



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 04:19 PM JST

PDB ID : 7F57  
EMDB ID : EMD-31460  
Title : Kainate-bound GluK2-1xNeto2 complex, at the desensitized state  
Authors : He, L.L.; Gao, Y.W.; Li, B.; Zhao, Y.  
Deposited on : 2021-06-21  
Resolution : 3.80 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:

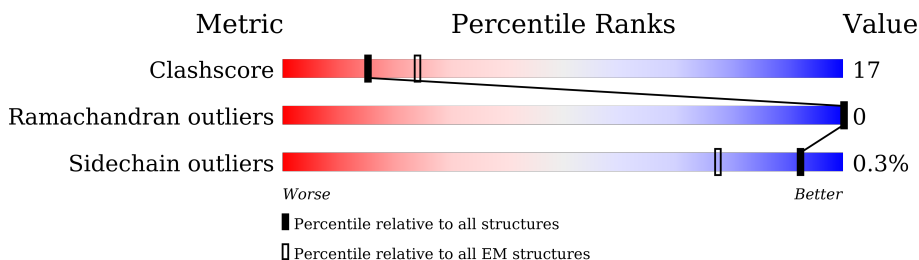
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.





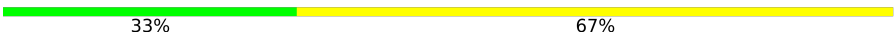
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	908	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">11% 57% 34% 8%</p>
1	B	908	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">14% 63% 29% 8%</p>
1	C	908	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">9% 59% 33% 8%</p>
1	D	908	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">12% 64% 26% 10%</p>
2	E	525	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">11% 14% 13% 72%</p>
3	F	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 10px;">33% 67%</p>
3	G	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 10px;">67% 33%</p>
3	H	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 10px;">33% 67%</p>

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Mol	Chain	Length	Quality of chain	
3	I	3	 33%	67%
3	J	3	 33%	67%
3	K	3	 33%	67%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	I	3	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27863 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, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	835	6614	4240	1102	1233	39	0	0
1	B	835	6611	4238	1102	1233	38	0	0
1	C	835	6611	4239	1102	1231	39	0	0
1	D	818	6467	4150	1077	1205	35	0	0

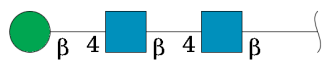
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	LEU	PHE	engineered mutation	UNP P42260
A	567	VAL	ILE	variant	UNP P42260
A	571	CYS	TYR	variant	UNP P42260
B	107	LEU	PHE	engineered mutation	UNP P42260
B	567	VAL	ILE	variant	UNP P42260
B	571	CYS	TYR	variant	UNP P42260
C	107	LEU	PHE	engineered mutation	UNP P42260
C	567	VAL	ILE	variant	UNP P42260
C	571	CYS	TYR	variant	UNP P42260
D	107	LEU	PHE	engineered mutation	UNP P42260
D	567	VAL	ILE	variant	UNP P42260
D	571	CYS	TYR	variant	UNP P42260

- Molecule 2 is a protein called Neuropilin and tolloid-like protein 2.

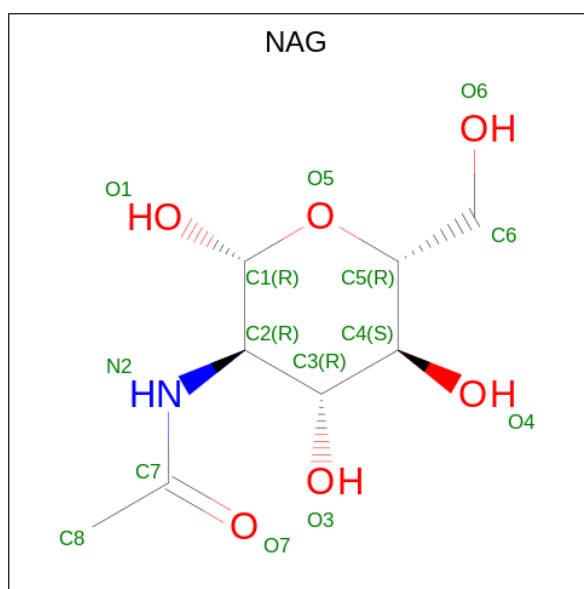
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	145	1172	760	199	207	6	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	Total	C	N	O	0
			56	32	4	20	
4	A	1	Total	C	N	O	0
			56	32	4	20	
4	A	1	Total	C	N	O	0
			56	32	4	20	

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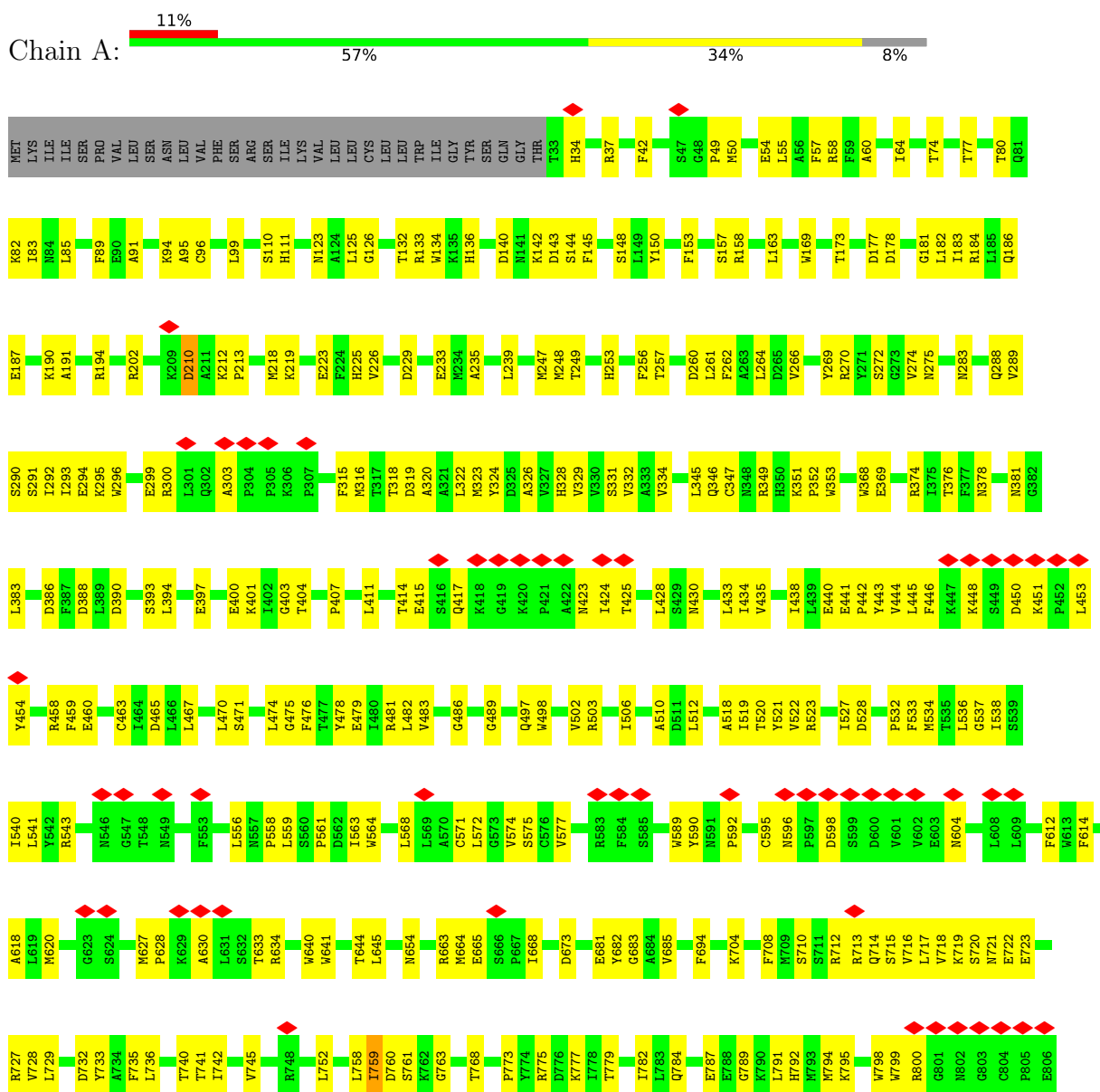
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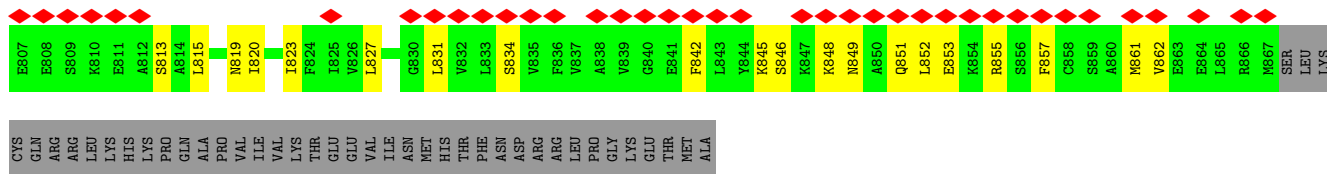
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
4	A	1	Total	C	N	O	0
			56	32	4	20	
4	B	1	Total	C	N	O	0
			28	16	2	10	
4	B	1	Total	C	N	O	0
			28	16	2	10	
4	C	1	Total	C	N	O	0
			42	24	3	15	
4	C	1	Total	C	N	O	0
			42	24	3	15	
4	C	1	Total	C	N	O	0
			42	24	3	15	
4	D	1	Total	C	N	O	0
			28	16	2	10	
4	D	1	Total	C	N	O	0
			28	16	2	10	

### 3 Residue-property plots

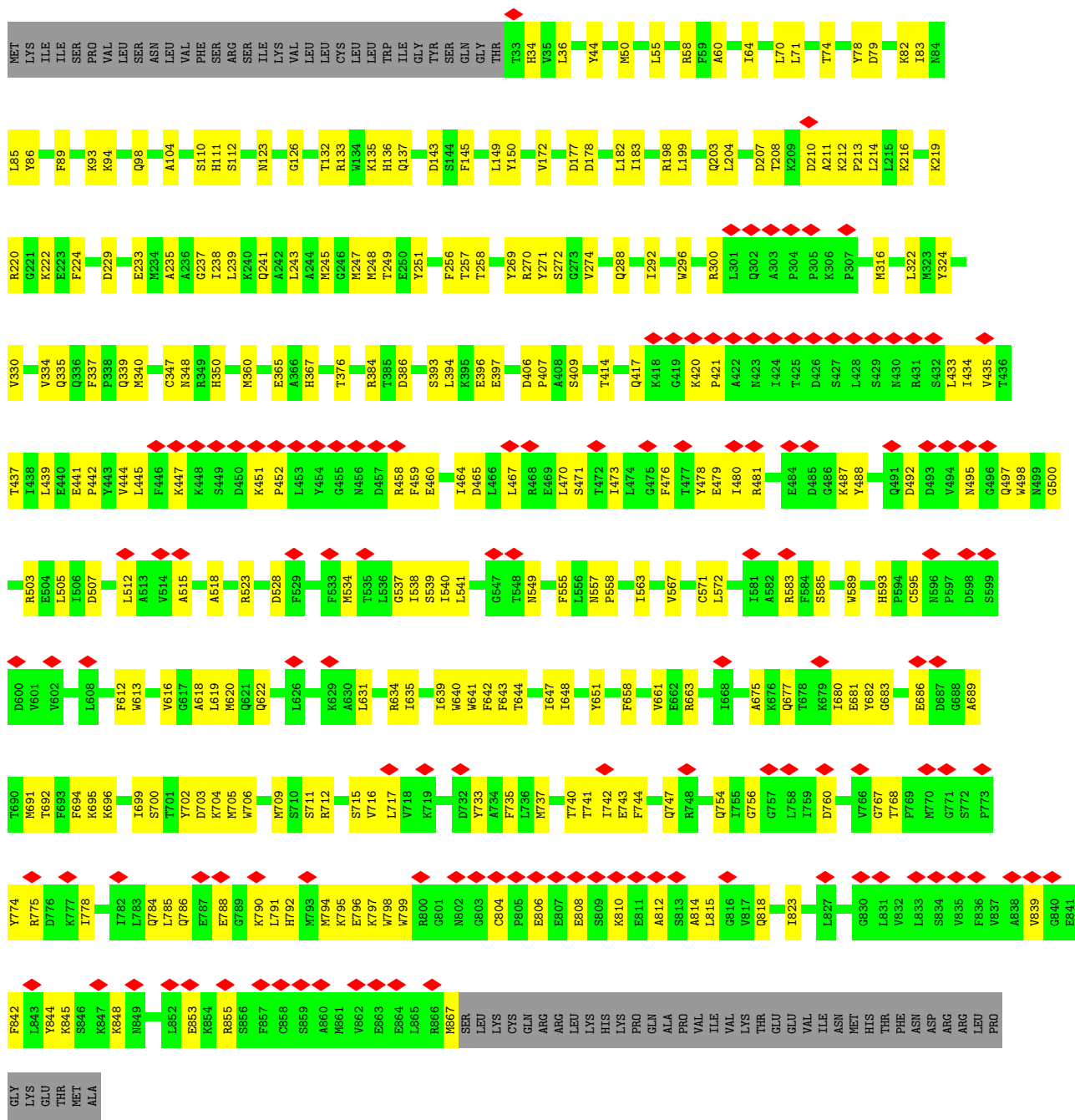
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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, kainate 2





• Molecule 1: Glutamate receptor ionotropic, kainate 2



• Molecule 1: Glutamate receptor ionotropic, kainate 2








MET  
ALA  
CYS  
LYS  
THR  
THR  
PHE  
ASN  
LYS  
THR  
THR  
PHE  
GLN  
GLU  
VAL  
PHE  
ASN  
PRO  
ASP  
PRO  
HIS  
TYR  
GLU  
LEU  
LEU  
PHE  
SER  
SER  
LEU  
ARG  
ASP  
PHE  
GLU  
LYS  
GLN  
GLU  
ILE  
SER  
ALA  
MET  
ASP  
THR  
PHE  
ASP  
LEU  
SER  
GLU  
PHE  
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LEU  
LYS  
ASP  
ASN  
TYR  
GLN  
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LYS  
ARG  
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SER  
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ALA  
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CYS  
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HIS  
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MET  
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GLU  
ASP

ASP  
ARG  
VAL  
MET  
GLU  
ILE  
PRO  
CYS  
ILE  
TYR  
VAL  
ARG  
GLY  
ASP  
ASP  
SER  
SER  
ALA  
GLN  
ALA  
SER  
ILE  
SER  
ILE  
PHE

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

Chain F:  33% 67%


MAG1  
MAG2  
BMA3

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

Chain G:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain H:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain I:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain J:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain K:  33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.621	Depositor
Minimum map value	-1.120	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.463	Depositor
Map size ( $\text{\AA}$ )	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/6763	0.55	0/9157
1	B	0.38	0/6760	0.51	0/9154
1	C	0.40	0/6760	0.54	0/9153
1	D	0.39	0/6615	0.53	0/8963
2	E	0.30	0/1204	0.51	0/1626
All	All	0.39	0/28102	0.53	0/38053

