Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 04:18 PM JST

PDB ID	:	7F56
EMDB ID	:	EMD-31459
Title	:	DNQX-bound GluK2-1xNeto2 complex, with asymmetric LBD
Authors	:	He, L.L.; Gao, Y.W.; Li, B.; Zhao, Y.
Deposited on	:	2021-06-21
Resolution	:	4.10 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:

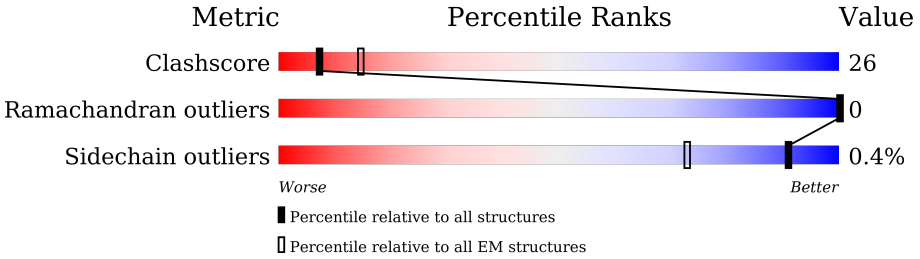
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

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 4.10 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	908	5%, 46%, 45%, 8%
1	B	908	7%, 50%, 42%, 8%
1	C	908	7%, 46%, 45%, 8%
1	D	908	6%, 49%, 41%, 10%
2	E	525	7%, 15%, 14%, 71%
3	F	3	33%, 67%
3	G	3	67%, 33%
3	H	3	100%

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Mol	Chain	Length	Quality of chain
3	I	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	NAG	G	1	-	-	X	-
3	NAG	H	1	X	-	-	-
4	NAG	B	1004	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27834 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	831	6578	4218	1095	1227	38	0	0
1	B	831	6575	4216	1095	1227	37	0	0
1	C	835	6604	4231	1102	1232	39	0	0
1	D	818	6471	4152	1077	1207	35	0	0

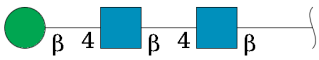
There are 12 discrepancies between the modelled and reference sequences:

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.

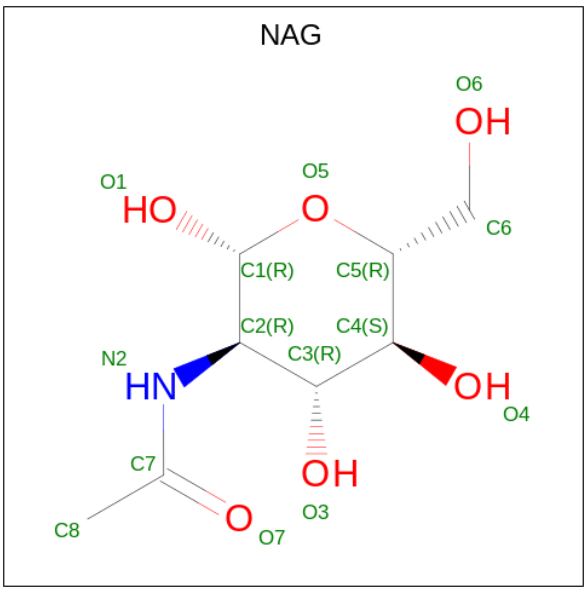
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	153	1226	793	208	217	8	0	0

- 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
3	H	3	Total 39	C 22	N 2	O 15	0	0
3	F	3	Total 39	C 22	N 2	O 15	0	0
3	G	3	Total 39	C 22	N 2	O 15	0	0
3	I	3	Total 39	C 22	N 2	O 15	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
4	A	1	Total 42	C 24	N 3	O 15	0
4	A	1	Total 42	C 24	N 3	O 15	0
4	A	1	Total 42	C 24	N 3	O 15	0
4	B	1	Total 56	C 32	N 4	O 20	0
4	B	1	Total 56	C 32	N 4	O 20	0

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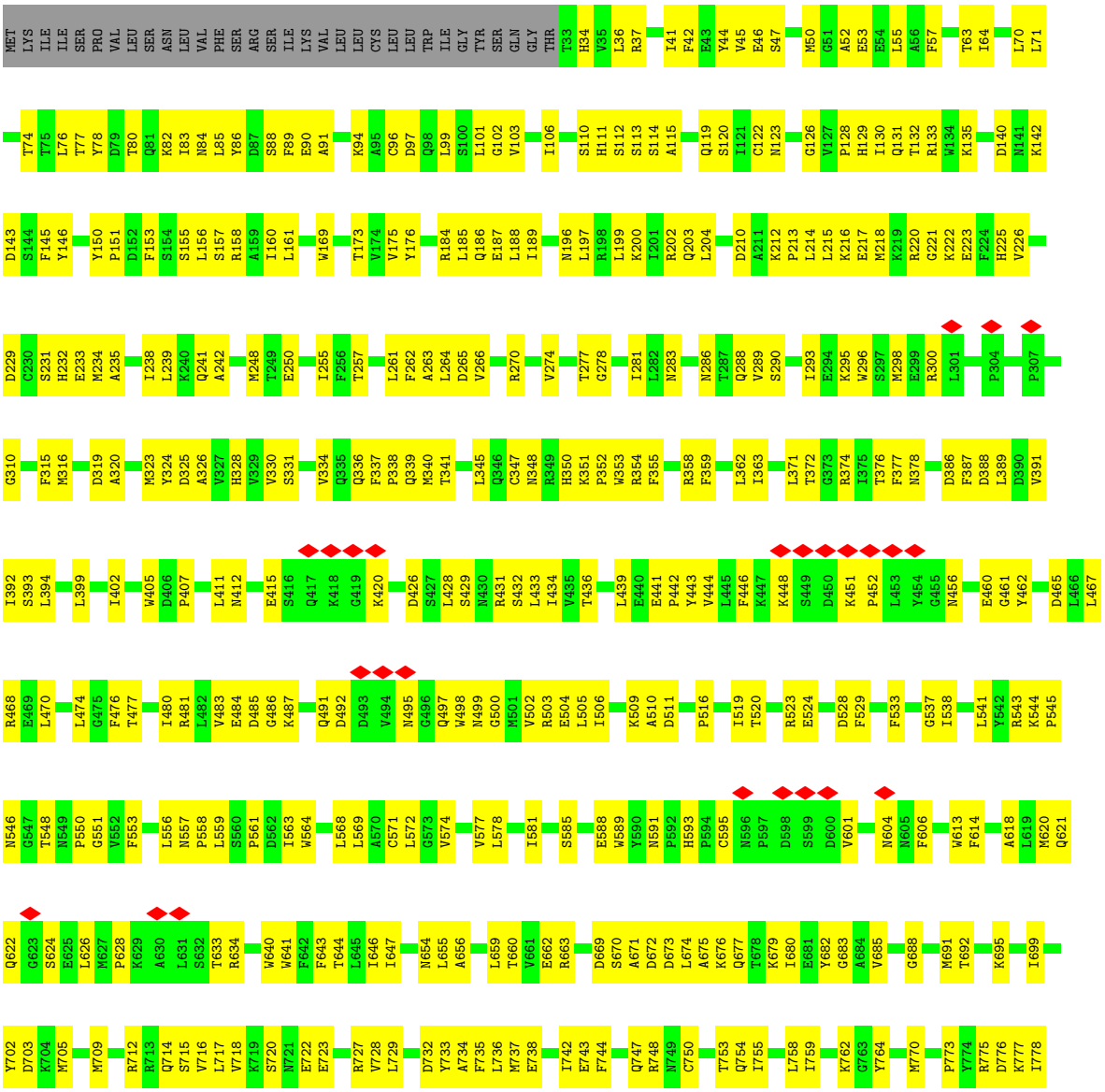
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	56	32	4	20	0
			Total	C	N	O	
4	B	1	56	32	4	20	0
			Total	C	N	O	
4	C	1	70	40	5	25	0
			Total	C	N	O	
4	C	1	70	40	5	25	0
			Total	C	N	O	
4	C	1	70	40	5	25	0
			Total	C	N	O	
4	C	1	70	40	5	25	0
			Total	C	N	O	
4	C	1	70	40	5	25	0
			Total	C	N	O	
4	D	1	56	32	4	20	0
			Total	C	N	O	
4	D	1	56	32	4	20	0
			Total	C	N	O	
4	D	1	56	32	4	20	0
			Total	C	N	O	
4	D	1	56	32	4	20	0

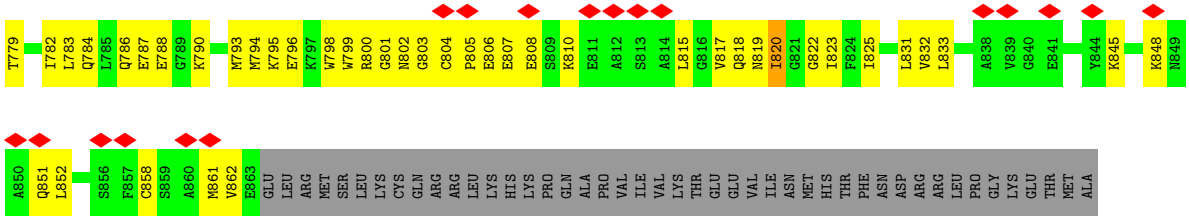
3 Residue-property plots (i)

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, kainate 2

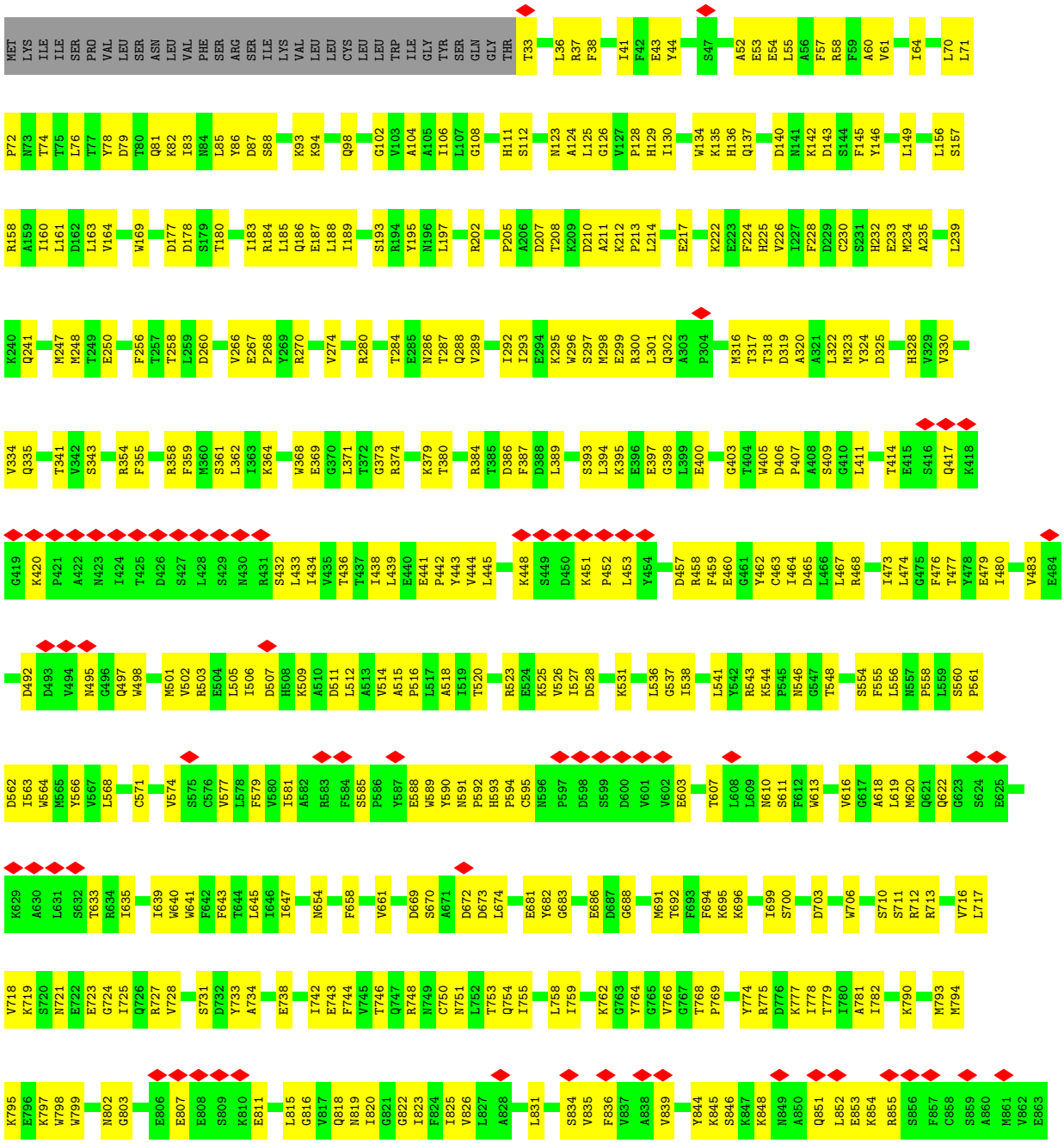
Chain A:

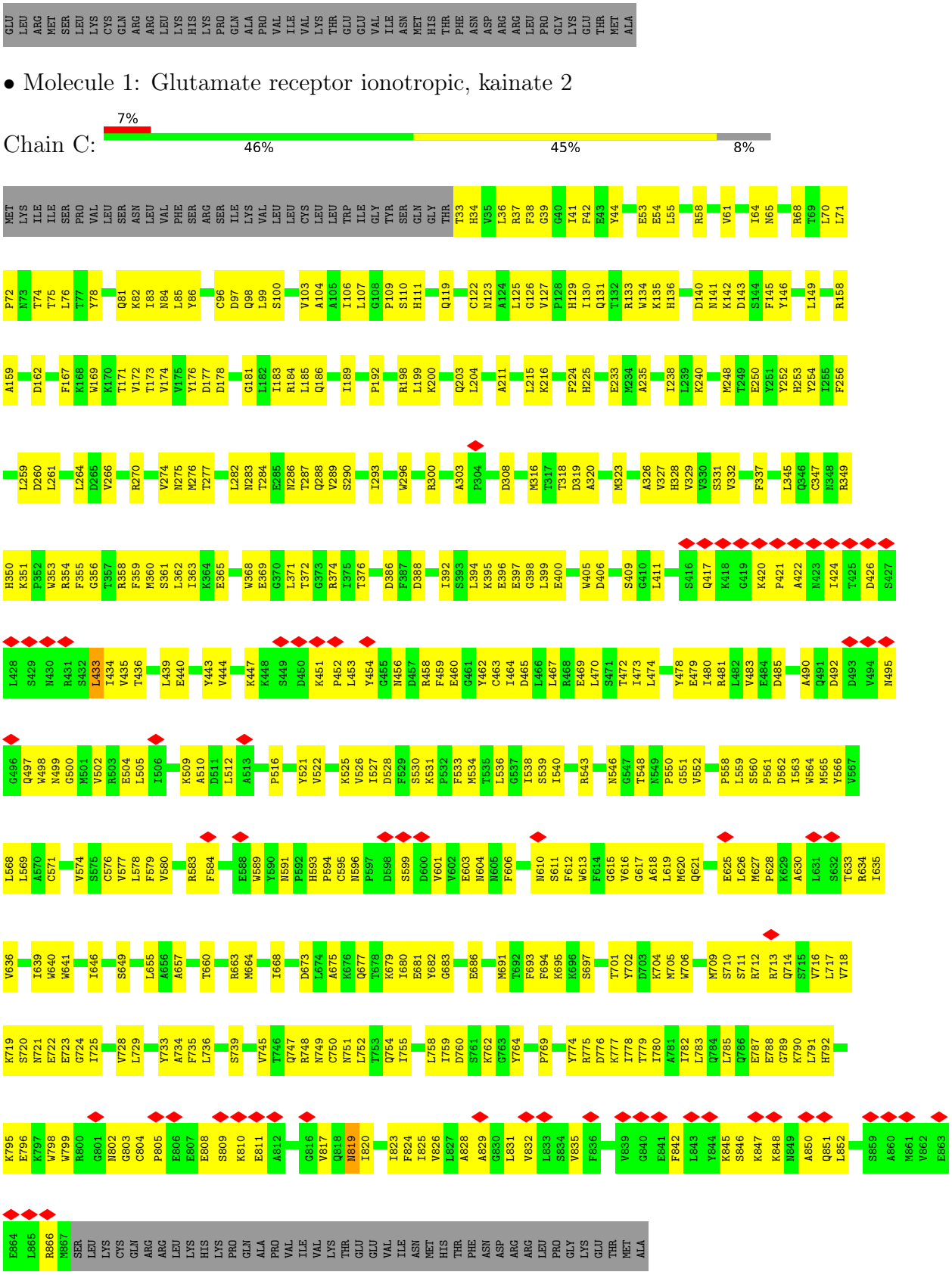




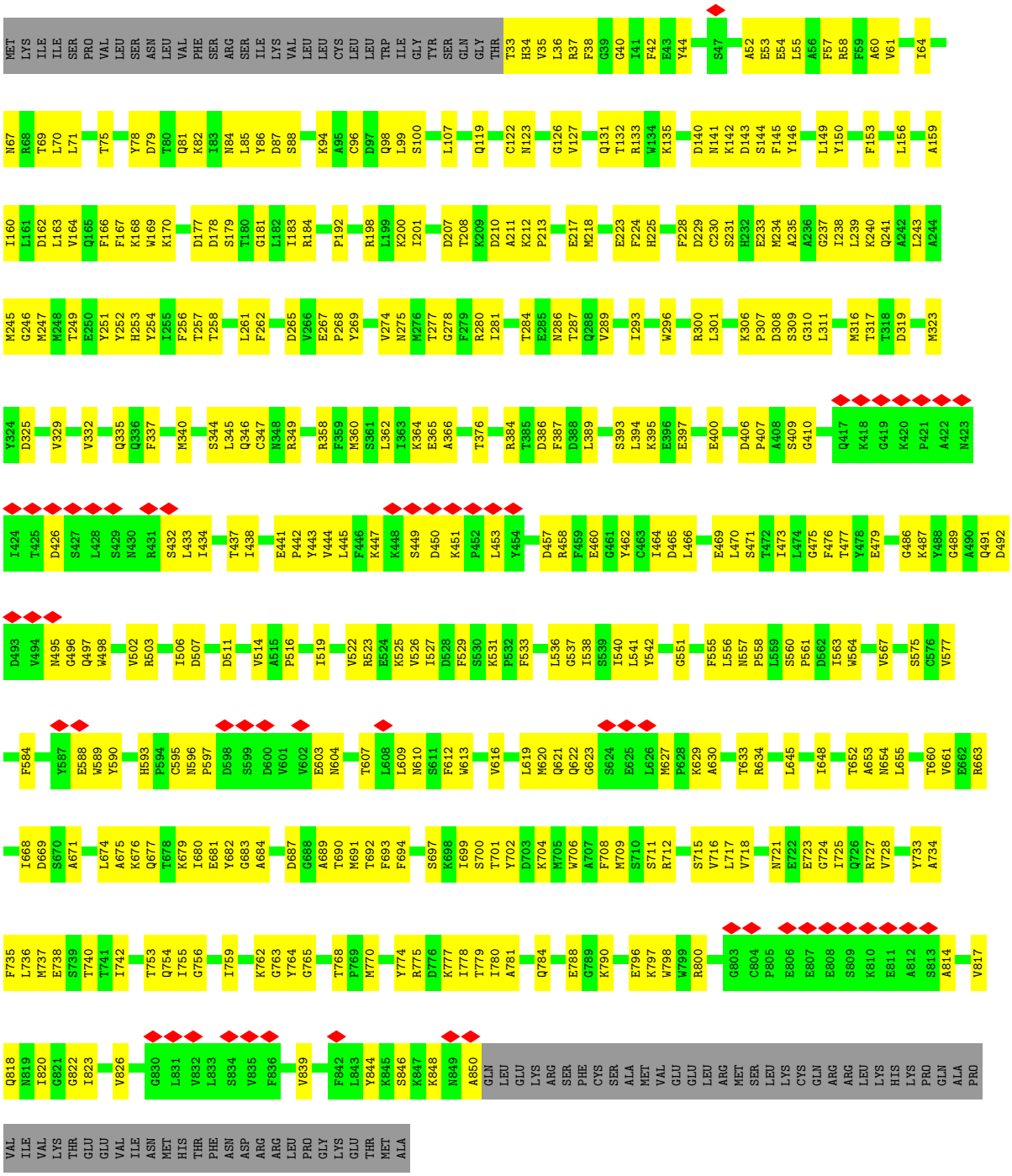
- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain B:



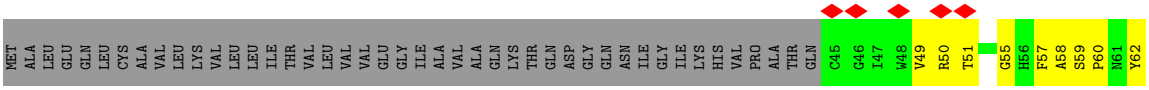

GLU LEU ARG MET SER LEU LYS CYS GLN ARG ARG LEU LYS HIS LYS PRO GLN ALA PRO VAL ILE VAL LYS THR GLU GLU VAL ILE ASN MET HIS THR PHE ASN ASP ARG ARG LEU PRO GLY LYS GLU THR MET ALA
• Molecule 1: Glutamate receptor ionotropic, kainate 2
Chain C:
7%
46%
45%
8%
• Molecule 1: Glutamate receptor ionotropic, kainate 2

