2	2:D:391:TRP:HE3	2.25	0.54
2:D:413:GLU:O	2:D:416:PHE:N	2.39	0.54
1:A:540:ILE:HG23	1:A:550:PHE:CE2	2.42	0.54
2:B:412:GLU:OE2	2:B:419:VAL:N	2.40	0.54
2:B:776:VAL:O	2:B:779:ALA:HB3	2.06	0.54
1:C:521:GLY:O	1:C:524:GLY:N	2.39	0.54
2:D:107:ALA:HA	2:D:110:GLN:HG3	1.89	0.54
1:A:38:HIS:O	1:A:42:PHE:CB	2.55	0.54
2:B:164:TYR:CE2	2:B:391:TRP:HE3	2.25	0.54
2:B:226:PRO:O	2:B:254:TYR:HA	2.07	0.54
2:D:817:ASN:O	2:D:820:GLY:N	2.40	0.54
2:B:364:ILE:N	2:B:377:GLY:O	2.40	0.54
2:D:364:ILE:N	2:D:377:GLY:O	2.40	0.54
1:C:360:GLU:O	1:C:367:ARG:HA	2.07	0.54
1:C:540:ILE:HG23	1:C:550:PHE:CE2	2.42	0.54
1:A:148:SER:HA	1:A:151:TRP:CG	2.43	0.54
1:A:360:GLU:O	1:A:367:ARG:HA	2.07	0.54
1:A:291:GLN:HB2	1:A:373:SER:HB2	1.89	0.54
1:C:806:MET:O	1:C:809:LEU:N	2.41	0.54
2:D:412:GLU:OE2	2:D:419:VAL:N	2.40	0.54
1:A:312:ALA:O	1:A:316:LEU:CB	2.56	0.54
2:B:320:SER:O	2:B:324:THR:HG23	2.08	0.54
1:C:153:GLU:OE1	1:C:156:ARG:HD3	2.07	0.54
2:D:38:ALA:H	2:D:97:VAL:HA	1.71	0.54
2:D:507:TYR:CD2	2:D:508:MET:HG3	2.43	0.54
2:B:227:ILE:HG12	2:B:255:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:743:ASP:OD1	2:D:744:GLU:N	2.41	0.54
1:A:74:MET:O	1:A:78:VAL:HG23	2.07	0.54
2:B:507:TYR:CD2	2:B:508:MET:HG3	2.43	0.54
2:D:227:ILE:HG12	2:D:255:THR:HB	1.90	0.54
2:D:251:GLY:O	2:D:254:TYR:HB2	2.07	0.54
2:D:408:ILE:HB	2:D:477:ASP:O	2.08	0.54
1:A:78:VAL:HG22	1:A:82:LEU:HD12	1.90	0.53
2:B:408:ILE:HB	2:B:477:ASP:O	2.08	0.53
2:D:152:GLN:HA	2:D:155:SER:HB3	1.89	0.53
2:B:430:MET:O	2:B:433:THR:OG1	2.12	0.53
1:C:38:HIS:O	1:C:42:PHE:CB	2.55	0.53
1:A:47:ASN:HA	1:A:50:ASN:ND2	2.23	0.53
1:A:562:LEU:O	1:A:749:ALA:HA	2.08	0.53
1:C:732:TYR:HE2	1:C:747:LEU:HD11	1.73	0.53
2:D:534:ILE:N	2:D:757:PHE:O	2.39	0.53
1:A:90:ILE:O	1:A:118:VAL:HG13	2.09	0.53
1:A:541:ASN:HD21	1:A:543:GLU:HB2	1.74	0.53
2:B:336:ASN:HA	2:B:339:LEU:HD12	1.90	0.53
2:B:743:ASP:OD1	2:B:744:GLU:N	2.41	0.53
1:C:127:ILE:HD11	1:C:133:ILE:HD12	1.91	0.53
1:A:297:ASN:HB3	1:A:301:HIS:CE1	2.44	0.53
1:A:693:LEU:HG	1:A:702:TYR:CE1	2.42	0.53
2:B:780:ILE:HA	2:B:783:LEU:HB2	1.91	0.53
1:C:148:SER:HA	1:C:151:TRP:CG	2.43	0.53
1:C:562:LEU:O	1:C:749:ALA:HA	2.08	0.53
2:D:320:SER:O	2:D:324:THR:HG23	2.08	0.53
1:A:32:VAL:N	1:A:91:LEU:O	2.37	0.53
1:A:587:VAL:O	1:A:591:VAL:CB	2.57	0.53
2:B:152:GLN:HA	2:B:155:SER:HB3	1.89	0.53
1:C:587:VAL:O	1:C:591:VAL:CB	2.57	0.53
2:D:272:GLU:OE1	2:D:272:GLU:N	2.34	0.53
2:D:533:GLY:O	2:D:733:ALA:N	2.40	0.53
2:D:780:ILE:HA	2:D:783:LEU:HB2	1.91	0.53
1:A:164:ILE:O	1:A:241:ILE:N	2.36	0.53
1:A:758:GLU:O	1:A:762:SER:CB	2.57	0.53
1:C:151:TRP:CD1	1:C:269:LEU:HD11	2.44	0.53
1:C:424:ILE:HG21	1:C:505:PHE:CE1	2.42	0.53
1:C:47:ASN:HA	1:C:50:ASN:ND2	2.23	0.53
1:C:78:VAL:HG22	1:C:82:LEU:HD12	1.90	0.53
1:C:297:ASN:HB3	1:C:301:HIS:CE1	2.44	0.53
1:C:723:MET:O	1:C:726:HIS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:GLU:N	2:D:456:CYS:HB2	2.19	0.53
1:A:127:ILE:HD11	1:A:133:ILE:HD12	1.91	0.53
1:A:151:TRP:CD1	1:A:269:LEU:HD11	2.44	0.53
1:A:796:SER:O	1:A:799:LYS:HB3	2.09	0.53
1:C:121:LEU:HD22	1:C:301:HIS:HB3	1.91	0.53
1:C:312:ALA:O	1:C:316:LEU:CB	2.56	0.53
1:C:796:SER:O	1:C:799:LYS:HB3	2.09	0.53
2:D:277:LEU:HD12	2:D:278:ILE:H	1.74	0.53
1:A:121:LEU:HD22	1:A:301:HIS:HB3	1.91	0.52
2:B:278:ILE:HG12	2:B:366:LEU:HD13	1.91	0.52
2:B:533:GLY:O	2:B:733:ALA:N	2.40	0.52
1:C:90:ILE:O	1:C:118:VAL:HG13	2.09	0.52
2:D:336:ASN:HA	2:D:339:LEU:HD12	1.90	0.52
1:A:168:SER:HB3	1:A:218:PHE:CE1	2.44	0.52
2:B:106:GLU:H	2:B:106:GLU:CD	2.11	0.52
2:B:277:LEU:HD12	2:B:278:ILE:H	1.74	0.52
1:A:732:TYR:HE2	1:A:747:LEU:HD11	1.73	0.52
2:B:107:ALA:HA	2:B:110:GLN:HG3	1.90	0.52
1:C:168:SER:HB3	1:C:218:PHE:CE1	2.44	0.52
1:C:793:VAL:O	1:C:797:ILE:HG12	2.10	0.52
1:A:422:VAL:HA	1:A:498:HIS:O	2.10	0.52
1:C:422:VAL:HA	1:C:498:HIS:O	2.10	0.52
1:C:766:ASP:OD1	1:C:766:ASP:N	2.41	0.52
1:A:806:MET:O	1:A:809:LEU:N	2.41	0.52
1:A:723:MET:O	1:A:726:HIS:N	2.40	0.52
2:B:460:PHE:HE1	2:B:792:LEU:HB3	1.75	0.52
2:B:465:LEU:HD12	2:B:468:ILE:HD11	1.92	0.52
1:C:541:ASN:HD21	1:C:543:GLU:HB2	1.74	0.52
2:D:278:ILE:HG12	2:D:366:LEU:HD13	1.91	0.52
2:D:562:MET:O	2:D:566:LEU:CB	2.58	0.52
1:A:342:PHE:CE2	1:A:346:LEU:HD11	2.44	0.52
1:C:139:ARG:HH22	1:C:143:PRO:HD3	1.74	0.52
1:C:805:PHE:O	1:C:808:ASP:HB2	2.10	0.52
1:A:703:ALA:HB1	1:A:731:ASN:OD1	2.10	0.52
2:B:114:PHE:O	2:B:118:GLN:HG2	2.10	0.52
2:B:321:CYS:O	2:B:324:THR:OG1	2.25	0.52
2:B:517:GLU:O	2:B:520:SER:OG	2.14	0.52
2:D:106:GLU:H	2:D:106:GLU:CD	2.11	0.52
2:D:114:PHE:O	2:D:118:GLN:HG2	2.10	0.52
2:D:149:SER:O	2:D:153:GLN:HG3	2.09	0.52
2:D:438:LYS:O	2:D:452:TYR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:460:PHE:HE1	2:D:792:LEU:HB3	1.75	0.52
1:A:78:VAL:HA	1:A:82:LEU:HD12	1.92	0.52
1:A:793:VAL:O	1:A:797:ILE:HG12	2.10	0.52
2:B:735:VAL:O	2:B:739:MET:HB3	2.10	0.52
1:C:342:PHE:CE2	1:C:346:LEU:HD11	2.44	0.52
2:B:149:SER:O	2:B:153:GLN:HG3	2.09	0.51
2:B:170:SER:N	2:B:228:ILE:HG12	2.25	0.51
2:B:408:ILE:HG12	2:B:508:MET:HB2	1.92	0.51
1:C:148:SER:HA	1:C:151:TRP:CD2	2.45	0.51
1:C:703:ALA:HB1	1:C:731:ASN:OD1	2.10	0.51
1:A:564:LYS:HA	1:A:767:LEU:HD23	1.92	0.51
1:A:805:PHE:O	1:A:808:ASP:HB2	2.10	0.51
1:C:316:LEU:HD12	1:C:345:VAL:HG21	1.93	0.51
2:D:430:MET:O	2:D:433:THR:OG1	2.12	0.51
1:A:148:SER:HA	1:A:151:TRP:CD2	2.45	0.51
1:A:809:LEU:O	1:A:812:THR:OG1	2.22	0.51
1:C:446:THR:OG1	1:C:450:ASP:N	2.30	0.51
1:A:554:PHE:N	1:A:779:PHE:O	2.29	0.51
2:B:562:MET:O	2:B:566:LEU:CB	2.58	0.51
1:C:78:VAL:HA	1:C:82:LEU:HD12	1.92	0.51
1:C:758:GLU:O	1:C:762:SER:CB	2.57	0.51
1:C:105:THR:HG23	1:C:134:HIS:HE1	1.76	0.51
1:C:541:ASN:ND2	1:C:543:GLU:HB2	2.26	0.51
2:D:465:LEU:HD12	2:D:468:ILE:HD11	1.92	0.51
1:C:153:GLU:OE1	1:C:156:ARG:NH1	2.40	0.51
1:A:139:ARG:HH22	1:A:143:PRO:HD3	1.74	0.51
1:A:766:ASP:N	1:A:766:ASP:OD1	2.41	0.51
2:B:169:PHE:HA	2:B:227:ILE:O	2.11	0.51
2:D:788:GLU:O	2:D:792:LEU:HG	2.11	0.51
1:A:126:SER:HB2	1:A:171:HIS:CD2	2.46	0.50
2:B:606:ILE:O	2:B:610:TRP:CB	2.54	0.50
2:B:788:GLU:O	2:B:792:LEU:HG	2.11	0.50
2:D:117:ALA:HB2	2:D:141:SER:HB2	1.93	0.50
2:D:169:PHE:HA	2:D:227:ILE:O	2.11	0.50
2:D:340:ILE:HD11	2:D:352:SER:HA	1.93	0.50
1:C:126:SER:HB2	1:C:171:HIS:CD2	2.46	0.50
2:D:170:SER:N	2:D:228:ILE:HG12	2.25	0.50
2:D:214:CYS:HB3	2:D:217:GLN:HB3	1.94	0.50
1:A:541:ASN:ND2	1:A:543:GLU:HB2	2.26	0.50
2:B:235:GLU:O	2:B:238:THR:OG1	2.18	0.50
2:D:606:ILE:O	2:D:610:TRP:CB	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:LYS:HA	1:C:767:LEU:HD23	1.92	0.50
2:D:149:SER:OG	2:D:152:GLN:HB3	2.11	0.50
2:D:735:VAL:O	2:D:739:MET:HB3	2.10	0.50
2:B:206:ASP:OD1	2:B:208:SER:N	2.44	0.50
1:C:151:TRP:CG	1:C:269:LEU:HD11	2.47	0.50
1:C:419:LEU:HA	1:C:532:ASP:OD2	2.12	0.50
2:D:321:CYS:O	2:D:324:THR:OG1	2.25	0.50
1:A:316:LEU:HD12	1:A:345:VAL:HG21	1.93	0.50
2:B:149:SER:OG	2:B:152:GLN:HB3	2.11	0.50
2:B:438:LYS:O	2:B:452:TYR:HA	2.10	0.50
1:C:270:VAL:HB	1:C:274:GLU:CD	2.32	0.50
2:D:408:ILE:HG12	2:D:508:MET:HB2	1.92	0.50
1:A:270:VAL:HB	1:A:274:GLU:CD	2.32	0.50
2:D:154:ALA:O	2:D:157:MET:HB2	2.12	0.50
2:D:532:THR:HG22	2:D:761:GLY:HA2	1.93	0.50
1:C:525:GLU:O	1:C:530:GLN:N	2.45	0.50
1:C:787:SER:OG	1:C:789:TRP:HD1	1.95	0.50
2:D:483:ASN:ND2	2:D:495:ASN:O	2.45	0.50
2:B:340:ILE:HD11	2:B:352:SER:HA	1.92	0.50
1:A:105:THR:HG23	1:A:134:HIS:HE1	1.76	0.49
1:A:424:ILE:HG21	1:A:505:PHE:CE1	2.42	0.49
2:B:101:ASP:OD2	2:B:103:THR:OG1	2.25	0.49
2:B:214:CYS:HB3	2:B:217:GLN:HB3	1.94	0.49
2:B:38:ALA:HB3	2:B:97:VAL:HG22	1.93	0.49
2:B:434:VAL:N	2:B:457:CYS:O	2.34	0.49
2:B:532:THR:HG22	2:B:761:GLY:HA2	1.93	0.49
1:C:739:ILE:O	1:C:743:ARG:CB	2.60	0.49
2:D:38:ALA:HB3	2:D:97:VAL:HG22	1.93	0.49
1:A:91:LEU:HA	1:A:119:LEU:O	2.13	0.49
1:A:165:LEU:HD23	1:A:215:VAL:HG12	1.94	0.49
1:C:408:GLU:O	1:C:410:PRO:HD3	2.12	0.49
2:D:418:ILE:O	2:D:457:CYS:HA	2.13	0.49
1:A:151:TRP:CG	1:A:269:LEU:HD11	2.46	0.49
1:C:736:ALA:HA	1:C:739:ILE:HD12	1.94	0.49
2:D:158:LEU:HD23	2:D:161:MET:CE	2.43	0.49
2:D:384:LEU:HD11	2:D:386:MET:SD	2.53	0.49
2:B:117:ALA:HB2	2:B:141:SER:HB2	1.93	0.49
2:B:154:ALA:O	2:B:157:MET:HB2	2.12	0.49
2:B:173:THR:O	2:B:204:LEU:HD12	2.13	0.49
1:C:545:ALA:HA	1:C:548:ILE:O	2.13	0.49
1:C:742:VAL:HB	1:C:747:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:HG22	1:A:502:ASP:H	1.78	0.49
1:A:408:GLU:O	1:A:410:PRO:HD3	2.12	0.49
1:A:736:ALA:HA	1:A:739:ILE:HD12	1.94	0.49
2:B:138:ASP:CG	2:B:140:SER:H	2.16	0.49
1:A:419:LEU:HA	1:A:532:ASP:OD2	2.12	0.49
1:C:91:LEU:HA	1:C:119:LEU:O	2.13	0.49
1:A:701:ILE:H	1:A:748:HIS:HB2	1.78	0.49
2:B:420:GLU:N	2:B:456:CYS:HB2	2.19	0.49
1:C:165:LEU:HD23	1:C:215:VAL:HG12	1.94	0.49
2:D:101:ASP:OD2	2:D:103:THR:OG1	2.25	0.49
2:D:173:THR:O	2:D:204:LEU:HD12	2.13	0.49
2:D:195:VAL:HB	2:D:197:TRP:CD1	2.48	0.49
2:D:685:THR:HB	2:D:730:ILE:HB	1.95	0.49
2:D:779:ALA:O	2:D:782:GLN:N	2.46	0.49
1:A:739:ILE:O	1:A:743:ARG:CB	2.60	0.48
2:B:157:MET:O	2:B:160:ILE:HB	2.13	0.48
1:C:466:GLY:H	1:C:469[A]:ARG:HH22	1.59	0.48
1:C:701:ILE:H	1:C:748:HIS:HB2	1.78	0.48
1:A:742:VAL:HB	1:A:747:LEU:HB2	1.94	0.48
1:A:787:SER:OG	1:A:789:TRP:HD1	1.95	0.48
2:B:195:VAL:HB	2:B:197:TRP:CD1	2.48	0.48
2:D:148:PRO:CB	2:D:153:GLN:HG2	2.40	0.48
2:D:157:MET:O	2:D:160:ILE:HB	2.14	0.48
2:B:158:LEU:HD23	2:B:161:MET:CE	2.43	0.48
2:B:411:LEU:HG	2:B:412:GLU:O	2.13	0.48
2:B:780:ILE:O	2:B:783:LEU:HB2	2.13	0.48
2:D:780:ILE:O	2:D:783:LEU:HB2	2.13	0.48
1:A:158:TYR:OH	1:A:400:ILE:HD13	2.14	0.48