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6614	0	6593	260	0
1	B	6611	0	6587	204	0
1	C	6611	0	6590	237	0
1	D	6467	0	6440	199	0
2	E	1172	0	1165	71	0
3	F	39	0	34	0	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	39	0	34	0	0
3	J	39	0	34	0	0
3	K	39	0	34	0	0
4	A	56	0	52	0	0
4	B	28	0	26	0	0
4	C	42	0	39	1	0
4	D	28	0	26	0	0
All	All	27863	0	27722	922	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (922) 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:D:482:LEU:HD12	1:D:482:LEU:O	1.18	1.29
1:A:518:ALA:CB	1:A:520:THR:HG23	1.85	1.07
1:D:544:LYS:NZ	1:D:808:GLU:HG2	1.70	1.06
1:A:518:ALA:HB3	1:A:520:THR:HG23	1.38	1.06
1:D:482:LEU:O	1:D:482:LEU:CD1	2.06	1.02
1:A:519:ILE:HG23	1:A:763:GLY:O	1.63	0.98
1:C:138:VAL:HG11	1:D:111:HIS:CE1	2.03	0.93
1:A:664:MET:O	1:A:665:GLU:HG3	1.71	0.89
1:D:544:LYS:HZ1	1:D:808:GLU:HG2	1.28	0.89
1:C:424:ILE:HG22	1:C:427:SER:O	1.75	0.87
1:B:806:GLU:HG2	1:B:808:GLU:H	1.40	0.86
1:D:804:CYS:SG	1:D:805:PRO:HD2	2.17	0.85
1:C:433:LEU:HD21	1:C:511:ASP:HB2	1.60	0.84
1:B:528:ASP:HB3	1:B:768:THR:HG23	1.58	0.83
1:A:54:GLU:OE1	1:A:82:LYS:HE3	1.80	0.81
1:C:610:ASN:HB3	1:C:626:LEU:HD11	1.62	0.81
1:A:518:ALA:HB3	1:A:520:THR:CG2	2.11	0.80
1:A:533:PHE:HB3	1:A:782:ILE:HD11	1.61	0.80
1:B:177:ASP:OD1	1:B:178:ASP:N	2.15	0.80
1:D:536:LEU:HD11	1:D:738:GLU:HB3	1.64	0.79
1:D:34:HIS:HB3	1:D:74:THR:HA	1.65	0.79
1:C:687:ASP:H	1:C:691:MET:HE2	1.47	0.79
1:B:683:GLY:HA2	1:B:716:VAL:HG13	1.66	0.78
1:C:483:VAL:HG12	1:C:486:GLY:H	1.47	0.78
1:A:414:THR:HG23	1:A:414:THR:O	1.83	0.77
1:D:544:LYS:HE3	1:D:808:GLU:CD	2.04	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:ARG:O	1:C:714:GLN:HG3	1.84	0.77
1:C:262:PHE:CE2	1:C:280:ARG:HD3	2.20	0.76
1:B:123:ASN:ND2	1:B:143:ASP:OD1	2.20	0.75
1:B:619:LEU:HD23	1:B:644:THR:HG22	1.66	0.75
1:A:440:GLU:HB2	1:A:443:TYR:HB2	1.67	0.75
1:D:676:LYS:HE3	1:D:704:LYS:NZ	2.02	0.75
1:B:136:HIS:HD2	1:B:183:ILE:HG21	1.51	0.75
1:C:44:TYR:CE1	1:C:82:LYS:HB3	2.22	0.75
2:E:73:ILE:HD13	2:E:140:LYS:HG3	1.68	0.74
1:D:628:PRO:HB3	1:D:633:THR:HG23	1.70	0.74
2:E:50:ARG:HG2	2:E:51:THR:HG23	1.70	0.74
1:D:169:TRP:HZ2	1:D:253:HIS:HD2	1.33	0.74
1:C:558:PRO:HG3	1:C:655:LEU:HD12	1.69	0.74
1:D:439:LEU:CD2	1:D:482:LEU:HD22	2.18	0.73
1:A:714:GLN:HA	1:A:717:LEU:HB2	1.71	0.73
1:C:36:LEU:HD11	1:C:104:ALA:HB2	1.69	0.73
1:D:540:ILE:HD13	1:D:736:LEU:HD21	1.69	0.73
1:B:248:MET:HG3	1:B:274:VAL:HG21	1.70	0.73
1:A:518:ALA:HB1	1:A:520:THR:HG23	1.68	0.73
1:A:83:ILE:HD13	1:A:91:ALA:HA	1.70	0.73
1:C:58:ARG:NH1	1:C:78:TYR:OH	2.21	0.73
1:C:728:VAL:HG22	1:C:733:TYR:HB3	1.71	0.73
1:B:406:ASP:OD1	1:B:409:SER:N	2.23	0.72
1:D:240:LYS:NZ	1:D:308:ASP:O	2.21	0.72
1:C:679:LYS:HE3	1:D:670:SER:OG	1.90	0.72
1:D:542:TYR:HB3	1:D:755:ILE:HD13	1.72	0.72
1:A:239:LEU:HD21	1:A:256:PHE:HZ	1.56	0.71
1:A:415:GLU:OE2	1:A:417:GLN:NE2	2.23	0.70
1:B:50:MET:SD	1:B:55:LEU:HG	2.31	0.70
1:C:138:VAL:HG11	1:D:111:HIS:HE1	1.53	0.70
1:D:169:TRP:CZ2	1:D:253:HIS:HD2	2.10	0.70
1:B:270:ARG:NH1	1:B:396:GLU:O	2.26	0.69
1:D:435:VAL:HG11	1:D:467:LEU:HD11	1.73	0.69
1:B:386:ASP:HA	1:B:407:PRO:HG2	1.75	0.69
1:B:470:LEU:HD21	1:B:778:ILE:HD11	1.75	0.69
1:A:518:ALA:CB	1:A:520:THR:CG2	2.67	0.68
1:D:126:GLY:HA2	1:D:145:PHE:CE2	2.29	0.68
1:D:528:ASP:OD1	1:D:775:ARG:NE	2.26	0.68
1:D:561:PRO:HA	1:D:564:TRP:HD1	1.57	0.68
1:C:140:ASP:H	1:D:86:TYR:HE2	1.42	0.68
1:B:337:PHE:HD2	1:B:340:MET:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:CYS:SG	1:D:805:PRO:CD	2.82	0.67
1:D:58:ARG:NH1	1:D:78:TYR:OH	2.28	0.67
2:E:85:GLU:HG2	2:E:157:SER:HB2	1.77	0.66
1:C:563:ILE:O	1:C:567:VAL:N	2.26	0.66
2:E:90:GLU:HB2	2:E:126:SER:HB2	1.76	0.66
1:B:518:ALA:HB3	1:B:523:ARG:HD2	1.78	0.66
1:A:50:MET:CE	1:A:55:LEU:HD13	2.26	0.66
1:A:438:ILE:HG12	1:A:483:VAL:HG11	1.78	0.66
1:B:445:LEU:N	1:B:460:GLU:O	2.30	0.65
1:D:440:GLU:HB3	1:D:443:TYR:HD2	1.61	0.65
1:C:712:ARG:HB3	1:C:715:SER:HB2	1.77	0.65
1:D:489:GLY:HA3	1:D:502:VAL:HG23	1.79	0.65
1:B:549:ASN:O	1:B:818:GLN:NE2	2.30	0.65
1:B:658:PHE:HE1	1:C:815:LEU:HD22	1.62	0.65
1:C:126:GLY:HA2	1:C:145:PHE:HE2	1.61	0.65
1:D:544:LYS:HZ2	1:D:808:GLU:HG2	1.60	0.64
1:A:823:ILE:O	1:A:827:LEU:N	2.24	0.64
1:C:540:ILE:HG22	1:C:736:LEU:HG	1.77	0.64
2:E:77:GLU:HG3	2:E:136:PHE:HE1	1.61	0.64
1:C:424:ILE:CG2	1:C:427:SER:O	2.44	0.64
1:A:54:GLU:CD	1:A:82:LYS:HE3	2.18	0.64
1:A:851:GLN:HG3	1:A:852:LEU:H	1.63	0.64
1:B:518:ALA:H	1:B:523:ARG:HH11	1.45	0.64
1:D:538:ILE:HG13	1:D:759:ILE:HB	1.80	0.64
1:C:220:ARG:HG3	2:E:102:PHE:CE1	2.33	0.64
1:A:319:ASP:OD1	1:A:320:ALA:N	2.31	0.64
1:D:249:THR:HG1	1:D:251:TYR:HD2	1.46	0.63
1:A:49:PRO:HG2	1:A:303:ALA:HB1	1.79	0.63
1:D:81:GLN:HG2	1:D:98:GLN:HE21	1.63	0.63
1:B:497:GLN:OE1	1:B:503:ARG:NE	2.31	0.63
2:E:87:THR:O	2:E:155:LYS:N	2.30	0.63
1:A:441:GLU:HB2	1:A:442:PRO:HD3	1.80	0.63
1:C:331:SER:HA	1:C:334:VAL:HG12	1.79	0.63
1:A:489:GLY:O	1:A:523:ARG:NH2	2.32	0.63
1:B:639:ILE:HD11	1:C:826:VAL:HG12	1.80	0.63
1:A:543:ARG:HD3	1:A:729:LEU:HD13	1.81	0.62
1:C:694:PHE:HB3	1:C:706:TRP:HB2	1.81	0.62
1:A:712:ARG:HG3	1:A:716:VAL:HG22	1.81	0.62
1:B:207:ASP:OD1	1:B:208:THR:N	2.32	0.62
1:C:177:ASP:OD1	1:C:178:ASP:N	2.31	0.62
2:E:362:LEU:O	2:E:366:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ARG:HD2	1:A:715:SER:HB2	1.80	0.62
1:A:543:ARG:HD3	1:A:729:LEU:HA	1.80	0.62
2:E:70:LYS:H	2:E:143:SER:HB2	1.64	0.62
1:D:544:LYS:HE3	1:D:808:GLU:OE2	1.99	0.62
1:A:819:ASN:OD1	1:A:819:ASN:O	2.18	0.61
1:D:537:GLY:HA3	1:D:758:LEU:HD11	1.82	0.61
1:B:487:LYS:HG3	1:B:488:TYR:H	1.65	0.61
1:C:300:ARG:O	1:C:300:ARG:NH1	2.30	0.61
1:D:677:GLN:NE2	1:D:679:LYS:HB3	2.14	0.61
2:E:107:VAL:HG12	2:E:118:ILE:HD12	1.81	0.61
1:C:538:ILE:HG13	1:C:759:ILE:HB	1.81	0.61
1:C:639:ILE:HG21	1:D:830:GLY:HA3	1.81	0.61
1:A:465:ASP:OD2	1:A:798:TRP:NE1	2.34	0.61
1:A:498:TRP:HH2	1:A:522:VAL:HG23	1.66	0.61
1:B:473:ILE:HD11	1:B:785:LEU:HD21	1.82	0.61
1:C:43:GLU:OE2	1:C:86:TYR:N	2.26	0.61
1:C:84:ASN:OD1	1:C:85:LEU:N	2.34	0.61
1:A:349:ARG:NH1	1:A:351:LYS:O	2.34	0.61
1:B:435:VAL:HG13	1:B:480:ILE:HG22	1.83	0.61
1:B:686:GLU:HG2	1:B:717:LEU:HD12	1.82	0.61
1:A:654:ASN:OD1	1:B:663:ARG:NH2	2.34	0.61
2:E:88:PHE:CE2	2:E:127:PRO:HD2	2.35	0.60
1:C:720:SER:HB2	1:C:723:GLU:HG3	1.83	0.60
1:C:691:MET:HA	1:C:694:PHE:HD2	1.65	0.60
1:D:523:ARG:HB3	1:D:527:ILE:HD12	1.82	0.60
1:D:528:ASP:OD2	1:D:775:ARG:NH2	2.29	0.60
1:A:815:LEU:HD22	1:A:819:ASN:ND2	2.16	0.60
1:A:853:GLU:OE2	1:A:855:ARG:NH1	2.34	0.60
1:B:296:TRP:HE1	1:B:300:ARG:HH11	1.50	0.60
1:B:439:LEU:HD12	1:B:444:VAL:HG23	1.84	0.60
1:A:434:ILE:HG23	1:A:510:ALA:HA	1.84	0.60
1:C:337:PHE:HD2	1:C:340:MET:HB2	1.65	0.60
1:C:628:PRO:HB2	1:C:634:ARG:HG3	1.84	0.60
1:C:36:LEU:O	1:C:77:THR:N	2.34	0.60
1:A:575:SER:HB2	1:A:612:PHE:HA	1.83	0.59
1:A:773:PRO:O	1:A:777:LYS:NZ	2.35	0.59
1:C:248:MET:HE3	1:C:274:VAL:HG11	1.82	0.59
1:B:528:ASP:OD2	1:B:775:ARG:NH1	2.35	0.59
1:C:44:TYR:CE2	1:C:46:GLU:HA	2.37	0.59
2:E:363:ILE:HA	2:E:366:ILE:HD12	1.83	0.59
1:C:563:ILE:HG22	1:C:567:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:ILE:HD11	1:C:825:ILE:HB	1.84	0.59
1:A:50:MET:HE3	1:A:55:LEU:HD13	1.84	0.59
1:B:794:MET:O	1:B:797:LYS:HG2	2.03	0.59
1:B:788:GLU:HB3	1:B:790:LYS:HG3	1.85	0.59
1:C:846:SER:HA	1:C:850:ALA:HB3	1.85	0.59
1:D:674:LEU:HD12	1:D:682:TYR:HD2	1.68	0.59
2:E:86:LEU:O	2:E:131:ARG:NH2	2.35	0.59
1:C:262:PHE:HE2	1:C:280:ARG:HD3	1.65	0.58
1:A:253:HIS:CD2	1:A:275:ASN:HB2	2.39	0.58
1:B:296:TRP:CZ2	1:B:300:ARG:HD3	2.38	0.58
1:B:692:THR:O	1:B:696:LYS:NZ	2.36	0.58
1:C:34:HIS:HB3	1:C:74:THR:HG23	1.85	0.58
1:C:544:LYS:N	1:C:751:ASN:O	2.33	0.58
1:D:676:LYS:HE3	1:D:704:LYS:HZ3	1.68	0.58
1:A:628:PRO:HB2	1:A:634:ARG:HG3	1.84	0.58
1:C:747:GLN:NE2	1:C:803:GLY:O	2.36	0.58
1:A:441:GLU:OE2	1:A:721:ASN:ND2	2.35	0.58
1:C:260:ASP:CG	1:C:318:THR:H	2.06	0.58
1:D:434:ILE:N	1:D:511:ASP:OD2	2.28	0.58
1:B:337:PHE:CD2	1:B:340:MET:HB2	2.38	0.58
1:A:497:GLN:NE2	1:A:503:ARG:HD2	2.19	0.58
1:C:128:PRO:HG2	1:C:359:PHE:HD2	1.69	0.58
1:C:646:ILE:HD13	1:D:823:ILE:HD11	1.85	0.58
1:C:248:MET:CE	1:C:274:VAL:HG11	2.34	0.57
1:A:34:HIS:H	1:A:74:THR:HA	1.70	0.57
1:A:182:LEU:HD23	1:B:182:LEU:HD22	1.87	0.57
1:D:471:SER:O	1:D:475:GLY:N	2.36	0.57
1:A:760:ASP:OD1	1:A:761:SER:N	2.37	0.57
1:B:703:ASP:OD1	1:B:704:LYS:N	2.36	0.57
1:C:589:TRP:HE3	1:C:603:GLU:HA	1.70	0.57
1:D:465:ASP:OD1	1:D:466:LEU:N	2.38	0.57
1:D:87:ASP:OD1	1:D:88:SER:N	2.37	0.57
1:D:531:LYS:H	1:D:779:THR:HG22	1.70	0.57
1:A:42:PHE:HE1	1:A:323:MET:HE1	1.69	0.57
1:D:44:TYR:HB2	1:D:82:LYS:HB3	1.87	0.57
1:A:641:TRP:HB3	1:B:620:MET:HG2	1.85	0.57
1:B:36:LEU:HD11	1:B:104:ALA:HB2	1.86	0.57
1:B:810:LYS:HG3	1:B:812:ALA:H	1.70	0.57
1:C:140:ASP:HB2	1:D:86:TYR:CE2	2.40	0.57
1:D:233:GLU:OE1	1:D:233:GLU:N	2.35	0.57
1:A:249:THR:O	1:A:274:VAL:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:HD12	1:B:70:LEU:HD23	1.86	0.56
1:C:184:ARG:NH1	1:C:229:ASP:OD1	2.37	0.56
1:D:519:ILE:HD11	1:D:765:GLY:HA3	1.87	0.56
1:A:126:GLY:HA2	1:A:145:PHE:HE2	1.70	0.56
1:A:191:ALA:HA	1:A:194:ARG:HH21	1.70	0.56
1:A:722:GLU:N	1:A:722:GLU:OE1	2.38	0.56
1:C:123:ASN:ND2	1:C:143:ASP:HA	2.21	0.56
1:C:586:PRO:HG2	1:C:587:TYR:HD1	1.70	0.56
1:A:483:VAL:HG22	1:A:486:GLY:H	1.70	0.56
1:B:563:ILE:HD11	1:C:817:VAL:HA	1.87	0.56
2:E:77:GLU:HG3	2:E:136:PHE:CE1	2.40	0.56
1:B:229:ASP:HA	1:B:257:THR:HG22	1.87	0.56
1:A:714:GLN:OE1	1:A:719:LYS:NZ	2.28	0.56
1:A:831:LEU:HD11	1:D:577:VAL:HG11	1.86	0.56
1:B:135:LYS:NZ	1:B:137:GLN:OE1	2.37	0.56
1:B:145:PHE:CD1	1:B:360:MET:HG2	2.41	0.56
1:D:300:ARG:HH12	1:D:315:PHE:C	2.09	0.56
1:B:754:GLN:NE2	1:B:756:GLY:O	2.38	0.56
1:D:846:SER:O	1:D:850:ALA:N	2.34	0.56
1:A:683:GLY:O	1:A:736:LEU:N	2.38	0.56
1:C:539:SER:OG	1:C:754:GLN:OE1	2.24	0.56
2:E:148:GLU:OE2	2:E:148:GLU:N	2.39	0.56
1:B:487:LYS:H	1:B:500:GLY:HA2	1.71	0.56
1:C:267:GLU:HB3	1:C:268:PRO:HD3	1.88	0.56
1:B:786:GLN:HB2	1:B:791:LEU:HD12	1.87	0.55
1:D:607:THR:H	1:D:610:ASN:HB2	1.70	0.55
1:A:349:ARG:NH1	1:A:352:PRO:O	2.39	0.55
1:C:558:PRO:HG2	1:C:651:TYR:CE1	2.42	0.55
1:D:169:TRP:HZ2	1:D:253:HIS:CD2	2.21	0.55
1:D:583:ARG:HD3	1:D:589:TRP:HZ2	1.72	0.55
1:B:136:HIS:CD2	1:B:183:ILE:HG21	2.39	0.55
1:B:663:ARG:CZ	1:B:814:ALA:HB1	2.36	0.55
1:B:492:ASP:HB2	1:B:497:GLN:HB3	1.88	0.55
1:B:661:VAL:HG21	1:C:663:ARG:HH11	1.71	0.55
1:C:153:PHE:HA	1:C:156:LEU:HB2	1.87	0.55
1:C:521:TYR:HB3	1:C:696:LYS:HE2	1.88	0.55
1:D:433:LEU:HD21	1:D:774:TYR:CZ	2.42	0.55
1:B:467:LEU:HD11	1:B:476:PHE:HZ	1.71	0.55
1:B:618:ALA:HB3	1:B:640:TRP:HE1	1.70	0.55
1:D:210:ASP:O	1:D:213:PRO:HD2	2.06	0.55
1:D:432:SER:HA	1:D:477:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:VAL:HG22	1:B:643:PHE:HZ	1.71	0.55
1:C:150:TYR:HE2	1:C:153:PHE:CZ	2.25	0.55
1:C:409:SER:OG	1:C:410:GLY:N	2.39	0.55
1:B:459:PHE:HD2	1:B:480:ILE:HD12	1.72	0.55
1:A:260:ASP:CG	1:A:318:THR:H	2.09	0.54
2:E:112:PHE:CE2	2:E:138:TRP:HB3	2.42	0.54
1:A:148:SER:HB3	1:A:383:LEU:HD12	1.89	0.54
2:E:75:ILE:HG23	2:E:138:TRP:NE1	2.23	0.54
1:A:57:PHE:HB2	1:A:323:MET:HE1	1.90	0.54
1:A:229:ASP:HA	1:A:257:THR:HG22	1.89	0.54
1:B:434:ILE:HG23	1:B:481:ARG:HH21	1.73	0.54
1:D:544:LYS:CE	1:D:808:GLU:OE2	2.55	0.54
2:E:92:TYR:HB2	2:E:150:LEU:HD22	1.88	0.54
1:D:439:LEU:HD22	1:D:482:LEU:HD22	1.90	0.54
1:A:42:PHE:HE2	1:A:80:THR:HB	1.72	0.54
1:A:218:MET:SD	1:A:223:GLU:HB2	2.48	0.54
1:B:558:PRO:HG2	1:B:651:TYR:HE1	1.71	0.54
1:B:743:GLU:OE1	1:B:743:GLU:N	2.36	0.54
1:C:845:LYS:O	1:C:850:ALA:N	2.39	0.54
1:A:471:SER:O	1:A:475:GLY:N	2.41	0.54
1:A:614:PHE:O	1:A:618:ALA:N	2.39	0.54
1:B:845:LYS:HA	1:B:848:LYS:HD2	1.90	0.54
1:A:543:ARG:HG3	1:A:728:VAL:HG12	1.89	0.54
1:A:37:ARG:HG3	1:A:77:THR:HG23	1.90	0.53
1:C:112:SER:O	1:C:115:ALA:N	2.41	0.53
1:D:126:GLY:HA2	1:D:145:PHE:HE2	1.72	0.53
1:A:136:HIS:CD2	1:A:183:ILE:HD13	2.43	0.53
1:A:291:SER:HA	1:A:294:GLU:OE1	2.07	0.53
1:B:467:LEU:HD23	1:B:478:TYR:HE1	1.72	0.53
1:C:628:PRO:O	1:C:634:ARG:NE	2.40	0.53
2:E:111:PRO:HA	2:E:138:TRP:CE3	2.43	0.53
1:A:664:MET:SD	1:D:661:VAL:HG12	2.48	0.53
1:A:261:LEU:HD12	1:A:264:LEU:HD13	1.91	0.53
1:C:491:GLN:OE1	1:C:492:ASP:N	2.41	0.53
1:A:235:ALA:O	1:A:239:LEU:HD23	2.08	0.53
1:C:731:SER:OG	1:C:732:ASP:N	2.41	0.53
1:A:177:ASP:OD1	1:A:178:ASP:N	2.41	0.53
1:A:386:ASP:HA	1:A:407:PRO:HG2	1.89	0.53
1:C:782:ILE:O	1:C:786:GLN:N	2.30	0.53
1:D:450:ASP:OD1	1:D:451:LYS:N	2.42	0.53
1:D:533:PHE:CD2	1:D:534:MET:HG2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:O	1:A:460:GLU:N	2.29	0.53
1:D:455:GLY:HA2	1:D:458:ARG:NH1	2.24	0.53
1:C:479:GLU:OE1	1:C:481:ARG:NH2	2.42	0.53
1:D:110:SER:OG	1:D:133:ARG:HG3	2.08	0.53
1:B:126:GLY:HA2	1:B:145:PHE:CE2	2.44	0.53
1:C:202:ARG:HB3	1:C:214:LEU:HD11	1.91	0.53
1:B:675:ALA:O	1:B:704:LYS:NZ	2.33	0.52
1:B:555:PHE:CD1	1:B:823:ILE:HD11	2.44	0.52
1:A:248:MET:HE3	1:A:274:VAL:HG11	1.90	0.52
1:A:668:ILE:HG23	1:A:673:ASP:HB2	1.92	0.52
1:C:846:SER:OG	1:C:852:LEU:O	2.27	0.52
1:A:110:SER:HB3	1:A:133:ARG:HG3	1.92	0.52
1:A:435:VAL:HG22	1:A:512:LEU:HB2	1.91	0.52
1:B:741:THR:HA	1:B:744:PHE:HD2	1.74	0.52
1:C:386:ASP:HA	1:C:407:PRO:HG3	1.91	0.52
1:A:184:ARG:NH1	1:A:229:ASP:OD2	2.42	0.52
1:A:414:THR:O	1:A:414:THR:CG2	2.56	0.52
1:B:488:TYR:HB2	1:B:523:ARG:HH22	1.73	0.52
1:B:709:MET:HB2	1:B:716:VAL:HG11	1.92	0.52
1:C:726:GLN:HA	1:C:729:LEU:HB2	1.90	0.52
1:D:720:SER:O	1:D:724:GLY:N	2.43	0.52
1:D:738:GLU:O	1:D:742:ILE:HG12	2.09	0.52
2:E:88:PHE:CZ	2:E:152:PHE:HB2	2.45	0.52
1:D:630:ALA:HB3	1:D:633:THR:HG22	1.91	0.52
1:C:126:GLY:HA2	1:C:145:PHE:CE2	2.42	0.52
1:C:544:LYS:HB2	1:C:753:THR:HG23	1.92	0.52
1:D:212:LYS:NZ	1:D:241:GLN:OE1	2.35	0.52
1:D:253:HIS:ND1	1:D:275:ASN:HB2	2.24	0.52
1:A:716:VAL:HA	1:A:727:ARG:NH1	2.25	0.52
1:D:702:TYR:HA	1:D:705:MET:HE2	1.91	0.52
1:C:583:ARG:HH11	1:C:604:ASN:HB2	1.75	0.52
1:D:136:HIS:CG	1:D:136:HIS:O	2.62	0.52
1:A:89:PHE:HE2	1:B:350:HIS:CD2	2.28	0.51
1:A:233:GLU:OE1	1:A:233:GLU:N	2.39	0.51
1:A:641:TRP:NE1	1:B:622:GLN:HG2	2.25	0.51
1:B:222:LYS:HB3	1:B:224:PHE:HE1	1.75	0.51