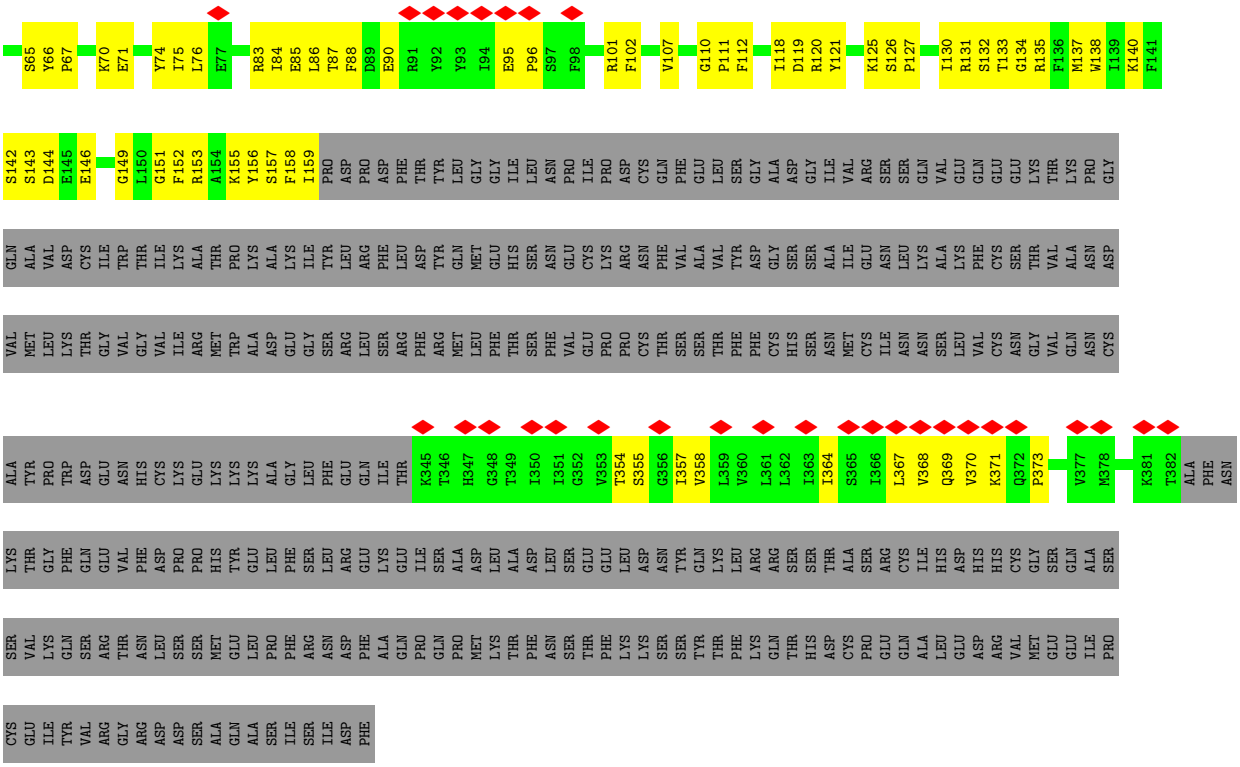
Chain D:



• Molecule 2: Neuropilin and tolloid-like protein 2

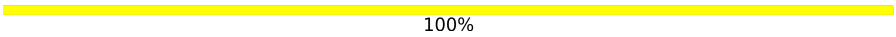
Chain E:





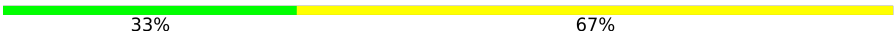
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• 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:



• 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:

• 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:

NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90580	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 ($e^-/Å^2$)	60	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	2.109	Depositor
Minimum map value	-0.620	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.455	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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, BMA

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	0.41	0/6727	0.58	0/9110
1	B	0.44	0/6724	0.57	0/9107
1	C	0.46	0/6752	0.59	0/9142
1	D	0.48	0/6619	0.59	0/8968
2	E	0.41	0/1258	0.55	0/1699
All	All	0.45	0/28080	0.58	0/38026

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	6578	0	6556	394	0
1	B	6575	0	6546	345	0
1	C	6604	0	6578	390	0
1	D	6471	0	6442	327	0
2	E	1226	0	1220	79	0
3	F	39	0	34	0	0
3	G	39	0	34	11	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	1	0
4	A	42	0	39	6	0
4	B	56	0	52	8	0
4	C	70	0	65	1	0
4	D	56	0	52	5	0
All	All	27834	0	27686	1460	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 26.