1:A:534:ILE:HB	1:A:782:GLY:HA3	1.95	0.48
2:B:164:TYR:HE1	2:B:390:VAL:HA	1.78	0.48
2:B:418:ILE:O	2:B:457:CYS:HA	2.13	0.48
2:B:779:ALA:O	2:B:782:GLN:N	2.46	0.48
1:A:545:ALA:HA	1:A:548:ILE:O	2.13	0.48
2:B:483:ASN:ND2	2:B:495:ASN:O	2.45	0.48
2:B:483:ASN:HD21	2:B:495:ASN:HB2	1.79	0.48
1:C:237:ALA:HA	1:C:412:GLY:O	2.14	0.48
1:C:689:ASN:OD1	1:C:694:ARG:NH2	2.46	0.48
1:A:466:GLY:H	1:A:469[A]:ARG:HH22	1.59	0.48
1:A:525:GLU:O	1:A:530:GLN:N	2.45	0.48
2:B:384:LEU:HD11	2:B:386:MET:SD	2.53	0.48
2:B:770:SER:OG	2:B:771:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:HA	1:A:366:ASP:O	2.14	0.48
2:B:289:LEU:HB3	2:B:290:PRO:HD3	1.96	0.48
2:D:411:LEU:HG	2:D:412:GLU:O	2.13	0.48
1:C:361:PHE:HA	1:C:366:ASP:O	2.14	0.48
1:C:534:ILE:HB	1:C:782:GLY:HA3	1.95	0.48
2:D:82:ILE:HA	2:D:85:ILE:HD12	1.96	0.48
1:A:167:VAL:HG12	1:A:243:SER:HB3	1.96	0.48
1:A:378:GLN:NE2	1:A:401:ILE:HD12	2.29	0.48
2:B:206:ASP:OD1	2:B:208:SER:OG	2.28	0.48
2:D:292:ARG:HA	2:D:295:ASP:OD2	2.13	0.48
1:A:33:LEU:HD13	1:A:38:HIS:HB3	1.95	0.47
1:A:92:VAL:H	1:A:120:GLY:CA	2.26	0.47
2:B:214:CYS:O	2:B:218:ASN:N	2.42	0.47
2:B:352:SER:N	2:B:356:TYR:O	2.46	0.47
1:C:33:LEU:HD13	1:C:38:HIS:HB3	1.95	0.47
1:C:167:VAL:HG12	1:C:243:SER:HB3	1.96	0.47
1:C:421:ILE:HA	1:C:533:MET:HB3	1.96	0.47
1:C:693:LEU:HG	1:C:702:TYR:CD1	2.49	0.47
2:D:303:ALA:O	2:D:306:ASP:N	2.45	0.47
2:D:483:ASN:HD21	2:D:495:ASN:HB2	1.79	0.47
2:D:732:ASP:O	2:D:736:LEU:HD13	2.14	0.47
1:A:139:ARG:HH12	1:A:143:PRO:HB3	1.79	0.47
2:B:82:ILE:HA	2:B:85:ILE:HD12	1.96	0.47
2:D:434:VAL:N	2:D:457:CYS:O	2.34	0.47
1:A:689:ASN:OD1	1:A:694:ARG:NH2	2.46	0.47
2:B:292:ARG:HA	2:B:295:ASP:OD2	2.13	0.47
1:C:27:VAL:HB	1:C:60:LEU:HA	1.97	0.47
1:C:158:TYR:OH	1:C:400:ILE:HD13	2.14	0.47
1:C:688:ILE:HD12	1:C:774:PHE:CE2	2.50	0.47
2:D:164:TYR:HE1	2:D:390:VAL:HA	1.78	0.47
2:D:259:PRO:HD2	2:D:262:VAL:HG21	1.95	0.47
1:A:434:PRO:HG3	1:A:474:GLN:NE2	2.30	0.47
1:A:446:THR:OG1	1:A:450:ASP:N	2.30	0.47
2:B:780:ILE:HG23	2:B:783:LEU:HD22	1.96	0.47
1:C:428:PRO:HD3	1:C:756:VAL:HG13	1.96	0.47
2:D:148:PRO:HG2	2:D:153:GLN:HE21	1.79	0.47
1:A:30:GLY:HA2	1:A:63:THR:O	2.15	0.47
1:A:688:ILE:HD12	1:A:774:PHE:CE2	2.50	0.47
2:B:732:ASP:O	2:B:736:LEU:HD13	2.15	0.47
1:C:30:GLY:HA2	1:C:63:THR:O	2.15	0.47
1:C:700:PHE:HA	1:C:748:HIS:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:LEU:HB3	2:D:290:PRO:HD3	1.96	0.47
2:D:352:SER:N	2:D:356:TYR:O	2.46	0.47
2:D:536:VAL:O	2:D:750:THR:OG1	2.23	0.47
1:A:105:THR:HG23	1:A:134:HIS:CE1	2.49	0.47
1:A:462:ASP:O	1:A:463:THR:OG1	2.27	0.47
1:A:693:LEU:HG	1:A:702:TYR:CD1	2.49	0.47
2:B:685:THR:HB	2:B:730:ILE:HB	1.95	0.47
1:C:331:GLY:HA2	2:D:75:GLU:OE1	2.14	0.47
2:D:40:ILE:N	2:D:98:VAL:O	2.47	0.47
2:D:138:ASP:CG	2:D:140:SER:H	2.16	0.47
1:A:228:LEU:O	1:A:231:GLU:HB2	2.15	0.47
1:A:237:ALA:HA	1:A:412:GLY:O	2.14	0.47
1:A:700:PHE:HA	1:A:748:HIS:CG	2.50	0.47
2:B:40:ILE:N	2:B:98:VAL:O	2.47	0.47
2:B:259:PRO:HD2	2:B:262:VAL:HG21	1.95	0.47
2:B:412:GLU:OE1	2:B:419:VAL:HB	2.14	0.47
1:C:139:ARG:HH12	1:C:143:PRO:HB3	1.79	0.47
2:D:89:MET:HB3	2:D:319:SER:HA	1.97	0.47
2:D:307:MET:O	2:D:311:HIS:N	2.45	0.47
1:A:421:ILE:HA	1:A:533:MET:HB3	1.96	0.47
1:A:700:PHE:HA	1:A:748:HIS:CD2	2.50	0.47
1:A:806:MET:HA	1:A:809:LEU:HG	1.97	0.47
2:B:148:PRO:HG2	2:B:153:GLN:HE21	1.79	0.47
1:C:719:GLU:HG3	1:C:720:LEU:N	2.30	0.47
2:D:176:PHE:CG	2:D:177:PRO:HD2	2.50	0.47
2:D:214:CYS:O	2:D:218:ASN:N	2.42	0.47
2:D:770:SER:OG	2:D:771:GLY:N	2.47	0.47
1:C:228:LEU:O	1:C:231:GLU:HB2	2.15	0.47
1:C:378:GLN:NE2	1:C:401:ILE:HD12	2.29	0.47
1:A:331:GLY:HA2	2:B:75:GLU:OE1	2.14	0.47
1:A:428:PRO:HD3	1:A:756:VAL:HG13	1.96	0.47
2:B:516:ASN:HD21	2:B:519:ARG:CG	2.28	0.47
1:C:253:TYR:CG	1:C:284:PRO:HD3	2.50	0.47
1:A:466:GLY:N	1:A:469[A]:ARG:HH22	2.13	0.46
2:B:148:PRO:CB	2:B:153:GLN:HG2	2.40	0.46
2:B:307:MET:O	2:B:311:HIS:N	2.45	0.46
2:B:686:VAL:HB	2:B:687:PRO:HD2	1.96	0.46
2:D:40:ILE:HB	2:D:99:PHE:HA	1.96	0.46
2:D:206:ASP:OD1	2:D:208:SER:OG	2.28	0.46
1:A:103:THR:O	1:A:106:PRO:HD2	2.15	0.46
1:C:434:PRO:HG3	1:C:474:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:GLY:N	1:C:469[A]:ARG:HH22	2.13	0.46
1:C:500:VAL:HG22	1:C:502:ASP:H	1.77	0.46
1:C:688:ILE:HB	1:C:774:PHE:CE1	2.50	0.46
2:D:412:GLU:OE1	2:D:419:VAL:HB	2.14	0.46
2:B:40:ILE:HB	2:B:99:PHE:HA	1.96	0.46
2:B:84:ARG:O	2:B:88:LEU:CB	2.63	0.46
2:B:89:MET:HB3	2:B:319:SER:HA	1.97	0.46
1:C:105:THR:HG23	1:C:134:HIS:CE1	2.49	0.46
1:C:700:PHE:HA	1:C:748:HIS:CD2	2.50	0.46
2:D:218:ASN:O	2:D:221:LYS:N	2.48	0.46
1:A:27:VAL:HB	1:A:60:LEU:HA	1.97	0.46
1:A:253:TYR:CG	1:A:284:PRO:HD3	2.50	0.46
1:A:562:LEU:HD21	1:A:767:LEU:HD13	1.97	0.46
2:B:407:SER:H	2:B:507:TYR:HB3	1.80	0.46
1:C:103:THR:O	1:C:106:PRO:HD2	2.15	0.46
2:D:737:ASN:O	2:D:740:ALA:HB3	2.16	0.46
1:A:626:SER:O	1:A:629:TRP:HB3	2.16	0.46
1:A:688:ILE:HB	1:A:774:PHE:CE1	2.50	0.46
2:B:218:ASN:O	2:B:221:LYS:N	2.48	0.46
2:D:524:ASP:OD2	2:D:769:ASP:N	2.48	0.46
1:A:719:GLU:HG3	1:A:720:LEU:N	2.30	0.46
2:B:148:PRO:HG2	2:B:153:GLN:NE2	2.31	0.46
2:D:516:ASN:HD21	2:D:519:ARG:CG	2.28	0.46
2:D:686:VAL:HB	2:D:687:PRO:HD2	1.96	0.46
2:D:780:ILE:HG23	2:D:783:LEU:HD22	1.96	0.46
2:B:272:GLU:OE1	2:B:272:GLU:N	2.34	0.46
2:B:337:ARG:O	2:B:340:ILE:HG22	2.16	0.46
2:D:499:GLY:HA2	2:D:502:VAL:HG12	1.98	0.46
1:A:149:SER:HG	1:A:179:ARG:HE	1.57	0.46
2:B:176:PHE:CG	2:B:177:PRO:HD2	2.50	0.46
2:D:84:ARG:O	2:D:88:LEU:CB	2.63	0.46
2:D:335:LEU:O	2:D:339:LEU:HG	2.16	0.46
1:A:244:ALA:N	1:A:273:ARG:HH21	2.14	0.46
1:A:389:ASN:CB	3:E:1:NAG:HN2	2.29	0.46
2:B:648:ALA:O	2:B:651:ALA:HB3	2.16	0.46
1:C:446:THR:OG1	1:C:449:GLY:N	2.49	0.46
1:A:77:SER:OG	1:A:81:ASP:OD2	2.28	0.45
1:A:591:VAL:HA	1:A:657:TRP:CH2	2.52	0.45
2:D:186:ILE:O	2:D:190:ILE:HG13	2.17	0.45
1:A:523:MET:CE	1:A:544:ARG:HG2	2.46	0.45
2:B:170:SER:H	2:B:228:ILE:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:SER:O	2:B:363:VAL:N	2.44	0.45
2:D:148:PRO:HG2	2:D:153:GLN:NE2	2.31	0.45
2:D:648:ALA:O	2:D:651:ALA:HB3	2.16	0.45
1:A:422:VAL:HB	1:A:498:HIS:CE1	2.51	0.45
1:A:446:THR:OG1	1:A:449:GLY:N	2.49	0.45
2:B:234:LYS:O	2:B:238:THR:HG23	2.17	0.45
1:C:244:ALA:N	1:C:273:ARG:HH21	2.14	0.45
1:C:502:ASP:CG	1:C:504:LYS:H	2.18	0.45
1:A:502:ASP:CG	1:A:504:LYS:H	2.18	0.45
2:B:507:TYR:HD2	2:B:508:MET:HG3	1.79	0.45
2:B:524:ASP:OD2	2:B:769:ASP:N	2.48	0.45
2:B:737:ASN:O	2:B:740:ALA:HB3	2.16	0.45
1:C:523:MET:CE	1:C:544:ARG:HG2	2.46	0.45
1:C:562:LEU:HD21	1:C:767:LEU:HD13	1.97	0.45
1:A:177:GLN:NE2	1:A:181:GLU:OE2	2.31	0.45
1:A:297:ASN:HB3	1:A:301:HIS:HE1	1.81	0.45
1:A:515:ASN:HD22	2:B:188:SER:HB2	1.82	0.45
2:B:276:GLY:N	2:B:367:LEU:HD23	2.31	0.45
2:B:461:CYS:HA	2:B:464:ILE:HG12	1.99	0.45
1:C:559:LEU:HD23	1:C:559:LEU:HA	1.72	0.45
2:D:407:SER:H	2:D:507:TYR:HB3	1.80	0.45
2:D:507:TYR:HD2	2:D:508:MET:HG3	1.80	0.45
1:A:147:GLN:CD	1:A:271:GLY:HA3	2.37	0.45
2:B:303:ALA:O	2:B:306:ASP:N	2.45	0.45
2:B:335:LEU:O	2:B:339:LEU:HG	2.16	0.45
2:B:532:THR:OG1	2:B:732:ASP:OD2	2.30	0.45
1:C:479:PHE:O	1:C:482:ASP:HB2	2.16	0.45
1:C:806:MET:HA	1:C:809:LEU:HG	1.97	0.45
2:D:483:ASN:ND2	2:D:495:ASN:HB2	2.32	0.45
2:B:225:SER:HB2	2:B:228:ILE:CG1	2.46	0.45
1:C:422:VAL:HB	1:C:498:HIS:CE1	2.51	0.45
1:C:626:SER:O	1:C:629:TRP:HB3	2.16	0.45
2:D:276:GLY:N	2:D:367:LEU:HD23	2.32	0.45
1:A:179:ARG:O	1:A:182:THR:HB	2.17	0.45
1:A:479:PHE:O	1:A:482:ASP:HB2	2.16	0.45
2:B:186:ILE:O	2:B:190:ILE:HG13	2.16	0.45
1:C:757:LEU:HA	1:C:757:LEU:HD23	1.66	0.45
2:D:234:LYS:O	2:D:238:THR:HG23	2.17	0.45
1:C:121:LEU:HD23	1:C:140:THR:HG21	1.99	0.45
1:C:591:VAL:HA	1:C:657:TRP:CH2	2.52	0.45
2:D:73:MET:HE3	2:D:81:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:HIS:CG	2:D:406:LEU:N	2.85	0.45
2:D:468:ILE:HG13	2:D:469:SER:N	2.32	0.45
2:B:325:HIS:CD2	2:B:326:GLU:HG2	2.52	0.45
2:B:405:HIS:CG	2:B:406:LEU:N	2.85	0.45
2:B:468:ILE:HG13	2:B:469:SER:N	2.32	0.45
2:D:129:GLY:HA2	2:D:132:MET:HG3	1.98	0.45
2:D:225:SER:HB2	2:D:228:ILE:CG1	2.46	0.45
2:D:325:HIS:CD2	2:D:326:GLU:HG2	2.52	0.45
2:D:461:CYS:HA	2:D:464:ILE:HG12	1.99	0.45
2:D:516:ASN:CG	2:D:519:ARG:H	2.21	0.45
2:B:311:HIS:HB3	2:B:313:PHE:CE2	2.52	0.44
1:C:389:ASN:CB	3:H:1:NAG:HN2	2.29	0.44
1:A:152:PHE:O	1:A:155:MET:HB2	2.18	0.44
1:A:757:LEU:HA	1:A:757:LEU:HD23	1.67	0.44
2:B:129:GLY:HA2	2:B:132:MET:HG3	1.98	0.44
2:B:499:GLY:HA2	2:B:502:VAL:HG12	1.98	0.44
2:B:789:MET:HA	2:B:792:LEU:HD12	1.99	0.44
1:C:92:VAL:H	1:C:120:GLY:CA	2.26	0.44
2:D:460:PHE:O	2:D:463:ASP:N	2.51	0.44
1:C:32:VAL:N	1:C:91:LEU:O	2.37	0.44
2:D:311:HIS:HB3	2:D:313:PHE:CE2	2.52	0.44
2:B:187:ARG:O	2:B:190:ILE:N	2.50	0.44
2:B:682:ARG:O	2:B:727:ASP:HB2	2.18	0.44
1:C:112:GLY:C	1:C:115:ARG:H	2.20	0.44
2:D:337:ARG:O	2:D:340:ILE:HG22	2.16	0.44
2:B:483:ASN:ND2	2:B:495:ASN:HB2	2.32	0.44
2:B:774:ARG:NH2	1:C:786:ASP:OD1	2.51	0.44
1:C:515:ASN:HD22	2:D:188:SER:HB2	1.82	0.44
2:D:187:ARG:O	2:D:190:ILE:N	2.50	0.44
2:D:782:GLN:C	2:D:785:GLY:H	2.21	0.44
1:A:121:LEU:HD23	1:A:140:THR:HG21	1.99	0.44
2:B:292:ARG:O	2:B:295:ASP:HB2	2.18	0.44
1:A:429:PHE:O	1:A:478:GLY:HA3	2.18	0.44
1:A:734:SER:O	1:A:737:GLU:HB2	2.18	0.44
1:A:786:ASP:OD1	2:D:774:ARG:NH2	2.51	0.44
1:C:147:GLN:CD	1:C:271:GLY:HA3	2.37	0.44
1:C:268:TRP:HB2	1:C:287:ILE:HG13	2.00	0.44
2:D:437:GLN:O	2:D:480:LEU:N	2.29	0.44
2:D:682:ARG:O	2:D:727:ASP:HB2	2.18	0.44
1:A:112:GLY:C	1:A:115:ARG:H	2.20	0.44
1:C:734:SER:O	1:C:737:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:ASN:O	2:D:520:SER:HB3	2.18	0.44