2:E:106:GLU:OE2	2:E:140:LYS:HE3	2.10	0.51
1:A:50:MET:HE1	1:A:55:LEU:HD13	1.91	0.51
1:A:663:ARG:HH12	1:A:813:SER:HA	1.75	0.51
1:B:844:TYR:O	1:B:848:LYS:HG3	2.09	0.51
1:C:270:ARG:NH2	1:C:271:TYR:OH	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:O	1:C:415:GLU:HG2	2.09	0.51
1:A:540:ILE:HG13	1:A:736:LEU:HD23	1.92	0.51
1:D:229:ASP:HA	1:D:257:THR:HG22	1.92	0.51
1:A:126:GLY:HA2	1:A:145:PHE:CE2	2.46	0.51
1:B:198:ARG:HB3	1:B:198:ARG:CZ	2.41	0.51
1:B:256:PHE:HB3	1:B:258:THR:HG22	1.93	0.51
1:D:694:PHE:O	1:D:697:SER:OG	2.23	0.51
1:A:376:THR:HG21	1:A:386:ASP:HB3	1.91	0.51
1:A:800:ARG:O	1:A:800:ARG:NH1	2.43	0.51
1:B:210:ASP:O	1:B:213:PRO:HD2	2.11	0.51
1:B:437:THR:HG23	1:B:515:ALA:HB2	1.92	0.51
1:C:426:ASP:HB2	1:C:777:LYS:HD3	1.92	0.51
1:C:427:SER:OG	1:C:430:ASN:N	2.43	0.51
1:D:85:LEU:HG	1:D:111:HIS:HB2	1.91	0.51
1:A:210:ASP:O	1:A:213:PRO:HD2	2.11	0.51
1:B:634:ARG:HH12	1:C:609:LEU:HB3	1.76	0.51
2:E:87:THR:HA	2:E:129:LEU:HD22	1.92	0.51
1:A:270:ARG:NH1	1:A:397:GLU:O	2.43	0.51
1:B:208:THR:O	1:B:211:ALA:N	2.44	0.51
1:B:593:HIS:CE1	1:B:595:CYS:HB2	2.46	0.51
1:C:646:ILE:O	1:C:650:SER:N	2.37	0.51
1:C:677:GLN:NE2	1:C:679:LYS:HB2	2.26	0.51
1:A:54:GLU:OE2	1:A:82:LYS:NZ	2.44	0.51
1:A:83:ILE:HG12	1:A:94:LYS:HG3	1.92	0.51
1:A:433:LEU:HD23	1:A:512:LEU:HD13	1.93	0.51
1:C:207:ASP:OD1	1:C:208:THR:N	2.44	0.51
1:C:528:ASP:OD1	1:C:775:ARG:NH1	2.44	0.51
2:E:70:LYS:HD3	2:E:72:CYS:SG	2.51	0.51
1:A:446:PHE:O	1:A:448:LYS:NZ	2.44	0.51
1:A:497:GLN:HE22	1:A:503:ARG:HD2	1.76	0.51
1:B:444:VAL:HG12	1:B:464:ILE:HG12	1.93	0.51
1:C:138:VAL:HG11	1:D:111:HIS:NE2	2.26	0.51
1:A:479:GLU:OE1	1:A:481:ARG:HG3	2.11	0.50
1:A:558:PRO:HB3	1:A:654:ASN:HB3	1.93	0.50
1:C:456:ASN:ND2	1:C:478:TYR:O	2.43	0.50
1:C:540:ILE:HG13	1:C:755:ILE:HB	1.91	0.50
1:D:528:ASP:HB3	1:D:768:THR:HG23	1.93	0.50
1:A:459:PHE:HZ	1:A:482:LEU:HG	1.77	0.50
1:D:438:ILE:HG21	1:D:488:TYR:HE1	1.75	0.50
1:A:627:MET:SD	1:A:627:MET:N	2.84	0.50
1:D:462:TYR:HB2	1:D:798:TRP:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:O	1:A:150:TYR:HB2	2.12	0.50
1:B:689:ALA:O	1:B:692:THR:OG1	2.23	0.50
1:D:299:GLU:C	1:D:302:GLN:HE22	2.14	0.50
1:D:441:GLU:HB3	1:D:442:PRO:HD3	1.93	0.50
1:B:434:ILE:HA	1:B:479:GLU:OE2	2.11	0.50
1:B:774:TYR:O	1:B:778:ILE:N	2.43	0.50
1:C:563:ILE:HG23	1:D:824:PHE:HZ	1.76	0.50
1:C:793:MET:HA	1:C:796:GLU:HG2	1.94	0.50
1:D:744:PHE:HB2	1:D:799:TRP:CD1	2.47	0.50
1:C:658:PHE:HD1	1:C:659:LEU:HD22	1.77	0.50
1:D:299:GLU:O	1:D:302:GLN:NE2	2.44	0.50
1:D:682:TYR:CE1	1:D:705:MET:HG3	2.45	0.50
1:A:64:ILE:HD11	1:A:328:HIS:CE1	2.47	0.50
1:A:390:ASP:OD1	1:A:390:ASP:N	2.45	0.50
1:B:89:PHE:CZ	1:B:93:LYS:HE3	2.47	0.50
1:B:288:GLN:O	1:B:292:ILE:HG12	2.12	0.50
1:C:440:GLU:HG3	1:C:516:PRO:HG2	1.94	0.50
1:A:210:ASP:C	1:A:212:LYS:H	2.14	0.50
1:B:702:TYR:O	1:B:706:TRP:N	2.40	0.50
2:E:362:LEU:O	2:E:366:ILE:N	2.44	0.50
1:A:173:THR:O	1:A:226:VAL:HG23	2.12	0.50
1:B:447:LYS:HG3	1:B:458:ARG:O	2.12	0.50
1:C:443:TYR:O	1:C:462:TYR:N	2.45	0.50
1:D:795:LYS:HD2	1:D:799:TRP:CE3	2.47	0.50
1:A:239:LEU:HD21	1:A:256:PHE:CZ	2.40	0.49
1:A:620:MET:HG2	1:D:645:LEU:HD12	1.92	0.49
1:A:831:LEU:O	1:A:834:SER:OG	2.23	0.49
1:B:512:LEU:HA	1:B:767:GLY:O	2.11	0.49
1:D:340:MET:HE1	1:D:359:PHE:CD1	2.47	0.49
1:D:540:ILE:HB	1:D:755:ILE:O	2.12	0.49
1:D:699:ILE:HG21	1:D:702:TYR:CD2	2.47	0.49
1:A:54:GLU:OE2	1:A:82:LYS:HE3	2.11	0.49
1:B:149:LEU:HB3	1:B:322:LEU:HD12	1.94	0.49
1:C:435:VAL:HG23	1:C:480:ILE:HG13	1.95	0.49
1:A:96:CYS:HG	1:A:347:CYS:CB	2.21	0.49
1:A:401:LYS:NZ	1:A:403:GLY:O	2.44	0.49
1:A:556:LEU:HD23	1:A:556:LEU:H	1.77	0.49
1:D:89:PHE:CE2	1:D:93:LYS:HE3	2.47	0.49
2:E:59:SER:HB3	2:E:152:PHE:CE2	2.47	0.49
1:C:229:ASP:HA	1:C:257:THR:HG22	1.93	0.49
1:D:37:ARG:HG2	1:D:103:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:HE2	1:B:220:ARG:HH22	1.77	0.49
1:B:487:LYS:N	1:B:500:GLY:HA2	2.28	0.49
1:B:523:ARG:NH2	1:B:689:ALA:HB2	2.28	0.49
2:E:55:GLY:O	2:E:155:LYS:HD2	2.12	0.49
1:A:49:PRO:CG	1:A:303:ALA:HB1	2.43	0.49
1:A:630:ALA:HB3	1:A:633:THR:HG22	1.95	0.49
1:B:212:LYS:HG2	1:B:245:MET:HE1	1.94	0.49
1:D:439:LEU:HD21	1:D:482:LEU:CD2	2.42	0.49
1:D:544:LYS:NZ	1:D:808:GLU:CG	2.61	0.49
2:E:54:GLY:HA3	2:E:155:LYS:HZ1	1.78	0.49
1:A:50:MET:SD	1:A:58:ARG:NH1	2.86	0.49
1:A:719:LYS:N	1:A:723:GLU:OE2	2.27	0.49
1:C:216:LYS:HZ2	2:E:147:LEU:HD12	1.78	0.49
1:A:572:LEU:O	1:A:575:SER:OG	2.29	0.49
1:A:716:VAL:HG23	1:A:716:VAL:O	2.13	0.49
1:B:505:LEU:HD21	1:B:768:THR:N	2.27	0.49
1:D:71:LEU:HD11	1:D:74:THR:HB	1.95	0.49
1:A:210:ASP:C	1:A:212:LYS:N	2.67	0.48
1:B:583:ARG:O	1:B:589:TRP:HZ2	1.96	0.48
1:B:585:SER:O	1:B:589:TRP:NE1	2.46	0.48
1:C:608:LEU:HB2	2:E:366:ILE:HG21	1.94	0.48
1:C:674:LEU:HG	1:C:682:TYR:CE1	2.48	0.48
1:D:498:TRP:HB3	1:D:502:VAL:HB	1.94	0.48
2:E:75:ILE:HG23	2:E:138:TRP:CE2	2.48	0.48
2:E:79:ALA:HB3	2:E:82:GLN:NE2	2.27	0.48
1:A:654:ASN:HD21	1:B:815:LEU:HD13	1.76	0.48
1:B:635:ILE:HD12	1:B:635:ILE:H	1.79	0.48
1:C:220:ARG:HG3	2:E:102:PHE:HE1	1.74	0.48
2:E:351:ILE:O	2:E:354:THR:OG1	2.24	0.48
1:B:677:GLN:HE22	1:B:680:ILE:HB	1.78	0.48
1:D:306:LYS:HD2	1:D:307:PRO:HD2	1.94	0.48
1:D:843:LEU:O	1:D:847:LYS:N	2.28	0.48
2:E:83:ARG:HB2	2:E:159:ILE:HG13	1.95	0.48
1:B:272:SER:HB2	1:B:274:VAL:HG23	1.96	0.48
1:B:641:TRP:HB3	1:C:620:MET:HE3	1.94	0.48
1:C:284:THR:HA	1:C:289:VAL:HG11	1.95	0.48
1:B:447:LYS:HE3	1:B:458:ARG:HA	1.94	0.48
1:B:695:LYS:O	1:B:696:LYS:HG2	2.13	0.48
1:C:792:HIS:O	1:C:795:LYS:HB2	2.13	0.48
1:D:177:ASP:OD1	1:D:178:ASP:N	2.42	0.48
1:A:441:GLU:CD	1:A:441:GLU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:ARG:NH1	1:C:604:ASN:HB2	2.28	0.48
1:A:564:TRP:O	1:A:568:LEU:HD23	2.13	0.48
1:B:694:PHE:CE1	1:B:702:TYR:HB3	2.49	0.48
1:C:110:SER:O	1:C:133:ARG:HG3	2.13	0.48
1:C:724:GLY:HA3	1:C:735:PHE:CZ	2.48	0.48
1:A:153:PHE:CD2	1:A:184:ARG:HG3	2.49	0.48
1:A:595:CYS:HB3	1:B:593:HIS:CE1	2.48	0.48
1:C:782:ILE:HA	1:C:785:LEU:HB2	1.95	0.48
1:D:439:LEU:HD21	1:D:482:LEU:HD22	1.96	0.48
1:B:110:SER:HB3	1:B:133:ARG:HG3	1.96	0.48
1:A:791:LEU:O	1:A:795:LYS:N	2.43	0.48
1:A:528:ASP:O	1:A:768:THR:N	2.42	0.47
1:B:111:HIS:CG	1:B:112:SER:N	2.82	0.47
1:D:68:ARG:HD2	1:D:72:PRO:HA	1.95	0.47
1:D:818:GLN:OE1	1:D:818:GLN:N	2.40	0.47
1:A:34:HIS:HB3	1:A:74:THR:HG23	1.97	0.47
1:A:140:ASP:OD1	1:A:142:LYS:NZ	2.48	0.47
1:A:536:LEU:HB3	1:A:740:THR:HG23	1.96	0.47
1:C:189:ILE:O	1:C:192:PRO:HD2	2.15	0.47
1:C:435:VAL:HG11	1:C:467:LEU:HD11	1.95	0.47
1:A:202:ARG:NH2	1:A:223:GLU:OE2	2.44	0.47
1:A:374:ARG:NE	1:A:388:ASP:OD2	2.28	0.47
1:D:337:PHE:HD2	1:D:340:MET:HE3	1.80	0.47
1:D:536:LEU:HD13	1:D:764:TYR:CE2	2.49	0.47
1:D:453:LEU:HD22	1:D:458:ARG:HA	1.95	0.47
1:A:498:TRP:CD2	1:A:502:VAL:HG11	2.49	0.47
1:C:679:LYS:CE	1:D:670:SER:OG	2.62	0.47
1:D:718:VAL:HG21	1:D:724:GLY:HA2	1.95	0.47
1:D:737:MET:SD	1:D:738:GLU:N	2.88	0.47
1:A:96:CYS:CB	1:A:347:CYS:SG	3.02	0.47
1:B:86:TYR:HE1	1:B:111:HIS:CD2	2.32	0.47
1:B:512:LEU:HD11	1:B:774:TYR:HB3	1.95	0.47
1:C:431:ARG:HG2	1:C:774:TYR:OH	2.15	0.47
1:D:488:TYR:O	1:D:489:GLY:C	2.52	0.47
2:E:350:ILE:O	2:E:354:THR:HG23	2.15	0.47
1:A:537:GLY:HA3	1:A:758:LEU:HG	1.96	0.47
1:B:518:ALA:H	1:B:523:ARG:NH1	2.10	0.47
1:B:677:GLN:NE2	1:B:682:TYR:OH	2.47	0.47
1:B:792:HIS:O	1:B:796:GLU:HG2	2.14	0.47
1:C:138:VAL:HG12	1:C:139:SER:N	2.29	0.47
1:C:341:THR:OG1	1:C:354:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:O	1:C:478:TYR:HA	2.15	0.47
1:C:443:TYR:HB3	1:C:463:CYS:SG	2.55	0.47
1:C:677:GLN:HE22	1:C:679:LYS:HB2	1.80	0.47
1:C:685:VAL:HA	1:C:718:VAL:O	2.15	0.47
1:C:750:CYS:SG	1:C:751:ASN:N	2.88	0.47
2:E:45:CYS:HB3	2:E:72:CYS:HB2	1.97	0.47
1:B:631:LEU:O	1:B:635:ILE:HD12	2.15	0.47
1:C:64:ILE:HD11	1:C:328:HIS:CE1	2.49	0.47
1:C:825:ILE:O	1:C:829:ALA:N	2.38	0.47
1:D:491:GLN:HB2	1:D:498:TRP:CH2	2.50	0.47
2:E:76:LEU:HB2	2:E:137:MET:O	2.13	0.47
2:E:142:SER:OG	2:E:143:SER:N	2.47	0.47
1:A:143:ASP:OD1	1:A:144:SER:N	2.47	0.47
1:B:233:GLU:OE1	1:B:233:GLU:N	2.29	0.47
1:D:60:ALA:HB2	1:D:324:TYR:CD1	2.50	0.47
1:D:296:TRP:HZ3	1:D:300:ARG:CZ	2.28	0.47
1:A:795:LYS:O	1:A:799:TRP:HB2	2.15	0.46
1:B:58:ARG:NH1	1:B:78:TYR:OH	2.48	0.46
1:B:249:THR:HG1	1:B:251:TYR:HD2	1.63	0.46
1:B:839:VAL:HA	1:B:842:PHE:HB3	1.97	0.46
1:C:634:ARG:HH22	1:D:610:ASN:HD21	1.62	0.46
1:D:699:ILE:HG23	1:D:701:THR:H	1.80	0.46
1:A:219:LYS:HB2	1:A:247:MET:HE1	1.96	0.46
1:A:454:TYR:HA	1:A:458:ARG:HB2	1.96	0.46
1:C:215:LEU:HD12	1:C:245:MET:CE	2.45	0.46
1:A:815:LEU:CD1	1:D:654:ASN:HD21	2.29	0.46
1:B:487:LYS:HG3	1:B:488:TYR:N	2.30	0.46
1:C:71:LEU:HD21	1:C:334:VAL:HG13	1.97	0.46
1:D:551:GLY:HA2	1:D:554:SER:HB2	1.96	0.46
1:B:145:PHE:HD1	1:B:360:MET:HG2	1.79	0.46
1:B:441:GLU:HB3	1:B:442:PRO:HD3	1.97	0.46
1:C:43:GLU:HB3	1:C:85:LEU:HD12	1.97	0.46
1:C:148:SER:HB3	1:C:383:LEU:HD12	1.98	0.46
1:D:237:GLY:O	1:D:241:GLN:HG2	2.15	0.46
2:E:155:LYS:NZ	2:E:156:TYR:O	2.45	0.46
1:A:153:PHE:CG	1:A:184:ARG:HG3	2.51	0.46
1:A:694:PHE:CE2	1:A:736:LEU:HD13	2.50	0.46
1:B:83:ILE:HG22	1:B:94:LYS:HG3	1.98	0.46
1:B:397:GLU:OE1	1:B:397:GLU:N	2.45	0.46
1:B:503:ARG:NH1	1:B:507:ASP:OD2	2.48	0.46
1:C:86:TYR:CE2	1:D:140:ASP:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD23	1:B:214:LEU:HD12	1.98	0.46
1:B:248:MET:CG	1:B:274:VAL:HG21	2.41	0.46
1:C:392:ILE:HD12	1:C:399:LEU:HD12	1.97	0.46
1:A:784:GLN:O	1:A:787:GLU:HG3	2.15	0.46
1:B:219:LYS:HB2	1:B:247:MET:CE	2.45	0.46
1:B:339:GLN:CD	1:B:339:GLN:H	2.18	0.46
1:C:86:TYR:CZ	1:C:111:HIS:HB3	2.50	0.46
1:C:435:VAL:HG12	1:C:512:LEU:HB2	1.98	0.46
1:C:827:LEU:O	1:C:831:LEU:HG	2.16	0.46
1:D:778:ILE:O	1:D:782:ILE:HG12	2.16	0.46
1:A:134:TRP:CD2	1:A:153:PHE:CE2	3.04	0.46
1:A:212:LYS:HB2	1:A:213:PRO:HD3	1.98	0.46
1:A:454:TYR:HD1	1:A:458:ARG:HE	1.63	0.46
1:A:543:ARG:HA	1:A:752:LEU:HA	1.98	0.46
1:C:54:GLU:CD	1:C:82:LYS:HZ1	2.19	0.46
1:C:283:ASN:O	1:C:289:VAL:HG11	2.16	0.46
1:C:441:GLU:O	1:C:445:LEU:HD11	2.15	0.46
1:D:71:LEU:H	1:D:335:GLN:NE2	2.14	0.46
1:D:389:LEU:HB2	1:D:405:TRP:HB3	1.97	0.46
1:D:536:LEU:HB3	1:D:762:LYS:HB2	1.96	0.46
1:A:266:VAL:HG21	1:A:394:LEU:HD13	1.98	0.46
1:A:390:ASP:HA	1:A:404:THR:HA	1.98	0.46
1:D:59:PHE:CD2	1:D:296:TRP:HD1	2.34	0.46
2:E:133:THR:HG22	2:E:133:THR:O	2.15	0.46
1:D:157:SER:OG	1:D:187:GLU:HB3	2.16	0.46
1:D:406:ASP:OD1	1:D:406:ASP:N	2.46	0.46
1:D:519:ILE:HD12	1:D:529:PHE:HB3	1.97	0.46
2:E:45:CYS:SG	2:E:72:CYS:CB	3.04	0.46
2:E:101:ARG:HD3	2:E:120:ARG:HH12	1.81	0.46
1:A:57:PHE:HB2	1:A:323:MET:CE	2.46	0.45
1:A:528:ASP:OD1	1:A:775:ARG:NH1	2.49	0.45
1:A:574:VAL:HA	1:A:577:VAL:HG12	1.98	0.45
1:A:845:LYS:HA	1:A:848:LYS:HE2	1.99	0.45
1:B:420:LYS:N	1:B:421:PRO:HD3	2.30	0.45
1:B:634:ARG:HD3	1:C:613:TRP:CD2	2.51	0.45
1:C:89:PHE:CZ	1:C:93:LYS:HE3	2.51	0.45
1:C:191:ALA:HA	1:C:194:ARG:HE	1.81	0.45
1:C:674:LEU:HG	1:C:682:TYR:HE1	1.80	0.45
1:C:825:ILE:O	1:C:825:ILE:HG22	2.16	0.45
1:D:670:SER:N	1:D:673:ASP:OD2	2.49	0.45
1:A:42:PHE:CE1	1:A:323:MET:HE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:O	1:A:329:VAL:HG12	2.17	0.45
1:A:400:GLU:N	1:A:400:GLU:OE1	2.48	0.45
1:A:556:LEU:HB2	1:A:564:TRP:CZ2	2.51	0.45
1:C:467:LEU:HD12	1:C:514:VAL:HG11	1.98	0.45
1:A:521:TYR:O	1:A:522:VAL:HG22	2.17	0.45
1:A:628:PRO:HB2	1:A:634:ARG:CG	2.46	0.45
1:B:71:LEU:H	1:B:335:GLN:NE2	2.14	0.45
1:B:85:LEU:HG	1:B:86:TYR:CD2	2.51	0.45
1:B:571:CYS:SG	1:B:616:VAL:HG22	2.56	0.45
1:C:487:LYS:HB3	1:C:487:LYS:HE2	1.75	0.45
1:C:678:THR:HG21	1:D:701:THR:HG21	1.97	0.45
1:D:440:GLU:HB3	1:D:443:TYR:CD2	2.46	0.45
1:D:561:PRO:HA	1:D:564:TRP:CD1	2.44	0.45
1:D:768:THR:HG1	1:D:772:SER:HG	1.55	0.45
1:A:664:MET:C	1:A:665:GLU:HG3	2.34	0.45
1:A:849:ASN:HB3	1:A:857:PHE:HZ	1.80	0.45
1:C:129:HIS:O	1:C:146:TYR:HA	2.15	0.45
1:C:226:VAL:HB	1:C:254:TYR:HD1	1.81	0.45
1:D:438:ILE:HG21	1:D:488:TYR:CE1	2.52	0.45
1:B:691:MET:HA	1:B:694:PHE:HB3	1.98	0.45
1:C:86:TYR:CE1	1:C:111:HIS:HB3	2.51	0.45
1:D:590:TYR:N	1:D:603:GLU:O	2.48	0.45
1:D:629:LYS:HA	1:D:629:LYS:HD3	1.79	0.45
1:D:677:GLN:HE22	1:D:679:LYS:HB3	1.79	0.45
1:A:54:GLU:OE2	1:A:82:LYS:CE	2.64	0.45
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.86	0.45
2:E:101:ARG:O	2:E:102:PHE:CD2	2.69	0.45
1:C:498:TRP:CE3	1:C:502:VAL:HG11	2.52	0.45
2:E:148:GLU:H	2:E:148:GLU:CD	2.19	0.45
1:A:85:LEU:HD12	1:A:111:HIS:HD2	1.81	0.45
1:A:450:ASP:OD1	1:A:451:LYS:N	2.49	0.45
1:A:541:LEU:HG	1:A:742:ILE:HG12	1.99	0.45
1:B:437:THR:HG21	1:B:444:VAL:HG11	1.98	0.45
1:D:72:PRO:HD3	1:D:335:GLN:NE2	2.31	0.45
1:D:300:ARG:HH12	1:D:316:MET:N	2.14	0.45
1:D:544:LYS:CE	1:D:808:GLU:CD	2.82	0.45
1:A:533:PHE:CE2	1:A:534:MET:HG2	2.52	0.45
1:B:237:GLY:O	1:B:241:GLN:HG2	2.17	0.45
1:B:537:GLY:HA3	1:B:760:ASP:O	2.17	0.45
1:C:552:VAL:O	1:C:553:PHE:CD1	2.70	0.45
1:A:239:LEU:HB3	1:A:269:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HA	1:A:448:LYS:HD3	1.62	0.45
1:A:519:ILE:HG21	1:A:532:PRO:HG3	1.98	0.45
1:A:681:GLU:HB3	1:A:716:VAL:HG11	1.99	0.45
1:B:747:GLN:HA	1:B:804:CYS:SG	2.57	0.45
1:D:482:LEU:O	1:D:482:LEU:CG	2.63	0.45
1:A:34:HIS:N	1:A:74:THR:HA	2.32	0.44
1:A:459:PHE:CZ	1:A:482:LEU:HG	2.51	0.44
1:B:177:ASP:OD1	1:B:178:ASP:OD1	2.34	0.44
1:B:465:ASP:OD2	1:B:798:TRP:NE1	2.36	0.44
1:D:466:LEU:O	1:D:470:LEU:N	2.46	0.44
2:E:59:SER:HB3	2:E:152:PHE:CD2	2.53	0.44
1:A:85:LEU:CD1	1:A:111:HIS:HD2	2.31	0.44
1:A:248:MET:O	1:A:272:SER:OG	2.34	0.44
1:B:788:GLU:C	1:B:790:LYS:N	2.70	0.44
1:C:473:ILE:HG23	1:C:474:LEU:HG	1.99	0.44
1:C:552:VAL:O	1:C:553:PHE:HD1	2.01	0.44
1:D:744:PHE:O	1:D:748:ARG:NH1	2.50	0.44
1:D:802:ASN:HD22	1:D:802:ASN:HA	1.62	0.44
2:E:109:ASP:HA	2:E:136:PHE:O	2.16	0.44
1:A:752:LEU:HD23	1:A:752:LEU:H	1.82	0.44
1:B:296:TRP:HE1	1:B:300:ARG:NH1	2.16	0.44
1:C:501:MET:O	1:C:504:GLU:HG3	2.17	0.44
1:C:722:GLU:OE1	1:C:722:GLU:N	2.42	0.44
1:A:453:LEU:HD12	1:A:458:ARG:HA	1.98	0.44
1:A:640:TRP:O	1:A:644:THR:HG23	2.18	0.44
1:B:34:HIS:H	1:B:74:THR:HA	1.82	0.44
1:B:79:ASP:OD2	1:B:98:GLN:NE2	2.50	0.44
1:A:716:VAL:HA	1:A:727:ARG:HH12	1.82	0.44
1:B:296:TRP:CD1	1:B:316:MET:SD	3.11	0.44