All (1460) 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:275:ASN:ND2	4:D:1003:NAG:C1	1.70	1.52
1:A:378:ASN:CG	3:G:1:NAG:C8	1.83	1.46
1:A:412:ASN:HD21	4:A:1003:NAG:C1	1.29	1.44
1:C:216:LYS:HE3	2:E:102:PHE:CE2	1.56	1.41
1:A:412:ASN:ND2	4:A:1003:NAG:C1	1.81	1.39
1:A:378:ASN:CG	3:G:1:NAG:H82	1.44	1.23
1:A:378:ASN:OD1	3:G:1:NAG:H83	1.09	1.20
1:A:432:SER:HA	1:A:477:THR:CG2	1.69	1.20
1:C:420:LYS:HD2	1:C:421:PRO:HD2	1.18	1.16
1:C:709:MET:SD	1:C:717:LEU:HD21	1.85	1.16
1:A:378:ASN:CG	3:G:1:NAG:H83	1.56	1.11
1:A:378:ASN:OD1	3:G:1:NAG:C8	1.93	1.09
1:A:378:ASN:ND2	3:G:1:NAG:H82	1.70	1.06
1:A:432:SER:HA	1:A:477:THR:HG22	1.36	1.05
1:B:417:GLN:HG3	4:B:1004:NAG:O6	1.57	1.03
1:A:432:SER:CA	1:A:477:THR:CG2	2.39	1.00
1:C:713:ARG:O	1:C:714:GLN:HG2	1.62	0.98
1:D:296:TRP:HE1	1:D:300:ARG:HH11	0.99	0.98
2:E:90:GLU:HB2	2:E:126:SER:HB2	1.46	0.97
1:A:432:SER:CB	1:A:477:THR:CG2	2.45	0.94
1:A:140:ASP:HB2	1:B:86:TYR:CZ	2.02	0.94
1:C:216:LYS:CE	2:E:102:PHE:CE2	2.51	0.93
1:C:136:HIS:HD2	1:C:183:ILE:HD13	1.33	0.92
1:C:216:LYS:HE3	2:E:102:PHE:HE2	1.30	0.91
1:A:378:ASN:CB	3:G:1:NAG:C8	2.49	0.91
1:A:432:SER:HA	1:A:477:THR:HG23	1.53	0.90
1:A:36:LEU:HB3	1:A:76:LEU:HD22	1.54	0.90
1:C:136:HIS:CD2	1:C:183:ILE:HD13	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:CB	3:G:1:NAG:H82	2.04	0.88
1:C:71:LEU:HB3	1:C:74:THR:HB	1.57	0.86
1:A:412:ASN:CG	4:A:1003:NAG:C1	2.42	0.86
1:B:434:ILE:H	1:B:511:ASP:HB2	1.40	0.86
1:A:533:PHE:HB3	1:A:782:ILE:HD11	1.55	0.85
1:D:817:VAL:HA	1:D:820:ILE:HG22	1.59	0.85
1:C:718:VAL:HG12	1:C:720:SER:H	1.40	0.85
1:A:432:SER:OG	1:A:477:THR:HG23	1.76	0.85
1:C:551:GLY:HA2	1:C:820:ILE:HA	1.59	0.84
1:C:568:LEU:O	1:C:571:CYS:SG	2.36	0.83
1:A:432:SER:CB	1:A:477:THR:HG21	2.08	0.83
1:C:107:LEU:HD23	1:C:130:ILE:HB	1.61	0.83
1:D:360:MET:HG3	1:D:364:LYS:HE3	1.60	0.82
1:A:432:SER:HB2	1:A:477:THR:HG21	1.62	0.82
1:C:483:VAL:HG11	1:C:500:GLY:HA2	1.62	0.81
1:A:520:THR:HG23	1:A:523:ARG:H	1.46	0.80
1:C:502:VAL:HG13	1:C:527:ILE:HD11	1.63	0.80
1:A:391:VAL:HG13	1:A:402:ILE:HG13	1.64	0.80
1:C:470:LEU:HD22	1:C:778:ILE:HD11	1.63	0.80
1:A:296:TRP:HE1	1:A:300:ARG:HH11	1.27	0.80
1:C:435:VAL:HG21	1:C:467:LEU:HD11	1.63	0.80
1:D:296:TRP:HE1	1:D:300:ARG:NH1	1.78	0.79
1:B:845:LYS:HA	1:B:848:LYS:HE2	1.65	0.79
1:A:606:PHE:CE1	1:A:626:LEU:HB3	2.17	0.79
1:A:548:THR:HG23	1:A:548:THR:O	1.81	0.79
2:E:112:PHE:HB2	2:E:138:TRP:HB3	1.64	0.79
1:A:432:SER:CB	1:A:477:THR:HG23	2.13	0.78
1:A:677:GLN:HE21	1:A:679:LYS:HB2	1.48	0.78
1:C:395:LYS:HG3	1:C:400:GLU:HB2	1.64	0.78
1:C:591:ASN:HB3	1:C:596:ASN:HD22	1.48	0.78
1:C:561:PRO:HA	1:C:564:TRP:HD1	1.49	0.77
1:B:498:TRP:H	1:B:503:ARG:HD3	1.48	0.77
1:C:420:LYS:CD	1:C:421:PRO:HD2	2.08	0.77
1:A:432:SER:CA	1:A:477:THR:HG23	2.11	0.77
1:C:216:LYS:HE3	2:E:102:PHE:CD2	2.17	0.77
1:C:808:GLU:HG2	1:C:809:SER:H	1.51	0.76
1:D:486:GLY:O	1:D:487:LYS:HG2	1.85	0.76
1:B:433:LEU:HD13	1:B:476:PHE:HB2	1.68	0.76
1:C:808:GLU:HG2	1:C:809:SER:N	2.01	0.76
1:D:486:GLY:O	1:D:487:LYS:HD3	1.86	0.76
1:C:61:VAL:HA	1:C:64:ILE:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:NH2	1:A:484:GLU:OE2	2.20	0.75
1:C:172:VAL:HG13	1:C:199:LEU:HD13	1.65	0.75
1:C:198:ARG:HG2	1:D:198:ARG:HH22	1.50	0.75
2:E:107:VAL:HG12	2:E:118:ILE:HD12	1.66	0.75
2:E:70:LYS:H	2:E:143:SER:HB2	1.52	0.74
1:B:85:LEU:HG	1:B:86:TYR:CD2	2.22	0.74
1:B:728:VAL:HA	1:B:733:TYR:HB3	1.68	0.74
1:D:486:GLY:O	1:D:487:LYS:CG	2.35	0.74
1:B:710:SER:HA	1:B:713:ARG:HE	1.51	0.74
1:D:607:THR:H	1:D:610:ASN:HB2	1.51	0.74
1:A:161:LEU:HD21	1:A:188:LEU:HA	1.70	0.74
1:A:845:LYS:HA	1:A:848:LYS:HE2	1.70	0.74
1:A:52:ALA:HA	1:A:55:LEU:HD12	1.69	0.74
1:D:486:GLY:O	1:D:487:LYS:CD	2.36	0.74
1:A:37:ARG:NH1	1:A:102:GLY:O	2.21	0.74
1:C:456:ASN:HA	1:C:480:ILE:HG22	1.69	0.74
1:C:434:ILE:HG23	1:C:479:GLU:HB3	1.70	0.73
1:D:35:VAL:HG22	1:D:75:THR:HB	1.70	0.73
1:B:300:ARG:NH1	1:B:316:MET:SD	2.62	0.73
1:C:823:ILE:HG13	1:C:826:VAL:HG13	1.70	0.73
1:A:99:LEU:HD11	1:A:345:LEU:HB2	1.70	0.73
1:C:596:ASN:O	1:D:593:HIS:NE2	2.20	0.73
1:C:34:HIS:HB3	1:C:74:THR:HG23	1.71	0.72
1:D:699:ILE:HG21	1:D:702:TYR:HD2	1.54	0.72
1:C:540:ILE:HG22	1:C:736:LEU:HG	1.71	0.72
1:B:543:ARG:NH1	1:B:544:LYS:O	2.21	0.72
1:A:683:GLY:O	1:A:736:LEU:N	2.22	0.72
1:A:718:VAL:HG13	1:A:723:GLU:HG3	1.71	0.72
1:B:744:PHE:O	1:B:748:ARG:NH1	2.23	0.71
1:C:774:TYR:HA	1:C:777:LYS:HD2	1.72	0.71
1:D:58:ARG:NH1	1:D:78:TYR:OH	2.23	0.71
1:A:436:THR:HG22	1:A:481:ARG:HH11	1.53	0.71
1:B:52:ALA:HA	1:B:55:LEU:HD12	1.73	0.71
1:B:140:ASP:O	1:B:142:LYS:NZ	2.21	0.71
1:D:309:SER:HB2	1:D:311:LEU:HD13	1.72	0.71
1:A:319:ASP:OD1	1:A:320:ALA:N	2.23	0.71
1:A:497:GLN:NE2	1:A:498:TRP:O	2.24	0.71
1:A:569:LEU:HA	1:A:572:LEU:HD12	1.72	0.71
1:D:233:GLU:OE1	1:D:233:GLU:N	2.17	0.71
1:D:700:SER:O	1:D:704:LYS:NZ	2.23	0.71
1:B:445:LEU:O	1:B:460:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ASN:ND2	1:C:817:VAL:HG21	2.06	0.71
1:D:306:LYS:HD2	1:D:307:PRO:HD2	1.72	0.71
1:D:433:LEU:HD13	1:D:477:THR:H	1.56	0.71
1:B:299:GLU:O	1:B:302:GLN:NE2	2.24	0.71
1:D:87:ASP:OD1	1:D:88:SER:N	2.24	0.71
1:A:358:ARG:HH11	1:A:362:LEU:HD11	1.56	0.70
1:C:39:GLY:HA3	1:C:106:ILE:HD13	1.73	0.70
1:C:465:ASP:OD2	1:C:798:TRP:NE1	2.22	0.70
1:C:713:ARG:O	1:C:714:GLN:CG	2.37	0.70
1:A:44:TYR:CE1	1:A:82:LYS:HB3	2.25	0.70
1:C:686:GLU:HA	1:C:691:MET:HG2	1.73	0.70
1:A:350:HIS:CD2	1:B:93:LYS:HZ3	2.09	0.70
1:D:79:ASP:OD2	1:D:81:GLN:NE2	2.24	0.69
2:E:87:THR:O	2:E:155:LYS:N	2.24	0.69
1:C:37:ARG:O	1:C:104:ALA:N	2.25	0.69
1:C:589:TRP:HE3	1:C:603:GLU:HA	1.57	0.69
2:E:50:ARG:HG2	2:E:51:THR:HG23	1.74	0.69
1:B:531:LYS:NZ	1:C:530:SER:O	2.25	0.69
1:B:661:VAL:HB	1:C:663:ARG:HH11	1.57	0.69
1:B:445:LEU:N	1:B:460:GLU:O	2.26	0.69
1:B:561:PRO:HA	1:B:564:TRP:HD1	1.56	0.69
1:D:275:ASN:OD1	4:D:1003:NAG:C7	2.41	0.69
1:D:492:ASP:N	1:D:497:GLN:O	2.21	0.69
1:A:393:SER:HB2	1:A:402:ILE:HD13	1.75	0.69
1:B:135:LYS:HZ1	1:B:137:GLN:HA	1.57	0.69
1:D:33:THR:HG22	1:D:33:THR:O	1.92	0.68
1:D:275:ASN:CG	4:D:1003:NAG:C1	2.58	0.68
1:B:233:GLU:OE1	1:B:233:GLU:N	2.24	0.68
1:D:64:ILE:HG23	1:D:70:LEU:HD23	1.74	0.68
1:C:107:LEU:CD2	1:C:130:ILE:HB	2.23	0.68
2:E:354:THR:HG22	2:E:357:ILE:HG13	1.75	0.68
1:B:202:ARG:NH1	1:B:217:GLU:OE1	2.27	0.68
1:D:489:GLY:O	1:D:523:ARG:NH1	2.26	0.68
2:E:83:ARG:HB2	2:E:159:ILE:HG13	1.74	0.68
1:A:822:GLY:HA2	1:A:825:ILE:HD13	1.76	0.68
1:A:217:GLU:O	1:A:221:GLY:N	2.23	0.68
1:A:331:SER:HA	1:A:334:VAL:HG12	1.75	0.68
1:C:433:LEU:HD21	1:C:512:LEU:HD22	1.76	0.68
1:A:817:VAL:HG12	1:A:820:ILE:HG12	1.77	0.67
1:C:250:GLU:N	1:C:250:GLU:OE1	2.26	0.67
1:C:360:MET:HA	1:C:363:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:SER:HB2	1:C:811:GLU:HG3	1.75	0.67
1:D:526:VAL:HG13	1:D:527:ILE:HG13	1.77	0.67
1:A:663:ARG:HH12	1:A:815:LEU:HD13	1.60	0.67
1:D:708:PHE:HB3	1:D:712:ARG:HH12	1.59	0.67
1:A:389:LEU:O	1:A:405:TRP:N	2.26	0.67
1:B:743:GLU:OE1	1:B:743:GLU:N	2.27	0.67
1:D:486:GLY:C	1:D:487:LYS:HG2	2.15	0.67
1:B:212:LYS:NZ	1:B:241:GLN:OE1	2.22	0.67
1:C:714:GLN:HA	1:C:717:LEU:HB2	1.75	0.67
1:D:122:CYS:SG	1:D:123:ASN:N	2.67	0.67
1:A:563:ILE:HG21	1:B:820:ILE:HD11	1.76	0.67
1:B:38:PHE:O	1:B:79:ASP:N	2.26	0.67
1:C:158:ARG:NH1	1:C:162:ASP:OD2	2.28	0.67
1:A:151:PRO:HB2	1:A:156:LEU:HD11	1.76	0.67
1:C:677:GLN:HE22	1:C:679:LYS:HB2	1.60	0.67
2:E:155:LYS:NZ	2:E:156:TYR:O	2.24	0.66
1:A:622:GLN:NE2	1:D:623:GLY:HA3	2.09	0.66
1:C:616:VAL:O	1:C:620:MET:HB2	1.95	0.66
1:A:509:LYS:O	1:A:509:LYS:NZ	2.25	0.66
1:D:81:GLN:HG2	1:D:98:GLN:HE21	1.60	0.66
1:D:99:LEU:HD11	1:D:127:VAL:HG21	1.76	0.66
1:B:177:ASP:OD1	1:B:178:ASP:N	2.27	0.66
1:D:489:GLY:HA3	1:D:502:VAL:HG23	1.77	0.66
2:E:85:GLU:HB2	2:E:157:SER:HB2	1.78	0.66
1:B:123:ASN:ND2	1:B:143:ASP:OD1	2.28	0.66
1:B:135:LYS:NZ	1:B:136:HIS:O	2.29	0.66
1:A:263:ALA:HB2	1:A:315:PHE:HD2	1.61	0.66
1:B:364:LYS:HD3	1:B:379:LYS:HA	1.76	0.66
1:C:694:PHE:HB3	1:C:706:TRP:HB2	1.76	0.66
1:B:585:SER:HB2	1:B:588:GLU:HG2	1.77	0.65
1:B:444:VAL:HG12	1:B:464:ILE:HG12	1.78	0.65
1:C:817:VAL:HG12	1:C:817:VAL:O	1.96	0.65
1:D:432:SER:HA	1:D:477:THR:HB	1.78	0.65
1:A:545:PRO:HA	4:A:1002:NAG:H82	1.78	0.65
1:B:87:ASP:OD1	1:B:88:SER:N	2.30	0.65
1:C:286:ASN:HB3	1:C:289:VAL:HG23	1.78	0.65
1:A:432:SER:OG	1:A:477:THR:CG2	2.43	0.65
1:C:785:LEU:O	1:C:789:GLY:N	2.28	0.65
2:E:86:LEU:O	2:E:131:ARG:NH2	2.29	0.65
1:A:790:LYS:HA	1:A:793:MET:HG2	1.77	0.65
1:C:551:GLY:HA3	1:C:819:ASN:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLN:HE22	1:A:680:ILE:H	1.42	0.65
1:B:541:LEU:HD13	1:B:742:ILE:HG23	1.79	0.65
2:E:96:PRO:HD2	2:E:125:LYS:HE3	1.78	0.65
1:B:53:GLU:HG2	1:B:54:GLU:N	2.11	0.65
1:C:211:ALA:O	1:C:215:LEU:N	2.21	0.65
1:D:52:ALA:HA	1:D:55:LEU:HD12	1.79	0.65
1:C:531:LYS:HB2	1:C:782:ILE:HD11	1.78	0.65
1:B:807:GLU:OE1	1:B:807:GLU:N	2.30	0.65
1:C:483:VAL:HG12	1:C:485:ASP:H	1.62	0.65
1:D:393:SER:OG	1:D:394:LEU:N	2.30	0.65
1:D:275:ASN:OD1	4:D:1003:NAG:O7	2.14	0.65
1:D:465:ASP:OD2	1:D:797:LYS:NZ	2.29	0.65
1:D:445:LEU:O	1:D:460:GLU:N	2.30	0.64
1:D:774:TYR:HA	1:D:777:LYS:HE3	1.79	0.64
1:D:784:GLN:HG2	2:E:135:ARG:HH21	1.61	0.64
1:A:374:ARG:NH2	1:A:388:ASP:OD1	2.25	0.64
1:C:248:MET:HE1	1:C:274:VAL:HG11	1.80	0.64
2:E:101:ARG:HA	2:E:120:ARG:HH22	1.63	0.64
1:A:677:GLN:NE2	1:A:680:ILE:H	1.95	0.64
1:D:149:LEU:O	1:D:384:ARG:HD3	1.98	0.64
1:A:392:ILE:HD12	1:A:399:LEU:HD23	1.79	0.64
1:A:654:ASN:OD1	1:A:655:LEU:N	2.32	0.63
1:C:533:PHE:CD1	1:C:534:MET:HG2	2.33	0.63
1:C:526:VAL:HG23	1:C:527:ILE:HD12	1.81	0.63
1:D:471:SER:O	1:D:475:GLY:N	2.23	0.63
1:B:433:LEU:HD13	1:B:476:PHE:CB	2.28	0.63
1:B:536:LEU:N	1:B:762:LYS:O	2.24	0.63
1:B:766:VAL:HG21	1:B:778:ILE:HD13	1.80	0.63
1:C:174:VAL:HG23	1:C:199:LEU:HD11	1.79	0.63
1:C:374:ARG:NE	1:C:388:ASP:OD2	2.21	0.63
1:A:405:TRP:HD1	1:A:411:LEU:HG	1.62	0.63
1:A:498:TRP:HB3	1:A:502:VAL:HB	1.80	0.63
1:D:281:ILE:HD13	1:D:389:LEU:HD23	1.81	0.63
1:B:79:ASP:OD2	1:B:98:GLN:NE2	2.32	0.63
1:C:58:ARG:NH1	1:C:78:TYR:OH	2.31	0.63
1:C:319:ASP:OD1	1:C:320:ALA:N	2.31	0.63
1:A:563:ILE:HD11	1:B:816:GLY:HA2	1.80	0.62
1:C:177:ASP:OD1	1:C:178:ASP:N	2.32	0.62
2:E:76:LEU:HB2	2:E:137:MET:HB2	1.80	0.62
1:C:286:ASN:HD21	1:C:288:GLN:HB2	1.64	0.62
1:C:550:PRO:HB2	1:C:552:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLN:HB3	1:D:94:LYS:NZ	2.14	0.62
1:D:441:GLU:HB3	1:D:442:PRO:HD3	1.82	0.62
1:D:53:GLU:HB3	1:D:323:MET:HE1	1.82	0.62
1:D:126:GLY:HA2	1:D:145:PHE:CE2	2.35	0.62
1:B:256:PHE:HB3	1:B:258:THR:HG22	1.82	0.62
1:A:378:ASN:ND2	3:G:1:NAG:C8	2.42	0.62
1:A:659:LEU:O	1:A:662:GLU:HG3	2.00	0.62
1:D:177:ASP:OD1	1:D:178:ASP:N	2.33	0.62
1:B:33:THR:HG22	1:B:33:THR:O	2.00	0.62
1:B:661:VAL:HG21	1:C:663:ARG:HB3	1.82	0.62
1:B:692:THR:HA	1:B:695:LYS:HZ2	1.64	0.62
1:D:387:PHE:O	1:D:407:PRO:HD3	2.00	0.62
1:C:349:ARG:HH11	1:C:351:LYS:HB3	1.65	0.62
1:A:266:VAL:HG12	1:A:266:VAL:O	2.00	0.62
1:B:853:GLU:OE2	1:B:855:ARG:NH1	2.33	0.61
1:D:590:TYR:N	1:D:603:GLU:O	2.27	0.61
1:B:38:PHE:H	1:B:78:TYR:HA	1.63	0.61
1:B:571:CYS:HA	1:B:574:VAL:HG12	1.82	0.61
1:D:337:PHE:CD2	1:D:340:MET:HB3	2.35	0.61
1:B:186:GLN:HA	1:B:189:ILE:HD12	1.81	0.61
1:D:300:ARG:CZ	1:D:316:MET:HA	2.30	0.61
2:E:84:ILE:HG23	2:E:158:PHE:HE1	1.65	0.61
1:B:43:GLU:OE1	1:B:111:HIS:HE1	1.83	0.61
1:A:441:GLU:HB2	1:A:442:PRO:HD3	1.83	0.61
1:D:668:ILE:HB	1:D:671:ALA:HB2	1.81	0.61
2:E:88:PHE:CD2	2:E:127:PRO:HD2	2.36	0.61
1:B:536:LEU:HD11	1:B:764:TYR:CE1	2.36	0.61
1:A:716:VAL:HB	1:A:733:TYR:HE1	1.66	0.61
1:D:498:TRP:H	1:D:503:ARG:HD3	1.66	0.61
1:D:536:LEU:HB3	1:D:762:LYS:H	1.66	0.61
1:A:36:LEU:HD23	1:A:76:LEU:HD13	1.83	0.61
1:C:70:LEU:HD21	1:C:331:SER:HB3	1.82	0.61
1:A:44:TYR:CE2	1:A:46:GLU:HA	2.35	0.61
1:B:156:LEU:O	1:B:160:ILE:HG12	2.01	0.61
1:B:374:ARG:NH2	1:B:386:ASP:OD1	2.31	0.61
1:C:183:ILE:HD11	1:D:183:ILE:CD1	2.31	0.61
1:C:405:TRP:HD1	1:C:411:LEU:HA	1.66	0.61
1:A:173:THR:HB	1:A:226:VAL:HG22	1.81	0.60
1:B:718:VAL:HB	1:B:723:GLU:HB3	1.83	0.60
1:C:808:GLU:CG	1:C:809:SER:H	2.13	0.60
1:A:796:GLU:HA	1:A:800:ARG:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:ND2	1:C:143:ASP:OD1	2.33	0.60
1:D:502:VAL:HG13	1:D:527:ILE:HD11	1.82	0.60
1:C:536:LEU:O	1:C:762:LYS:N	2.35	0.60
1:C:795:LYS:O	1:C:799:TRP:HB2	2.00	0.60
1:C:266:VAL:HG11	1:C:394:LEU:HD13	1.82	0.60
1:C:172:VAL:HA	1:C:225:HIS:HB2	1.83	0.60
1:C:613:TRP:HA	1:C:616:VAL:HB	1.84	0.60
1:D:561:PRO:HA	1:D:564:TRP:HB2	1.83	0.60
1:B:531:LYS:H	1:B:779:THR:HG22	1.66	0.60
1:C:34:HIS:N	1:C:74:THR:HA	2.17	0.60
1:C:41:ILE:HD11	1:C:83:ILE:HG12	1.84	0.60
1:C:540:ILE:HG13	1:C:755:ILE:HB	1.84	0.60
1:D:447:LYS:N	1:D:458:ARG:O	2.26	0.60
1:A:270:ARG:HA	1:A:394:LEU:HD21	1.83	0.59
1:A:718:VAL:HG12	1:A:720:SER:H	1.66	0.59
1:B:319:ASP:OD1	1:B:320:ALA:N	2.35	0.59
1:B:451:LYS:HB2	1:B:452:PRO:HD3	1.83	0.59
1:C:171:THR:OG1	1:C:198:ARG:NH2	2.35	0.59
1:A:439:LEU:HA	1:A:444:VAL:HB	1.83	0.59
1:C:224:PHE:HA	1:C:252:TYR:CD2	2.37	0.59
1:C:579:PHE:HD2	1:C:611:SER:HG	1.50	0.59
1:A:618:ALA:HB3	1:A:640:TRP:HE1	1.67	0.59
1:A:628:PRO:HB3	1:A:633:THR:HG23	1.82	0.59
1:A:699:ILE:O	1:A:703:ASP:N	2.28	0.59
1:B:85:LEU:HG	1:B:86:TYR:HD2	1.64	0.59
1:D:590:TYR:HB3	1:D:603:GLU:HB3	1.84	0.59
1:A:202:ARG:NH2	1:A:223:GLU:OE2	2.25	0.59
1:B:518:ALA:HB1	1:B:520:THR:HG23	1.84	0.59
1:C:842:PHE:HA	1:C:845:LYS:NZ	2.17	0.59
1:A:255:ILE:HG12	1:A:277:THR:HB	1.84	0.59
1:A:428:LEU:HD13	1:A:431:ARG:HH21	1.67	0.59
1:B:654:ASN:ND2	1:C:817:VAL:CG2	2.66	0.59
1:C:677:GLN:NE2	1:C:680:ILE:H	2.01	0.59
1:A:663:ARG:HG2	1:D:661:VAL:HG21	1.83	0.59
1:C:39:GLY:HA3	1:C:106:ILE:HA	1.83	0.59
1:C:282:LEU:HA	1:C:372:THR:HG22	1.84	0.59
2:E:87:THR:N	2:E:155:LYS:O	2.20	0.59
1:A:470:LEU:HD13	1:A:778:ILE:HD11	1.85	0.59
1:B:158:ARG:NH1	1:B:407:PRO:O	2.34	0.59
1:D:682:TYR:OH	1:D:708:PHE:HB2	2.01	0.59
1:A:460:GLU:OE2	1:A:461:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:TYR:HB3	1:C:824:PHE:HE2	1.67	0.59
1:A:83:ILE:HG22	1:A:94:LYS:HG3	1.84	0.59
1:B:44:TYR:HB3	1:B:82:LYS:HD3	1.84	0.59
1:B:691:MET:SD	1:B:695:LYS:NZ	2.74	0.59
1:A:543:ARG:HD3	1:A:729:LEU:HD13	1.84	0.59
1:B:681:GLU:HG2	1:B:733:TYR:HA	1.84	0.59
1:C:454:TYR:HA	1:C:458:ARG:HD2	1.84	0.58
1:C:616:VAL:O	1:C:620:MET:CB	2.51	0.58
1:B:692:THR:HA	1:B:695:LYS:HG2	1.85	0.58
1:C:122:CYS:SG	1:C:129:HIS:HB2	2.43	0.58
1:A:497:GLN:HE21	1:A:503:ARG:HD2	1.68	0.58
1:C:439:LEU:HD23	1:C:444:VAL:HG12	1.85	0.58
1:B:661:VAL:HG11	1:C:663:ARG:HG2	1.85	0.58
1:C:543:ARG:NH1	1:C:728:VAL:O	2.35	0.58
1:C:657:ALA:HA	1:D:660:THR:HG22	1.85	0.58
1:D:141:ASN:ND2	1:D:143:ASP:OD2	2.36	0.58
1:B:81:GLN:HB3	1:B:94:LYS:NZ	2.18	0.58
1:B:325:ASP:OD1	1:B:371:LEU:HG	2.04	0.58
1:D:768:THR:HG21	1:D:775:ARG:HB2	1.85	0.58
2:E:87:THR:HB	2:E:155:LYS:HB3	1.85	0.58
1:A:123:ASN:ND2	1:A:143:ASP:HA	2.19	0.58
1:A:796:GLU:O	1:A:801:GLY:N	2.26	0.58
1:D:319:ASP:OD1	1:D:319:ASP:N	2.35	0.58
1:A:156:LEU:O	1:A:160:ILE:HG12	2.04	0.58
1:A:503:ARG:HA	1:A:506:ILE:HG22	1.85	0.58
1:B:123:ASN:HD22	1:B:143:ASP:CG	2.07	0.58
1:D:275:ASN:ND2	4:D:1003:NAG:O5	2.32	0.58
2:E:49:VAL:HB	2:E:156:TYR:CZ	2.39	0.58
1:B:300:ARG:HH22	1:B:317:THR:H	1.51	0.58
1:C:722:GLU:OE1	1:C:722:GLU:N	2.25	0.58
1:A:88:SER:OG	1:A:89:PHE:N	2.35	0.57
1:A:123:ASN:HD22	1:A:143:ASP:HA	1.69	0.57
1:C:434:ILE:HB	1:C:510:ALA:HB2	1.85	0.57
2:E:75:ILE:HG12	2:E:138:TRP:CE3	2.39	0.57
1:D:589:TRP:CZ3	1:D:604:ASN:HB3	2.38	0.57
1:A:793:MET:O	1:A:796:GLU:HG2	2.05	0.57
1:A:795:LYS:O	1:A:799:TRP:N	2.31	0.57
1:B:157:SER:OG	1:B:188:LEU:N	2.37	0.57
1:B:536:LEU:HB2	1:B:762:LYS:HB2	1.85	0.57
1:C:270:ARG:NH1	1:C:396:GLU:O	2.32	0.57
1:A:45:VAL:HG12	1:A:47:SER:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:VAL:HG11	1:B:831:LEU:HD11	1.87	0.57
1:B:417:GLN:HG3	4:B:1004:NAG:C6	2.34	0.57
1:B:686:GLU:HG2	1:B:717:LEU:HB3	1.85	0.57
1:B:795:LYS:HD2	1:B:799:TRP:CD1	2.40	0.57
1:C:718:VAL:HG12	1:C:719:LYS:N	2.18	0.57
1:D:207:ASP:OD1	1:D:208:THR:N	2.38	0.57
1:A:176:TYR:OH	1:A:203:GLN:HB2	2.05	0.57
1:A:487:LYS:HD3	1:A:499:ASN:OD1	2.05	0.57
1:A:286:ASN:ND2	1:A:288:GLN:HB2	2.19	0.57
1:B:417:GLN:HG3	4:B:1004:NAG:HO6	1.67	0.57
1:D:536:LEU:HD22	1:D:762:LYS:HB2	1.85	0.57
1:A:348:ASN:HA	1:A:350:HIS:CE1	2.40	0.57
1:A:537:GLY:HA3	1:A:758:LEU:HG	1.87	0.57
1:A:818:GLN:HG3	1:A:819:ASN:N	2.20	0.57
1:C:356:GLY:HA2	1:C:359:PHE:HB3	1.86	0.57