2:B:516:ASN:O	2:B:520:SER:HB3	2.18	0.44
2:B:782:GLN:C	2:B:785:GLY:H	2.21	0.43
2:B:132:MET:HB3	2:B:261:LEU:HD22	2.00	0.43
2:B:279:SER:OG	2:B:280:VAL:N	2.50	0.43
2:B:717:ALA:O	2:B:720:SER:OG	2.23	0.43
1:C:152:PHE:O	1:C:155:MET:HB2	2.17	0.43
1:C:179:ARG:O	1:C:182:THR:HB	2.17	0.43
2:D:170:SER:H	2:D:228:ILE:HG12	1.81	0.43
2:D:279:SER:OG	2:D:280:VAL:N	2.50	0.43
1:A:166:LEU:HD23	1:A:242:LEU:HD13	1.99	0.43
1:A:701:ILE:H	1:A:748:HIS:CG	2.37	0.43
2:B:460:PHE:CE1	2:B:792:LEU:HB3	2.53	0.43
1:C:302:ILE:O	1:C:306:VAL:HG23	2.19	0.43
1:C:752:TRP:CG	1:C:753:ASP:N	2.87	0.43
2:D:303:ALA:HB1	2:D:339:LEU:HD23	2.01	0.43
1:A:754:SER:O	1:A:757:LEU:N	2.52	0.43
1:C:429:PHE:O	1:C:478:GLY:HA3	2.18	0.43
2:B:107:ALA:HA	2:B:110:GLN:CG	2.49	0.43
2:B:460:PHE:O	2:B:463:ASP:N	2.51	0.43
1:C:701:ILE:H	1:C:748:HIS:CG	2.37	0.43
1:C:787:SER:OG	1:C:788:PRO:HD2	2.19	0.43
2:D:460:PHE:CE1	2:D:792:LEU:HB3	2.53	0.43
2:D:789:MET:HA	2:D:792:LEU:HD12	1.99	0.43
3:H:1:NAG:O3	3:H:2:NAG:O5	2.37	0.43
1:A:30:GLY:O	1:A:90:ILE:HA	2.18	0.43
1:A:302:ILE:O	1:A:306:VAL:HG23	2.19	0.43
2:B:170:SER:O	2:B:228:ILE:HG23	2.18	0.43
2:B:303:ALA:HB1	2:B:339:LEU:HD23	2.01	0.43
2:B:782:GLN:O	2:B:785:GLY:N	2.52	0.43
1:C:297:ASN:HB3	1:C:301:HIS:HE1	1.81	0.43
2:D:160:ILE:HD11	2:D:280:VAL:HG21	2.01	0.43
1:A:137:PHE:O	1:A:138:LEU:HD12	2.19	0.43
2:B:793:GLU:O	2:B:797:LEU:N	2.51	0.43
1:C:166:LEU:HD23	1:C:242:LEU:HD13	1.99	0.43
1:C:384:GLN:O	1:C:396:ASN:ND2	2.52	0.43
2:D:292:ARG:O	2:D:295:ASP:HB2	2.18	0.43
2:D:793:GLU:O	2:D:797:LEU:N	2.51	0.43
2:B:429:CYS:SG	2:B:433:THR:OG1	2.77	0.43
1:C:705:VAL:HG12	1:C:706:LYS:O	2.19	0.43
1:A:787:SER:OG	1:A:788:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:SER:C	2:B:228:ILE:HG23	2.40	0.43
2:B:389:TYR:CD2	2:B:390:VAL:HG23	2.51	0.43
1:C:286:GLY:N	1:C:377:LEU:HD23	2.33	0.43
3:E:1:NAG:O3	3:E:2:NAG:O5	2.37	0.43
1:C:30:GLY:O	1:C:90:ILE:HA	2.18	0.43
2:D:132:MET:HB3	2:D:261:LEU:HD22	2.00	0.43
2:D:717:ALA:O	2:D:720:SER:OG	2.23	0.43
1:A:268:TRP:HB2	1:A:287:ILE:HG13	2.00	0.42
1:A:732:TYR:CE2	1:A:747:LEU:HD11	2.54	0.42
2:D:133:ILE:HG22	2:D:261:LEU:CD2	2.48	0.42
2:D:171:ILE:HG21	2:D:182:PHE:CE1	2.54	0.42
2:D:782:GLN:O	2:D:785:GLY:N	2.52	0.42
1:A:362:ASN:H	1:A:366:ASP:N	2.13	0.42
2:B:409:VAL:HB	2:B:479:TYR:CE1	2.54	0.42
2:D:429:CYS:SG	2:D:433:THR:OG1	2.77	0.42
1:C:36:ARG:O	1:C:39:GLU:HB2	2.19	0.42
2:B:171:ILE:HG21	2:B:182:PHE:CE1	2.54	0.42
1:C:36:ARG:HA	1:C:39:GLU:HG3	2.01	0.42
1:C:272:GLU:OE1	1:C:292:LEU:N	2.52	0.42
2:D:409:VAL:HB	2:D:479:TYR:CE1	2.54	0.42
2:D:533:GLY:N	2:D:732:ASP:OD1	2.52	0.42
1:A:654:GLY:O	1:A:657:TRP:HB3	2.19	0.42
2:B:78:PRO:HA	2:B:81:ILE:HD12	2.01	0.42
1:C:180:LEU:O	1:C:184:LEU:HG	2.19	0.42
2:D:170:SER:C	2:D:228:ILE:HG23	2.40	0.42
2:D:281:SER:O	2:D:363:VAL:N	2.44	0.42
1:A:108:SER:HG	1:A:134:HIS:HD1	1.66	0.42
1:A:272:GLU:OE1	1:A:292:LEU:N	2.52	0.42
2:B:508:MET:HG2	2:B:766:ILE:HG22	2.01	0.42
2:D:124:LEU:CD2	2:D:144:PHE:HB2	2.49	0.42
2:D:519:ARG:O	2:D:522:VAL:HG22	2.20	0.42
1:A:36:ARG:O	1:A:39:GLU:HB2	2.19	0.42
1:A:286:GLY:N	1:A:377:LEU:HD23	2.33	0.42
1:A:672:LEU:O	1:A:675:PHE:N	2.53	0.42
2:B:160:ILE:HD11	2:B:280:VAL:HG21	2.01	0.42
2:D:78:PRO:HA	2:D:81:ILE:HD12	2.00	0.42
2:D:206:ASP:OD1	2:D:208:SER:N	2.44	0.42
1:A:336:TRP:CH2	1:A:338:THR:HB	2.55	0.42
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.72	0.42
1:C:32:VAL:HG12	1:C:65:VAL:HG23	2.01	0.42
1:C:654:GLY:O	1:C:657:TRP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:672:LEU:O	1:C:675:PHE:N	2.53	0.42
2:D:179:TYR:CG	2:D:180:GLN:N	2.88	0.42
1:A:705:VAL:HG12	1:A:706:LYS:O	2.19	0.42
1:A:752:TRP:CG	1:A:753:ASP:N	2.87	0.42
2:B:519:ARG:O	2:B:522:VAL:HG22	2.20	0.42
2:B:519:ARG:O	2:B:523:VAL:HG22	2.20	0.42
2:B:533:GLY:N	2:B:732:ASP:OD1	2.52	0.42
1:C:137:PHE:O	1:C:138:LEU:HD12	2.19	0.42
1:C:249:ALA:HA	1:C:252:VAL:HG22	2.02	0.42
2:D:170:SER:O	2:D:228:ILE:HG23	2.19	0.42
2:D:508:MET:HG2	2:D:766:ILE:HG22	2.01	0.42
1:A:27:VAL:N	1:A:59:GLN:O	2.53	0.42
1:A:106:PRO:HG3	2:B:114:PHE:CZ	2.55	0.42
1:A:180:LEU:O	1:A:184:LEU:HG	2.19	0.42
1:A:249:ALA:HA	1:A:252:VAL:HG22	2.02	0.42
1:A:384:GLN:O	1:A:396:ASN:ND2	2.52	0.42
2:B:256:TRP:O	2:B:278:ILE:HB	2.20	0.42
1:C:311:GLN:NE2	1:C:350:LYS:O	2.43	0.42
2:D:559:TRP:O	2:D:562:MET:N	2.53	0.42
1:A:421:ILE:O	1:A:498:HIS:ND1	2.53	0.41
2:B:295:ASP:O	2:B:299:ILE:HG13	2.20	0.41
1:C:27:VAL:N	1:C:59:GLN:O	2.53	0.41
1:C:106:PRO:HG3	2:D:114:PHE:CZ	2.55	0.41
2:B:364:ILE:HD12	2:B:378:LYS:N	2.34	0.41
1:C:78:VAL:HG11	1:C:110:THR:HG21	2.02	0.41
1:C:272:GLU:HB2	1:C:291:GLN:HA	2.02	0.41
1:C:754:SER:O	1:C:757:LEU:N	2.52	0.41
2:D:535:SER:HB2	2:D:736:LEU:HD22	2.02	0.41
1:A:36:ARG:HA	1:A:39:GLU:HG3	2.01	0.41
2:B:124:LEU:CD2	2:B:144:PHE:HB2	2.49	0.41
2:B:143:PHE:CZ	2:B:145:GLN:HG3	2.56	0.41
2:D:295:ASP:O	2:D:299:ILE:HG13	2.20	0.41
2:D:547:PRO:C	2:D:549:ALA:H	2.23	0.41
1:A:32:VAL:HG12	1:A:65:VAL:HG23	2.01	0.41
1:A:78:VAL:HG11	1:A:110:THR:HG21	2.02	0.41
1:C:92:VAL:HG21	1:C:107:VAL:HG11	2.02	0.41
1:C:421:ILE:O	1:C:498:HIS:ND1	2.54	0.41
2:D:519:ARG:O	2:D:523:VAL:HG22	2.20	0.41
1:A:92:VAL:HG21	1:A:107:VAL:HG11	2.02	0.41
1:A:151:TRP:HE1	1:A:290:LEU:HD11	1.85	0.41
1:C:309:VAL:O	1:C:313:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PHE:O	1:C:346:LEU:HG	2.21	0.41
2:D:143:PHE:CZ	2:D:145:GLN:HG3	2.56	0.41
2:D:364:ILE:HD12	2:D:378:LYS:N	2.34	0.41
1:A:241:ILE:HG12	1:A:269:LEU:HB3	2.03	0.41
2:B:536:VAL:HA	2:B:729:PHE:O	2.21	0.41
2:B:609:LEU:O	2:B:612:LEU:N	2.54	0.41
2:B:715:ASP:N	2:B:715:ASP:OD1	2.53	0.41
1:C:241:ILE:HG12	1:C:269:LEU:HB3	2.03	0.41
2:D:405:HIS:O	2:D:406:LEU:HD23	2.21	0.41
1:A:291:GLN:HG3	1:A:375:MET:HG3	2.03	0.41
1:A:309:VAL:O	1:A:313:VAL:HG23	2.21	0.41
1:C:239:VAL:HG22	1:C:267:VAL:HG21	2.03	0.41
1:A:166:LEU:O	1:A:242:LEU:HD12	2.21	0.41
1:A:272:GLU:HB2	1:A:291:GLN:HA	2.02	0.41
1:A:424:ILE:O	1:A:430:VAL:HG21	2.21	0.41
2:B:535:SER:HB2	2:B:736:LEU:HD22	2.02	0.41
2:B:547:PRO:C	2:B:549:ALA:H	2.23	0.41
1:C:111:ALA:HB1	1:C:116:ILE:O	2.21	0.41
1:C:166:LEU:O	1:C:242:LEU:HD12	2.21	0.41
1:A:791:GLN:O	1:A:795:LEU:HG	2.21	0.41
2:B:133:ILE:HG22	2:B:261:LEU:CD2	2.48	0.41
2:B:175:TYR:CE1	2:B:204:LEU:HD21	2.56	0.41
2:B:229:LEU:CD2	2:B:257:ILE:HB	2.51	0.41
2:B:255:THR:HG22	2:B:256:TRP:H	1.86	0.41
2:B:423:ASP:OD2	2:B:425:LEU:HB2	2.21	0.41
2:B:559:TRP:O	2:B:562:MET:N	2.53	0.41
2:B:669:LYS:O	2:B:672:GLN:N	2.39	0.41
1:C:77:SER:OG	1:C:81:ASP:OD2	2.28	0.41
1:C:336:TRP:CH2	1:C:338:THR:HB	2.55	0.41
1:C:424:ILE:O	1:C:430:VAL:HG21	2.21	0.41
1:C:756:VAL:O	1:C:759:PHE:HB3	2.21	0.41
2:D:107:ALA:HA	2:D:110:GLN:CG	2.49	0.41
2:D:111:ILE:O	2:D:114:PHE:HB3	2.20	0.41
2:D:175:TYR:CE1	2:D:204:LEU:HD21	2.56	0.41
2:D:406:LEU:HD22	2:D:507:TYR:CD2	2.56	0.41
2:D:513:LEU:HD21	2:D:525:PHE:CE1	2.52	0.41
2:B:516:ASN:CG	2:B:519:ARG:H	2.21	0.41
2:B:520:SER:OG	2:B:521:GLU:N	2.54	0.41
2:D:229:LEU:CD2	2:D:257:ILE:HB	2.51	0.41
1:A:423:THR:OG1	1:A:424:ILE:N	2.54	0.40
1:A:458:THR:HG22	1:A:473:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ILE:O	2:B:114:PHE:HB3	2.20	0.40
2:B:179:TYR:CG	2:B:180:GLN:N	2.88	0.40
1:C:344:ARG:HD3	2:D:209:LEU:HD22	2.03	0.40
1:C:498:HIS:CE1	1:C:531:ALA:HB2	2.56	0.40
2:D:143:PHE:CG	2:D:144:PHE:N	2.89	0.40
1:A:143:PRO:HD2	1:A:146:HIS:ND1	2.37	0.40
1:A:360:GLU:HG2	1:A:361:PHE:N	2.36	0.40
1:A:417:THR:O	1:A:493:PHE:HB2	2.21	0.40
1:A:431:TYR:O	1:A:476:CYS:HA	2.22	0.40
1:A:717:GLN:CD	1:A:719:GLU:HG2	2.41	0.40
2:B:155:SER:O	2:B:158:LEU:HB2	2.21	0.40
2:B:179:TYR:O	2:B:182:PHE:HB3	2.21	0.40
1:C:291:GLN:HG3	1:C:375:MET:HG3	2.03	0.40
1:C:717:GLN:CD	1:C:719:GLU:HG2	2.41	0.40
2:D:609:LEU:O	2:D:612:LEU:N	2.54	0.40
2:D:679:PRO:HA	2:D:680:PRO:HD3	1.97	0.40
1:A:117:PRO:HG2	1:A:342:PHE:CD2	2.51	0.40
1:A:342:PHE:O	1:A:346:LEU:HG	2.21	0.40
1:A:344:ARG:HD3	2:B:209:LEU:HD22	2.03	0.40
1:A:756:VAL:O	1:A:759:PHE:HB3	2.21	0.40
2:B:405:HIS:O	2:B:406:LEU:HD23	2.20	0.40
2:B:513:LEU:HD21	2:B:525:PHE:CE1	2.52	0.40
2:D:155:SER:O	2:D:158:LEU:HB2	2.22	0.40
2:D:361:LYS:O	2:D:362:LEU:HD23	2.21	0.40
2:D:774:ARG:O	2:D:777:ASP:HB2	2.21	0.40
1:A:239:VAL:HG22	1:A:267:VAL:HG21	2.03	0.40
1:A:480:CYS:HB3	1:A:535:VAL:HG12	2.04	0.40
2:B:280:VAL:HG13	2:B:363:VAL:C	2.41	0.40
2:B:437:GLN:O	2:B:480:LEU:N	2.29	0.40
1:C:151:TRP:HE1	1:C:290:LEU:HD11	1.85	0.40
1:C:362:ASN:H	1:C:366:ASP:N	2.13	0.40
1:C:462:ASP:C	1:C:464:SER:H	2.25	0.40
1:C:541:ASN:ND2	1:C:543:GLU:OE1	2.54	0.40
2:D:113:ASP:O	2:D:116:SER:HB3	2.21	0.40
2:D:520:SER:OG	2:D:521:GLU:N	2.54	0.40
2:D:547:PRO:O	2:D:549:ALA:N	2.55	0.40
2:B:361:LYS:O	2:B:362:LEU:HD23	2.21	0.40
1:C:158:TYR:HB3	1:C:160:TRP:CE2	2.56	0.40
1:C:376:ASN:ND2	1:C:401:ILE:O	2.55	0.40
1:C:417:THR:O	1:C:493:PHE:HB2	2.22	0.40
2:D:131:SER:HB2	2:D:146:PHE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:ILE:HG12	2:D:278:ILE:CG2	2.52	0.40
2:D:389:TYR:CD2	2:D:390:VAL:HG23	2.51	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	785/838 (94%)	702 (89%)	83 (11%)	0	100	100
1	C	785/838 (94%)	704 (90%)	81 (10%)	0	100	100
2	B	779/812 (96%)	706 (91%)	69 (9%)	4 (0%)	29	68
2	D	779/812 (96%)	706 (91%)	69 (9%)	4 (0%)	29	68
All	All	3128/3300 (95%)	2818 (90%)	302 (10%)	8 (0%)	44	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	808	VAL
2	D	808	VAL
2	B	396	PRO
2	D	396	PRO
2	B	655	ILE
2	D	186	ILE
2	D	655	ILE
2	B	186	ILE