1:C:434:ILE:HG21	1:C:481:ARG:HE	1.82	0.44
1:C:561:PRO:HA	1:C:564:TRP:HD1	1.82	0.44
1:D:83:ILE:HG13	1:D:83:ILE:O	2.17	0.44
1:A:474:LEU:HD13	1:A:476:PHE:CE2	2.52	0.44
1:A:519:ILE:HG13	1:A:520:THR:N	2.32	0.44
1:B:126:GLY:HA2	1:B:145:PHE:HE2	1.83	0.44
1:B:149:LEU:O	1:B:384:ARG:HD3	2.18	0.44
1:C:132:THR:HG21	1:C:323:MET:CE	2.48	0.44
1:C:471:SER:HA	1:C:476:PHE:HD2	1.82	0.44
1:D:747:GLN:O	1:D:803:GLY:HA3	2.18	0.44
1:A:393:SER:OG	1:A:394:LEU:N	2.50	0.44
1:B:712:ARG:HH11	1:B:715:SER:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:SER:H	1:C:673:ASP:HB3	1.83	0.44
1:D:68:ARG:HH21	1:D:72:PRO:HB3	1.81	0.44
2:E:85:GLU:OE1	2:E:159:ILE:HG12	2.17	0.44
1:A:169:TRP:CE2	1:A:225:HIS:HB3	2.53	0.44
1:A:664:MET:O	1:A:665:GLU:CG	2.57	0.44
1:B:784:GLN:NE2	1:B:785:LEU:HG	2.33	0.44
1:C:469:GLU:HB3	1:C:785:LEU:HD11	1.99	0.44
1:C:749:ASN:OD1	1:C:750:CYS:N	2.51	0.44
1:A:295:LYS:O	1:A:299:GLU:HG2	2.18	0.44
1:A:331:SER:HA	1:A:334:VAL:HG12	1.99	0.44
1:A:470:LEU:HD12	1:A:471:SER:N	2.32	0.44
1:C:770:MET:SD	1:C:770:MET:N	2.91	0.44
1:C:779:THR:O	1:C:783:LEU:HD23	2.18	0.44
1:D:527:ILE:HA	1:D:770:MET:HE1	1.99	0.44
2:E:140:LYS:NZ	2:E:142:SER:HB2	2.33	0.44
1:A:571:CYS:HA	1:A:574:VAL:HG22	2.00	0.43
1:C:87:ASP:HB3	1:C:90:GLU:HB3	2.00	0.43
1:C:300:ARG:NH1	1:C:303:ALA:HB3	2.33	0.43
1:C:433:LEU:HD12	1:C:434:ILE:H	1.83	0.43
1:A:186:GLN:O	1:A:190:LYS:HG3	2.18	0.43
1:A:556:LEU:HD12	1:A:564:TRP:CD1	2.52	0.43
1:B:111:HIS:CG	1:B:112:SER:H	2.36	0.43
1:B:132:THR:O	1:B:150:TYR:HB2	2.18	0.43
1:B:414:THR:HA	1:B:417:GLN:HG2	2.00	0.43
1:B:705:MET:HG3	1:B:709:MET:HE3	2.00	0.43
1:C:33:THR:N	1:C:73:ASN:O	2.51	0.43
1:C:647:ILE:O	1:C:651:TYR:N	2.49	0.43
1:C:750:CYS:HB3	4:C:1003:NAG:HN2	1.82	0.43
1:C:795:LYS:O	1:C:799:TRP:HB2	2.18	0.43
1:C:795:LYS:HD2	1:C:799:TRP:CZ3	2.52	0.43
1:D:563:ILE:O	1:D:567:VAL:HG22	2.18	0.43
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.92	0.43
1:A:541:LEU:HA	1:A:541:LEU:HD23	1.77	0.43
1:A:604:ASN:OD1	1:B:867:MET:HG2	2.18	0.43
1:A:718:VAL:HG13	1:A:723:GLU:HG3	2.01	0.43
1:B:86:TYR:CE1	1:B:111:HIS:CD2	3.06	0.43
1:C:579:PHE:CE2	2:E:366:ILE:HG12	2.53	0.43
1:D:556:LEU:HG	1:D:564:TRP:CZ2	2.53	0.43
1:A:559:LEU:HD13	1:A:563:ILE:HG21	2.00	0.43
1:B:270:ARG:NH2	1:B:271:TYR:OH	2.50	0.43
1:B:367:HIS:HD2	1:B:376:THR:OG1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD12	1:C:264:LEU:HD23	2.00	0.43
1:D:578:LEU:HD13	1:D:636:VAL:HG11	2.00	0.43
1:D:714:GLN:HG2	1:D:715:SER:N	2.33	0.43
2:E:356:GLY:HA2	2:E:359:LEU:HG	2.00	0.43
1:A:157:SER:OG	1:A:187:GLU:HB3	2.19	0.43
1:B:447:LYS:HD2	1:B:458:ARG:HD3	2.00	0.43
1:C:714:GLN:N	1:C:717:LEU:HD12	2.34	0.43
2:E:45:CYS:SG	2:E:60:PRO:HG3	2.58	0.43
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.64	0.43
1:B:699:ILE:HG13	1:B:700:SER:N	2.33	0.43
1:C:639:ILE:HG13	1:C:640:TRP:N	2.33	0.43
1:A:300:ARG:NH1	1:A:303:ALA:HB3	2.34	0.43
1:A:378:ASN:HB3	1:A:381:ASN:OD1	2.19	0.43
1:A:434:ILE:HG23	1:A:434:ILE:O	2.18	0.43
1:C:336:GLN:N	1:C:336:GLN:OE1	2.51	0.43
1:D:153:PHE:CG	1:D:184:ARG:HG3	2.54	0.43
2:E:129:LEU:HB3	2:E:131:ARG:NH2	2.34	0.43
1:A:283:ASN:O	1:A:289:VAL:HG11	2.19	0.43
1:A:704:LYS:HE3	1:B:700:SER:HA	1.99	0.43
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.74	0.43
1:C:539:SER:OG	1:C:540:ILE:N	2.52	0.43
1:D:297:SER:HA	1:D:300:ARG:CD	2.49	0.43
1:B:330:VAL:O	1:B:334:VAL:HG23	2.19	0.43
1:C:160:ILE:HD13	1:C:160:ILE:HA	1.91	0.43
1:C:239:LEU:HD12	1:C:239:LEU:HA	1.59	0.43
1:C:450:ASP:OD1	1:C:451:LYS:N	2.49	0.43
1:C:706:TRP:HA	1:C:709:MET:HE2	2.01	0.43
1:D:442:PRO:HD2	1:D:443:TYR:CD2	2.53	0.43
1:D:536:LEU:HD12	1:D:537:GLY:H	1.83	0.43
1:A:561:PRO:HA	1:A:564:TRP:CD1	2.54	0.43
1:A:789:GLY:O	1:A:792:HIS:HB3	2.19	0.43
1:B:44:TYR:CD1	1:B:82:LYS:HB3	2.54	0.43
1:B:541:LEU:HD13	1:B:742:ILE:HG23	2.01	0.43
1:C:216:LYS:NZ	2:E:147:LEU:HD12	2.34	0.43
1:C:483:VAL:HG21	1:C:501:MET:SD	2.59	0.43
1:C:565:MET:O	1:C:569:LEU:HG	2.19	0.43
1:C:683:GLY:HA3	1:C:733:TYR:CE2	2.54	0.43
1:D:441:GLU:OE1	1:D:748:ARG:NH2	2.40	0.43
1:D:537:GLY:HA2	1:D:760:ASP:O	2.19	0.43
2:E:49:VAL:HB	2:E:156:TYR:CZ	2.54	0.43
1:A:561:PRO:HA	1:A:564:TRP:HD1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:GLU:C	1:B:790:LYS:H	2.21	0.42
1:D:145:PHE:CD1	1:D:360:MET:HG2	2.54	0.42
1:A:169:TRP:HZ2	1:A:253:HIS:ND1	2.17	0.42
1:A:556:LEU:HD12	1:A:564:TRP:NE1	2.34	0.42
1:A:590:TYR:CE2	1:A:592:PRO:HG3	2.54	0.42
1:B:433:LEU:HD13	1:B:476:PHE:CG	2.55	0.42
1:C:340:MET:HA	1:C:355:PHE:CE2	2.53	0.42
1:D:426:ASP:OD1	1:D:427:SER:N	2.51	0.42
2:E:367:LEU:HD12	2:E:367:LEU:HA	1.88	0.42
1:B:711:SER:OG	1:B:712:ARG:N	2.52	0.42
1:C:654:ASN:ND2	1:D:815:LEU:HG	2.35	0.42
1:C:790:LYS:HD2	1:C:793:MET:HE3	1.99	0.42
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.83	0.42
1:D:655:LEU:HD12	1:D:655:LEU:HA	1.86	0.42
2:E:88:PHE:CD2	2:E:127:PRO:HD2	2.55	0.42
1:A:89:PHE:HE2	1:B:350:HIS:NE2	2.17	0.42
1:A:248:MET:HE1	1:A:274:VAL:HG21	2.00	0.42
1:B:495:ASN:ND2	1:B:497:GLN:HB2	2.34	0.42
1:A:716:VAL:HG12	1:A:727:ARG:NH2	2.35	0.42
1:B:348:ASN:HD22	1:B:348:ASN:HA	1.56	0.42
1:B:539:SER:OG	1:B:540:ILE:N	2.50	0.42
1:C:591:ASN:HD21	1:C:599:SER:HB2	1.84	0.42
1:C:601:VAL:HG12	1:C:601:VAL:O	2.19	0.42
1:C:748:ARG:NH1	1:C:802:ASN:HB2	2.33	0.42
1:D:215:LEU:HD21	1:D:238:ILE:HD11	2.00	0.42
1:D:294:GLU:O	1:D:297:SER:HB2	2.20	0.42
1:D:299:GLU:HA	1:D:302:GLN:HE22	1.84	0.42
2:E:358:VAL:O	2:E:361:LEU:HG	2.20	0.42
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.84	0.42
1:A:428:LEU:HA	1:A:474:LEU:O	2.19	0.42
1:A:443:TYR:HB3	1:A:463:CYS:SG	2.60	0.42
1:A:596:ASN:O	1:A:598:ASP:N	2.49	0.42
1:A:628:PRO:HB3	1:A:633:THR:HG23	2.01	0.42
1:A:720:SER:OG	1:A:723:GLU:HG2	2.20	0.42
1:B:644:THR:O	1:B:647:ILE:N	2.53	0.42
1:C:433:LEU:HD22	1:C:774:TYR:HE2	1.85	0.42
1:C:580:VAL:HG11	2:E:362:LEU:HD22	2.01	0.42
1:C:714:GLN:H	1:C:717:LEU:HD12	1.84	0.42
1:A:60:ALA:HA	1:A:324:TYR:CE1	2.55	0.42
1:A:150:TYR:HA	1:A:322:LEU:HD21	2.02	0.42
1:A:292:ILE:HA	1:A:295:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ILE:HG22	1:A:528:ASP:N	2.35	0.42
1:C:360:MET:HE3	1:C:360:MET:O	2.19	0.42
1:C:726:GLN:HG3	1:C:729:LEU:HD12	2.01	0.42
1:D:60:ALA:O	1:D:64:ILE:HG12	2.19	0.42
1:D:406:ASP:OD1	1:D:409:SER:HB2	2.20	0.42
1:D:589:TRP:CE3	1:D:604:ASN:HB3	2.55	0.42
1:A:60:ALA:HA	1:A:324:TYR:HE1	1.84	0.42
1:A:433:LEU:O	1:A:479:GLU:N	2.47	0.42
1:A:645:LEU:HD21	1:B:648:ILE:HD12	2.02	0.42
1:B:60:ALA:HB2	1:B:324:TYR:CD1	2.54	0.42
1:D:558:PRO:O	1:D:559:LEU:HG	2.20	0.42
1:D:675:ALA:HB2	1:D:705:MET:SD	2.59	0.42
1:D:689:ALA:O	1:D:692:THR:OG1	2.36	0.42
1:A:42:PHE:CE2	1:A:80:THR:HB	2.54	0.42
1:A:123:ASN:HB2	1:A:143:ASP:OD2	2.19	0.42
1:A:733:TYR:CE2	1:A:735:PHE:HB2	2.55	0.42
1:B:235:ALA:HA	1:B:238:ILE:HG22	2.01	0.42
1:B:788:GLU:CB	1:B:790:LYS:HG3	2.49	0.42
1:B:853:GLU:CD	1:B:855:ARG:H	2.22	0.42
1:C:339:GLN:CD	1:C:339:GLN:H	2.22	0.42
1:C:555:PHE:O	1:C:651:TYR:OH	2.28	0.42
1:C:677:GLN:NE2	1:C:680:ILE:HG12	2.34	0.42
2:E:87:THR:HB	2:E:155:LYS:HB3	2.02	0.42
1:A:158:ARG:CZ	1:A:158:ARG:HB2	2.49	0.42
1:A:842:PHE:O	1:A:846:SER:OG	2.23	0.42
1:B:549:ASN:HB3	1:B:818:GLN:HE22	1.85	0.42
1:B:740:THR:HB	1:B:799:TRP:CZ3	2.55	0.42
1:C:716:VAL:HG12	1:C:727:ARG:HH21	1.85	0.42
1:C:774:TYR:O	1:C:778:ILE:HG12	2.20	0.42
1:D:470:LEU:HD13	1:D:778:ILE:HD11	2.02	0.42
2:E:121:TYR:CE1	2:E:127:PRO:HB3	2.54	0.42
1:A:296:TRP:CD1	1:A:316:MET:CG	3.03	0.41
1:A:563:ILE:HD12	1:A:563:ILE:H	1.85	0.41
1:A:710:SER:O	1:A:713:ARG:HB2	2.19	0.41
1:A:779:THR:HA	1:A:782:ILE:HG22	2.00	0.41
1:B:717:LEU:H	1:B:717:LEU:HD23	1.85	0.41
1:B:735:PHE:CE2	1:B:737:MET:HG2	2.55	0.41
1:C:247:MET:O	1:C:249:THR:N	2.53	0.41
1:C:266:VAL:HG21	1:C:399:LEU:HD23	2.02	0.41
1:C:712:ARG:HD3	1:C:712:ARG:HA	1.83	0.41
1:D:36:LEU:HB3	1:D:76:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:LYS:CE	1:D:808:GLU:HG2	2.47	0.41
1:D:711:SER:OG	1:D:712:ARG:N	2.53	0.41
1:A:181:GLY:HA2	1:A:184:ARG:NH1	2.35	0.41
1:A:288:GLN:O	1:A:291:SER:OG	2.26	0.41
1:A:332:VAL:HG21	1:A:368:TRP:CE3	2.56	0.41
1:A:815:LEU:HD13	1:A:820:ILE:HD11	2.02	0.41
1:B:219:LYS:HB2	1:B:247:MET:HE1	2.02	0.41
1:C:723:GLU:HA	1:C:726:GLN:OE1	2.19	0.41
1:D:744:PHE:HB2	1:D:799:TRP:NE1	2.35	0.41
2:E:146:GLU:HG3	2:E:147:LEU:HG	2.03	0.41
1:A:440:GLU:N	1:A:444:VAL:O	2.49	0.41
1:A:732:ASP:N	1:A:732:ASP:OD1	2.53	0.41
1:C:218:MET:HE2	1:C:218:MET:HB2	1.94	0.41
1:C:443:TYR:CD2	1:C:516:PRO:HG3	2.55	0.41
1:C:709:MET:O	1:C:713:ARG:N	2.43	0.41
1:D:740:THR:O	1:D:743:GLU:HG2	2.20	0.41
1:D:792:HIS:O	1:D:796:GLU:N	2.42	0.41
1:A:518:ALA:HB1	1:A:520:THR:CG2	2.41	0.41
1:B:212:LYS:NZ	1:B:241:GLN:OE1	2.52	0.41
1:B:451:LYS:HB2	1:B:452:PRO:HD3	2.01	0.41
1:B:558:PRO:HA	1:B:658:PHE:CE2	2.56	0.41
1:B:642:PHE:HA	1:C:620:MET:HE1	2.01	0.41
1:C:359:PHE:CE2	1:C:363:ILE:HD11	2.56	0.41
2:E:144:ASP:OD1	2:E:144:ASP:N	2.40	0.41
1:B:534:MET:CB	1:B:795:LYS:NZ	2.84	0.41
1:C:634:ARG:HG2	1:D:613:TRP:CZ2	2.56	0.41
1:C:701:THR:O	1:C:705:MET:HB2	2.20	0.41
1:D:536:LEU:HD13	1:D:764:TYR:HE2	1.84	0.41
1:D:575:SER:O	1:D:578:LEU:HB3	2.21	0.41
2:E:85:GLU:OE1	2:E:85:GLU:N	2.52	0.41
2:E:88:PHE:HD1	2:E:154:ALA:HB2	1.86	0.41
1:A:95:ALA:O	1:A:99:LEU:HD23	2.21	0.41
1:A:682:TYR:HD2	1:A:708:PHE:CD1	2.38	0.41
1:B:172:VAL:O	1:B:199:LEU:HA	2.21	0.41
1:B:534:MET:HB3	1:B:795:LYS:NZ	2.35	0.41
1:C:541:LEU:HB2	1:C:742:ILE:HD11	2.03	0.41
1:C:679:LYS:HE2	1:C:679:LYS:HA	2.03	0.41
1:C:682:TYR:HA	1:C:734:ALA:HB3	2.01	0.41
1:C:683:GLY:O	1:C:736:LEU:N	2.52	0.41
1:C:714:GLN:HA	1:C:717:LEU:HB2	2.03	0.41
1:D:438:ILE:O	1:D:440:GLU:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:GLU:HG2	1:D:744:PHE:HE2	1.85	0.41
1:D:654:ASN:O	1:D:657:ALA:N	2.53	0.41
1:D:783:LEU:HD23	2:E:111:PRO:HD2	2.02	0.41
1:A:685:VAL:HG23	1:A:718:VAL:O	2.20	0.41
1:B:555:PHE:CG	1:B:823:ILE:HD11	2.56	0.41
1:C:157:SER:OG	1:C:187:GLU:HB3	2.21	0.41
1:C:253:HIS:CD2	1:C:275:ASN:O	2.74	0.41
1:D:267:GLU:HB3	1:D:268:PRO:HD3	2.03	0.41
1:D:493:ASP:N	1:D:493:ASP:OD1	2.53	0.41
1:D:504:GLU:HB3	1:D:510:ALA:HB3	2.03	0.41
1:A:538:ILE:HG13	1:A:759:ILE:HB	2.02	0.41
1:C:44:TYR:CZ	1:C:82:LYS:HB3	2.55	0.41
1:C:632:SER:O	1:C:635:ILE:HG22	2.20	0.41
1:C:820:ILE:O	1:C:820:ILE:HG13	2.20	0.41
1:C:832:VAL:HG23	1:C:833:LEU:HD12	2.02	0.41
1:D:195:TYR:N	1:D:195:TYR:CD1	2.89	0.41
1:D:469:GLU:O	1:D:473:ILE:HG12	2.20	0.41
1:A:423:ASN:OD1	1:A:425:THR:HB	2.21	0.41
1:B:365:GLU:O	1:B:365:GLU:HG2	2.21	0.41
1:B:557:ASN:N	1:B:558:PRO:HD2	2.35	0.41
1:B:663:ARG:NH2	1:B:814:ALA:HB1	2.36	0.41
1:C:71:LEU:H	1:C:335:GLN:NE2	2.19	0.41
1:C:406:ASP:OD1	1:C:406:ASP:N	2.54	0.41
1:C:603:GLU:HG2	1:C:604:ASN:N	2.36	0.41
1:D:64:ILE:HD12	1:D:70:LEU:HD23	2.03	0.41
2:E:70:LYS:CD	2:E:72:CYS:SG	3.09	0.41
2:E:84:ILE:HD12	2:E:137:MET:HG2	2.03	0.41
1:A:467:LEU:HD21	1:A:478:TYR:CG	2.56	0.41
1:B:498:TRP:O	1:B:503:ARG:HB2	2.21	0.41
1:B:572:LEU:HD13	1:B:612:PHE:CE1	2.55	0.41
1:C:345:LEU:HD11	1:C:353:TRP:HB2	2.03	0.41
1:C:668:ILE:O	1:C:668:ILE:HG13	2.21	0.41
1:D:443:TYR:CG	1:D:516:PRO:HG3	2.56	0.41
2:E:75:ILE:HG23	2:E:138:TRP:CD1	2.56	0.41
1:A:741:THR:O	1:A:745:VAL:N	2.43	0.40
1:B:681:GLU:HG2	1:B:733:TYR:HA	2.02	0.40
1:B:740:THR:HB	1:B:799:TRP:CH2	2.56	0.40
1:C:710:SER:O	1:C:713:ARG:HB2	2.21	0.40
1:D:36:LEU:HA	1:D:36:LEU:HD12	1.90	0.40
1:D:536:LEU:N	1:D:762:LYS:O	2.54	0.40
1:A:248:MET:HE3	1:A:274:VAL:CG1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HD11	1:A:353:TRP:CD1	2.55	0.40
1:B:136:HIS:CD2	1:B:183:ILE:HD13	2.57	0.40
1:B:467:LEU:O	1:B:471:SER:N	2.50	0.40
1:C:140:ASP:N	1:D:86:TYR:HE2	2.14	0.40
1:C:578:LEU:HD23	1:C:611:SER:HB2	2.03	0.40
1:C:591:ASN:OD1	1:C:592:PRO:HD2	2.21	0.40
1:D:368:TRP:CG	1:D:369:GLU:N	2.89	0.40
1:A:163:LEU:HA	1:A:411:LEU:HD11	2.03	0.40
1:A:262:PHE:HB3	1:A:315:PHE:CZ	2.56	0.40
1:A:290:SER:O	1:A:293:ILE:HB	2.21	0.40
1:A:346:GLN:HB2	1:A:349:ARG:HB3	2.04	0.40
1:A:498:TRP:CH2	1:A:522:VAL:HG23	2.50	0.40
1:A:503:ARG:HA	1:A:506:ILE:HG22	2.02	0.40
1:A:634:ARG:HB3	1:B:613:TRP:CZ3	2.57	0.40
1:A:791:LEU:HA	1:A:794:MET:HE2	2.04	0.40
1:A:861:MET:SD	1:A:862:VAL:HG23	2.61	0.40
1:B:393:SER:OG	1:B:394:LEU:N	2.54	0.40
1:B:634:ARG:HB3	1:C:613:TRP:CZ2	2.57	0.40
1:C:331:SER:O	1:C:334:VAL:HG12	2.21	0.40
1:C:504:GLU:HB2	1:C:509:LYS:HE2	2.03	0.40
1:C:722:GLU:HG2	1:C:723:GLU:N	2.36	0.40
1:D:432:SER:H	1:D:477:THR:HB	1.85	0.40
1:D:522:VAL:O	1:D:525:LYS:HG2	2.20	0.40
2:E:49:VAL:HB	2:E:156:TYR:OH	2.21	0.40
2:E:366:ILE:O	2:E:370:VAL:HG23	2.21	0.40
1:A:368:TRP:CG	1:A:369:GLU:N	2.89	0.40
1:B:243:LEU:HD22	1:B:269:TYR:CE1	2.56	0.40
1:B:538:ILE:HD12	1:B:760:ASP:OD2	2.21	0.40
1:C:169:TRP:CE3	1:C:225:HIS:HB3	2.57	0.40
1:C:286:ASN:ND2	1:C:288:GLN:HB2	2.37	0.40
2:E:347:HIS:HB3	2:E:350:ILE:HB	2.03	0.40
1:A:589:TRP:HZ3	1:A:604:ASN:HA	1.87	0.40
1:B:203:GLN:O	1:B:214:LEU:HD11	2.21	0.40
1:B:539:SER:OG	1:B:754:GLN:NE2	2.39	0.40
1:C:128:PRO:HG2	1:C:359:PHE:CD2	2.52	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	833/908 (92%)	768 (92%)	65 (8%)	0	100	100
1	B	833/908 (92%)	754 (90%)	79 (10%)	0	100	100
1	C	833/908 (92%)	771 (93%)	62 (7%)	0	100	100
1	D	816/908 (90%)	744 (91%)	72 (9%)	0	100	100
2	E	141/525 (27%)	128 (91%)	13 (9%)	0	100	100
All	All	3456/4157 (83%)	3165 (92%)	291 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/794 (91%)	722 (99%)	4 (1%)	86	92
1	B	725/794 (91%)	724 (100%)	1 (0%)	93	97
1	C	725/794 (91%)	725 (100%)	0	100	100
1	D	708/794 (89%)	704 (99%)	4 (1%)	86	92
2	E	128/465 (28%)	128 (100%)	0	100	100
All	All	3012/3641 (83%)	3003 (100%)	9 (0%)	92	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	A	424	ILE
1	A	430	ASN
1	A	759	ILE
1	B	347	CYS
1	D	33	THR
1	D	484	GLU
1	D	487	LYS
1	D	548	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	253	HIS
1	A	497	GLN
1	A	593	HIS
1	B	111	HIS
1	B	136	HIS
1	B	348	ASN
1	B	367	HIS
1	B	792	HIS
1	C	129	HIS
1	C	131	GLN
1	C	253	HIS
1	C	499	ASN
1	D	98	GLN
1	D	302	GLN
1	D	747	GLN
1	D	802	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