1:B:669:ASP:OD1	1:B:670:SER:N	2.37	0.57
1:B:683:GLY:N	1:B:734:ALA:O	2.37	0.57
1:C:521:TYR:CZ	1:C:525:LYS:HE3	2.40	0.57
1:D:491:GLN:HB2	1:D:498:TRP:CE2	2.40	0.57
1:A:428:LEU:HB3	1:A:431:ARG:HD3	1.86	0.57
1:C:85:LEU:HD11	1:C:111:HIS:CE1	2.39	0.57
1:B:248:MET:HG3	1:B:274:VAL:HG21	1.85	0.57
1:B:457:ASP:OD2	1:B:458:ARG:NH2	2.37	0.57
1:C:583:ARG:NH1	1:C:604:ASN:HB2	2.19	0.57
2:E:60:PRO:O	2:E:67:PRO:HD3	2.05	0.57
1:A:677:GLN:HE22	1:A:680:ILE:HG23	1.70	0.56
1:C:460:GLU:C	1:C:464:ILE:HD13	2.25	0.56
1:A:290:SER:O	1:A:293:ILE:N	2.39	0.56
1:B:374:ARG:O	1:B:384:ARG:NH2	2.37	0.56
1:A:34:HIS:HB3	1:A:74:THR:HG23	1.86	0.56
1:A:42:PHE:CE2	1:A:80:THR:HB	2.40	0.56
1:A:265:ASP:HB2	1:A:310:GLY:O	2.06	0.56
1:A:443:TYR:O	1:A:462:TYR:N	2.38	0.56
1:A:556:LEU:HD23	1:A:556:LEU:H	1.70	0.56
1:A:669:ASP:HA	1:A:673:ASP:HB2	1.87	0.56
1:B:355:PHE:O	1:B:359:PHE:N	2.24	0.56
1:B:721:ASN:O	1:B:725:ILE:HG12	2.05	0.56
1:C:183:ILE:HD11	1:D:183:ILE:HD11	1.87	0.56
1:C:189:ILE:O	1:C:192:PRO:HD2	2.05	0.56
1:D:300:ARG:HH22	1:D:317:THR:H	1.50	0.56
1:A:233:GLU:OE1	1:A:233:GLU:N	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASP:OD2	1:C:318:THR:N	2.20	0.56
1:D:224:PHE:CE1	1:D:251:TYR:HB3	2.40	0.56
1:D:449:SER:OG	1:D:450:ASP:N	2.36	0.56
1:A:585:SER:HB3	1:A:588:GLU:HG2	1.86	0.56
1:B:85:LEU:HD12	1:B:111:HIS:CE1	2.41	0.56
1:B:746:THR:OG1	1:B:753:THR:HA	2.06	0.56
1:C:84:ASN:OD1	1:C:85:LEU:N	2.35	0.56
1:C:167:PHE:HE2	1:C:253:HIS:NE2	2.03	0.56
1:C:171:THR:HG1	1:C:198:ARG:HH21	1.51	0.56
1:C:695:LYS:HG2	1:C:706:TRP:CZ2	2.41	0.56
1:D:715:SER:HB2	1:D:727:ARG:NH2	2.20	0.56
1:A:250:GLU:OE1	1:A:250:GLU:N	2.34	0.56
1:A:326:ALA:O	1:A:330:VAL:HG23	2.04	0.56
1:A:546:ASN:H	4:A:1002:NAG:H82	1.70	0.56
1:B:126:GLY:HA2	1:B:145:PHE:CE2	2.41	0.56
1:D:228:PHE:HE2	1:D:254:TYR:HD2	1.54	0.56
1:D:267:GLU:HB2	1:D:268:PRO:HD3	1.87	0.56
1:C:619:LEU:HB2	1:C:640:TRP:CZ2	2.40	0.56
1:C:709:MET:SD	1:C:717:LEU:CD2	2.77	0.56
1:D:34:HIS:O	1:D:75:THR:N	2.39	0.56
1:A:277:THR:HG23	1:A:402:ILE:HD11	1.87	0.56
1:C:149:LEU:HD12	1:C:149:LEU:H	1.71	0.56
1:A:266:VAL:HG11	1:A:394:LEU:HD13	1.86	0.55
1:B:37:ARG:HD3	1:B:79:ASP:HB2	1.87	0.55
1:D:630:ALA:O	1:D:633:THR:OG1	2.21	0.55
2:E:369:GLN:O	2:E:373:PRO:HD3	2.06	0.55
1:C:473:ILE:HG23	1:C:474:LEU:HG	1.88	0.55
1:C:591:ASN:HB3	1:C:596:ASN:ND2	2.20	0.55
1:D:519:ILE:HG12	1:D:763:GLY:O	2.06	0.55
2:E:75:ILE:HG12	2:E:138:TRP:CZ3	2.40	0.55
1:B:300:ARG:NH1	1:B:316:MET:HA	2.21	0.55
1:C:252:TYR:O	1:C:274:VAL:HG23	2.06	0.55
2:E:85:GLU:O	2:E:157:SER:N	2.34	0.55
1:B:497:GLN:OE1	1:B:503:ARG:NE	2.39	0.55
1:C:211:ALA:HB3	1:C:238:ILE:HD11	1.89	0.55
1:C:677:GLN:HE22	1:C:680:ILE:H	1.54	0.55
1:D:131:GLN:HE22	1:D:135:LYS:HE2	1.70	0.55
1:D:519:ILE:HD12	1:D:529:PHE:HB3	1.87	0.55
1:A:286:ASN:HD21	1:A:288:GLN:HB2	1.70	0.55
1:A:359:PHE:HA	1:A:362:LEU:HD12	1.88	0.55
1:B:681:GLU:O	1:B:734:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:ASN:OD1	1:B:803:GLY:N	2.39	0.55
1:C:177:ASP:HB3	1:C:204:LEU:HD12	1.87	0.55
1:C:551:GLY:CA	1:C:820:ILE:HA	2.35	0.55
1:D:551:GLY:HA3	1:D:818:GLN:O	2.07	0.55
1:A:263:ALA:HB2	1:A:315:PHE:CD2	2.42	0.55
1:A:456:ASN:HB2	1:A:480:ILE:HD12	1.89	0.55
1:C:123:ASN:HD22	1:C:143:ASP:CG	2.09	0.55
1:D:60:ALA:O	1:D:64:ILE:HG12	2.07	0.55
1:A:85:LEU:HG	1:A:86:TYR:CD2	2.42	0.55
1:A:432:SER:CA	1:A:477:THR:HG22	2.21	0.55
1:B:296:TRP:O	1:B:300:ARG:HB2	2.06	0.55
1:D:536:LEU:HD13	1:D:762:LYS:HB2	1.89	0.55
1:D:588:GLU:OE2	1:D:630:ALA:N	2.38	0.55
1:C:284:THR:HA	1:C:289:VAL:HG11	1.88	0.55
1:A:184:ARG:NH1	1:A:229:ASP:OD1	2.40	0.54
1:B:448:LYS:NZ	1:B:460:GLU:OE2	2.40	0.54
1:C:353:TRP:CH2	1:C:355:PHE:HB2	2.43	0.54
1:D:269:TYR:CD1	1:D:269:TYR:N	2.73	0.54
1:D:179:SER:O	1:D:181:GLY:N	2.40	0.54
1:D:434:ILE:HA	1:D:479:GLU:HB3	1.89	0.54
2:E:84:ILE:HD13	2:E:137:MET:HG2	1.89	0.54
1:A:210:ASP:O	1:A:213:PRO:HD2	2.08	0.54
1:B:444:VAL:HG13	1:B:463:CYS:HB3	1.89	0.54
1:C:492:ASP:OD1	1:C:499:ASN:ND2	2.41	0.54
1:C:610:ASN:HB3	1:C:626:LEU:HD22	1.90	0.54
1:C:630:ALA:HB3	1:C:633:THR:HG22	1.89	0.54
1:A:129:HIS:O	1:A:146:TYR:HA	2.07	0.54
1:C:185:LEU:O	1:C:189:ILE:HG13	2.06	0.54
1:C:725:ILE:O	1:C:729:LEU:HG	2.07	0.54
1:A:483:VAL:HG13	1:A:486:GLY:H	1.73	0.54
1:B:205:PRO:HD3	1:B:214:LEU:HD11	1.89	0.54
1:A:795:LYS:HG3	1:A:799:TRP:CE3	2.43	0.54
1:D:716:VAL:HG23	1:D:717:LEU:HD12	1.90	0.54
1:B:459:PHE:HD2	1:B:480:ILE:HD12	1.72	0.54
1:B:846:SER:HB3	1:B:854:LYS:HE2	1.90	0.54
1:C:290:SER:O	1:C:293:ILE:HB	2.08	0.54
1:C:533:PHE:HD1	1:C:534:MET:HG2	1.72	0.54
1:C:583:ARG:HH11	1:C:604:ASN:HB2	1.72	0.54
1:D:453:LEU:HD23	1:D:457:ASP:HB3	1.89	0.54
1:A:218:MET:O	1:A:222:LYS:N	2.40	0.54
1:C:326:ALA:O	1:C:329:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:ARG:HH22	1:D:814:ALA:HA	1.72	0.54
1:A:250:GLU:HG3	1:A:773:PRO:HG3	1.90	0.53
1:A:262:PHE:HA	1:A:399:LEU:HD22	1.89	0.53
1:C:395:LYS:N	1:C:398:GLY:O	2.40	0.53
1:D:140:ASP:O	1:D:142:LYS:NZ	2.36	0.53
1:D:445:LEU:N	1:D:460:GLU:O	2.23	0.53
1:B:393:SER:OG	1:B:394:LEU:N	2.41	0.53
1:B:593:HIS:NE2	1:B:595:CYS:HB2	2.23	0.53
1:D:470:LEU:HD13	1:D:778:ILE:HD11	1.89	0.53
1:A:41:ILE:HG13	1:A:106:ILE:HD11	1.89	0.53
1:A:674:LEU:O	1:A:682:TYR:OH	2.25	0.53
1:B:439:LEU:HD13	1:B:459:PHE:HE1	1.74	0.53
1:C:290:SER:HA	1:C:293:ILE:HD12	1.91	0.53
1:D:84:ASN:OD1	1:D:85:LEU:HG	2.09	0.53
1:A:64:ILE:HA	1:A:70:LEU:HD11	1.89	0.53
1:A:641:TRP:HB3	1:B:620:MET:HE2	1.91	0.53
1:B:248:MET:SD	1:B:274:VAL:HG21	2.47	0.53
1:B:683:GLY:HA3	1:B:733:TYR:CZ	2.44	0.53
1:C:492:ASP:N	1:C:497:GLN:O	2.23	0.53
1:C:748:ARG:HD2	1:C:802:ASN:CG	2.28	0.53
1:D:376:THR:CG2	1:D:386:ASP:HB3	2.38	0.53
1:A:185:LEU:O	1:A:188:LEU:HB3	2.08	0.53
1:A:744:PHE:CZ	1:A:748:ARG:HD3	2.44	0.53
1:B:436:THR:HG22	1:B:501:MET:HE1	1.89	0.53
1:C:34:HIS:H	1:C:74:THR:HA	1.74	0.53
1:C:53:GLU:OE2	1:C:110:SER:OG	2.21	0.53
1:C:776:ASP:O	1:C:779:THR:OG1	2.23	0.53
1:D:689:ALA:O	1:D:692:THR:OG1	2.25	0.53
1:A:528:ASP:OD2	1:A:775:ARG:HG3	2.07	0.53
1:B:492:ASP:HB2	1:B:497:GLN:HB3	1.90	0.53
1:C:289:VAL:O	1:C:293:ILE:HG13	2.09	0.53
1:A:621:GLN:HG3	1:D:621:GLN:HG2	1.90	0.53
1:B:672:ASP:OD1	1:B:673:ASP:N	2.41	0.53
1:C:565:MET:SD	1:C:565:MET:N	2.81	0.53
1:A:628:PRO:O	1:A:634:ARG:NE	2.42	0.53
1:A:831:LEU:HD11	1:D:577:VAL:HG11	1.91	0.53
1:C:440:GLU:HB2	1:C:443:TYR:HB2	1.89	0.53
1:D:708:PHE:HB3	1:D:712:ARG:NH1	2.23	0.53
1:A:213:PRO:O	1:A:216:LYS:HB3	2.08	0.53
1:A:465:ASP:O	1:A:468:ARG:N	2.42	0.53
1:A:748:ARG:HH11	1:A:802:ASN:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HG11	1:B:228:PHE:CZ	2.44	0.53
1:D:788:GLU:OE1	1:D:790:LYS:N	2.42	0.53
2:E:364:ILE:O	2:E:368:VAL:HG22	2.09	0.53
1:A:444:VAL:HA	1:A:461:GLY:HA3	1.90	0.53
1:C:119:GLN:HE22	1:C:141:ASN:HD21	1.55	0.53
1:C:300:ARG:NH1	1:C:303:ALA:HB3	2.24	0.53
1:D:677:GLN:NE2	1:D:679:LYS:HB3	2.23	0.53
1:A:155:SER:HA	1:A:158:ARG:NH1	2.23	0.52
1:A:200:LYS:HD3	1:B:193:SER:HA	1.91	0.52
1:A:699:ILE:HA	1:D:708:PHE:HE1	1.74	0.52
1:D:207:ASP:HB3	1:D:210:ASP:OD2	2.09	0.52
1:D:230:CYS:SG	1:D:234:MET:HB3	2.49	0.52
1:D:536:LEU:HD23	1:D:537:GLY:N	2.24	0.52
1:D:728:VAL:HG22	1:D:733:TYR:O	2.08	0.52
1:A:175:VAL:HG22	1:A:202:ARG:HB2	1.90	0.52
1:A:674:LEU:HB3	1:A:682:TYR:HE1	1.74	0.52
1:A:714:GLN:HA	1:A:717:LEU:HB2	1.91	0.52
1:B:654:ASN:HD21	1:C:817:VAL:CG2	2.23	0.52
1:C:37:ARG:HB3	1:C:103:VAL:HG12	1.92	0.52
1:C:216:LYS:HG3	2:E:102:PHE:CZ	2.45	0.52
1:C:539:SER:OG	1:C:754:GLN:OE1	2.25	0.52
1:C:615:GLY:HA2	1:C:640:TRP:HE1	1.75	0.52
1:C:792:HIS:O	1:C:796:GLU:HG2	2.08	0.52
1:D:300:ARG:NH1	1:D:316:MET:HA	2.24	0.52
1:D:450:ASP:OD1	1:D:451:LYS:N	2.42	0.52
1:D:538:ILE:HG13	1:D:759:ILE:HB	1.91	0.52
1:D:699:ILE:HG21	1:D:702:TYR:CD2	2.40	0.52
2:E:354:THR:CG2	2:E:357:ILE:HG13	2.38	0.52
1:C:123:ASN:OD1	1:C:145:PHE:CD2	2.62	0.52
2:E:76:LEU:HD12	2:E:137:MET:HB2	1.90	0.52
1:A:42:PHE:HE2	1:A:80:THR:HB	1.73	0.52
1:A:42:PHE:HD2	1:A:82:LYS:HG2	1.74	0.52
1:A:796:GLU:HB2	1:A:800:ARG:HB3	1.90	0.52
1:B:595:CYS:HB3	1:C:593:HIS:CE1	2.45	0.52
1:D:239:LEU:HD21	1:D:256:PHE:HZ	1.74	0.52
1:D:555:PHE:CZ	1:D:820:ILE:HD12	2.45	0.52
1:B:556:LEU:HD23	1:B:556:LEU:H	1.73	0.52
1:B:566:TYR:HB3	1:C:824:PHE:CE2	2.44	0.52
2:E:370:VAL:O	2:E:373:PRO:HD2	2.10	0.52
1:B:528:ASP:HB3	1:B:768:THR:HG23	1.91	0.52
1:B:744:PHE:HB2	1:B:799:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLY:HA2	1:C:145:PHE:CE2	2.44	0.52
1:C:200:LYS:HE2	1:D:192:PRO:O	2.09	0.52
1:C:358:ARG:HD2	1:C:362:LEU:HG	1.91	0.52
1:C:635:ILE:O	1:C:639:ILE:HG12	2.10	0.52
1:D:126:GLY:HA2	1:D:145:PHE:CD2	2.44	0.52
1:D:329:VAL:O	1:D:332:VAL:HG12	2.09	0.52
1:D:337:PHE:HD2	1:D:340:MET:HB3	1.75	0.52
1:A:78:TYR:HD2	1:A:80:THR:HG23	1.75	0.52
1:A:266:VAL:O	1:A:266:VAL:CG1	2.57	0.52
1:B:403:GLY:HA2	1:B:414:THR:HG23	1.90	0.52
1:B:727:ARG:HB3	1:B:733:TYR:CD2	2.45	0.52
1:C:531:LYS:HG2	1:C:779:THR:HG22	1.91	0.52
1:A:212:LYS:HB2	1:A:213:PRO:HD3	1.92	0.52
1:B:498:TRP:N	1:B:503:ARG:HD3	2.21	0.52
1:B:790:LYS:O	1:B:794:MET:HG3	2.09	0.52
1:B:797:LYS:HD2	1:B:798:TRP:CZ3	2.44	0.52
1:C:668:ILE:HG13	1:C:673:ASP:OD2	2.10	0.52
1:D:239:LEU:HB3	1:D:269:TYR:CE2	2.44	0.52
1:D:560:SER:HB3	1:D:563:ILE:CD1	2.40	0.52
1:A:412:ASN:OD1	4:A:1003:NAG:C1	2.57	0.52
1:A:628:PRO:HB2	1:A:634:ARG:HG3	1.92	0.52
1:A:776:ASP:OD1	1:A:777:LYS:N	2.43	0.52
1:B:505:LEU:O	1:B:769:PRO:HG3	2.09	0.52
1:C:728:VAL:HG22	1:C:733:TYR:HB3	1.91	0.52
1:D:84:ASN:OD1	1:D:85:LEU:N	2.42	0.52
1:D:159:ALA:HA	1:D:162:ASP:OD2	2.09	0.52
1:A:571:CYS:HA	1:A:574:VAL:HG12	1.92	0.52
1:B:358:ARG:O	1:B:361:SER:HB3	2.09	0.52
1:C:775:ARG:O	1:C:779:THR:HG23	2.10	0.52
1:D:132:THR:OG1	1:D:133:ARG:N	2.42	0.52
1:D:486:GLY:C	1:D:487:LYS:CG	2.79	0.52
1:A:446:PHE:O	1:A:448:LYS:NZ	2.43	0.51
1:A:656:ALA:O	1:A:660:THR:OG1	2.21	0.51
1:B:548:THR:HB	1:B:818:GLN:NE2	2.24	0.51
1:C:349:ARG:HD3	1:C:351:LYS:HB3	1.93	0.51
1:C:641:TRP:HB3	1:D:620:MET:HG2	1.91	0.51
1:C:649:SER:OG	1:D:652:THR:OG1	2.20	0.51
1:C:702:TYR:CZ	1:C:759:ILE:HG23	2.45	0.51
1:D:495:ASN:O	1:D:497:GLN:NE2	2.42	0.51
1:D:778:ILE:HD12	1:D:781:ALA:HB3	1.92	0.51
1:D:796:GLU:O	1:D:800:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:CYS:CB	1:A:347:CYS:HG	2.13	0.51
1:A:491:GLN:OE1	1:A:492:ASP:N	2.42	0.51
1:B:58:ARG:NH1	1:B:78:TYR:OH	2.43	0.51
1:B:134:TRP:NE1	1:B:135:LYS:O	2.44	0.51
1:B:498:TRP:C	1:B:503:ARG:HB2	2.31	0.51
1:C:675:ALA:HB2	1:C:705:MET:SD	2.50	0.51
1:C:729:LEU:HD21	1:C:752:LEU:HD11	1.92	0.51
1:D:44:TYR:CE1	1:D:82:LYS:HB3	2.44	0.51
1:D:218:MET:HG3	1:D:223:GLU:OE1	2.10	0.51
1:D:240:LYS:NZ	1:D:308:ASP:O	2.43	0.51
1:D:406:ASP:OD1	1:D:410:GLY:N	2.34	0.51
1:D:542:TYR:O	1:D:753:THR:HB	2.10	0.51
1:A:386:ASP:HA	1:A:407:PRO:HG2	1.91	0.51
1:A:589:TRP:CZ3	1:A:604:ASN:HA	2.46	0.51
1:A:682:TYR:OH	1:A:705:MET:SD	2.63	0.51
1:A:801:GLY:HA2	1:A:804:CYS:SG	2.50	0.51
1:C:186:GLN:O	1:C:189:ILE:N	2.42	0.51
1:C:546:ASN:OD1	1:C:548:THR:HG23	2.10	0.51
1:D:677:GLN:NE2	1:D:680:ILE:HG12	2.25	0.51
1:A:330:VAL:HA	1:A:363:ILE:HD11	1.92	0.51
1:A:806:GLU:HB2	1:A:808:GLU:HG3	1.93	0.51
1:B:61:VAL:HG11	1:B:78:TYR:HD1	1.76	0.51
1:B:267:GLU:HB3	1:B:268:PRO:HD3	1.92	0.51
1:B:560:SER:O	1:B:562:ASP:N	2.43	0.51
1:A:426:ASP:HB3	1:A:429:SER:HB3	1.92	0.51
1:B:81:GLN:HB3	1:B:94:LYS:HZ2	1.76	0.51
1:B:207:ASP:OD1	1:B:208:THR:N	2.39	0.51
1:C:417:GLN:HG3	1:C:421:PRO:HA	1.93	0.51
1:A:720:SER:OG	1:A:723:GLU:HG2	2.11	0.51
1:B:210:ASP:O	1:B:213:PRO:HD2	2.11	0.51
1:B:222:LYS:HB3	1:B:224:PHE:CE2	2.46	0.51
1:B:324:TYR:HH	1:B:328:HIS:HE2	1.57	0.51
1:B:439:LEU:HD11	1:B:445:LEU:HA	1.93	0.51
1:B:822:GLY:HA2	1:B:825:ILE:HD13	1.92	0.51
1:C:233:GLU:OE1	1:C:233:GLU:N	2.30	0.51
1:D:184:ARG:NH1	1:D:229:ASP:OD1	2.42	0.51
1:B:38:PHE:HE1	1:B:104:ALA:HB3	1.76	0.51
1:B:280:ARG:NH1	1:B:284:THR:OG1	2.43	0.51
1:C:559:LEU:HB3	1:C:564:TRP:CZ2	2.46	0.51
1:C:847:LYS:HD3	1:C:848:LYS:HZ2	1.76	0.51
1:D:677:GLN:HE22	1:D:679:LYS:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD13	1:D:86:TYR:HD2	1.76	0.51
1:D:438:ILE:HD13	1:D:486:GLY:HA2	1.93	0.51
1:D:737:MET:SD	1:D:738:GLU:N	2.84	0.51
2:E:102:PHE:O	2:E:144:ASP:HB3	2.11	0.51
1:A:161:LEU:HD11	1:A:187:GLU:HG3	1.91	0.51
1:A:196:ASN:O	1:A:197:LEU:HD12	2.10	0.51
1:C:256:PHE:HE1	1:C:276:MET:HG3	1.76	0.51
1:C:277:THR:HG23	1:C:392:ILE:O	2.10	0.51
1:C:747:GLN:HB3	1:C:803:GLY:HA3	1.92	0.51
1:D:261:LEU:HD23	1:D:278:GLY:HA3	1.93	0.51
2:E:62:TYR:CE1	2:E:153:ARG:HB2	2.46	0.51
1:A:589:TRP:HZ3	1:A:604:ASN:HA	1.77	0.50
1:A:750:CYS:HB2	1:A:807:GLU:HB3	1.92	0.50
1:B:53:GLU:HG2	1:B:54:GLU:H	1.75	0.50
1:C:64:ILE:HD13	1:C:76:LEU:HD12	1.93	0.50
1:C:97:ASP:O	1:C:100:SER:HB3	2.12	0.50
1:C:693:PHE:O	1:C:697:SER:N	2.44	0.50
1:D:519:ILE:HD11	1:D:765:GLY:H	1.75	0.50
1:A:528:ASP:OD1	1:A:775:ARG:NH1	2.43	0.50
1:A:614:PHE:HD1	1:A:624:SER:HB3	1.75	0.50
1:A:784:GLN:HA	1:A:787:GLU:CD	2.31	0.50
1:B:495:ASN:HD21	1:B:497:GLN:HB2	1.77	0.50
1:A:36:LEU:O	1:A:77:THR:N	2.44	0.50
1:B:330:VAL:O	1:B:334:VAL:HG23	2.11	0.50
1:B:443:TYR:O	1:B:463:CYS:N	2.43	0.50
1:D:132:THR:O	1:D:150:TYR:HB2	2.11	0.50
1:D:694:PHE:HB3	1:D:706:TRP:HB2	1.93	0.50
1:B:561:PRO:HA	1:B:564:TRP:CD1	2.42	0.50
1:C:96:CYS:CB	1:C:347:CYS:SG	2.98	0.50
1:D:123:ASN:ND2	1:D:143:ASP:HA	2.27	0.50
1:A:339:GLN:CD	1:A:339:GLN:H	2.14	0.50
1:A:443:TYR:HA	1:A:462:TYR:HB3	1.93	0.50
1:C:296:TRP:CD1	1:C:316:MET:SD	3.05	0.50
1:C:286:ASN:OD1	1:C:287:THR:N	2.45	0.50
1:C:337:PHE:CZ	1:C:355:PHE:HB3	2.47	0.50
1:D:53:GLU:HB3	1:D:323:MET:CE	2.41	0.50
1:A:248:MET:HB3	1:A:274:VAL:HG11	1.94	0.50
1:A:300:ARG:NH1	1:A:316:MET:HA	2.26	0.50
1:A:563:ILE:HD12	1:A:563:ILE:H	1.75	0.50
1:C:216:LYS:CE	2:E:102:PHE:CD2	2.87	0.50
1:C:253:HIS:CE1	1:C:275:ASN:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:TRP:CG	1:C:354:ARG:N	2.80	0.50
1:A:36:LEU:CB	1:A:76:LEU:HD22	2.35	0.50
1:A:817:VAL:HG23	1:D:654:ASN:ND2	2.27	0.50
1:C:565:MET:HA	1:C:568:LEU:HD12	1.93	0.50
1:C:634:ARG:HD3	1:D:613:TRP:CD2	2.47	0.50
2:E:121:TYR:CE1	2:E:127:PRO:HB3	2.47	0.50
1:B:325:ASP:CG	1:B:371:LEU:H	2.16	0.50
1:C:558:PRO:HG3	1:C:655:LEU:HD13	1.94	0.50
2:E:88:PHE:CZ	2:E:152:PHE:HB2	2.46	0.50
1:A:120:SER:OG	1:B:87:ASP:OD1	2.29	0.49
1:C:41:ILE:HD11	1:C:83:ILE:HG23	1.93	0.49
1:A:53:GLU:O	1:A:323:MET:HE1	2.12	0.49
1:A:732:ASP:N	1:A:732:ASP:OD1	2.43	0.49
1:C:528:ASP:OD1	1:C:775:ARG:NH1	2.46	0.49
1:D:301:LEU:HD23	1:D:301:LEU:H	1.76	0.49
1:A:538:ILE:O	1:A:759:ILE:HG12	2.13	0.49
1:A:775:ARG:O	1:A:778:ILE:HG22	2.12	0.49
1:C:240:LYS:NZ	1:C:308:ASP:O	2.46	0.49
1:A:528:ASP:HB2	1:A:770:MET:HA	1.93	0.49
1:B:797:LYS:HD2	1:B:798:TRP:CE3	2.48	0.49
1:C:739:SER:HB2	1:C:758:LEU:HD11	1.94	0.49
1:C:846:SER:HA	1:C:850:ALA:HB3	1.95	0.49
1:A:235:ALA:O	1:A:239:LEU:HG	2.13	0.49
1:B:443:TYR:CE2	1:B:516:PRO:HG3	2.47	0.49
1:B:453:LEU:O	1:B:458:ARG:HG3	2.11	0.49
1:C:683:GLY:HA3	1:C:733:TYR:CE2	2.47	0.49
1:D:444:VAL:HG22	1:D:464:ILE:HG23	1.93	0.49
2:E:101:ARG:HE	2:E:120:ARG:NH2	2.11	0.49
2:E:132:SER:HB3	2:E:137:MET:HE1	1.94	0.49
1:A:374:ARG:NE	1:A:388:ASP:OD2	2.44	0.49
1:B:61:VAL:HG11	1:B:78:TYR:CD1	2.47	0.49
1:C:211:ALA:CB	1:C:238:ILE:HD11	2.43	0.49
1:A:817:VAL:HG23	1:D:654:ASN:HD22	1.76	0.49
1:B:71:LEU:HD21	1:B:74:THR:HB	1.94	0.49
1:B:195:TYR:HB2	1:B:197:LEU:HD13	1.95	0.49
1:B:593:HIS:CD2	1:B:595:CYS:HB2	2.47	0.49
1:C:129:HIS:CE1	1:C:131:GLN:HE21	2.30	0.49
1:C:516:PRO:HB3	1:C:764:TYR:CZ	2.48	0.49
1:D:325:ASP:O	1:D:329:VAL:HG23	2.13	0.49
2:E:119:ASP:OD1	2:E:120:ARG:N	2.46	0.49
1:A:262:PHE:HB3	1:A:315:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:HG2	4:B:1004:NAG:H61	1.94	0.49
1:B:738:GLU:O	1:B:742:ILE:HG13	2.13	0.49
1:B:136:HIS:CD2	1:B:183:ILE:HD13	2.47	0.49
1:B:618:ALA:HB3	1:B:640:TRP:NE1	2.28	0.49
1:C:576:CYS:SG	2:E:368:VAL:HG21	2.53	0.49
1:A:37:ARG:NH1	1:A:101:LEU:O	2.46	0.49
1:A:186:GLN:HA	1:A:189:ILE:HD12	1.93	0.49
1:A:516:PRO:HB3	1:A:764:TYR:CE2	2.48	0.49
1:D:306:LYS:HZ2	1:D:308:ASP:H	1.59	0.48
2:E:355:SER:O	2:E:358:VAL:N	2.46	0.48
1:C:536:LEU:HD12	1:C:739:SER:HB3	1.94	0.48
1:D:337:PHE:CE2	1:D:340:MET:HB3	2.48	0.48
1:D:531:LYS:H	1:D:779:THR:HG22	1.78	0.48
1:D:701:THR:HA	1:D:704:LYS:NZ	2.28	0.48
1:A:295:LYS:HA	1:A:298:MET:CE	2.43	0.48
1:A:378:ASN:HB2	3:G:1:NAG:H82	1.89	0.48
1:A:557:ASN:N	1:A:558:PRO:HD2	2.29	0.48
1:B:301:LEU:HD23	1:B:301:LEU:H	1.78	0.48
1:B:442:PRO:HD2	1:B:443:TYR:CD1	2.49	0.48