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	437/724 (60%)	437 (100%)	0	100	100
1	C	437/724 (60%)	437 (100%)	0	100	100
2	B	404/709 (57%)	404 (100%)	0	100	100
2	D	404/709 (57%)	404 (100%)	0	100	100
All	All	1682/2866 (59%)	1682 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	695	ASN
2	B	483	ASN
2	B	486	HIS
1	C	146	HIS
1	C	695	ASN
2	D	483	ASN
2	D	486	HIS

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)

12 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	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.44	0
3	NAG	F	1	3,1	14,14,15	1.17	2 (14%)	17,19,21	0.87	1 (5%)
3	NAG	F	2	3	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	G	1	2,3	14,14,15	0.80	1 (7%)	17,19,21	0.46	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	H	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	H	2	3	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	I	1	3,1	14,14,15	1.15	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	I	2	3	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	J	1	2,3	14,14,15	0.81	1 (7%)	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.31	0	17,19,21	0.56	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	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	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	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O5-C1	3.73	1.49	1.43
3	I	1	NAG	O5-C1	3.68	1.49	1.43
3	J	1	NAG	O5-C1	-2.82	1.39	1.43
3	G	1	NAG	O5-C1	-2.78	1.39	1.43
3	F	1	NAG	C1-C2	2.17	1.55	1.52
3	I	1	NAG	C1-C2	2.14	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	C1-O5-C5	2.92	116.14	112.19
3	F	1	NAG	C1-O5-C5	2.91	116.13	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7