18 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	F	1	1,3	14,14,15	0.41	0	17,19,21	1.09	2 (11%)
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	1.74	4 (23%)
3	BMA	F	3	3	11,11,12	0.22	0	15,15,17	0.61	0
3	NAG	G	1	1,3	14,14,15	0.56	0	17,19,21	0.82	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.76	0
3	BMA	G	3	3	11,11,12	0.32	0	15,15,17	0.89	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.63	0	17,19,21	1.53	3 (17%)
3	NAG	H	2	3	14,14,15	0.52	0	17,19,21	1.55	3 (17%)
3	BMA	H	3	3	11,11,12	0.31	0	15,15,17	0.80	0
3	NAG	I	1	1,3	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
3	NAG	I	2	3	14,14,15	0.45	0	17,19,21	1.48	3 (17%)
3	BMA	I	3	3	11,11,12	0.22	0	15,15,17	0.82	0
3	NAG	J	1	1,3	14,14,15	0.52	0	17,19,21	1.27	2 (11%)
3	NAG	J	2	3	14,14,15	0.51	0	17,19,21	0.93	0
3	BMA	J	3	3	11,11,12	0.37	0	15,15,17	1.04	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.40	0	17,19,21	1.01	1 (5%)
3	NAG	K	2	3	14,14,15	0.26	0	17,19,21	1.17	2 (11%)
3	BMA	K	3	3	11,11,12	0.24	0	15,15,17	0.60	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	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C2-N2-C7	-4.75	116.14	122.90
3	F	2	NAG	C2-N2-C7	4.07	128.69	122.90
3	H	1	NAG	O5-C1-C2	-3.69	105.46	111.29
3	H	1	NAG	C2-N2-C7	-3.40	118.06	122.90
3	I	1	NAG	O4-C4-C5	-3.32	101.06	109.30
3	K	1	NAG	O4-C4-C5	-3.24	101.25	109.30
3	I	2	NAG	O3-C3-C2	-3.24	102.77	109.47
3	F	2	NAG	C1-C2-N2	3.20	115.96	110.49
3	I	2	NAG	C1-O5-C5	3.07	116.36	112.19
3	F	2	NAG	O5-C1-C2	-3.05	106.47	111.29
3	J	1	NAG	C2-N2-C7	3.01	127.19	122.90
3	I	1	NAG	C2-N2-C7	2.91	127.05	122.90
3	K	2	NAG	C1-O5-C5	2.84	116.05	112.19
3	H	2	NAG	O5-C1-C2	-2.46	107.41	111.29
3	F	1	NAG	C3-C4-C5	-2.41	105.94	110.24
3	H	1	NAG	C4-C3-C2	-2.41	107.49	111.02
3	F	1	NAG	O5-C1-C2	-2.40	107.50	111.29
3	K	2	NAG	C2-N2-C7	2.38	126.29	122.90
3	F	2	NAG	C4-C3-C2	-2.31	107.64	111.02
3	H	2	NAG	C4-C3-C2	-2.30	107.64	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	O5-C1-C2	2.18	114.73	111.29
3	J	1	NAG	C4-C3-C2	-2.11	107.92	111.02
3	J	3	BMA	O2-C2-C3	-2.07	106.00	110.14
3	I	1	NAG	C1-O5-C5	2.05	114.98	112.19
3	G	3	BMA	O5-C5-C6	2.03	110.38	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	3	BMA	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C1-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	F	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C4-C5-C6-O6