1:B:443:TYR:CZ	1:B:516:PRO:HG3	2.48	0.48
1:B:558:PRO:HA	1:B:658:PHE:CE2	2.48	0.48
1:C:198:ARG:HG2	1:D:198:ARG:NH2	2.25	0.48
1:A:551:GLY:HA2	1:A:819:ASN:C	2.33	0.48
1:A:568:LEU:O	1:A:572:LEU:HG	2.13	0.48
1:A:677:GLN:NE2	1:A:679:LYS:HB2	2.24	0.48
1:A:702:TYR:OH	1:A:759:ILE:HB	2.13	0.48
1:B:112:SER:OG	1:B:135:LYS:HB2	2.12	0.48
1:B:710:SER:HB2	1:B:713:ARG:HH21	1.78	0.48
1:B:811:GLU:N	1:B:811:GLU:OE2	2.46	0.48
1:C:498:TRP:CE3	1:C:502:VAL:HG11	2.49	0.48
1:C:618:ALA:HB3	1:C:640:TRP:NE1	2.29	0.48
1:C:748:ARG:HD2	1:C:802:ASN:ND2	2.29	0.48
1:D:432:SER:OG	1:D:479:GLU:HB2	2.13	0.48
2:E:130:ILE:O	2:E:131:ARG:NE	2.45	0.48
1:A:231:SER:OG	1:A:234:MET:HG2	2.13	0.48
1:A:622:GLN:HE22	1:D:623:GLY:CA	2.26	0.48
1:B:439:LEU:HD13	1:B:459:PHE:CE1	2.48	0.48
2:E:83:ARG:HG2	2:E:133:THR:HG22	1.96	0.48
1:A:126:GLY:HA2	1:A:145:PHE:HE2	1.78	0.48
1:A:175:VAL:CG1	1:A:204:LEU:HG	2.44	0.48
1:A:670:SER:OG	1:A:671:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:MET:CE	1:A:717:LEU:HG	2.44	0.48
1:B:232:HIS:O	1:B:235:ALA:N	2.46	0.48
1:C:122:CYS:HB3	1:C:127:VAL:O	2.13	0.48
1:C:443:TYR:HA	1:C:462:TYR:HB3	1.95	0.48
1:A:128:PRO:HA	1:A:145:PHE:HB3	1.96	0.48
1:A:460:GLU:HG3	1:A:798:TRP:HH2	1.79	0.48
1:A:622:GLN:NE2	1:D:623:GLY:CA	2.76	0.48
1:C:70:LEU:HG	1:C:71:LEU:HG	1.94	0.48
1:C:326:ALA:HA	1:C:329:VAL:HG12	1.96	0.48
2:E:83:ARG:N	2:E:159:ILE:O	2.38	0.48
1:B:60:ALA:O	1:B:64:ILE:HG12	2.14	0.48
1:B:83:ILE:HG22	1:B:94:LYS:HG3	1.96	0.48
1:B:439:LEU:HD12	1:B:444:VAL:HG23	1.94	0.48
1:B:595:CYS:SG	1:C:594:PRO:HD3	2.54	0.48
1:C:463:CYS:SG	1:C:516:PRO:HD3	2.54	0.48
1:C:704:LYS:HE3	1:D:700:SER:HB3	1.94	0.48
1:C:713:ARG:C	1:C:714:GLN:HG2	2.32	0.48
1:D:346:GLN:HB2	1:D:349:ARG:HG3	1.95	0.48
1:D:434:ILE:N	1:D:511:ASP:OD2	2.31	0.48
1:A:150:TYR:CD1	1:A:151:PRO:HD2	2.48	0.48
1:A:485:ASP:C	1:A:487:LYS:H	2.17	0.48
1:A:543:ARG:NE	1:A:728:VAL:O	2.30	0.48
1:C:85:LEU:HG	1:C:86:TYR:CD2	2.49	0.48
1:C:169:TRP:CZ2	1:C:253:HIS:HD2	2.32	0.48
1:C:361:SER:O	1:C:365:GLU:HG3	2.13	0.48
1:C:577:VAL:HA	1:C:580:VAL:HG12	1.96	0.48
1:D:160:ILE:O	1:D:164:VAL:HG23	2.14	0.48
1:D:691:MET:HG3	1:D:709:MET:SD	2.54	0.48
2:E:95:GLU:HA	2:E:125:LYS:HE3	1.96	0.48
1:A:634:ARG:HD3	1:B:613:TRP:CD2	2.49	0.48
1:B:681:GLU:OE2	1:B:731:SER:OG	2.32	0.48
1:D:286:ASN:OD1	1:D:287:THR:N	2.47	0.48
1:D:406:ASP:CG	1:D:409:SER:H	2.16	0.48
1:A:281:ILE:HG13	1:A:388:ASP:O	2.14	0.47
1:B:467:LEU:HD13	1:B:514:VAL:HG11	1.96	0.47
1:C:41:ILE:HG21	1:C:109:PRO:HD3	1.96	0.47
1:A:564:TRP:O	1:A:568:LEU:HD23	2.13	0.47
1:B:696:LYS:O	1:B:696:LYS:HG2	2.14	0.47
1:C:286:ASN:HB3	1:C:289:VAL:CG2	2.42	0.47
1:C:601:VAL:HG12	1:C:601:VAL:O	2.14	0.47
1:C:779:THR:O	1:C:783:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:SER:HA	1:A:115:ALA:HB3	1.96	0.47
1:A:129:HIS:CE1	1:A:131:GLN:HE21	2.33	0.47
1:A:593:HIS:NE2	1:A:595:CYS:HB2	2.29	0.47
1:A:788:GLU:HB3	1:A:790:LYS:HE3	1.96	0.47
1:B:851:GLN:HG3	1:B:852:LEU:H	1.79	0.47
1:C:453:LEU:O	1:C:454:TYR:HD1	1.97	0.47
1:D:211:ALA:HB3	1:D:241:GLN:HG3	1.97	0.47
1:D:346:GLN:HG2	1:D:349:ARG:NH1	2.29	0.47
1:D:675:ALA:O	1:D:676:LYS:HG2	2.14	0.47
1:A:90:GLU:O	1:A:94:LYS:HG2	2.14	0.47
1:B:579:PHE:HB2	1:B:611:SER:OG	2.14	0.47
1:B:686:GLU:HA	1:B:717:LEU:HD22	1.96	0.47
1:C:433:LEU:HD11	1:C:512:LEU:HD13	1.96	0.47
1:C:782:ILE:HG13	1:C:783:LEU:N	2.28	0.47
1:D:469:GLU:O	1:D:473:ILE:HG12	2.14	0.47
1:D:687:ASP:H	1:D:691:MET:HE1	1.79	0.47
1:D:721:ASN:O	1:D:725:ILE:HG23	2.13	0.47
1:A:831:LEU:HD21	1:D:577:VAL:HG21	1.96	0.47
1:B:686:GLU:CG	1:B:717:LEU:HB3	2.45	0.47
1:A:591:ASN:HA	1:A:601:VAL:O	2.13	0.47
1:B:525:LYS:HE3	1:C:780:ILE:HD13	1.95	0.47
1:C:842:PHE:HA	1:C:845:LYS:HZ2	1.78	0.47
2:E:132:SER:HB3	2:E:137:MET:CE	2.44	0.47
1:A:286:ASN:O	1:A:289:VAL:HB	2.15	0.47
1:A:387:PHE:O	1:A:407:PRO:HD3	2.14	0.47
1:A:646:ILE:HD13	1:B:823:ILE:HG12	1.96	0.47
1:A:735:PHE:CE2	1:A:737:MET:HG2	2.50	0.47
1:A:779:THR:O	1:A:783:LEU:HD23	2.14	0.47
1:A:861:MET:O	1:D:584:PHE:HE1	1.98	0.47
1:B:178:ASP:OD1	1:B:180:THR:OG1	2.32	0.47
1:B:507:ASP:HB2	1:B:509:LYS:HD3	1.96	0.47
1:B:619:LEU:HB2	1:B:640:TRP:HZ2	1.78	0.47
1:B:775:ARG:O	1:B:779:THR:HG23	2.15	0.47
1:B:844:TYR:CZ	1:B:848:LYS:HD3	2.50	0.47
1:C:169:TRP:CZ3	1:C:225:HIS:HB3	2.50	0.47
1:C:718:VAL:CG1	1:C:719:LYS:N	2.78	0.47
1:D:57:PHE:O	1:D:61:VAL:HG23	2.15	0.47
1:D:309:SER:OG	1:D:311:LEU:HB2	2.14	0.47
1:D:376:THR:HG21	1:D:386:ASP:HB3	1.95	0.47
1:D:542:TYR:HB3	1:D:755:ILE:HG13	1.97	0.47
1:C:619:LEU:HB2	1:C:640:TRP:HZ2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:O	1:D:33:THR:CG2	2.61	0.47
1:D:235:ALA:HA	1:D:238:ILE:HG22	1.96	0.47
1:D:443:TYR:CD1	1:D:516:PRO:HG3	2.49	0.47
1:D:677:GLN:CD	1:D:680:ILE:HG12	2.34	0.47
2:E:354:THR:HG22	2:E:354:THR:O	2.15	0.47
1:A:541:LEU:HD21	1:A:742:ILE:HG23	1.96	0.47
1:B:134:TRP:HZ3	1:B:184:ARG:HH21	1.62	0.47
1:B:300:ARG:HH12	1:B:316:MET:HA	1.80	0.47
1:D:40:GLY:H	1:D:98:GLN:HE22	1.62	0.47
1:D:179:SER:C	1:D:181:GLY:N	2.67	0.47
2:E:101:ARG:HE	2:E:120:ARG:NH1	2.13	0.47
1:A:674:LEU:HB3	1:A:682:TYR:CE1	2.50	0.47
1:C:721:ASN:O	1:C:725:ILE:HG12	2.15	0.47
1:D:200:LYS:O	1:D:201:ILE:HG13	2.15	0.47
1:D:237:GLY:O	1:D:241:GLN:HG2	2.15	0.47
1:D:465:ASP:OD1	1:D:466:LEU:N	2.48	0.47
1:D:541:LEU:N	1:D:735:PHE:O	2.42	0.47
2:E:84:ILE:HD11	2:E:135:ARG:C	2.35	0.47
1:A:126:GLY:HA2	1:A:145:PHE:CE2	2.50	0.46
1:A:202:ARG:HB3	1:A:214:LEU:HD11	1.97	0.46
1:A:242:ALA:HB3	1:A:248:MET:HE2	1.96	0.46
1:A:561:PRO:HA	1:A:564:TRP:HD1	1.80	0.46
1:B:54:GLU:HA	1:B:57:PHE:HB3	1.97	0.46
1:B:432:SER:OG	1:B:479:GLU:HB2	2.15	0.46
1:B:574:VAL:HA	1:B:577:VAL:HG12	1.97	0.46
1:B:682:TYR:HA	1:B:734:ALA:HB3	1.97	0.46
1:B:699:ILE:HG13	1:B:700:SER:H	1.79	0.46
1:C:44:TYR:CD1	1:C:82:LYS:HB3	2.50	0.46
1:C:261:LEU:HD12	1:C:264:LEU:HD13	1.97	0.46
1:C:691:MET:SD	1:C:695:LYS:HE2	2.55	0.46
1:D:365:GLU:OE1	1:D:365:GLU:N	2.48	0.46
1:D:556:LEU:HG	1:D:564:TRP:CZ2	2.51	0.46
1:D:754:GLN:NE2	1:D:756:GLY:O	2.36	0.46
1:A:84:ASN:OD1	1:A:85:LEU:N	2.47	0.46
1:A:122:CYS:SG	1:A:129:HIS:HB2	2.55	0.46
1:A:820:ILE:O	1:A:823:ILE:HG12	2.16	0.46
1:B:136:HIS:CG	1:B:183:ILE:HD13	2.50	0.46
1:B:286:ASN:OD1	1:B:287:THR:N	2.48	0.46
1:C:817:VAL:O	1:C:817:VAL:CG1	2.62	0.46
1:D:44:TYR:CD1	1:D:82:LYS:HB3	2.50	0.46
1:D:100:SER:HB2	1:D:346:GLN:HE22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ASP:O	1:D:213:PRO:HD2	2.15	0.46
1:A:405:TRP:CH2	1:A:407:PRO:HA	2.50	0.46
1:A:606:PHE:HE1	1:A:626:LEU:HB3	1.75	0.46
1:A:699:ILE:HA	1:D:708:PHE:CE1	2.50	0.46
1:B:394:LEU:HD12	1:B:398:GLY:O	2.14	0.46
1:B:417:GLN:CG	4:B:1004:NAG:C6	2.93	0.46
1:B:443:TYR:HB3	1:B:463:CYS:HB2	1.98	0.46
1:B:502:VAL:O	1:B:506:ILE:HG23	2.15	0.46
1:C:538:ILE:HD12	1:C:760:ASP:HB2	1.97	0.46
1:D:846:SER:O	1:D:850:ALA:N	2.27	0.46
1:A:96:CYS:CB	1:A:347:CYS:SG	3.03	0.46
1:A:153:PHE:CG	1:A:184:ARG:HG3	2.51	0.46
1:A:220:ARG:O	1:A:222:LYS:HE3	2.16	0.46
1:A:232:HIS:NE2	1:A:233:GLU:OE2	2.49	0.46
1:A:283:ASN:O	1:A:289:VAL:HG11	2.14	0.46
1:A:491:GLN:HB2	1:A:498:TRP:CZ3	2.50	0.46
1:A:634:ARG:HD3	1:B:613:TRP:CE3	2.51	0.46
1:A:643:PHE:O	1:A:647:ILE:HG12	2.16	0.46
1:B:433:LEU:HD23	1:B:511:ASP:HB3	1.97	0.46
1:B:512:LEU:HD11	1:B:774:TYR:HB3	1.97	0.46
1:C:286:ASN:ND2	1:C:288:GLN:HB2	2.30	0.46
1:C:347:CYS:O	1:C:350:HIS:HD2	1.98	0.46
1:C:406:ASP:OD1	1:C:409:SER:N	2.41	0.46
1:C:618:ALA:HB3	1:C:640:TRP:HE1	1.79	0.46
1:D:541:LEU:O	1:D:735:PHE:N	2.36	0.46
1:D:822:GLY:O	1:D:826:VAL:HG23	2.15	0.46
1:A:286:ASN:HB3	1:A:289:VAL:HG23	1.97	0.46
1:A:578:LEU:HA	1:A:581:ILE:HG22	1.97	0.46
1:A:685:VAL:HG13	1:A:688:GLY:HA3	1.97	0.46
1:B:64:ILE:HG23	1:B:70:LEU:HD23	1.98	0.46
1:B:222:LYS:HB3	1:B:224:PHE:HE2	1.79	0.46
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.64	0.46
1:C:42:PHE:CE2	1:C:54:GLU:HG3	2.51	0.46
1:C:584:PHE:HE2	1:D:839:VAL:HG12	1.81	0.46
3:I:1:NAG:H4	3:I:2:NAG:H2	1.81	0.46
1:A:431:ARG:HD2	1:A:431:ARG:N	2.31	0.46
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.67	0.46
1:B:473:ILE:HD11	1:B:781:ALA:HB1	1.98	0.46
1:C:283:ASN:O	1:C:289:VAL:HG21	2.16	0.46
1:C:376:THR:HG21	1:C:386:ASP:HB3	1.97	0.46
1:D:437:THR:HG22	1:D:514:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:HA	1:A:257:THR:HG22	1.96	0.46
1:A:709:MET:HE2	1:A:717:LEU:HG	1.98	0.46
1:A:804:CYS:HB2	1:A:805:PRO:HD3	1.97	0.46
1:B:169:TRP:CZ3	1:B:225:HIS:HB3	2.50	0.46
1:B:288:GLN:O	1:B:292:ILE:HG12	2.16	0.46
1:B:498:TRP:HB3	1:B:502:VAL:HG12	1.97	0.46
1:C:579:PHE:CE2	1:C:606:PHE:HB3	2.51	0.46
1:D:247:MET:HG3	1:D:252:TYR:CE2	2.51	0.46
1:D:693:PHE:O	1:D:697:SER:HB3	2.15	0.46
1:D:770:MET:SD	1:D:770:MET:N	2.88	0.46
1:A:36:LEU:HD22	1:A:340:MET:HE2	1.97	0.46
1:A:389:LEU:HB2	1:A:405:TRP:HB3	1.97	0.46
1:A:682:TYR:HA	1:A:734:ALA:HB3	1.98	0.46
1:A:743:GLU:O	1:A:747:GLN:HG2	2.14	0.46
1:C:140:ASP:HB3	1:C:142:LYS:NZ	2.30	0.46
1:C:566:TYR:HA	1:C:569:LEU:HG	1.96	0.46
1:D:709:MET:HA	1:D:716:VAL:HG21	1.98	0.46
1:D:844:TYR:CE2	1:D:848:LYS:HD2	2.51	0.46
2:E:88:PHE:CE2	2:E:127:PRO:HD2	2.51	0.46
1:A:672:ASP:O	1:A:676:LYS:HG2	2.16	0.46
1:A:691:MET:HE2	1:A:709:MET:HB3	1.97	0.46
1:B:694:PHE:HD2	1:B:706:TRP:HD1	1.64	0.46
1:C:374:ARG:HH21	1:C:388:ASP:CG	2.19	0.46
1:D:470:LEU:HD22	1:D:778:ILE:HD11	1.97	0.46
1:A:186:GLN:HG3	1:A:187:GLU:N	2.31	0.46
1:A:350:HIS:CD2	1:B:93:LYS:NZ	2.83	0.46
1:A:794:MET:O	1:A:798:TRP:HD1	1.99	0.46
1:B:293:ILE:HA	1:B:316:MET:HE2	1.97	0.46
1:B:318:THR:O	1:B:322:LEU:HD23	2.16	0.46
1:B:563:ILE:H	1:B:563:ILE:HD12	1.81	0.46
1:B:589:TRP:HE3	1:B:603:GLU:O	1.98	0.46
1:B:620:MET:O	1:B:622:GLN:N	2.45	0.46
1:B:754:GLN:NE2	1:B:755:ILE:O	2.49	0.46
1:C:534:MET:HE3	1:C:791:LEU:HB2	1.96	0.46
1:C:722:GLU:O	1:C:725:ILE:HB	2.16	0.46
1:D:706:TRP:HA	1:D:709:MET:HG2	1.97	0.46
2:E:66:TYR:HD2	2:E:151:GLY:HA2	1.80	0.46
1:A:42:PHE:O	1:A:44:TYR:HD1	1.98	0.45
1:A:669:ASP:N	1:A:673:ASP:OD2	2.49	0.45
1:B:248:MET:CG	1:B:274:VAL:HG21	2.47	0.45
1:B:432:SER:HA	1:B:477:THR:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:VAL:HG23	1:B:527:ILE:HG23	1.97	0.45
1:C:625:GLU:HG3	1:C:626:LEU:CD1	2.46	0.45
1:C:810:LYS:O	1:C:810:LYS:HG2	2.15	0.45
1:B:822:GLY:O	1:B:826:VAL:HG23	2.17	0.45
1:D:243:LEU:O	1:D:246:GLY:N	2.38	0.45
1:D:332:VAL:HG11	1:D:366:ALA:CB	2.45	0.45
1:D:462:TYR:HB2	1:D:798:TRP:CD1	2.51	0.45
1:D:491:GLN:HB2	1:D:498:TRP:CZ2	2.52	0.45
1:D:621:GLN:NE2	1:D:648:ILE:HG13	2.31	0.45
2:E:101:ARG:HE	2:E:120:ARG:CZ	2.29	0.45
1:A:132:THR:O	1:A:150:TYR:HB2	2.16	0.45
1:A:692:THR:HA	1:A:695:LYS:HG2	1.98	0.45
1:A:722:GLU:OE1	1:A:722:GLU:N	2.45	0.45
1:C:125:LEU:HD23	1:C:345:LEU:HB3	1.99	0.45
1:C:612:PHE:HD2	1:C:613:TRP:CD2	2.34	0.45
1:D:96:CYS:CB	1:D:347:CYS:SG	3.02	0.45
1:A:261:LEU:O	1:A:264:LEU:HD13	2.15	0.45
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.80	0.45
1:A:779:THR:O	1:A:782:ILE:HG22	2.17	0.45
1:B:230:CYS:HB2	1:B:234:MET:HB3	1.97	0.45
1:B:296:TRP:HE1	1:B:300:ARG:NH1	2.15	0.45
1:C:68:ARG:HA	1:C:68:ARG:NE	2.31	0.45
1:C:591:ASN:HD21	1:C:599:SER:H	1.64	0.45
1:D:555:PHE:C	1:D:557:ASN:H	2.19	0.45
1:B:417:GLN:CG	4:B:1004:NAG:O6	2.47	0.45
1:B:641:TRP:HE3	1:C:620:MET:HG2	1.82	0.45
1:C:159:ALA:HB2	1:C:405:TRP:CH2	2.51	0.45
1:C:595:CYS:SG	1:D:595:CYS:HB2	2.56	0.45
1:C:646:ILE:HD11	1:D:555:PHE:CD1	2.51	0.45
1:D:358:ARG:NH2	1:D:362:LEU:HD11	2.32	0.45
1:A:86:TYR:HH	1:A:111:HIS:CE1	2.28	0.45
1:A:204:LEU:HD23	1:A:214:LEU:HD23	1.98	0.45
1:B:495:ASN:ND2	1:B:497:GLN:HB2	2.31	0.45
1:B:516:PRO:HB3	1:B:764:TYR:CZ	2.52	0.45
1:C:677:GLN:CD	1:C:680:ILE:H	2.19	0.45
1:C:787:GLU:OE1	1:C:788:GLU:HG3	2.17	0.45
1:D:289:VAL:O	1:D:293:ILE:HG13	2.17	0.45
1:A:71:LEU:HB3	1:A:74:THR:HB	1.97	0.45
1:A:113:SER:OG	1:A:114:SER:N	2.50	0.45
1:A:351:LYS:HA	1:A:352:PRO:HD3	1.87	0.45
1:A:548:THR:O	1:A:548:THR:CG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HG12	1:B:820:ILE:HD11	1.99	0.45
1:B:293:ILE:HA	1:B:316:MET:CE	2.47	0.45
1:B:585:SER:O	1:B:589:TRP:NE1	2.49	0.45
1:B:674:LEU:HD13	1:B:682:TYR:CE1	2.52	0.45
1:C:434:ILE:HG21	1:C:481:ARG:HE	1.82	0.45
1:D:57:PHE:CE1	1:D:107:LEU:HD12	2.52	0.45
1:D:71:LEU:HD13	1:D:335:GLN:HA	1.98	0.45
1:D:119:GLN:NE2	1:D:146:TYR:CD1	2.85	0.45
1:D:163:LEU:HD21	1:D:277:THR:HG21	1.98	0.45
1:D:684:ALA:HB2	1:D:736:LEU:HB3	1.99	0.45
1:A:88:SER:HA	1:A:114:SER:OG	2.17	0.45
1:A:428:LEU:HB3	1:A:431:ARG:HB2	1.98	0.45
1:A:675:ALA:HA	1:A:705:MET:SD	2.57	0.45
1:B:445:LEU:O	1:B:460:GLU:HG3	2.17	0.45
1:C:464:ILE:H	1:C:464:ILE:HD12	1.82	0.45
1:A:53:GLU:OE1	1:A:53:GLU:N	2.48	0.45
1:A:169:TRP:CE3	1:A:225:HIS:HB3	2.52	0.45
1:A:199:LEU:HD12	1:A:199:LEU:O	2.17	0.45
1:A:337:PHE:CE1	1:A:339:GLN:HB2	2.52	0.45
1:B:36:LEU:HB3	1:B:76:LEU:HD23	1.98	0.45
1:C:110:SER:HB3	1:C:133:ARG:HG3	1.99	0.45
1:C:444:VAL:HA	1:C:464:ILE:CD1	2.47	0.45
1:C:456:ASN:ND2	1:C:478:TYR:O	2.47	0.45
1:D:669:ASP:HB3	1:D:674:LEU:HD11	1.99	0.45
1:D:718:VAL:HG21	1:D:724:GLY:HA2	1.98	0.45
1:D:724:GLY:O	1:D:728:VAL:HG23	2.17	0.45
1:A:63:THR:HG21	1:A:324:TYR:OH	2.16	0.45
1:A:88:SER:O	1:A:91:ALA:N	2.50	0.45
1:A:215:LEU:HD11	1:A:238:ILE:HD11	1.99	0.45
1:A:295:LYS:HA	1:A:298:MET:HE3	1.99	0.45
1:A:500:GLY:O	1:A:504:GLU:HG2	2.16	0.45
1:C:368:TRP:CG	1:C:369:GLU:N	2.84	0.45
1:C:615:GLY:HA2	1:C:640:TRP:NE1	2.31	0.45
1:A:37:ARG:HB3	1:A:103:VAL:HG12	1.99	0.44
1:A:434:ILE:HG23	1:A:510:ALA:HA	2.00	0.44
1:A:620:MET:HA	1:D:645:LEU:HD11	1.98	0.44
1:B:41:ILE:CD1	1:B:81:GLN:HB2	2.47	0.44
1:B:160:ILE:O	1:B:164:VAL:HG23	2.16	0.44
1:B:531:LYS:HA	1:B:531:LYS:HD3	1.84	0.44
1:C:436:THR:OG1	1:C:483:VAL:HG23	2.17	0.44
1:C:439:LEU:HD21	1:C:459:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:LEU:HD11	1:C:769:PRO:HD3	1.99	0.44
1:C:683:GLY:C	1:C:735:PHE:HA	2.38	0.44
1:C:825:ILE:O	1:C:825:ILE:HG22	2.16	0.44
1:C:828:ALA:O	1:C:831:LEU:HG	2.17	0.44
1:A:550:PRO:CB	1:A:553:PHE:HB2	2.46	0.44
1:A:685:VAL:HA	1:A:718:VAL:O	2.17	0.44
1:B:795:LYS:HD2	1:B:799:TRP:NE1	2.32	0.44
1:C:55:LEU:HD23	1:C:296:TRP:CH2	2.53	0.44
1:C:254:TYR:HB3	1:C:256:PHE:CE1	2.52	0.44
1:C:778:ILE:O	1:C:782:ILE:HG23	2.17	0.44
1:D:36:LEU:HD12	1:D:37:ARG:H	1.81	0.44
2:E:101:ARG:HH21	2:E:120:ARG:HH12	1.64	0.44
2:E:110:GLY:C	2:E:138:TRP:CD1	2.91	0.44
1:A:296:TRP:CD1	1:A:300:ARG:HB2	2.53	0.44
1:A:316:MET:SD	1:A:320:ALA:HB3	2.56	0.44
1:B:124:ALA:C	1:B:125:LEU:HD12	2.37	0.44
1:C:282:LEU:HD11	1:C:371:LEU:HB3	1.98	0.44
1:C:721:ASN:HA	1:C:735:PHE:CE2	2.52	0.44
1:A:50:MET:SD	1:A:55:LEU:HG	2.57	0.44
1:B:389:LEU:O	1:B:405:TRP:N	2.49	0.44
1:B:645:LEU:HD11	1:C:621:GLN:HB3	1.99	0.44
1:C:123:ASN:HA	1:C:145:PHE:HD2	1.82	0.44
1:C:745:VAL:O	1:C:749:ASN:HB2	2.18	0.44
2:E:367:LEU:O	2:E:371:LYS:HG3	2.17	0.44
1:A:261:LEU:HD22	1:A:278:GLY:HA3	2.00	0.44
1:A:712:ARG:O	1:A:715:SER:OG	2.27	0.44
1:B:128:PRO:HG2	1:B:359:PHE:CD2	2.53	0.44
1:B:538:ILE:HG22	1:B:759:ILE:HD12	1.98	0.44
1:C:447:LYS:HG3	1:C:459:PHE:C	2.38	0.44
1:C:561:PRO:HA	1:C:564:TRP:CD1	2.39	0.44
1:D:563:ILE:O	1:D:567:VAL:HG23	2.17	0.44
1:D:616:VAL:O	1:D:619:LEU:HB3	2.18	0.44
1:A:325:ASP:OD1	1:A:371:LEU:N	2.50	0.44
1:A:495:ASN:OD1	1:A:497:GLN:HB3	2.16	0.44
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.90	0.44
1:B:417:GLN:CG	4:B:1004:NAG:H61	2.47	0.44
1:C:99:LEU:HD23	1:C:99:LEU:HA	1.71	0.44
1:C:420:LYS:HG3	1:C:422:ALA:H	1.82	0.44
1:D:471:SER:CB	1:D:476:PHE:HB2	2.47	0.44
1:A:699:ILE:HD13	1:A:702:TYR:HD2	1.82	0.44
1:B:129:HIS:O	1:B:146:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HA	1:B:411:LEU:HD11	2.00	0.44
1:C:434:ILE:HG21	1:C:481:ARG:HH21	1.83	0.44
1:C:579:PHE:CE1	1:C:583:ARG:HG2	2.52	0.44
1:D:728:VAL:HA	1:D:733:TYR:HB3	1.99	0.44
1:A:462:TYR:HD1	1:A:794:MET:HB3	1.83	0.44
1:B:128:PRO:HG2	1:B:359:PHE:CE2	2.53	0.44
1:B:442:PRO:O	1:B:462:TYR:HB3	2.18	0.44
1:C:81:GLN:HG2	1:C:98:GLN:HE21	1.83	0.44
1:C:186:GLN:HA	1:C:189:ILE:HD12	2.00	0.44
1:C:847:LYS:HB3	1:C:848:LYS:HZ3	1.82	0.44
1:D:280:ARG:NH1	1:D:284:THR:OG1	2.50	0.44
1:D:462:TYR:HB2	1:D:798:TRP:CG	2.53	0.44
1:D:522:VAL:O	1:D:525:LYS:HG2	2.17	0.44
2:E:159:ILE:HG13	2:E:159:ILE:O	2.18	0.44
1:A:825:ILE:HD12	1:A:825:ILE:H	1.83	0.44
1:A:851:GLN:HG3	1:A:852:LEU:H	1.83	0.44
1:B:108:GLY:N	1:B:130:ILE:O	2.51	0.44
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.83	0.44
1:B:607:THR:N	1:B:610:ASN:HB2	2.33	0.44
1:B:635:ILE:O	1:B:639:ILE:HG12	2.18	0.44