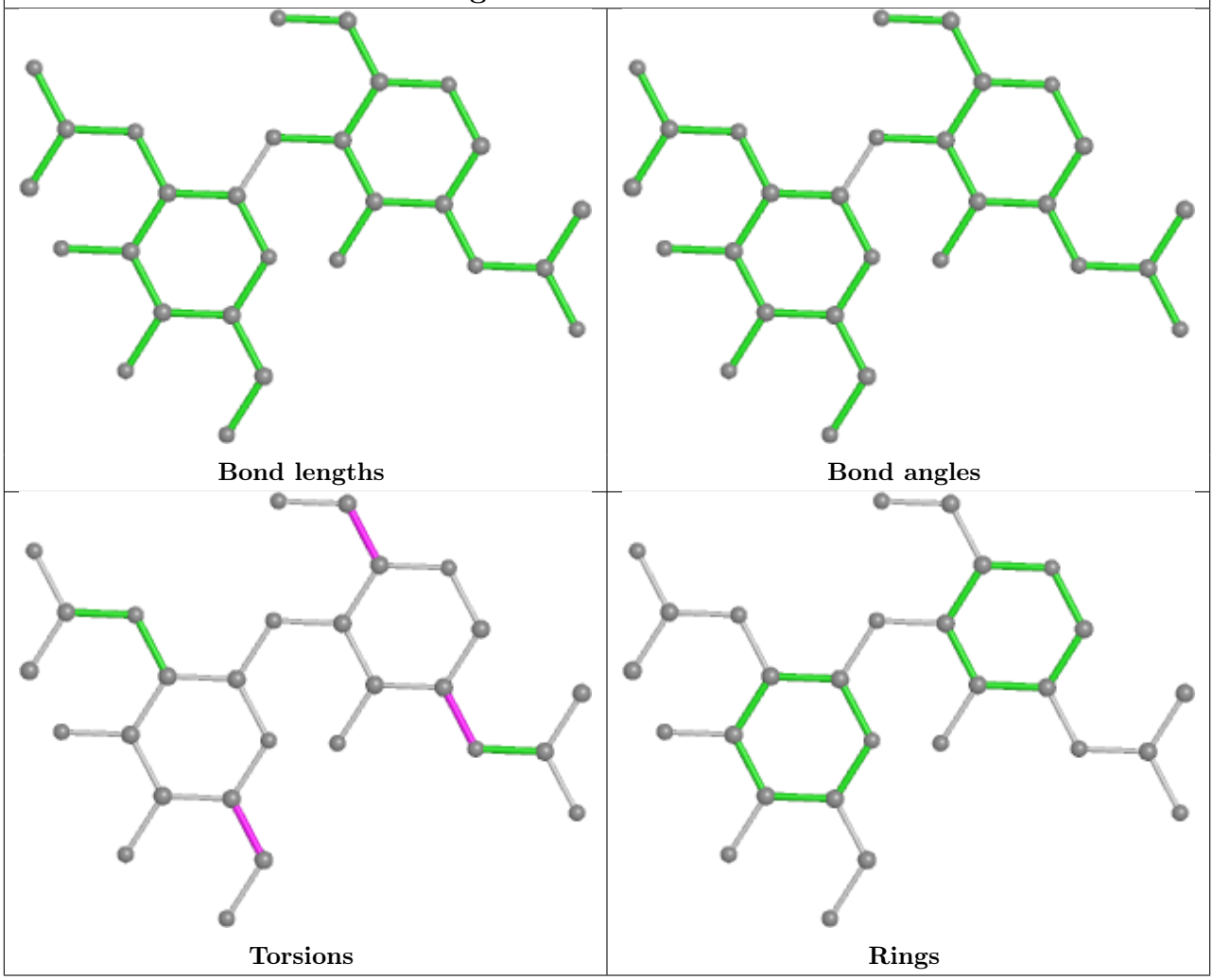
There are no ring outliers.

4 monomers are involved in 6 short contacts:

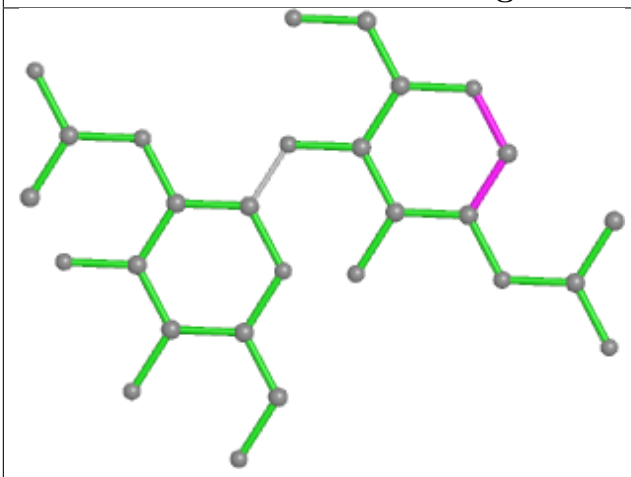
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	3	0
3	H	2	NAG	1	0
3	E	2	NAG	1	0
3	E	1	NAG	3	0