*Continued on next page...*

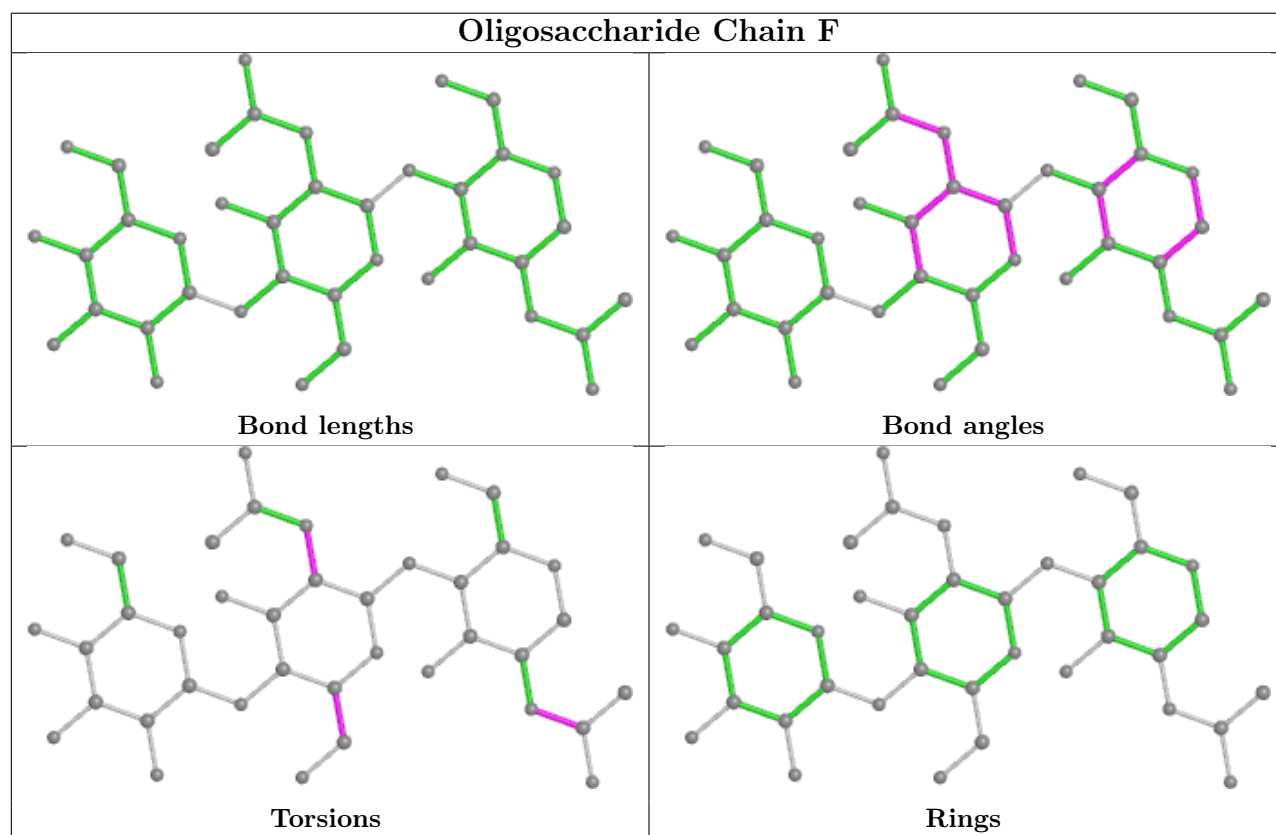
Continued from previous page...

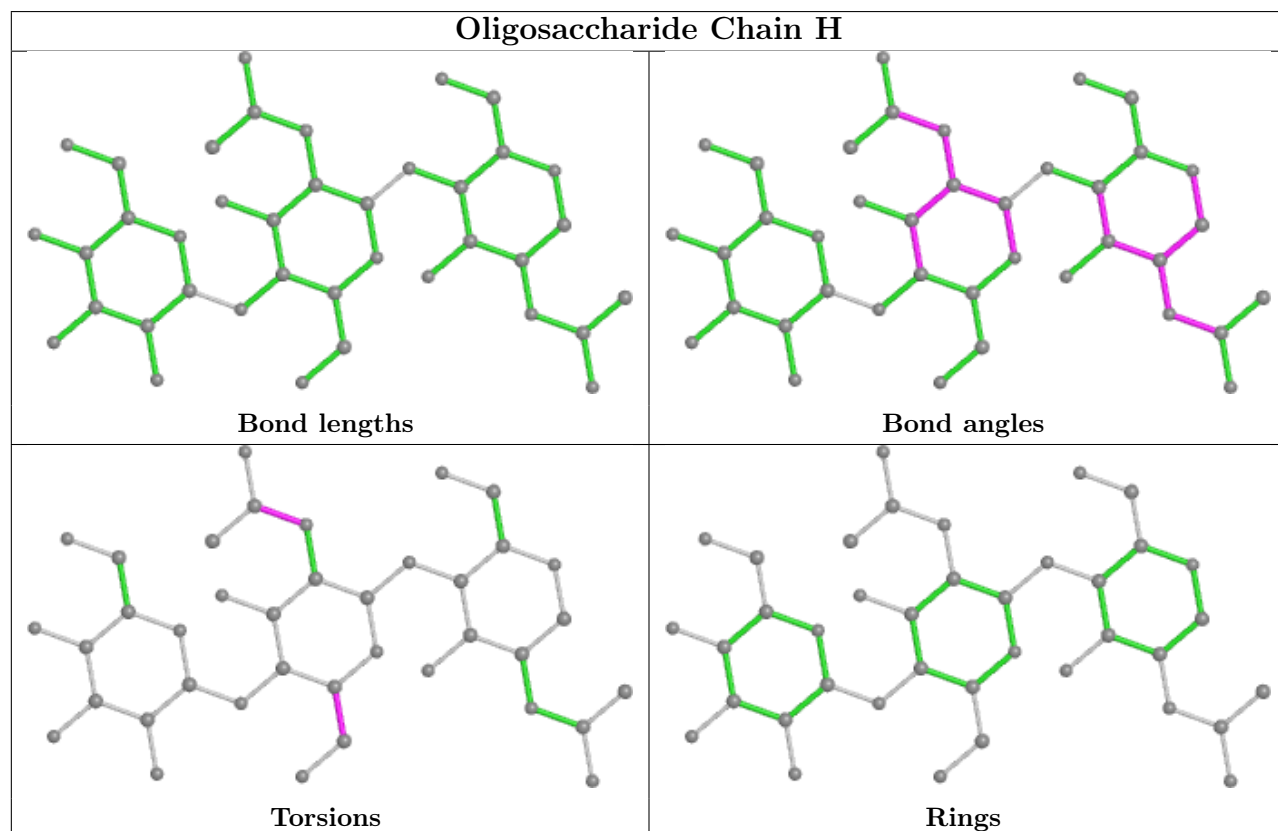
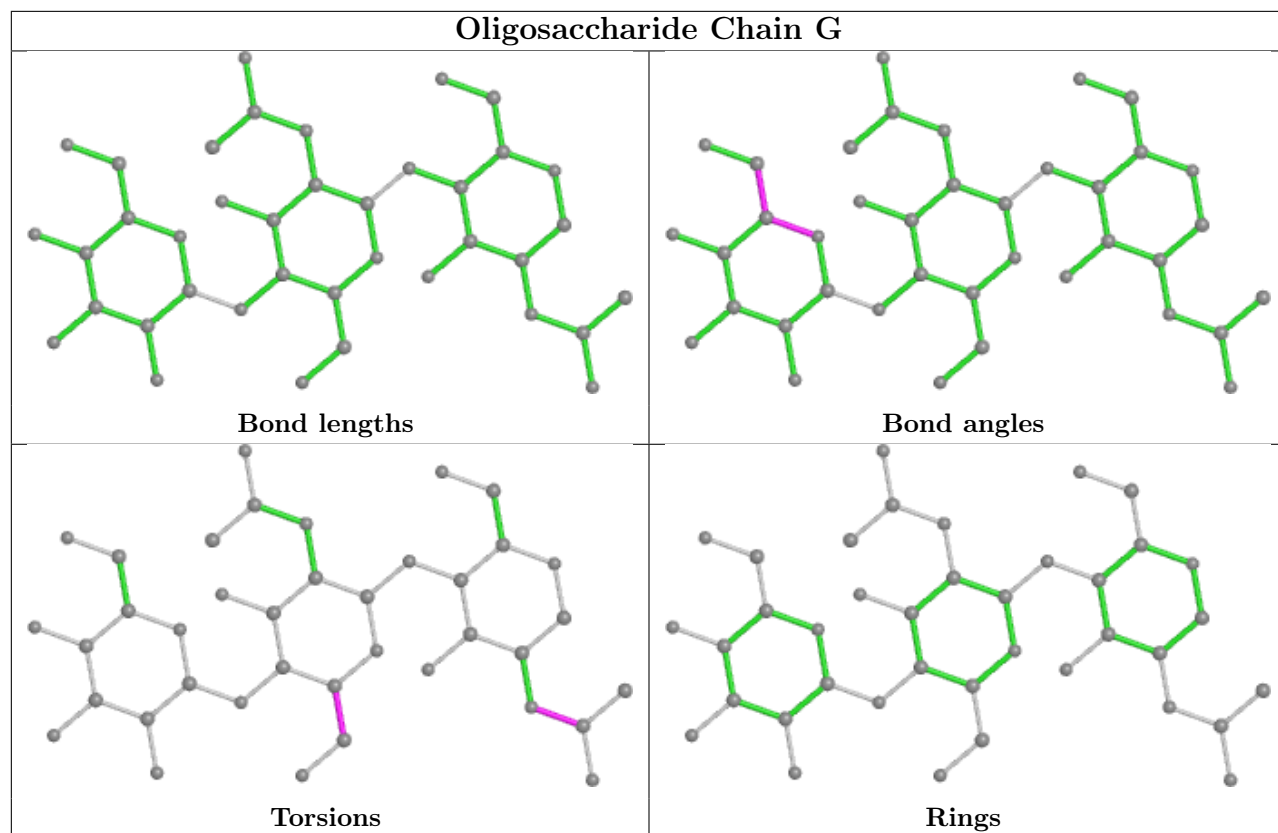
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7

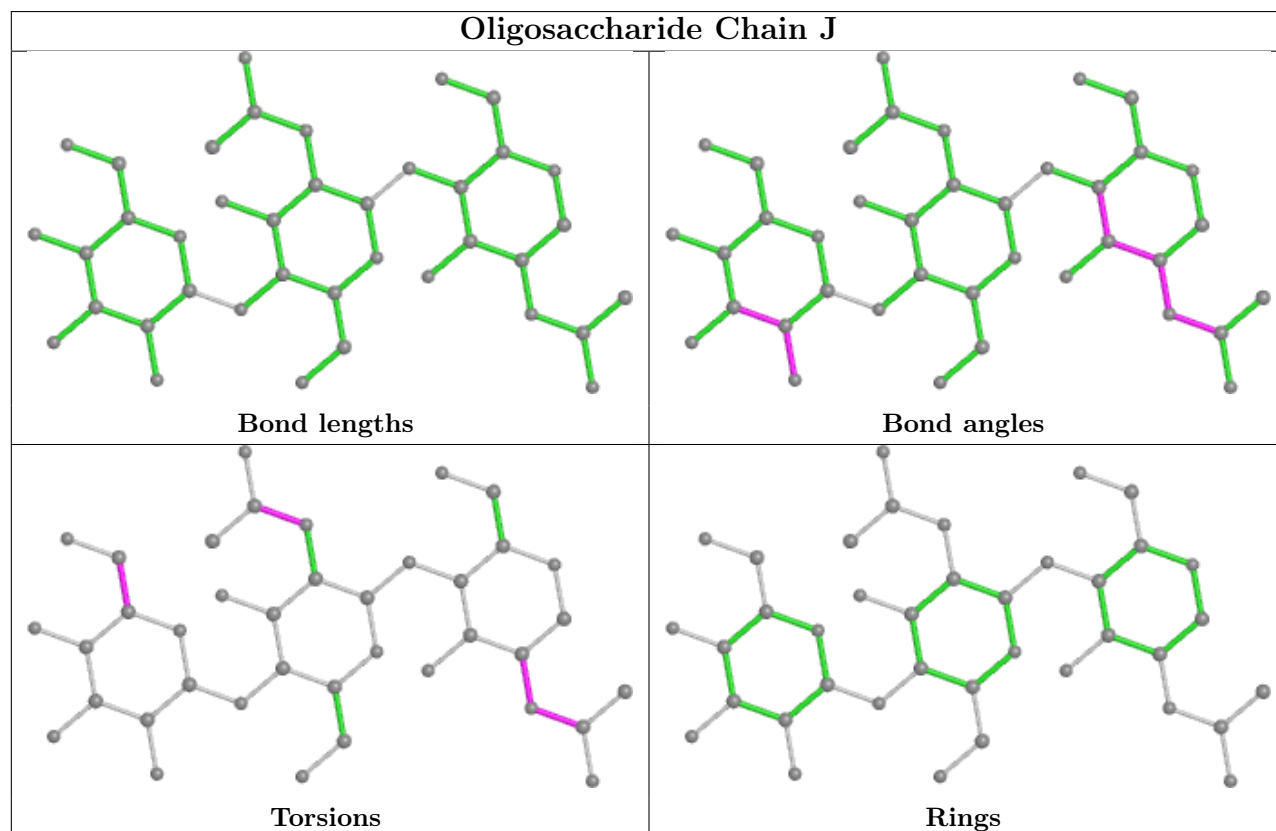
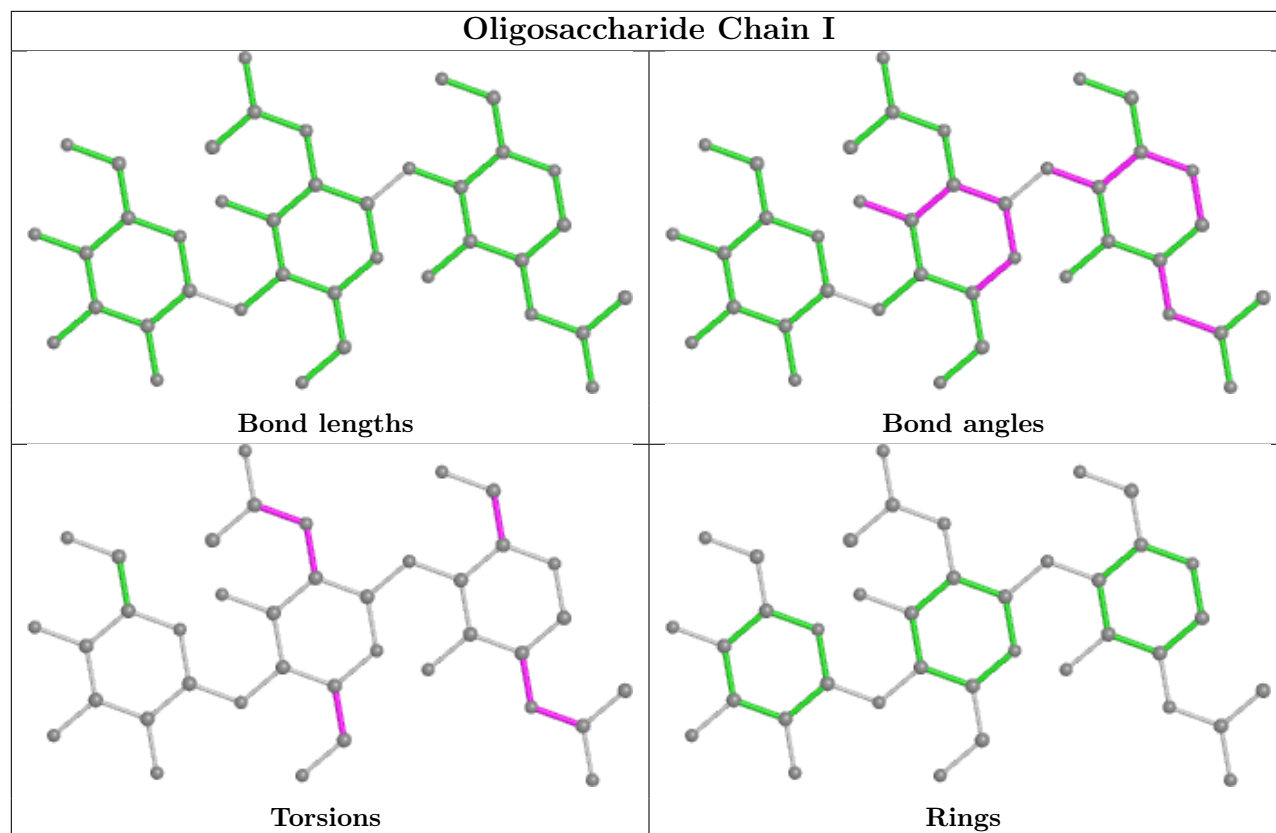
There are no ring outliers.