1:B:775:ARG:O	1:B:778:ILE:HG22	2.17	0.44
1:D:40:GLY:H	1:D:98:GLN:NE2	2.15	0.44
2:E:49:VAL:HB	2:E:156:TYR:OH	2.17	0.44
1:A:434:ILE:HD11	1:A:481:ARG:HD2	2.00	0.43
1:A:656:ALA:HA	1:D:653:ALA:HB1	2.00	0.43
1:A:832:VAL:HG23	1:A:833:LEU:HD22	1.98	0.43
1:B:71:LEU:HD11	1:B:74:THR:HB	1.99	0.43
1:B:369:GLU:HA	1:B:373:GLY:O	2.18	0.43
1:D:40:GLY:O	1:D:98:GLN:NE2	2.44	0.43
1:D:498:TRP:HB3	1:D:502:VAL:HB	1.99	0.43
2:E:58:ALA:HB2	2:E:153:ARG:HD2	2.00	0.43
1:B:505:LEU:HD21	1:B:768:THR:N	2.34	0.43
1:B:640:TRP:HZ3	1:B:643:PHE:HD2	1.65	0.43
1:B:710:SER:HB2	1:B:713:ARG:NH2	2.33	0.43
1:C:683:GLY:HA3	1:C:733:TYR:CZ	2.53	0.43
1:C:795:LYS:HD2	1:C:799:TRP:CZ3	2.53	0.43
1:D:395:LYS:HG3	1:D:400:GLU:OE1	2.18	0.43
1:A:290:SER:O	1:A:293:ILE:HB	2.18	0.43
1:A:296:TRP:CD1	1:A:316:MET:HB2	2.53	0.43
1:A:747:GLN:OE1	1:A:803:GLY:HA3	2.19	0.43
1:B:643:PHE:O	1:B:647:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ASP:OD1	1:B:703:ASP:N	2.52	0.43
1:C:61:VAL:O	1:C:64:ILE:HB	2.18	0.43
1:C:129:HIS:O	1:C:146:TYR:HA	2.18	0.43
1:C:181:GLY:O	1:C:184:ARG:HG2	2.18	0.43
1:C:495:ASN:OD1	1:C:495:ASN:N	2.51	0.43
1:C:574:VAL:HG21	1:C:640:TRP:CE3	2.53	0.43
1:C:832:VAL:O	1:C:835:VAL:HG12	2.17	0.43
1:D:306:LYS:NZ	1:D:308:ASP:H	2.17	0.43
1:D:471:SER:HB2	1:D:476:PHE:HB2	1.99	0.43
1:A:341:THR:OG1	1:A:354:ARG:HD3	2.19	0.43
1:B:836:PHE:O	1:B:839:VAL:HG12	2.18	0.43
1:D:492:ASP:O	1:D:496:GLY:N	2.49	0.43
1:D:502:VAL:HG22	1:D:527:ILE:HD11	2.00	0.43
1:D:655:LEU:HD12	1:D:655:LEU:HA	1.80	0.43
1:D:682:TYR:HB3	1:D:734:ALA:HB3	2.00	0.43
1:D:690:THR:OG1	1:D:691:MET:N	2.52	0.43
2:E:125:LYS:HA	2:E:125:LYS:HE2	2.00	0.43
1:A:541:LEU:HD12	1:A:735:PHE:HD2	1.82	0.43
1:B:250:GLU:OE1	1:B:250:GLU:N	2.43	0.43
1:B:523:ARG:O	1:B:527:ILE:HG12	2.17	0.43
1:C:578:LEU:HD13	1:C:636:VAL:HB	2.00	0.43
1:C:716:VAL:HB	1:C:733:TYR:HE1	1.83	0.43
1:D:238:ILE:HG23	1:D:239:LEU:HD22	2.00	0.43
1:D:645:LEU:HD23	1:D:645:LEU:HA	1.90	0.43
1:D:844:TYR:OH	1:D:848:LYS:NZ	2.36	0.43
2:E:140:LYS:HZ2	2:E:142:SER:HB2	1.83	0.43
1:C:443:TYR:HB3	1:C:463:CYS:SG	2.59	0.43
1:C:538:ILE:HB	1:C:759:ILE:HB	1.99	0.43
1:C:634:ARG:NH1	1:D:609:LEU:HG	2.33	0.43
1:D:81:GLN:HB3	1:D:94:LYS:HZ2	1.81	0.43
1:D:228:PHE:CE1	1:D:238:ILE:HG12	2.54	0.43
1:D:231:SER:O	1:D:233:GLU:N	2.51	0.43
1:D:434:ILE:HG23	1:D:479:GLU:OE1	2.18	0.43
1:D:683:GLY:N	1:D:734:ALA:O	2.51	0.43
1:C:42:PHE:CD2	1:C:54:GLU:HG3	2.53	0.43
1:C:469:GLU:HA	1:C:472:THR:OG1	2.19	0.43
1:C:695:LYS:HA	1:C:706:TRP:CD1	2.53	0.43
1:C:701:THR:OG1	1:C:702:TYR:N	2.52	0.43
1:D:126:GLY:HA2	1:D:145:PHE:HE2	1.80	0.43
1:D:144:SER:O	1:D:364:LYS:NZ	2.51	0.43
1:D:489:GLY:HA3	1:D:502:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:HG2	1:A:529:PHE:HD2	1.83	0.43
1:B:284:THR:HA	1:B:289:VAL:HG11	2.00	0.43
1:B:358:ARG:CZ	1:B:362:LEU:HD21	2.48	0.43
1:C:216:LYS:HD3	2:E:146:GLU:OE2	2.19	0.43
1:D:541:LEU:HB2	1:D:742:ILE:HD12	2.01	0.43
2:E:67:PRO:HB2	2:E:70:LYS:HG3	2.00	0.43
1:A:110:SER:HB3	1:A:133:ARG:HG3	2.00	0.43
1:A:320:ALA:HA	1:A:323:MET:HG3	2.01	0.43
1:A:420:LYS:HD3	1:A:420:LYS:HA	1.83	0.43
1:A:712:ARG:HB3	1:A:715:SER:HB2	2.01	0.43
1:B:38:PHE:CE1	1:B:104:ALA:HB3	2.54	0.43
1:B:55:LEU:HB3	1:B:296:TRP:HH2	1.83	0.43
1:B:711:SER:OG	1:B:712:ARG:N	2.52	0.43
1:C:332:VAL:HG21	1:C:368:TRP:CE3	2.54	0.43
1:C:394:LEU:HA	1:C:399:LEU:HD23	2.00	0.43
1:C:724:GLY:O	1:C:728:VAL:HG23	2.19	0.43
1:A:348:ASN:HA	1:A:350:HIS:HE1	1.82	0.43
1:B:387:PHE:HE2	1:B:389:LEU:HD11	1.83	0.43
1:B:438:ILE:HG22	1:B:515:ALA:HB1	2.01	0.43
1:B:564:TRP:O	1:B:568:LEU:HD23	2.19	0.43
1:B:692:THR:HA	1:B:695:LYS:NZ	2.33	0.43
1:C:65:ASN:OD1	1:C:75:THR:HG23	2.19	0.43
1:D:386:ASP:OD1	1:D:387:PHE:N	2.52	0.43
1:D:540:ILE:O	1:D:755:ILE:HB	2.19	0.43
2:E:88:PHE:HZ	2:E:152:PHE:HB2	1.84	0.43
1:A:296:TRP:CD1	1:A:300:ARG:HD2	2.54	0.42
1:A:654:ASN:HD22	1:B:815:LEU:HD12	1.84	0.42
1:B:462:TYR:O	1:B:465:ASP:HB2	2.19	0.42
1:B:474:LEU:HD13	1:B:777:LYS:HE3	2.01	0.42
1:B:555:PHE:CE1	1:B:556:LEU:HD22	2.54	0.42
1:D:556:LEU:HA	1:D:564:TRP:CZ2	2.53	0.42
1:A:140:ASP:HB2	1:B:86:TYR:CE1	2.53	0.42
1:A:784:GLN:HA	1:A:787:GLU:OE2	2.18	0.42
1:B:185:LEU:O	1:B:189:ILE:HG13	2.19	0.42
1:B:595:CYS:HB3	1:C:593:HIS:ND1	2.34	0.42
1:C:38:PHE:CD1	1:C:104:ALA:HB3	2.54	0.42
1:C:266:VAL:HG21	1:C:399:LEU:HD11	2.01	0.42
1:C:560:SER:C	1:C:562:ASP:H	2.22	0.42
1:C:804:CYS:HB3	1:C:805:PRO:HD3	2.01	0.42
2:E:57:PHE:CE1	2:E:74:TYR:CG	3.07	0.42
1:A:669:ASP:O	1:A:755:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:ND2	1:B:288:GLN:HB2	2.34	0.42
1:B:618:ALA:HB3	1:B:640:TRP:HE1	1.84	0.42
1:C:718:VAL:HG11	1:C:723:GLU:HB3	2.01	0.42
1:D:167:PHE:CE2	1:D:253:HIS:CE1	3.06	0.42
1:D:589:TRP:CE3	1:D:604:ASN:HB3	2.54	0.42
1:D:683:GLY:HA3	1:D:733:TYR:CE1	2.53	0.42
1:A:443:TYR:HD1	1:A:462:TYR:HD2	1.68	0.42
1:B:149:LEU:HB3	1:B:322:LEU:HD12	2.01	0.42
1:B:247:MET:O	1:B:247:MET:HG3	2.19	0.42
1:B:536:LEU:HD21	1:B:764:TYR:CE2	2.54	0.42
1:B:554:SER:HB3	1:B:819:ASN:O	2.19	0.42
1:C:248:MET:CE	1:C:274:VAL:HG11	2.47	0.42
1:D:169:TRP:CE2	1:D:225:HIS:ND1	2.88	0.42
1:A:94:LYS:HA	1:A:97:ASP:OD2	2.19	0.42
1:A:140:ASP:HB2	1:B:86:TYR:CE2	2.51	0.42
1:A:621:GLN:HG3	1:D:621:GLN:CG	2.49	0.42
1:A:692:THR:O	1:A:695:LYS:HG2	2.20	0.42
1:B:72:PRO:HD3	1:B:335:GLN:NE2	2.34	0.42
1:B:395:LYS:HB2	1:B:400:GLU:OE2	2.20	0.42
1:B:483:VAL:HB	1:B:501:MET:CE	2.49	0.42
1:B:618:ALA:HB1	1:B:641:TRP:CD1	2.54	0.42
1:B:681:GLU:H	1:B:681:GLU:CD	2.23	0.42
1:C:64:ILE:HD11	1:C:327:VAL:HG12	2.00	0.42
1:C:574:VAL:HG11	1:C:640:TRP:CD2	2.55	0.42
1:D:67:ASN:O	1:D:69:THR:N	2.53	0.42
1:D:166:PHE:O	1:D:168:LYS:HG3	2.19	0.42
1:D:397:GLU:OE1	1:D:397:GLU:N	2.36	0.42
1:A:99:LEU:HG	1:A:345:LEU:O	2.19	0.42
1:A:738:GLU:H	1:A:738:GLU:CD	2.23	0.42
1:B:368:TRP:NE1	1:B:369:GLU:O	2.53	0.42
1:B:451:LYS:H	1:B:451:LYS:HD2	1.84	0.42
1:D:230:CYS:O	1:D:258:THR:HB	2.20	0.42
1:D:249:THR:O	1:D:274:VAL:HG22	2.19	0.42
1:D:265:ASP:N	1:D:310:GLY:O	2.51	0.42
1:A:262:PHE:HA	1:A:399:LEU:CD2	2.49	0.42
1:A:325:ASP:CG	1:A:371:LEU:H	2.22	0.42
1:A:559:LEU:O	1:A:564:TRP:NE1	2.52	0.42
1:B:33:THR:O	1:B:33:THR:CG2	2.67	0.42
1:B:260:ASP:OD1	1:B:318:THR:OG1	2.34	0.42
1:B:710:SER:CB	1:B:713:ARG:HH21	2.32	0.42
1:B:743:GLU:HA	1:B:746:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:HIS:ND1	1:C:275:ASN:HB2	2.34	0.42
1:C:270:ARG:NH1	1:C:397:GLU:HA	2.33	0.42
1:C:349:ARG:NH1	1:C:351:LYS:O	2.52	0.42
1:C:677:GLN:OE1	1:C:680:ILE:N	2.51	0.42
1:C:686:GLU:HG2	1:C:719:LYS:NZ	2.34	0.42
2:E:65:SER:HA	2:E:149:GLY:O	2.20	0.42
1:A:119:GLN:OE1	1:A:135:LYS:HE2	2.19	0.42
1:A:336:GLN:C	1:A:338:PRO:HD3	2.40	0.42
1:A:391:VAL:HG22	1:A:402:ILE:HD11	2.02	0.42
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.88	0.42
1:A:585:SER:O	1:A:588:GLU:HG3	2.19	0.42
1:A:618:ALA:O	1:A:644:THR:HG21	2.20	0.42
1:B:106:ILE:HG23	1:B:129:HIS:HD2	1.85	0.42
1:B:266:VAL:HG11	1:B:394:LEU:HD21	2.02	0.42
1:B:300:ARG:HH22	1:B:317:THR:N	2.17	0.42
1:B:434:ILE:HG13	1:B:511:ASP:OD2	2.18	0.42
1:C:36:LEU:HB3	1:C:76:LEU:HD22	2.02	0.42
1:C:37:ARG:HB2	1:C:103:VAL:HA	2.02	0.42
1:C:411:LEU:HA	1:C:411:LEU:HD23	1.93	0.42
1:D:443:TYR:OH	1:D:740:THR:HG21	2.19	0.42
1:A:57:PHE:HE2	1:A:78:TYR:CD2	2.38	0.42
1:A:157:SER:OG	1:A:187:GLU:HB3	2.20	0.42
1:A:544:LYS:HG2	1:A:753:THR:HB	2.01	0.42
1:A:793:MET:HE2	1:A:793:MET:N	2.35	0.42
1:B:616:VAL:O	1:B:619:LEU:HB3	2.19	0.42
1:C:625:GLU:HG3	1:C:626:LEU:HD13	2.01	0.42
1:D:239:LEU:HD13	1:D:239:LEU:HA	1.84	0.42
1:D:558:PRO:HB2	1:D:654:ASN:HB3	2.02	0.42
1:A:281:ILE:HG12	1:A:372:THR:HB	2.01	0.42
1:B:467:LEU:HD12	1:B:467:LEU:HA	1.82	0.42
1:B:591:ASN:OD1	1:B:594:PRO:HG3	2.19	0.42
1:B:712:ARG:CZ	1:B:716:VAL:HG23	2.49	0.42
1:B:831:LEU:O	1:B:834:SER:OG	2.26	0.42
1:C:790:LYS:HD2	1:C:790:LYS:HA	1.77	0.42
1:C:866:ARG:HA	1:C:866:ARG:HD3	1.85	0.42
1:D:506:ILE:HG22	1:D:507:ASP:OD1	2.20	0.42
1:D:718:VAL:HG22	1:D:723:GLU:HG3	2.02	0.42
2:E:112:PHE:CZ	2:E:140:LYS:HB2	2.55	0.42
1:B:778:ILE:O	1:B:782:ILE:HG13	2.20	0.41
1:C:235:ALA:O	1:C:238:ILE:HG22	2.20	0.41
1:C:563:ILE:O	1:C:566:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HD22	1:D:340:MET:HE3	2.01	0.41
1:D:38:PHE:H	1:D:78:TYR:HA	1.85	0.41
1:D:344:SER:O	1:D:345:LEU:HD23	2.20	0.41
1:D:681:GLU:HG2	1:D:716:VAL:HG12	2.02	0.41
2:E:59:SER:HB3	2:E:152:PHE:CD2	2.54	0.41
1:A:129:HIS:O	1:A:130:ILE:HD13	2.20	0.41
1:A:433:LEU:HD11	1:A:476:PHE:CG	2.55	0.41
1:A:810:LYS:HD3	1:A:810:LYS:HA	1.90	0.41
1:B:205:PRO:HD3	1:B:214:LEU:CD1	2.49	0.41
1:B:695:LYS:HB3	1:B:706:TRP:CE2	2.55	0.41
1:D:629:LYS:HA	1:D:634:ARG:HH21	1.85	0.41
1:A:238:ILE:HD12	1:A:241:GLN:HG3	2.02	0.41
1:A:762:LYS:HB3	1:A:762:LYS:HE2	1.80	0.41
1:B:126:GLY:HA2	1:B:145:PHE:HE2	1.85	0.41
1:B:270:ARG:NH1	1:B:397:GLU:HA	2.35	0.41
1:B:688:GLY:O	1:B:692:THR:HG23	2.20	0.41
1:C:296:TRP:O	1:C:300:ARG:CB	2.68	0.41
1:C:490:ALA:H	1:C:499:ASN:HB2	1.85	0.41
1:C:504:GLU:OE1	1:C:509:LYS:HE3	2.20	0.41
1:C:617:GLY:HA2	1:C:620:MET:HB3	2.02	0.41
1:C:829:ALA:HA	1:C:832:VAL:HG22	2.02	0.41
1:D:596:ASN:HA	1:D:597:PRO:HD3	1.93	0.41
1:D:702:TYR:OH	1:D:759:ILE:HD12	2.20	0.41
1:D:711:SER:OG	1:D:712:ARG:HG3	2.21	0.41
2:E:71:GLU:HA	2:E:140:LYS:HE2	2.02	0.41
2:E:155:LYS:NZ	2:E:157:SER:OG	2.53	0.41
1:A:716:VAL:HA	1:A:727:ARG:NH2	2.35	0.41
1:B:157:SER:CB	1:B:187:GLU:HB2	2.50	0.41
1:B:358:ARG:NH1	1:B:362:LEU:HD21	2.35	0.41
1:B:546:ASN:ND2	4:B:1002:NAG:O7	2.53	0.41
1:C:337:PHE:HZ	1:C:355:PHE:HB3	1.84	0.41
1:C:420:LYS:HG2	1:C:424:ILE:O	2.21	0.41
1:C:498:TRP:HB3	1:C:502:VAL:HB	2.03	0.41
1:C:820:ILE:H	1:C:820:ILE:HG12	1.62	0.41
1:D:213:PRO:O	1:D:217:GLU:HG2	2.20	0.41
1:D:438:ILE:HD12	1:D:438:ILE:HA	1.92	0.41
1:D:445:LEU:HD12	1:D:460:GLU:HB3	2.03	0.41
1:D:797:LYS:NZ	1:D:798:TRP:HE1	2.18	0.41
1:A:467:LEU:O	1:A:470:LEU:HG	2.20	0.41
1:A:543:ARG:HD3	1:A:729:LEU:HA	2.03	0.41
1:B:57:PHE:HB2	1:B:323:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASP:O	1:B:468:ARG:NH2	2.54	0.41
1:C:345:LEU:HD21	1:C:353:TRP:CD1	2.55	0.41
1:C:451:LYS:HA	1:C:452:PRO:HD3	1.93	0.41
1:C:579:PHE:HD2	1:C:611:SER:CB	2.34	0.41
1:C:750:CYS:HB3	4:C:1001:NAG:N2	2.36	0.41
1:D:536:LEU:HD22	1:D:762:LYS:HG3	2.03	0.41
2:E:111:PRO:HA	2:E:138:TRP:CD1	2.54	0.41
1:A:558:PRO:HB3	1:A:654:ASN:OD1	2.21	0.41
1:A:574:VAL:HG11	1:A:640:TRP:CZ3	2.55	0.41
1:B:208:THR:O	1:B:211:ALA:N	2.52	0.41
1:B:343:SER:OG	1:B:354:ARG:NH1	2.53	0.41
1:C:129:HIS:HD2	1:C:130:ILE:N	2.19	0.41
1:C:183:ILE:CD1	1:D:183:ILE:HD11	2.49	0.41
1:C:323:MET:O	1:C:327:VAL:HG23	2.21	0.41
1:D:254:TYR:CD1	1:D:254:TYR:N	2.87	0.41
1:D:560:SER:HB3	1:D:563:ILE:HD13	2.03	0.41
1:D:575:SER:HB3	1:D:612:PHE:HD1	1.85	0.41
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.86	0.41
1:B:57:PHE:HB2	1:B:323:MET:CE	2.51	0.41
1:B:724:GLY:O	1:B:728:VAL:HG12	2.21	0.41
1:B:815:LEU:HD23	1:B:815:LEU:HA	1.91	0.41
1:C:68:ARG:HE	1:C:72:PRO:HA	1.85	0.41
1:D:85:LEU:HB2	1:D:86:TYR:CD2	2.56	0.41
1:D:170:LYS:HE2	1:D:170:LYS:HA	2.03	0.41
1:D:224:PHE:HE1	1:D:251:TYR:HB3	1.84	0.41
1:D:780:ILE:HD11	2:E:134:GLY:HA3	2.03	0.41
1:A:142:LYS:HD3	1:A:142:LYS:HA	1.83	0.41
1:A:324:TYR:CZ	1:A:328:HIS:NE2	2.89	0.41
1:B:750:CYS:SG	1:B:751:ASN:N	2.94	0.41
1:C:172:VAL:HG22	1:C:173:THR:H	1.86	0.41
1:C:253:HIS:HD1	1:C:275:ASN:HB2	1.85	0.41
1:D:42:PHE:CG	1:D:54:GLU:HB2	2.56	0.41
1:A:376:THR:OG1	1:A:377:PHE:N	2.53	0.41
1:A:451:LYS:HA	1:A:452:PRO:HD3	1.96	0.41
1:A:613:TRP:CZ3	1:D:634:ARG:HB3	2.56	0.41
1:A:737:MET:SD	1:A:742:ILE:HG13	2.61	0.41
1:A:858:CYS:O	1:A:862:VAL:HG23	2.21	0.41
1:B:295:LYS:HA	1:B:298:MET:CE	2.51	0.41
1:B:537:GLY:HA3	1:B:758:LEU:HD22	2.03	0.41
1:B:719:LYS:N	1:B:723:GLU:OE2	2.43	0.41
1:B:793:MET:SD	1:B:794:MET:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:THR:HB	1:C:75:THR:HB	2.03	0.41
1:C:70:LEU:HD21	1:C:331:SER:CB	2.48	0.41
1:C:145:PHE:HD1	1:C:145:PHE:HA	1.75	0.41
1:C:453:LEU:O	1:C:458:ARG:HB3	2.21	0.41
1:C:563:ILE:HD11	1:D:817:VAL:N	2.35	0.41
1:C:627:MET:HE1	1:C:628:PRO:O	2.20	0.41
1:C:682:TYR:HA	1:C:734:ALA:HB3	2.03	0.41
1:C:751:ASN:O	1:C:752:LEU:HD23	2.20	0.41
1:C:775:ARG:O	1:C:778:ILE:HG22	2.21	0.41
1:C:791:LEU:HD12	1:C:792:HIS:N	2.35	0.41
1:D:35:VAL:HA	1:D:75:THR:O	2.21	0.41
1:D:212:LYS:HG2	1:D:245:MET:CE	2.50	0.41
1:D:533:PHE:CZ	1:D:764:TYR:HB3	2.56	0.41
1:D:607:THR:H	1:D:610:ASN:CB	2.27	0.41
1:D:627:MET:SD	1:D:627:MET:N	2.94	0.41
1:D:718:VAL:CG2	1:D:723:GLU:HG3	2.51	0.41
2:E:142:SER:OG	2:E:143:SER:N	2.53	0.41
1:A:161:LEU:CD1	1:A:187:GLU:HG3	2.51	0.41
1:A:378:ASN:CA	3:G:1:NAG:C8	2.99	0.41
1:A:783:LEU:O	1:A:786:GLN:HB3	2.20	0.41
1:B:289:VAL:O	1:B:293:ILE:HG13	2.21	0.41
1:B:325:ASP:OD2	1:B:371:LEU:N	2.51	0.41
1:B:590:TYR:CE2	1:B:592:PRO:HG3	2.56	0.41
1:C:172:VAL:HG22	1:C:173:THR:N	2.36	0.41
1:C:349:ARG:HH11	1:C:351:LYS:CB	2.33	0.41
1:C:683:GLY:O	1:C:736:LEU:N	2.50	0.41
2:E:101:ARG:HA	2:E:120:ARG:NH2	2.33	0.41
1:A:788:GLU:O	1:A:790:LYS:N	2.54	0.40
1:B:71:LEU:H	1:B:335:GLN:NE2	2.18	0.40
1:B:531:LYS:HA	1:C:531:LYS:HZ1	1.86	0.40
1:B:831:LEU:O	1:B:835:VAL:HG23	2.21	0.40
1:C:169:TRP:HZ2	1:C:253:HIS:HD2	1.69	0.40
1:D:85:LEU:HD13	1:D:86:TYR:CD2	2.55	0.40
1:D:153:PHE:CD1	1:D:156:LEU:HD12	2.56	0.40
2:E:84:ILE:HG23	2:E:158:PHE:CE1	2.52	0.40
1:A:460:GLU:OE2	1:A:798:TRP:HZ2	2.04	0.40
1:A:491:GLN:OE1	1:A:497:GLN:N	2.54	0.40
1:B:531:LYS:HZ3	1:C:531:LYS:HA	1.86	0.40
1:C:522:VAL:O	1:C:525:LYS:HB2	2.21	0.40
1:D:228:PHE:HE2	1:D:254:TYR:CD2	2.37	0.40
1:D:434:ILE:HD12	1:D:511:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:PHE:CE2	1:D:823:ILE:HG12	2.56	0.40
1:B:98:GLN:O	1:B:102:GLY:N	2.54	0.40
1:B:224:PHE:O	1:B:225:HIS:CG	2.74	0.40
1:C:561:PRO:CA	1:C:564:TRP:HD1	2.28	0.40
1:D:229:ASP:HA	1:D:257:THR:HG22	2.02	0.40
1:D:231:SER:O	1:D:234:MET:N	2.40	0.40
1:D:274:VAL:HG12	1:D:275:ASN:N	2.36	0.40
1:D:563:ILE:HD12	1:D:563:ILE:H	1.86	0.40
1:D:699:ILE:HD13	1:D:702:TYR:CD2	2.56	0.40
1:A:289:VAL:O	1:A:293:ILE:HG13	2.22	0.40
1:A:353:TRP:CZ2	1:A:355:PHE:HB2	2.56	0.40
1:A:551:GLY:HA2	1:A:819:ASN:O	2.21	0.40
1:A:628:PRO:HB3	1:A:633:THR:CG2	2.51	0.40
1:B:57:PHE:O	1:B:61:VAL:HG23	2.21	0.40
1:B:297:SER:O	1:B:301:LEU:HD22	2.21	0.40
1:C:81:GLN:HG2	1:C:98:GLN:NE2	2.36	0.40
1:C:134:TRP:NE1	1:C:135:LYS:O	2.55	0.40
1:C:176:TYR:CE1	1:C:203:GLN:HG3	2.56	0.40
1:C:591:ASN:HD21	1:C:599:SER:N	2.18	0.40
1:C:660:THR:O	1:C:664:MET:HG3	2.21	0.40
1:C:851:GLN:O	1:C:852:LEU:HG	2.21	0.40
1:A:433:LEU:HA	1:A:511:ASP:OD2	2.21	0.40
1:A:682:TYR:CZ	1:A:705:MET:SD	3.15	0.40
1:B:70:LEU:HD12	1:B:335:GLN:OE1	2.22	0.40
1:B:341:THR:O	1:B:354:ARG:NH2	2.54	0.40
1:B:406:ASP:OD1	1:B:409:SER:N	2.32	0.40
1:B:441:GLU:HB3	1:B:442:PRO:HD3	2.04	0.40
1:B:443:TYR:HA	1:B:462:TYR:HB3	2.03	0.40
1:B:581:ILE:HG22	1:B:633:THR:HG22	2.04	0.40
1:C:65:ASN:CG	1:C:75:THR:HG23	2.41	0.40
1:C:169:TRP:HZ2	1:C:253:HIS:CD2	2.40	0.40
1:C:259:LEU:O	1:C:261:LEU:N	2.55	0.40
1:C:328:HIS:O	1:C:332:VAL:HG23	2.20	0.40
1:C:681:GLU:HG2	1:C:716:VAL:HG11	2.04	0.40
1:C:712:ARG:HA	1:C:712:ARG:HD3	1.80	0.40
1:D:622:GLN:OE1	1:D:622:GLN:N	2.55	0.40
1:D:675:ALA:C	1:D:677:GLN:H	2.24	0.40
2:E:55:GLY:O	2:E:155:LYS:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	829/908 (91%)	757 (91%)	72 (9%)	0	100	100
1	B	829/908 (91%)	736 (89%)	93 (11%)	0	100	100
1	C	833/908 (92%)	754 (90%)	79 (10%)	0	100	100
1	D	816/908 (90%)	706 (86%)	110 (14%)	0	100	100
2	E	149/525 (28%)	137 (92%)	12 (8%)	0	100	100
All	All	3456/4157 (83%)	3090 (89%)	366 (11%)	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	722/794 (91%)	718 (99%)	4 (1%)	86	92
1	B	721/794 (91%)	719 (100%)	2 (0%)	92	95
1	C	724/794 (91%)	719 (99%)	5 (1%)	84	90
1	D	709/794 (89%)	707 (100%)	2 (0%)	92	95
2	E	134/465 (29%)	134 (100%)	0	100	100
All	All	3010/3641 (83%)	2997 (100%)	13 (0%)	91	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
1	A	519	ILE
1	A	754	GLN
1	A	820	ILE
1	B	380	THR
1	B	420	LYS
1	C	426	ASP
1	C	433	LEU
1	C	710	SER
1	C	711	SER
1	C	819	ASN
1	D	262	PHE
1	D	426	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	129	HIS
1	A	131	GLN
1	A	137	GLN
1	A	497	GLN
1	A	622	GLN
1	A	677	GLN
1	A	818	GLN
1	B	34	HIS
1	B	111	HIS
1	B	350	HIS
1	B	654	ASN
1	B	819	ASN
1	C	119	GLN
1	C	123	ASN
1	C	131	GLN
1	C	136	HIS
1	D	98	GLN
1	D	123	ASN
1	D	253	HIS
1	D	499	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)