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

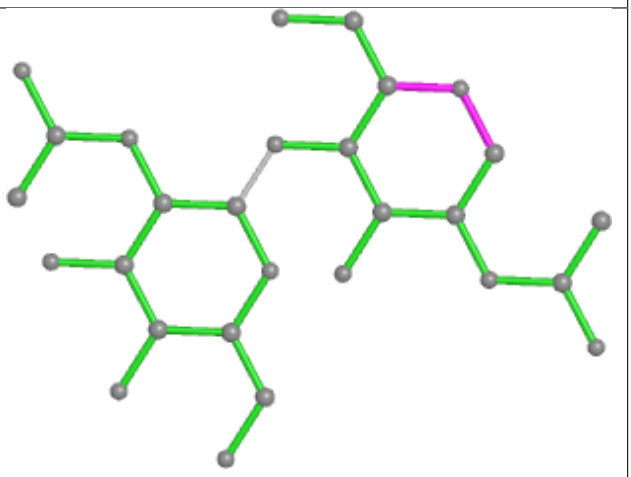
Oligosaccharide Chain E



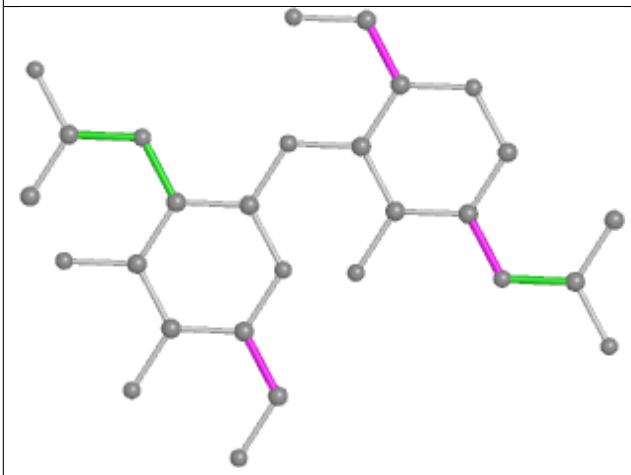
Oligosaccharide Chain F



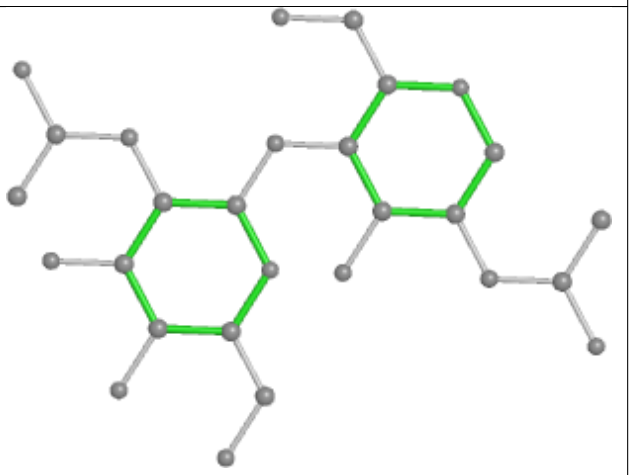
Bond lengths



Bond angles

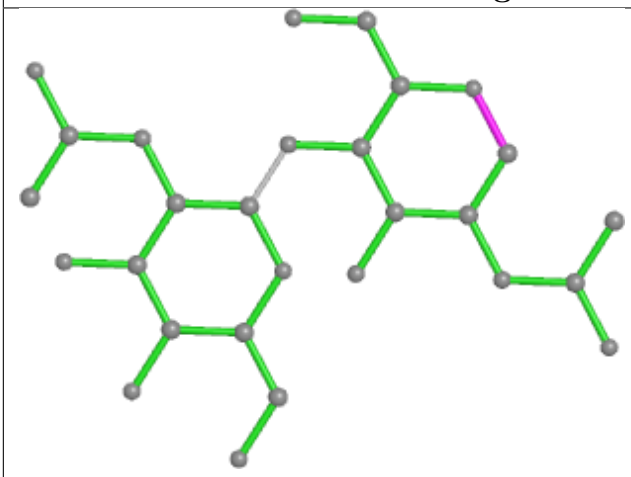


Torsions

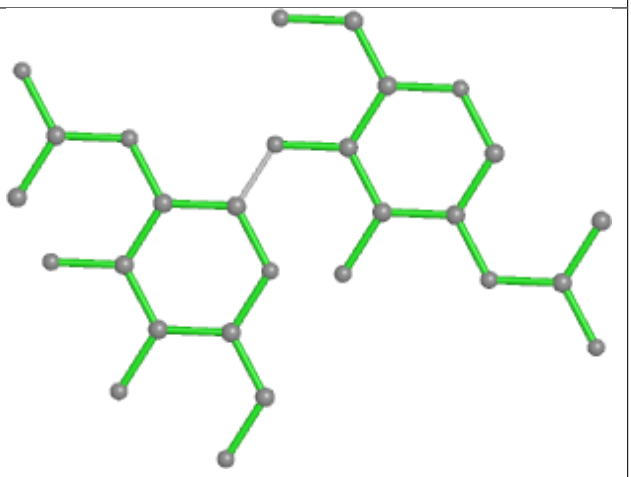


Rings

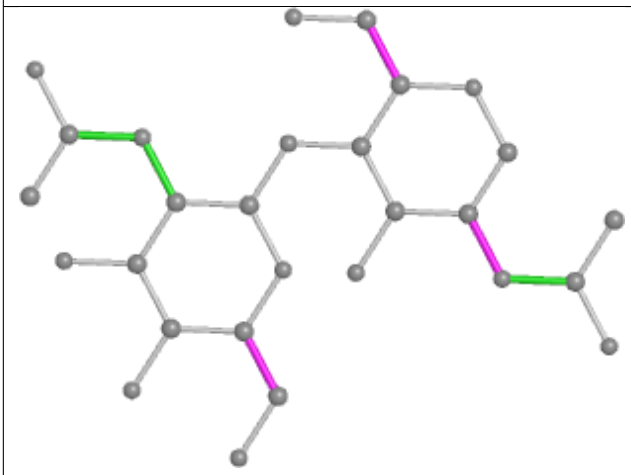
Oligosaccharide Chain G



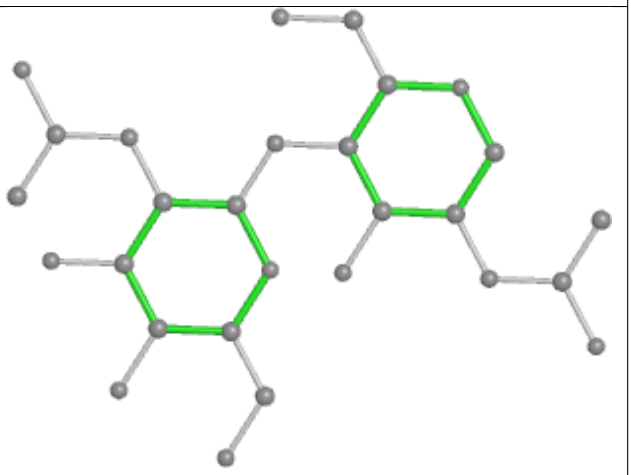
Bond lengths



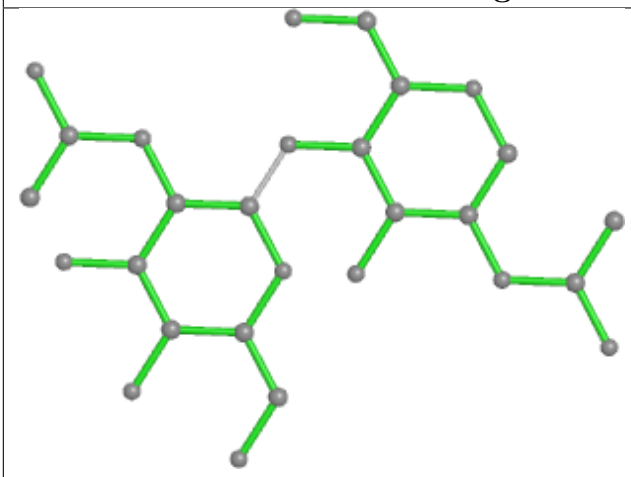
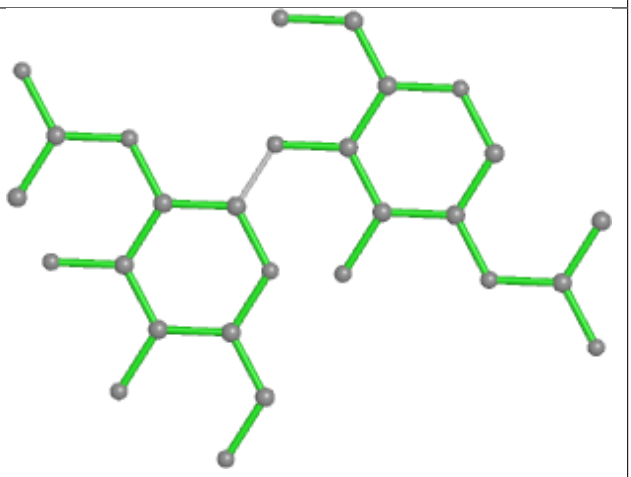
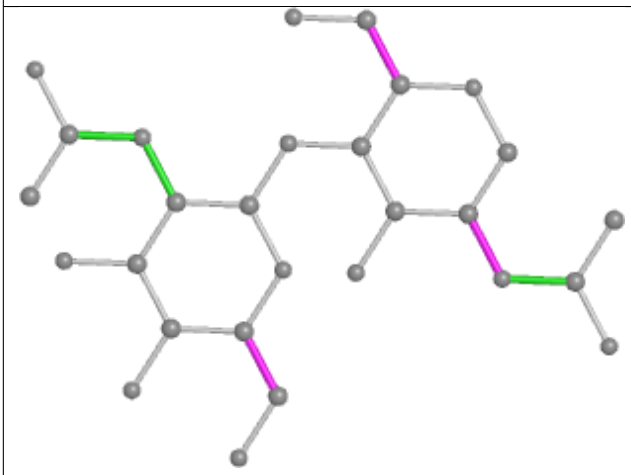
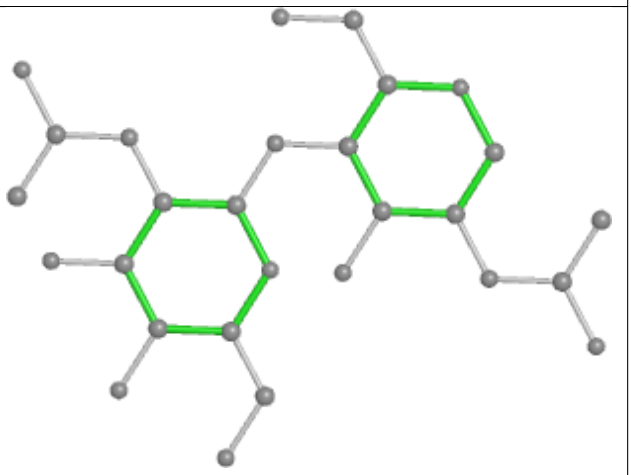
Bond angles



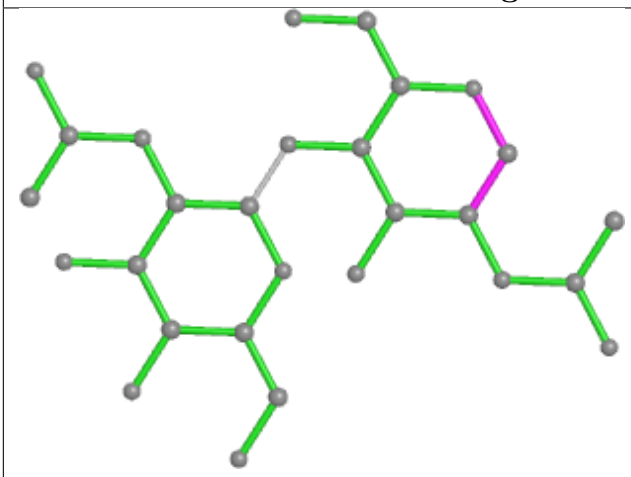
Torsions



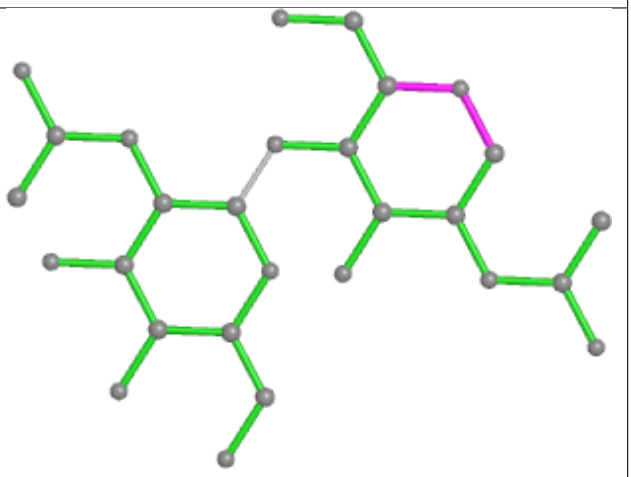
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

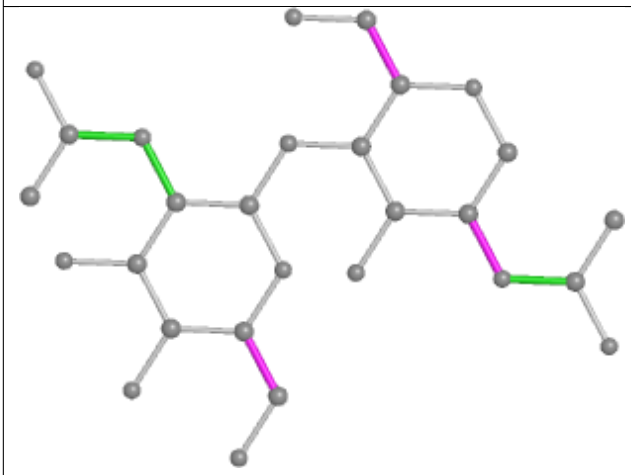
Oligosaccharide Chain I



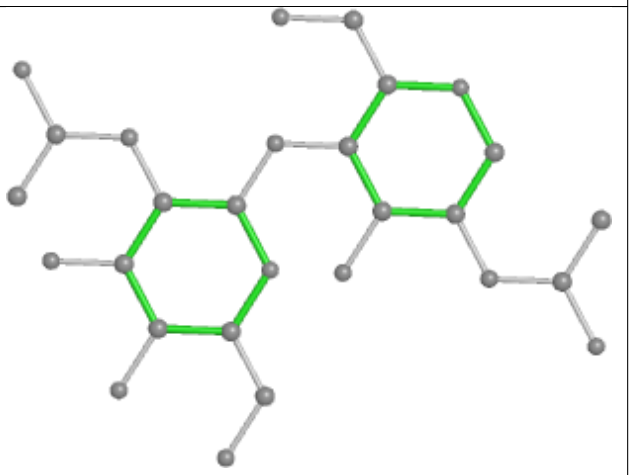
Bond lengths



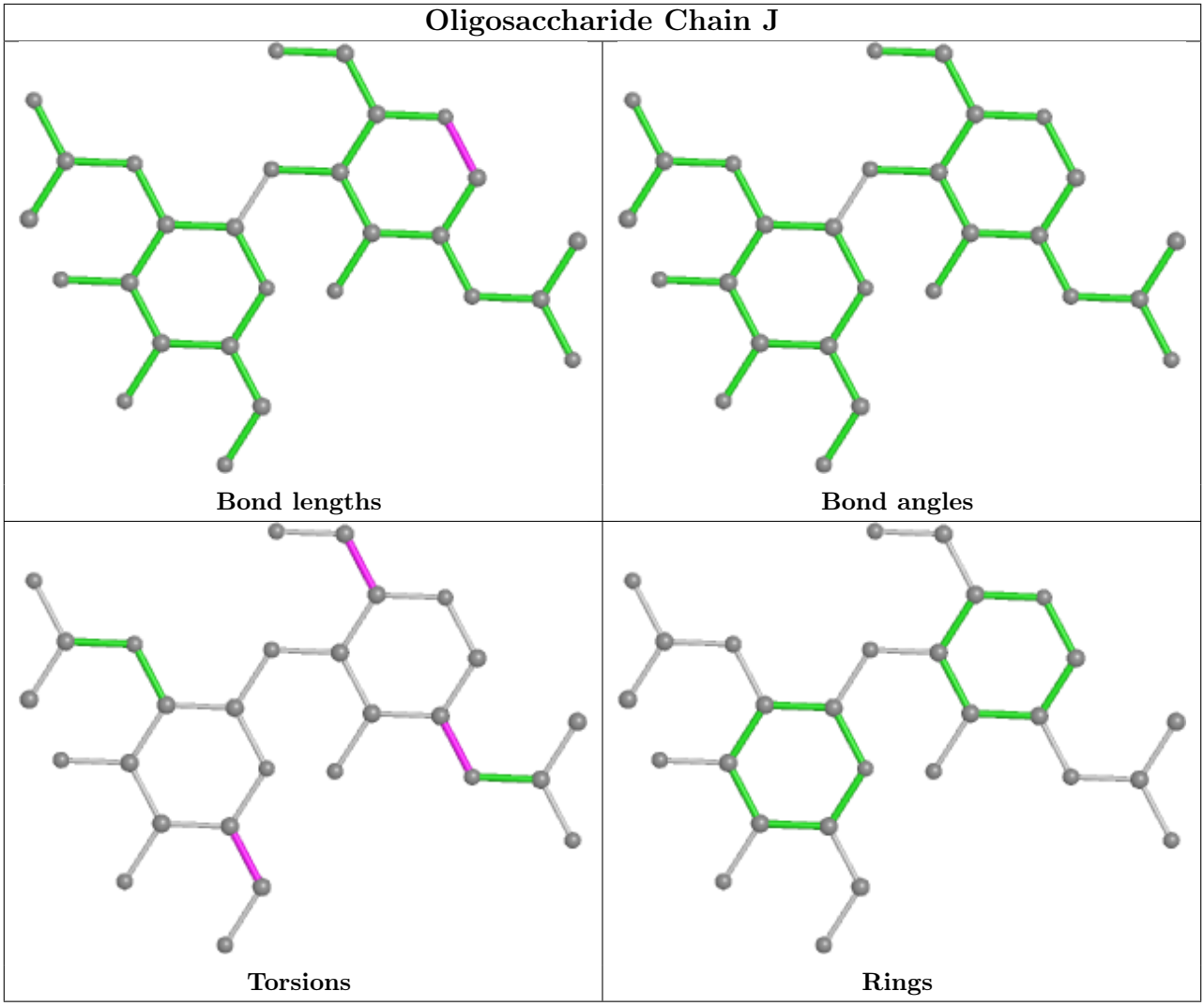
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

10 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	904	2	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	D	903	2	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	C	901	-	14,14,15	0.50	0	17,19,21	0.34	0
4	NAG	C	904	1	14,14,15	0.24	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	A	904	1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	B	904	2	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	A	905	1	14,14,15	0.36	0	17,19,21	0.35	0
4	NAG	B	903	2	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	A	901	-	14,14,15	0.49	0	17,19,21	0.35	0
4	NAG	C	905	1	14,14,15	0.36	0	17,19,21	0.35	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	904	2	-	2/6/23/26	0/1/1/1
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	901	-	-	0/6/23/26	0/1/1/1
4	NAG	C	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	904	1	-	1/6/23/26	0/1/1/1
4	NAG	B	904	2	-	2/6/23/26	0/1/1/1
4	NAG	A	905	1	-	1/6/23/26	0/1/1/1
4	NAG	B	903	2	-	2/6/23/26	0/1/1/1
4	NAG	A	901	-	-	0/6/23/26	0/1/1/1
4	NAG	C	905	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	903	NAG	O5-C5-C6-O6
4	D	903	NAG	O5-C5-C6-O6
4	B	903	NAG	C4-C5-C6-O6
4	B	904	NAG	C4-C5-C6-O6
4	D	903	NAG	C4-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	A	905	NAG	C1-C2-N2-C7
4	C	905	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	904	NAG	C1-C2-N2-C7
4	C	904	NAG	C1-C2-N2-C7
4	C	905	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

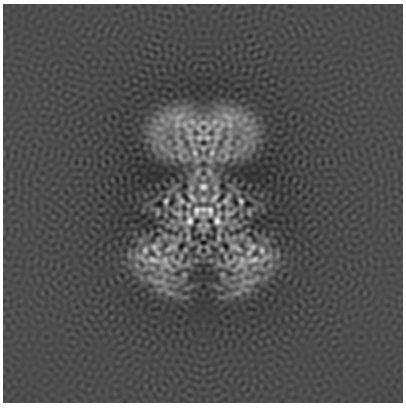
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7529. These allow visual inspection of the internal detail of the map and identification of artifacts.