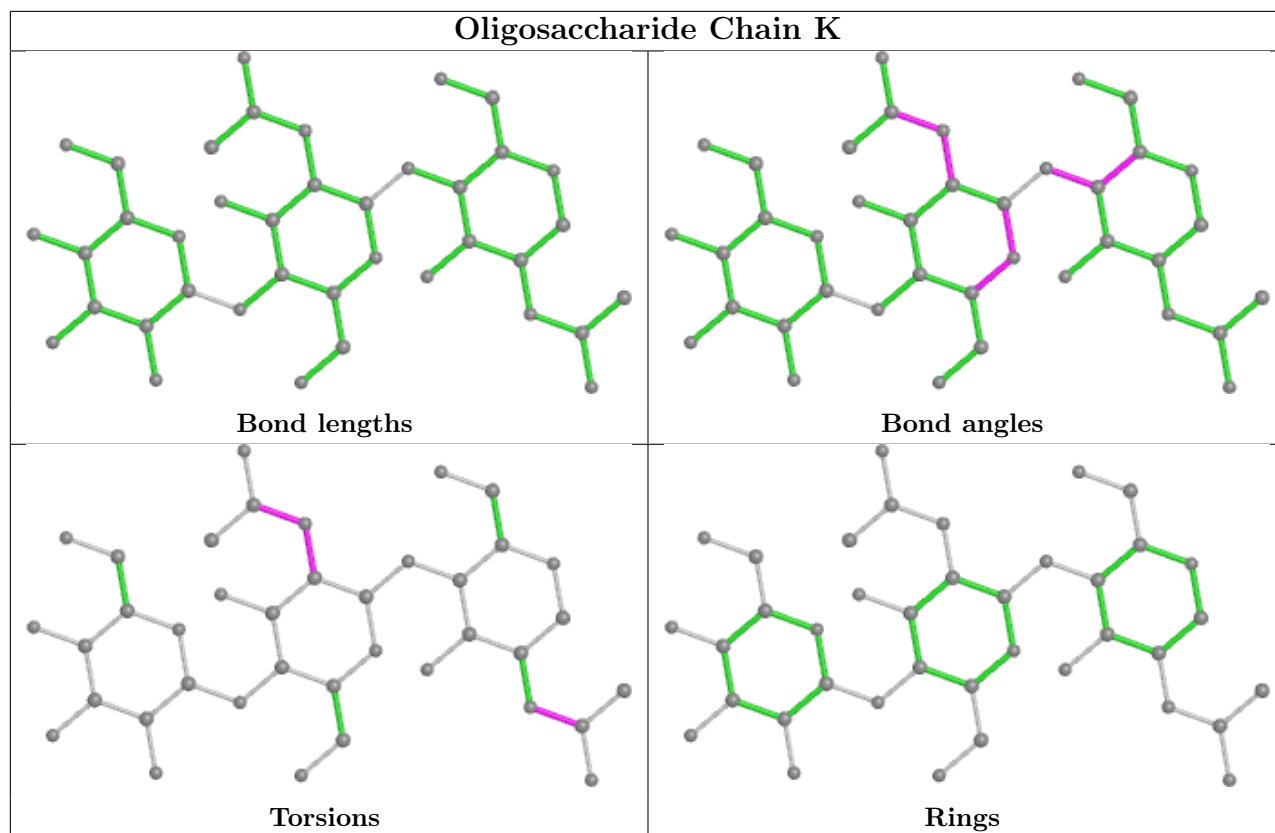
No monomer is involved in short contacts.

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](#)

11 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	1002	1	14,14,15	0.43	0	17,19,21	1.00	1 (5%)
4	NAG	A	1003	1	14,14,15	0.26	0	17,19,21	1.03	2 (11%)
4	NAG	C	1002	1	14,14,15	0.36	0	17,19,21	0.68	0
4	NAG	A	1004	1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
4	NAG	A	1001	1	14,14,15	0.30	0	17,19,21	0.72	0
4	NAG	B	1001	1	14,14,15	0.28	0	17,19,21	0.95	1 (5%)
4	NAG	A	1002	1	14,14,15	0.33	0	17,19,21	1.08	2 (11%)
4	NAG	C	1003	1	14,14,15	0.29	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1001	1	14,14,15	0.39	0	17,19,21	1.05	2 (11%)
4	NAG	B	1002	1	14,14,15	0.32	0	17,19,21	1.04	1 (5%)
4	NAG	D	1001	1	14,14,15	0.29	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
4	NAG	D	1002	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1004	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	NAG	C1-O5-C5	3.00	116.25	112.19
4	A	1002	NAG	C1-O5-C5	2.83	116.03	112.19
4	D	1002	NAG	C2-N2-C7	-2.58	119.22	122.90
4	C	1001	NAG	C2-N2-C7	-2.54	119.28	122.90
4	B	1001	NAG	C2-N2-C7	2.49	126.44	122.90
4	A	1003	NAG	C1-O5-C5	2.45	115.51	112.19
4	C	1001	NAG	C4-C3-C2	-2.40	107.50	111.02
4	A	1003	NAG	C2-N2-C7	2.33	126.22	122.90
4	A	1002	NAG	O5-C1-C2	-2.09	107.99	111.29
4	A	1004	NAG	O5-C1-C2	2.08	114.58	111.29
4	C	1003	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	C8-C7-N2-C2
4	A	1002	NAG	O7-C7-N2-C2
4	A	1003	NAG	C8-C7-N2-C2
4	A	1003	NAG	O7-C7-N2-C2
4	A	1004	NAG	C3-C2-N2-C7
4	A	1004	NAG	O7-C7-N2-C2
4	B	1001	NAG	C8-C7-N2-C2
4	B	1001	NAG	O7-C7-N2-C2
4	C	1003	NAG	C8-C7-N2-C2
4	C	1003	NAG	O7-C7-N2-C2
4	A	1004	NAG	C8-C7-N2-C2
4	C	1003	NAG	C1-C2-N2-C7
4	C	1001	NAG	C8-C7-N2-C2
4	C	1001	NAG	O7-C7-N2-C2
4	C	1002	NAG	C8-C7-N2-C2
4	B	1001	NAG	C1-C2-N2-C7
4	B	1002	NAG	C8-C7-N2-C2
4	C	1002	NAG	O7-C7-N2-C2
4	B	1002	NAG	O7-C7-N2-C2
4	A	1002	NAG	O5-C5-C6-O6
4	A	1004	NAG	O5-C5-C6-O6
4	D	1002	NAG	O5-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	A	1003	NAG	C3-C2-N2-C7
4	C	1003	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



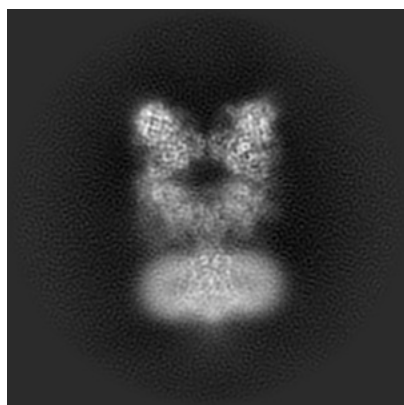
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31460. These allow visual inspection of the internal detail of the map and identification of artifacts.

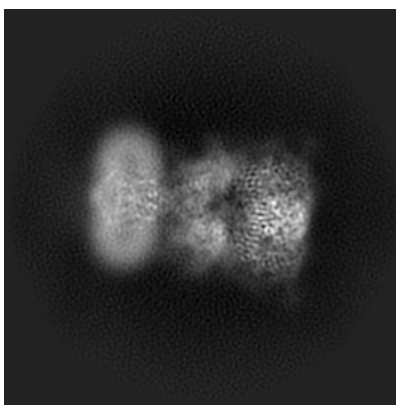
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

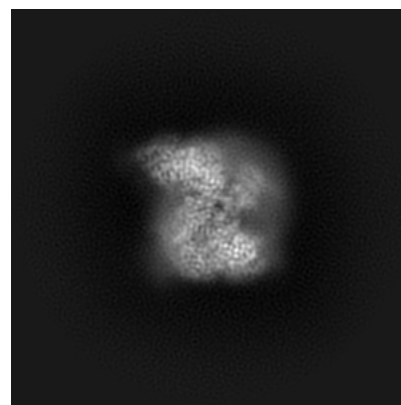
#### 6.1.1 Primary map



X



Y

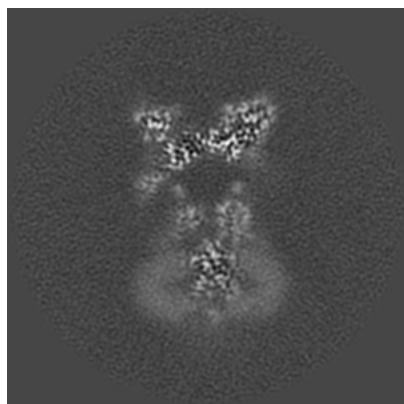


Z

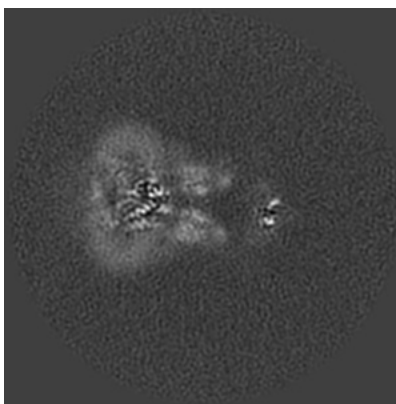
The images above show the map projected in three orthogonal directions.

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

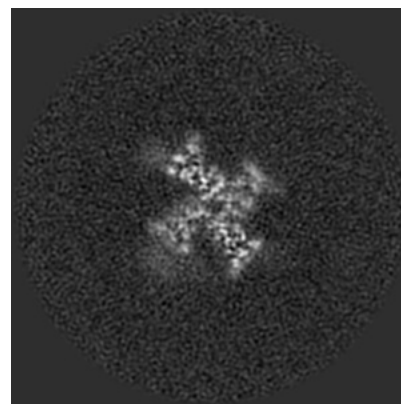
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

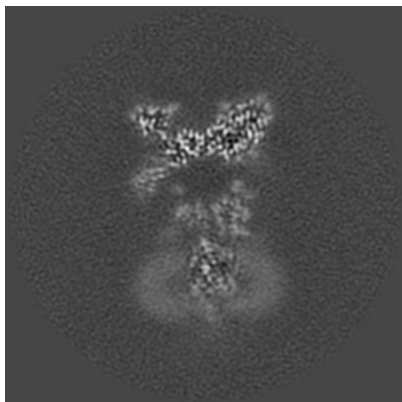


Z Index: 128

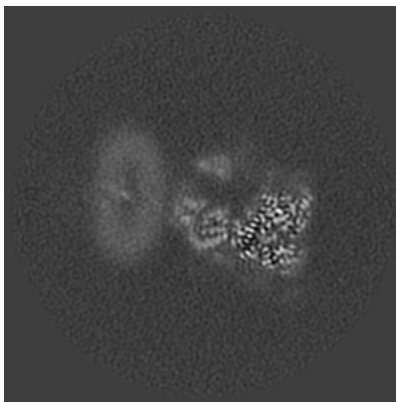
The images above show central slices of the map in three orthogonal directions.

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

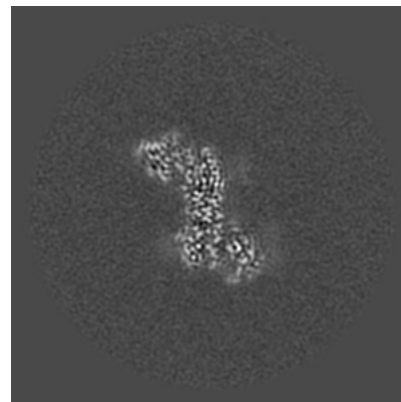
### 6.3.1 Primary map



X Index: 126



Y Index: 152

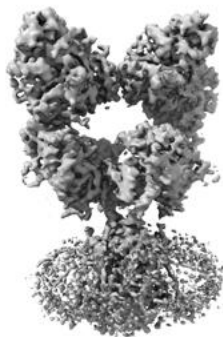


Z Index: 172

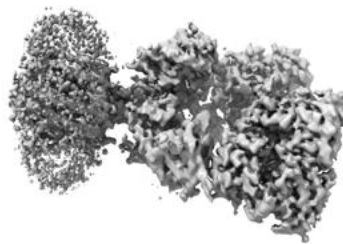
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.463. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

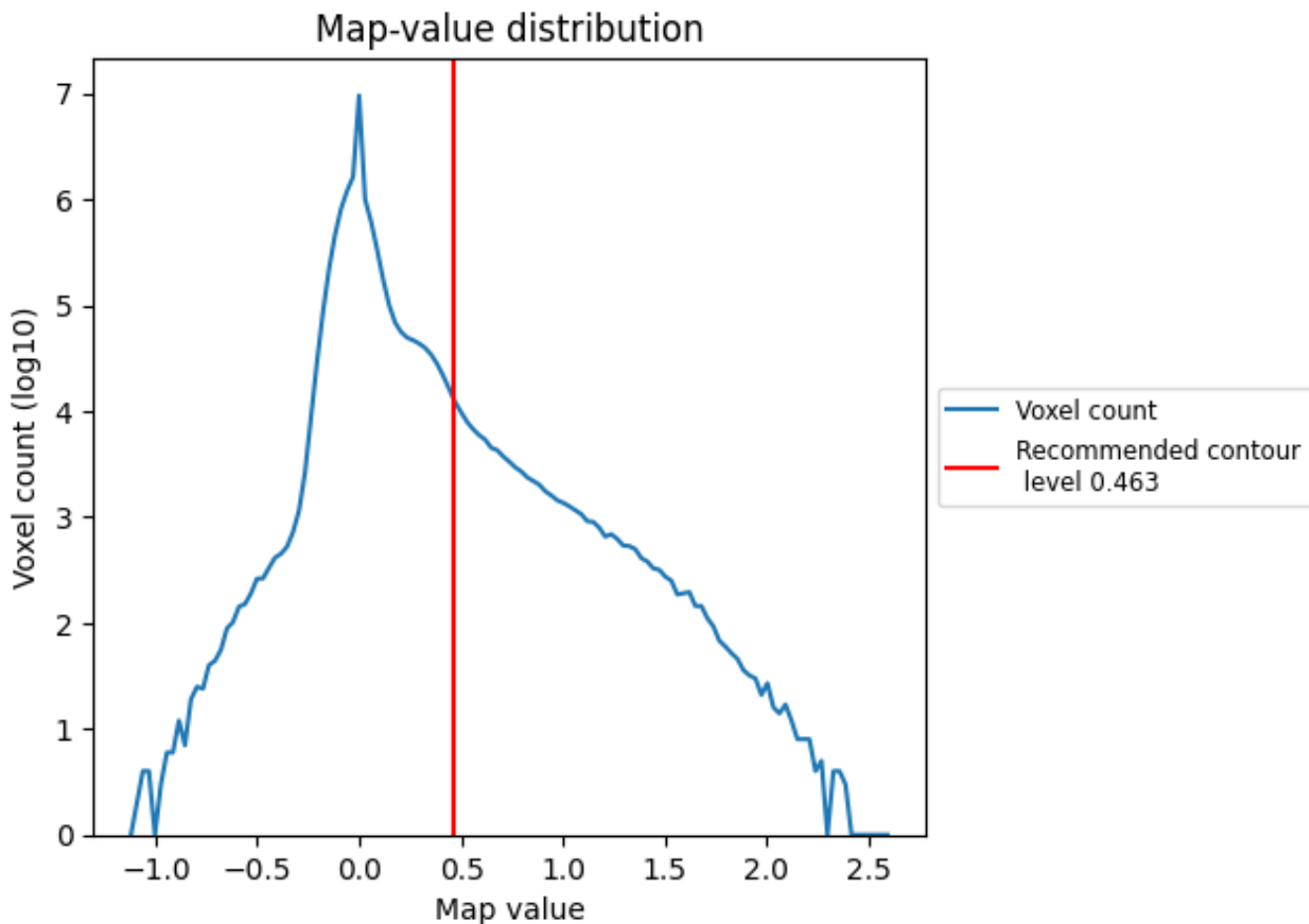
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