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	F	1	1,3	14,14,15	0.38	0	17,19,21	1.16	2 (11%)
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	1.73	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	0.31	0	17,19,21	0.88	1 (5%)
3	NAG	G	2	3	14,14,15	0.33	0	17,19,21	0.58	0
3	BMA	G	3	3	11,11,12	0.22	0	15,15,17	0.60	0
3	NAG	H	1	1,3	14,14,15	0.53	0	17,19,21	1.45	2 (11%)
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.86	1 (5%)
3	BMA	H	3	3	11,11,12	0.32	0	15,15,17	1.06	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
3	NAG	I	2	3	14,14,15	0.46	0	17,19,21	1.16	2 (11%)
3	BMA	I	3	3	11,11,12	0.20	0	15,15,17	0.67	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	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	-4.50	106.09	112.19
3	F	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	I	2	NAG	C1-O5-C5	3.46	116.87	112.19
3	F	2	NAG	C1-C2-N2	3.30	116.12	110.49
3	F	2	NAG	O5-C1-C2	-3.14	106.33	111.29
3	H	3	BMA	C1-C2-C3	2.70	112.98	109.67
3	F	1	NAG	C3-C4-C5	-2.67	105.48	110.24
3	H	1	NAG	C2-N2-C7	2.48	126.43	122.90
3	F	2	NAG	C4-C3-C2	-2.38	107.54	111.02
3	H	2	NAG	C1-O5-C5	2.28	115.28	112.19
3	F	1	NAG	O5-C5-C6	2.21	110.67	107.20
3	G	1	NAG	C1-O5-C5	2.20	115.17	112.19
3	I	1	NAG	O4-C4-C5	2.17	114.69	109.30
3	I	2	NAG	C1-C2-N2	2.01	113.93	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2