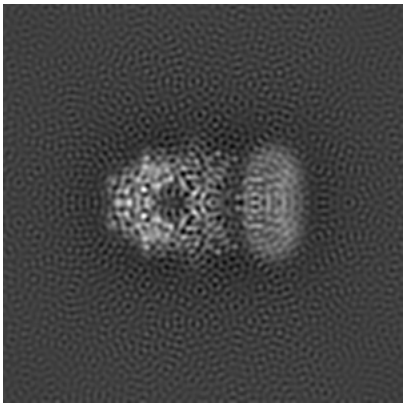
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

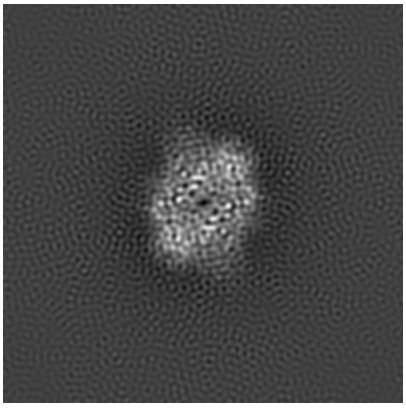
6.1.1 Primary map



X



Y

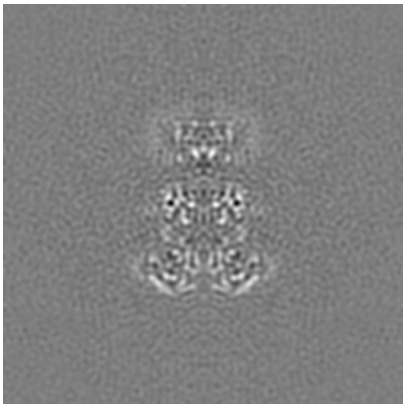


Z

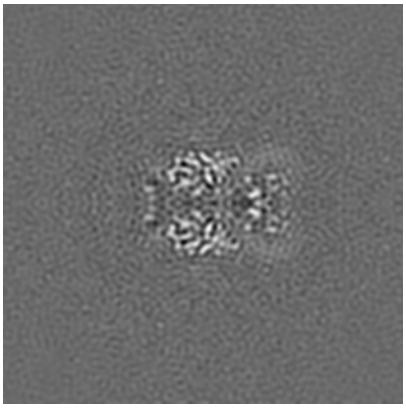
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

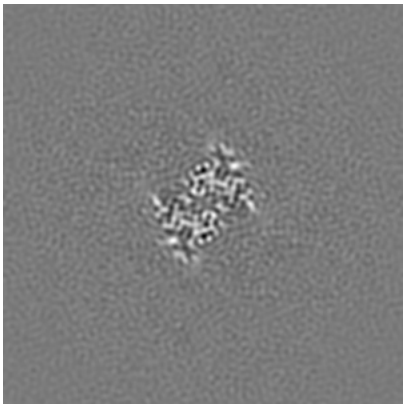
6.2.1 Primary map



X Index: 128



Y Index: 128

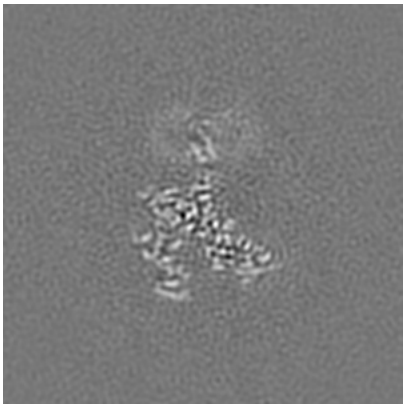


Z Index: 128

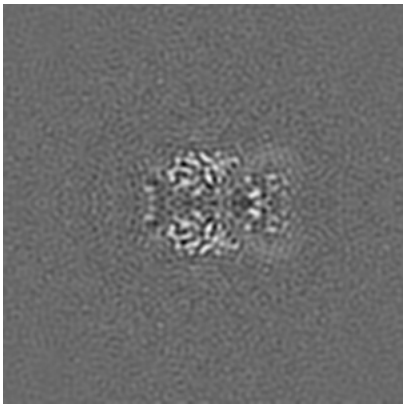
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

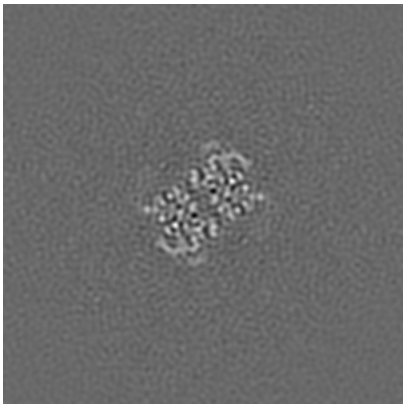
6.3.1 Primary map



X Index: 113



Y Index: 128

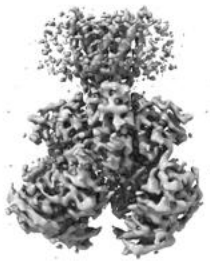


Z Index: 122

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 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

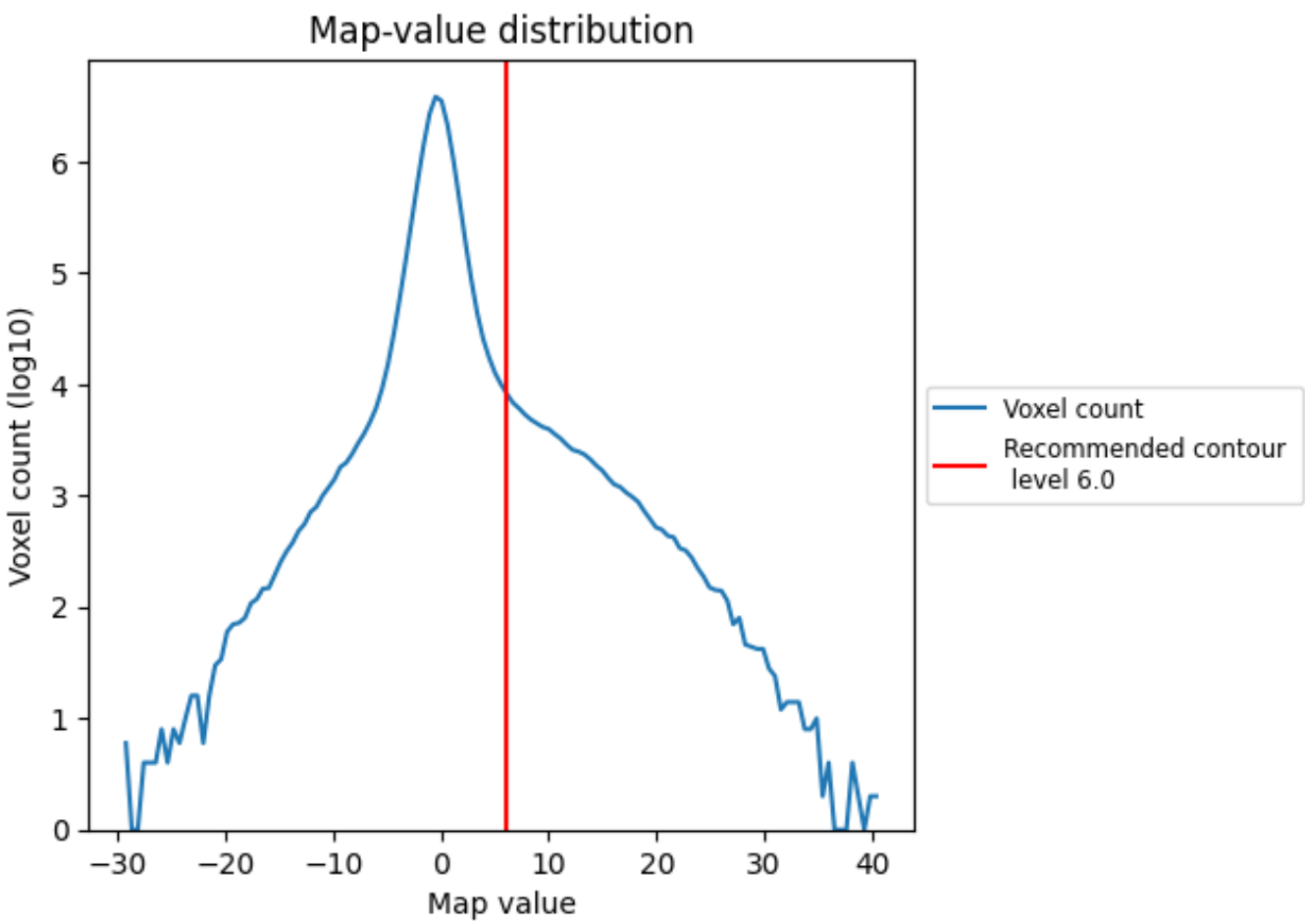
6.5 Mask visualisation (i)

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

7 Map analysis (i)

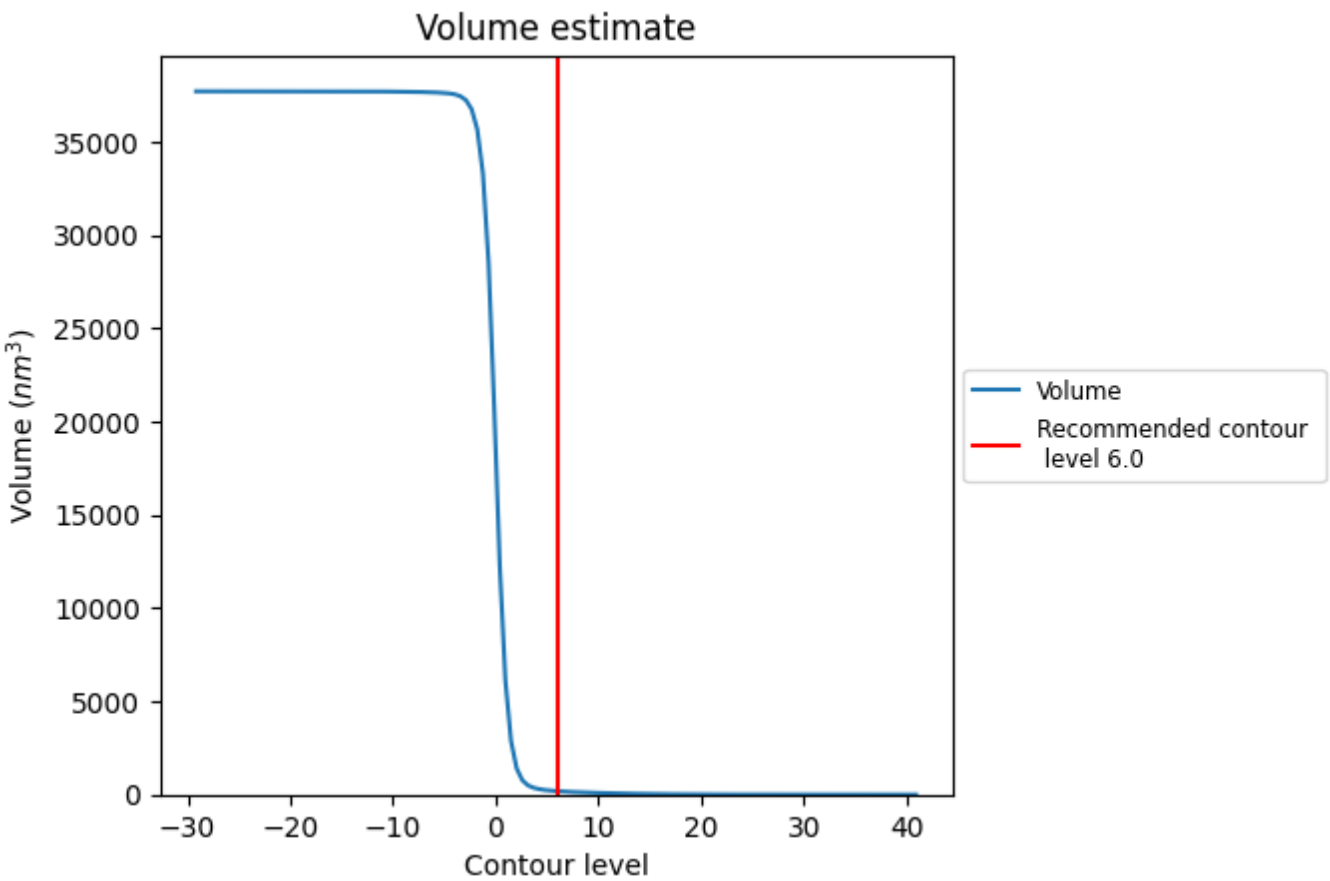
This section contains the results of statistical analysis of the map.