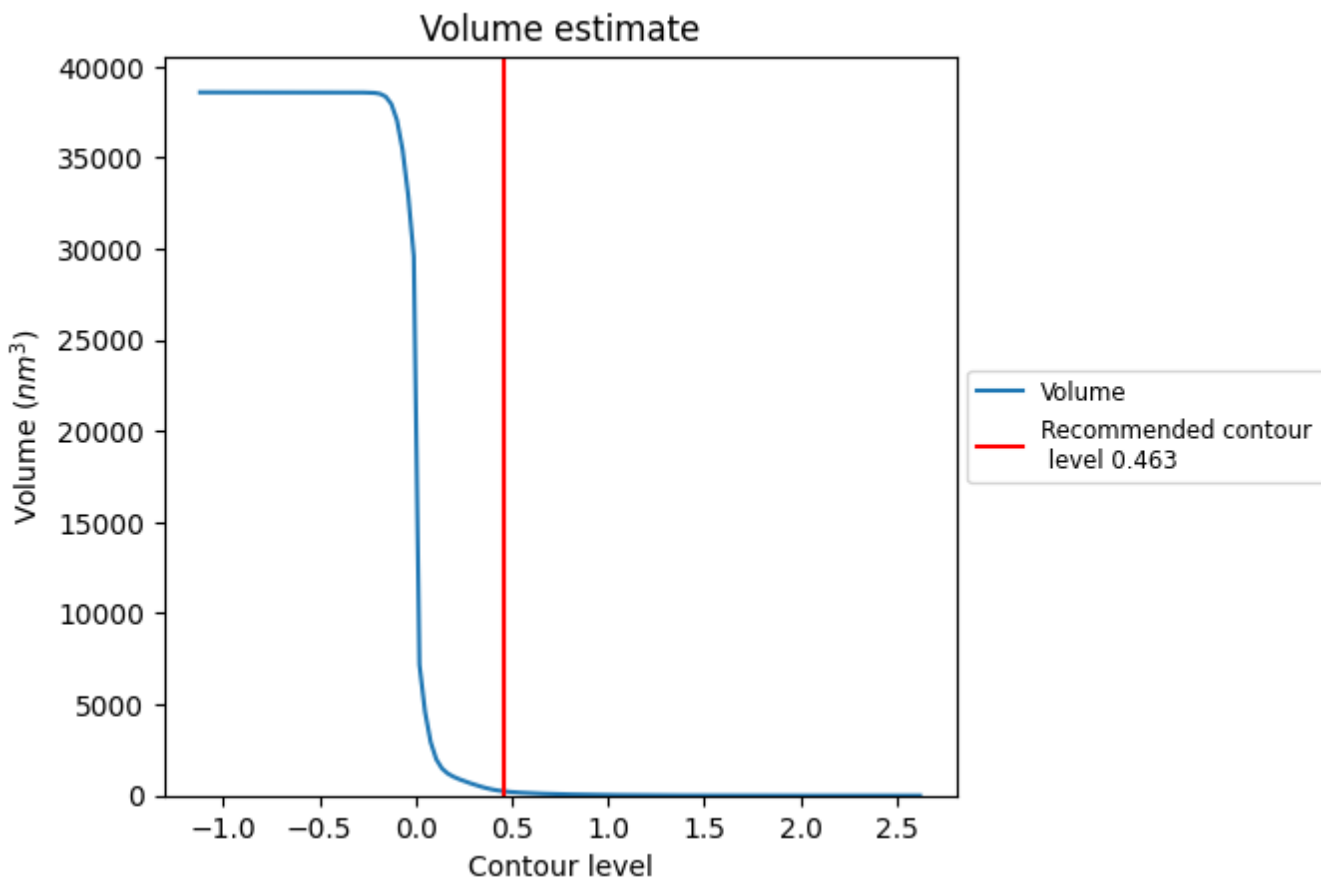
This section contains the results of statistical analysis of the map.

### 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.

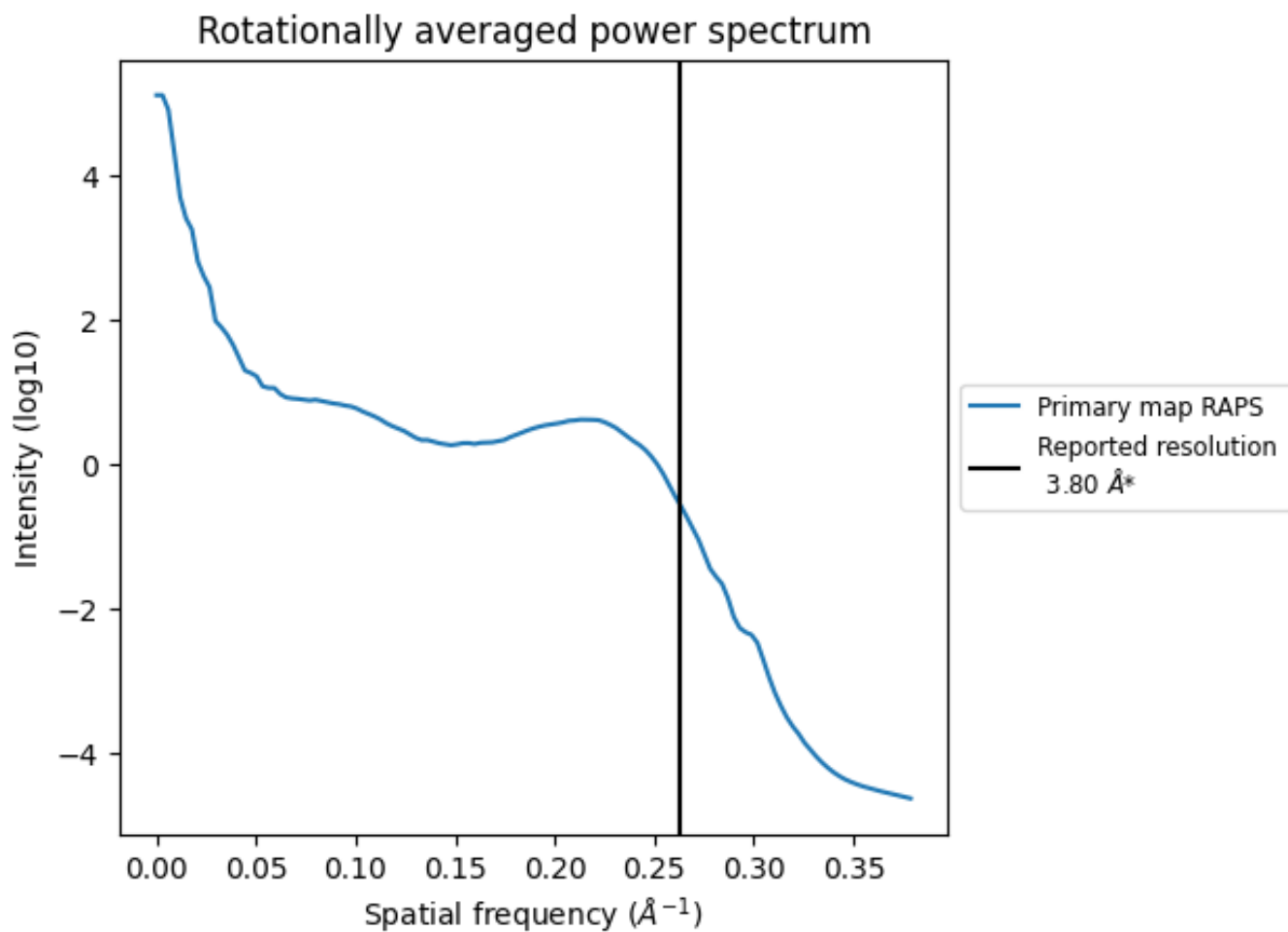
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm<sup>3</sup>; this corresponds to an approximate mass of 207 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 0.263 Å<sup>-1</sup>

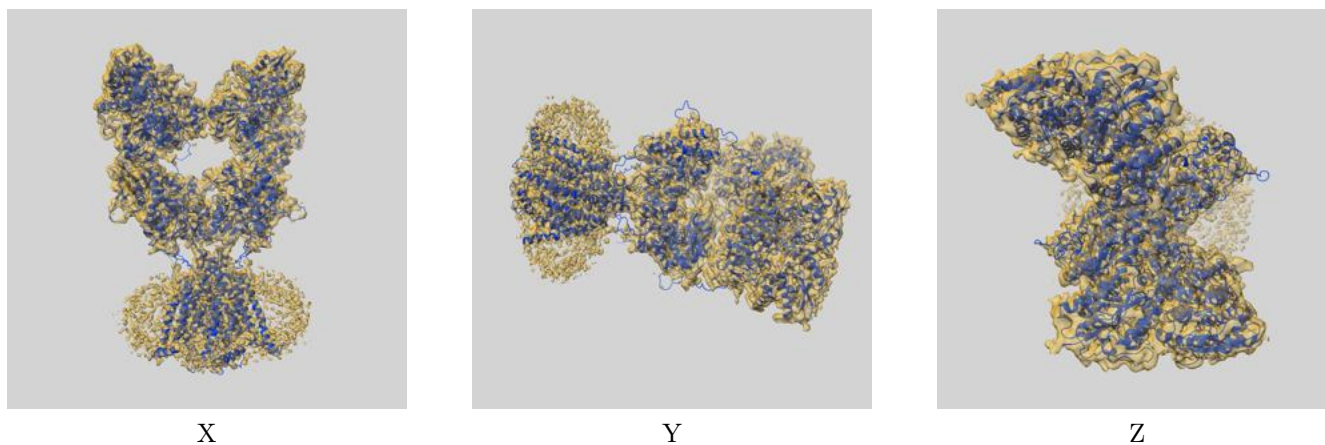
## 8 Fourier-Shell correlation

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-31460 and PDB model 7F57. Per-residue inclusion information can be found in section 3 on page 7.

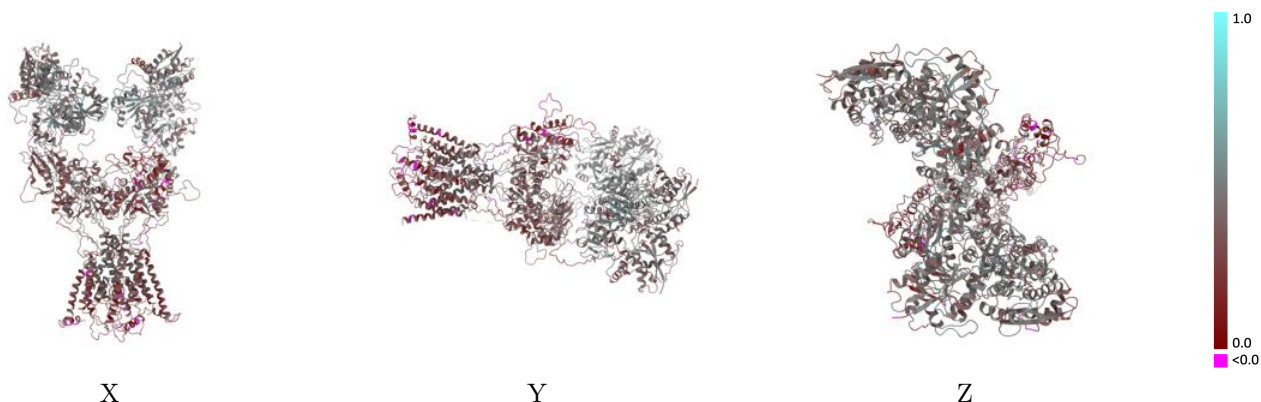
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.463 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

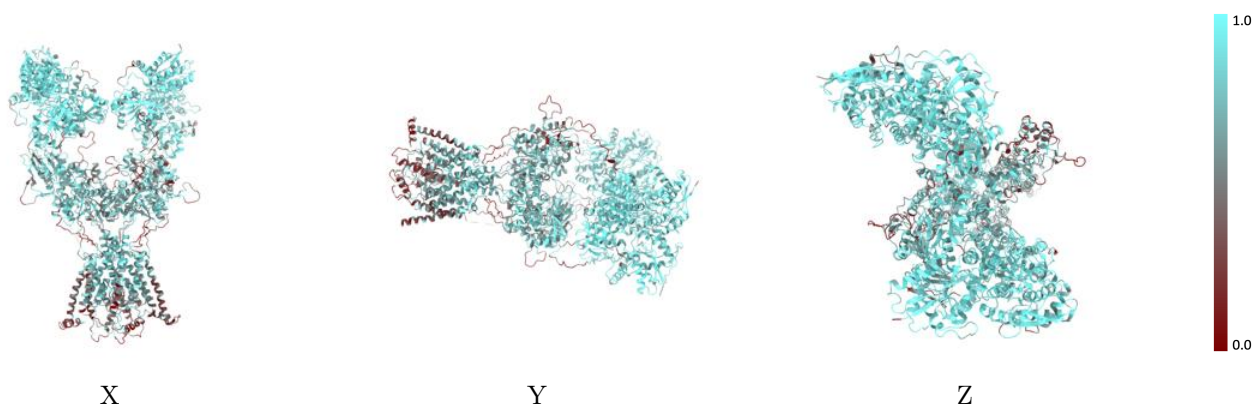


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



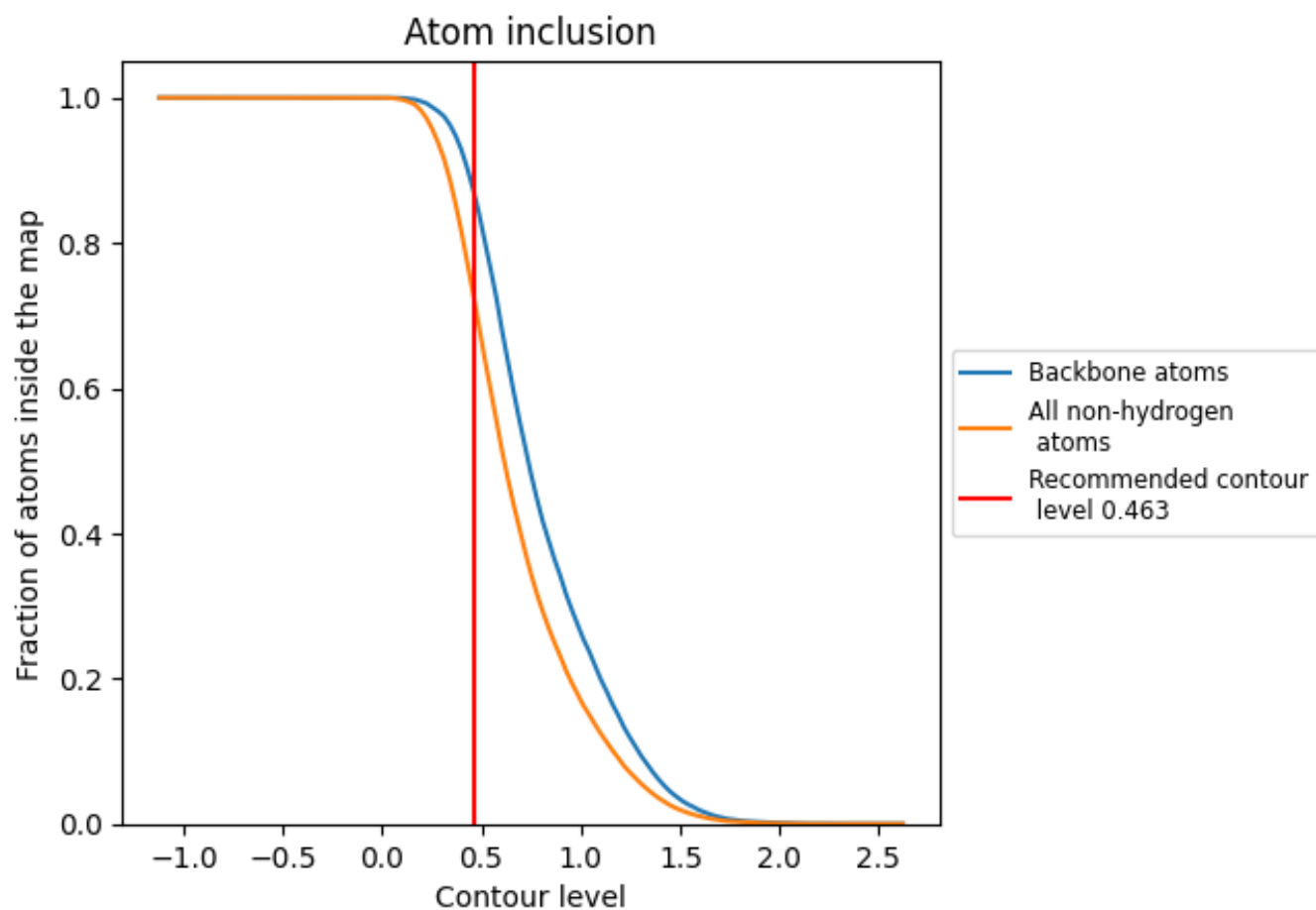
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.463).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.463) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7235	 0.3730
A	 0.7471	 0.3760
B	 0.7026	 0.3600
C	 0.7642	 0.3950
D	 0.7160	 0.3780
E	 0.5180	 0.2840
F	 0.6923	 0.4190
G	 0.7436	 0.3980
H	 0.8718	 0.4320
I	 0.6923	 0.4100
J	 0.6923	 0.4350
K	 0.6154	 0.2560