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.

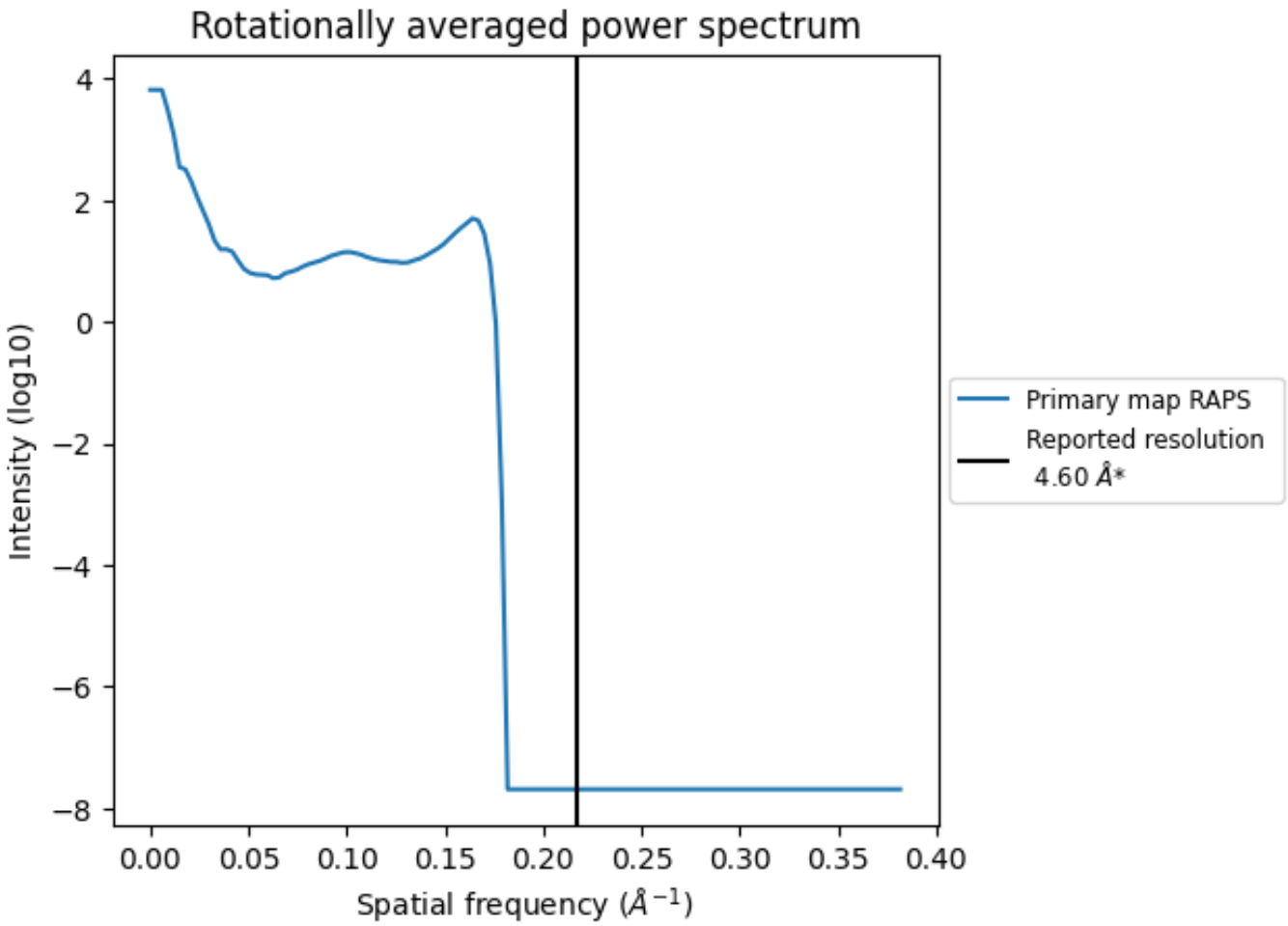
7.2 Volume estimate (i)



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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 0.217 Å^{-1}

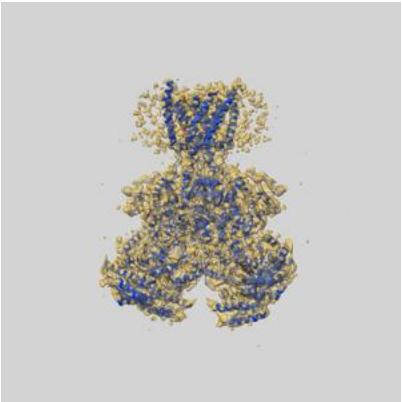
8 Fourier-Shell correlation (i)

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

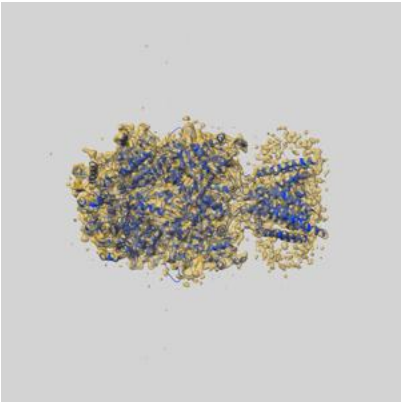
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7529 and PDB model 6CNA. Per-residue inclusion information can be found in section 3 on page 7.

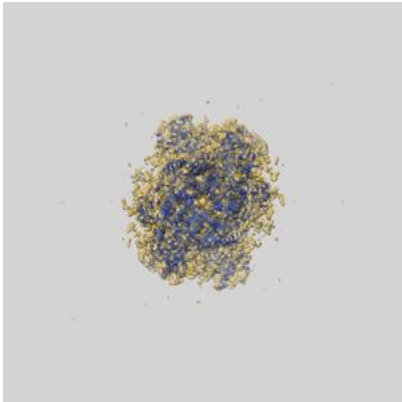
9.1 Map-model overlay (i)



X



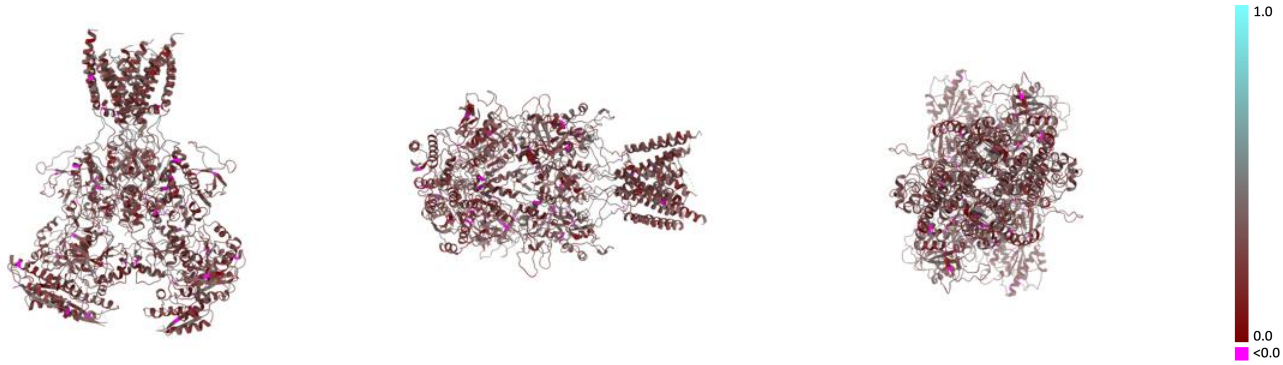
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

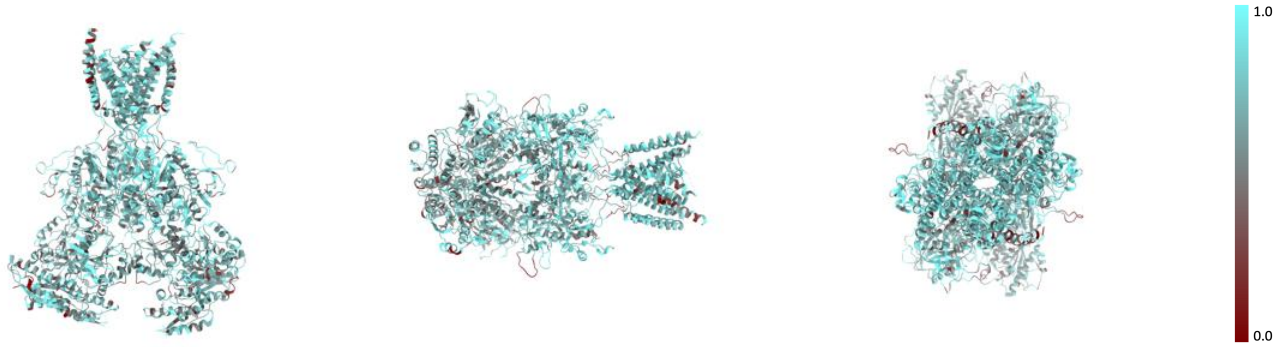
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

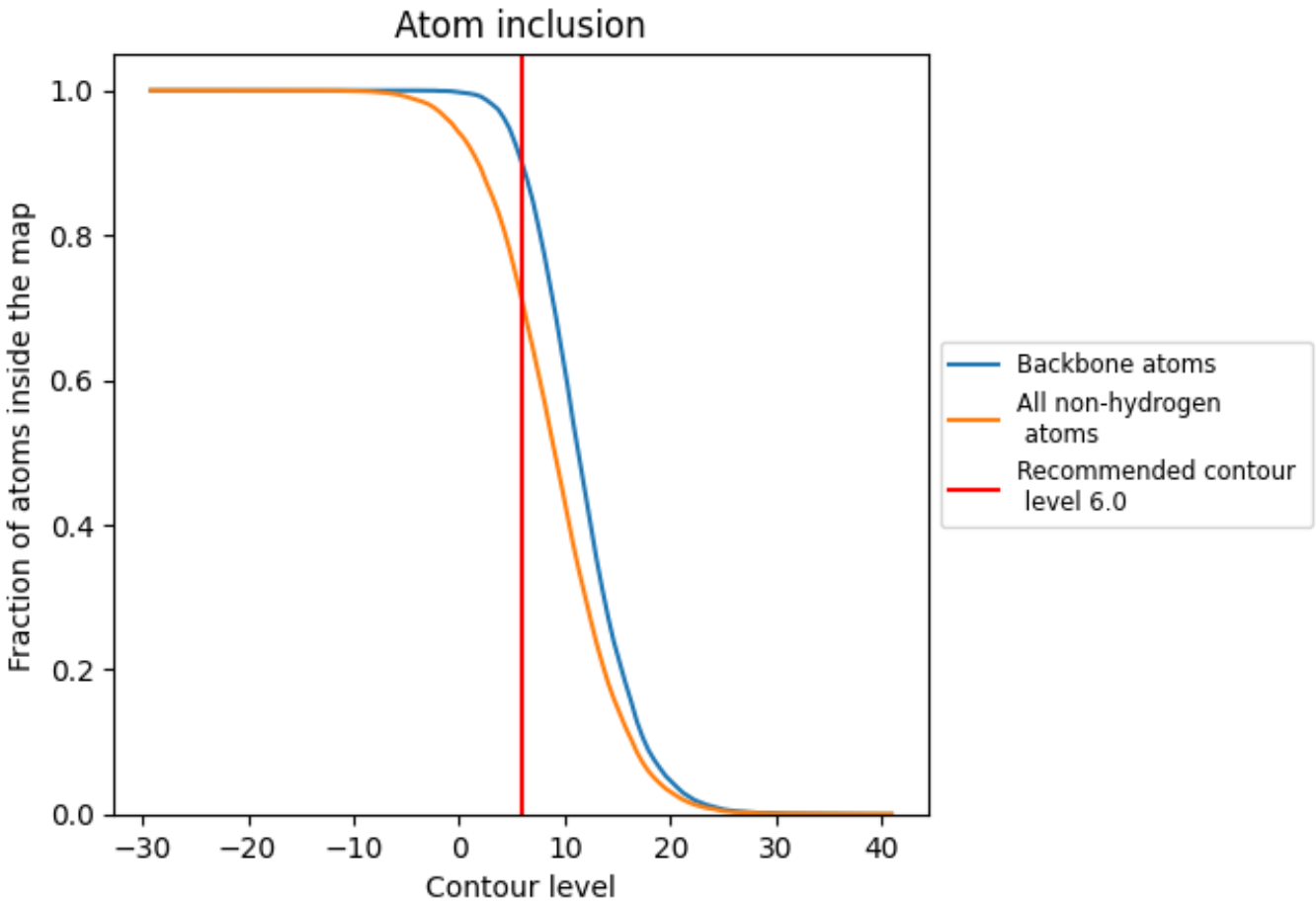
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7066	0.2960
A	0.7022	0.2930
B	0.7136	0.2970
C	0.7005	0.2950
D	0.7142	0.2960
E	0.5357	0.3890
F	0.6071	0.4870
G	0.6429	0.3900
H	0.5357	0.3980
I	0.6071	0.4900
J	0.6429	0.3930