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

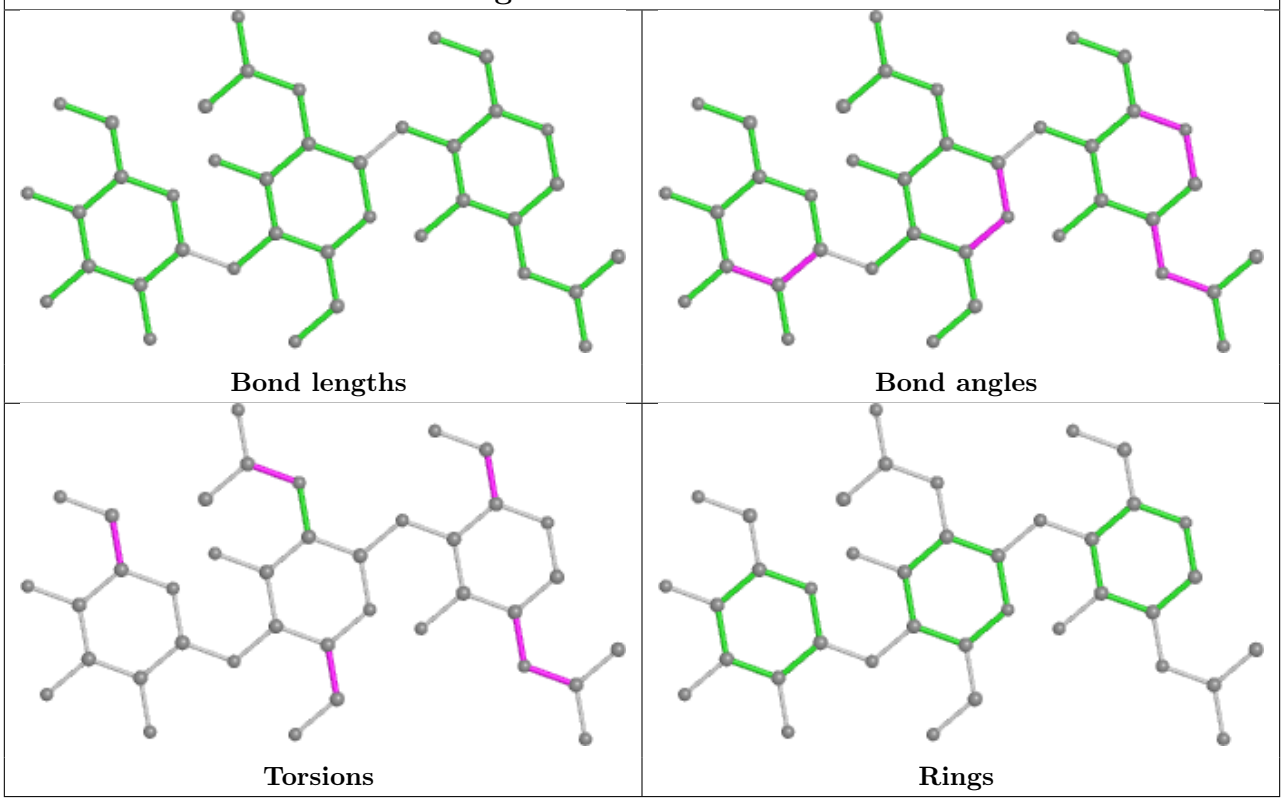
There are no ring outliers.

3 monomers are involved in 12 short contacts:

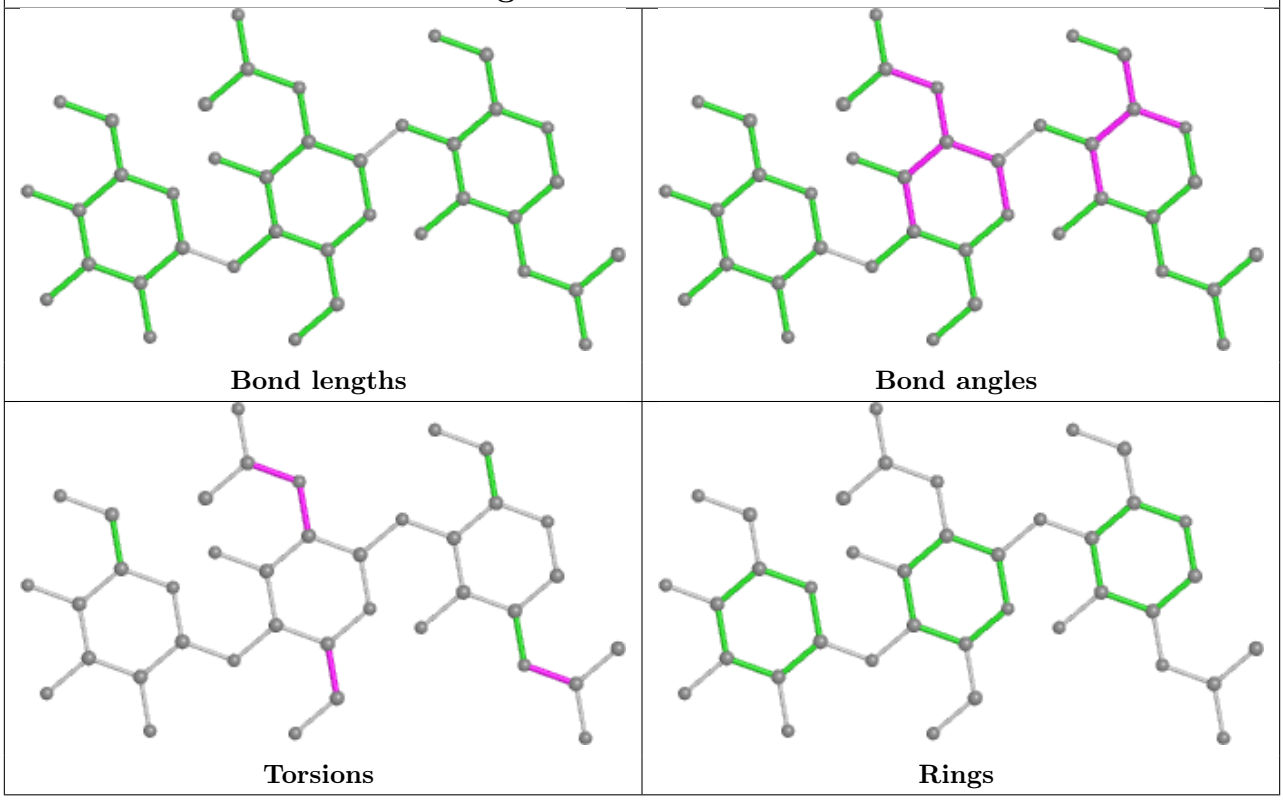
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	11	0
3	I	1	NAG	1	0
3	I	2	NAG	1	0

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

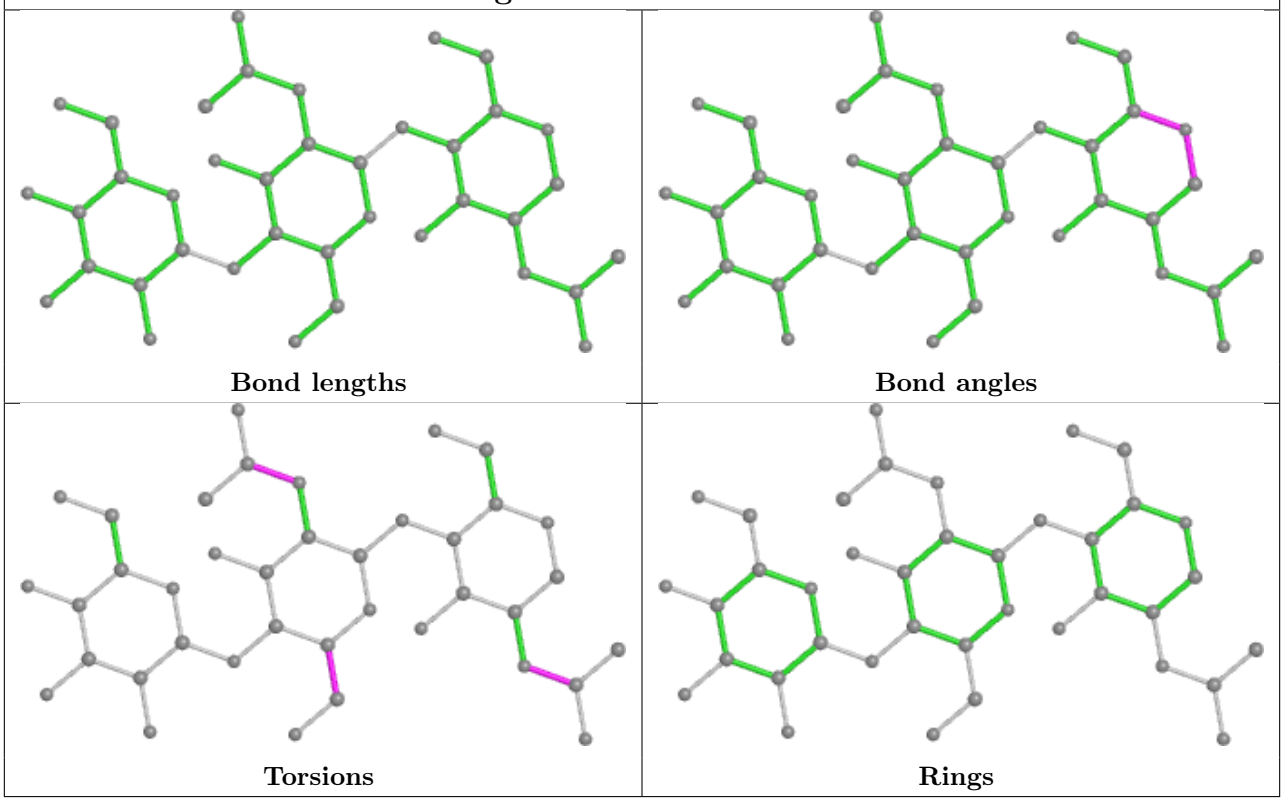
Oligosaccharide Chain H



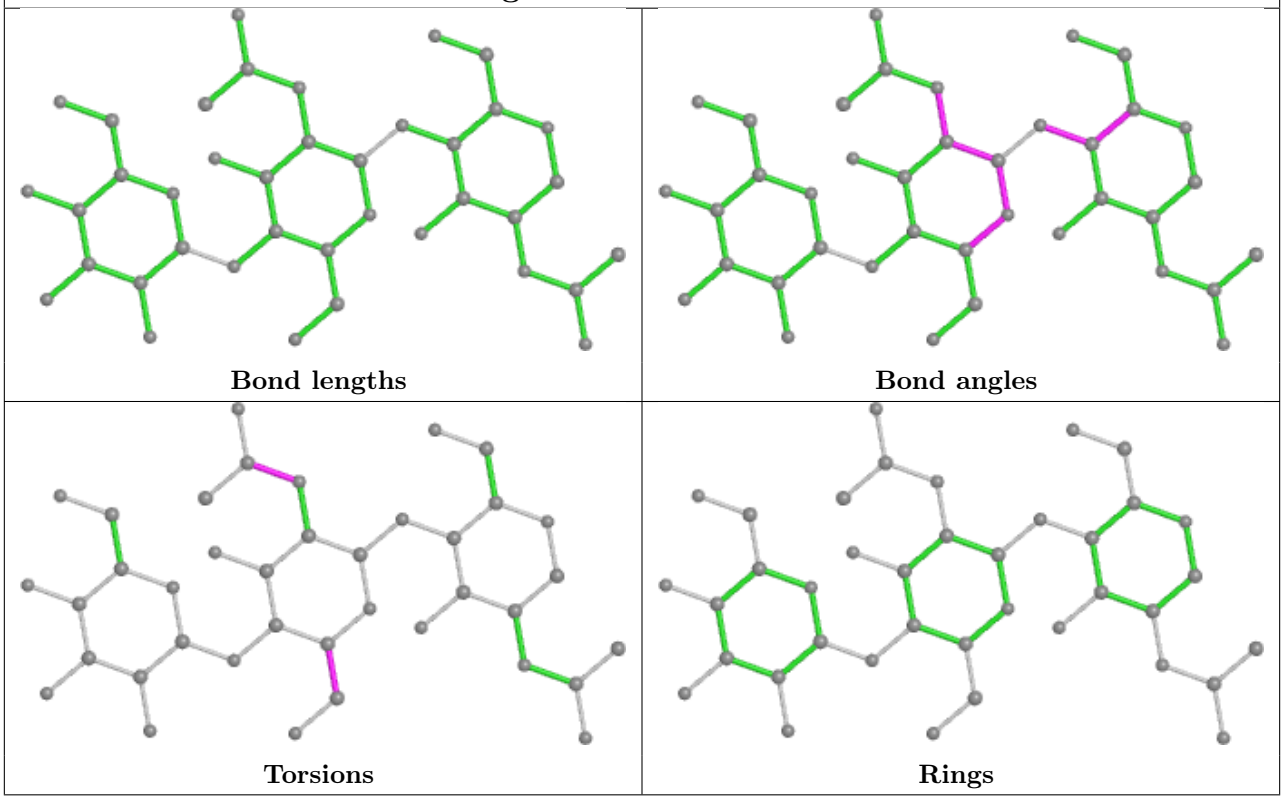
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain I



5.6 Ligand geometry (i)

16 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	A	1001	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	D	1004	1	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	B	1001	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	C	1005	1	14,14,15	0.24	0	17,19,21	0.79	0
4	NAG	A	1002	1	14,14,15	0.46	0	17,19,21	0.38	0
4	NAG	C	1003	1	14,14,15	0.23	0	17,19,21	0.84	0
4	NAG	C	1004	1	14,14,15	0.24	0	17,19,21	1.01	2 (11%)
4	NAG	D	1001	1	14,14,15	0.23	0	17,19,21	0.65	0
4	NAG	A	1003	-	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	B	1002	1	14,14,15	0.51	0	17,19,21	0.41	0
4	NAG	C	1002	1	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
4	NAG	B	1004	1	14,14,15	0.24	0	17,19,21	0.96	1 (5%)
4	NAG	D	1002	1	14,14,15	0.74	1 (7%)	17,19,21	0.77	0
4	NAG	D	1003	-	14,14,15	0.34	0	17,19,21	1.12	2 (11%)
4	NAG	B	1003	1	14,14,15	0.26	0	17,19,21	0.92	1 (5%)
4	NAG	C	1001	1	14,14,15	0.18	0	17,19,21	0.38	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	A	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1004	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1005	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1003	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1001	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1003	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1002	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1003	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	NAG	O5-C1	-2.60	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1003	NAG	C1-O5-C5	2.86	116.06	112.19
4	B	1003	NAG	C2-N2-C7	2.57	126.57	122.90
4	B	1004	NAG	C2-N2-C7	2.57	126.57	122.90
4	C	1004	NAG	C2-N2-C7	2.37	126.27	122.90
4	D	1003	NAG	O5-C1-C2	2.29	114.90	111.29
4	C	1002	NAG	C1-O5-C5	2.17	115.13	112.19
4	C	1004	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	NAG	C8-C7-N2-C2
4	B	1003	NAG	O7-C7-N2-C2
4	B	1004	NAG	C3-C2-N2-C7
4	B	1004	NAG	C8-C7-N2-C2
4	B	1004	NAG	O7-C7-N2-C2
4	C	1003	NAG	C8-C7-N2-C2
4	C	1003	NAG	O7-C7-N2-C2
4	C	1005	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	1005	NAG	O7-C7-N2-C2
4	B	1001	NAG	C4-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	C	1004	NAG	C8-C7-N2-C2
4	C	1004	NAG	O7-C7-N2-C2
4	C	1002	NAG	O5-C5-C6-O6
4	B	1001	NAG	O5-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	D	1002	NAG	O5-C5-C6-O6
4	C	1001	NAG	C8-C7-N2-C2
4	C	1001	NAG	O7-C7-N2-C2
4	D	1004	NAG	C8-C7-N2-C2
4	D	1001	NAG	C4-C5-C6-O6
4	B	1003	NAG	C1-C2-N2-C7
4	C	1003	NAG	C1-C2-N2-C7
4	C	1004	NAG	C1-C2-N2-C7
4	D	1004	NAG	O7-C7-N2-C2
4	D	1003	NAG	C8-C7-N2-C2
4	C	1002	NAG	C4-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	D	1003	NAG	O7-C7-N2-C2
4	D	1004	NAG	O5-C5-C6-O6
4	A	1003	NAG	O5-C5-C6-O6
4	B	1004	NAG	O5-C5-C6-O6
4	C	1004	NAG	O5-C5-C6-O6
4	C	1005	NAG	O5-C5-C6-O6
4	D	1002	NAG	C4-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	C	1002	NAG	C3-C2-N2-C7
4	D	1001	NAG	C3-C2-N2-C7
4	D	1002	NAG	C3-C2-N2-C7
4	D	1001	NAG	C1-C2-N2-C7
4	D	1002	NAG	C1-C2-N2-C7
4	C	1005	NAG	C3-C2-N2-C7
4	A	1002	NAG	C1-C2-N2-C7
4	C	1005	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	NAG	2	0
4	A	1003	NAG	4	0
4	B	1002	NAG	1	0
4	B	1004	NAG	7	0
4	D	1003	NAG	5	0
4	C	1001	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.

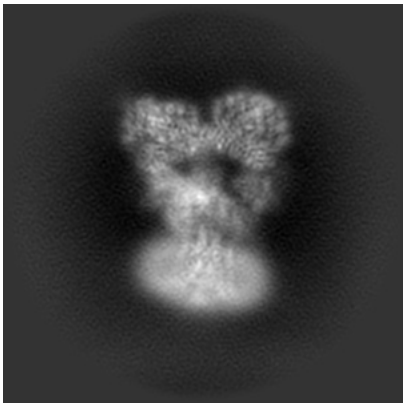
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31459. These allow visual inspection of the internal detail of the map and identification of artifacts.

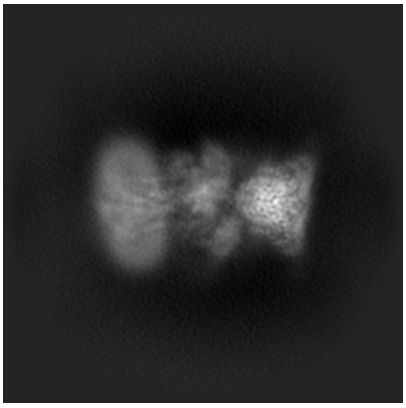
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

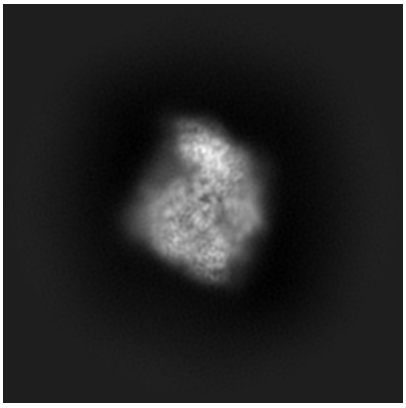
6.1.1 Primary map



X



Y

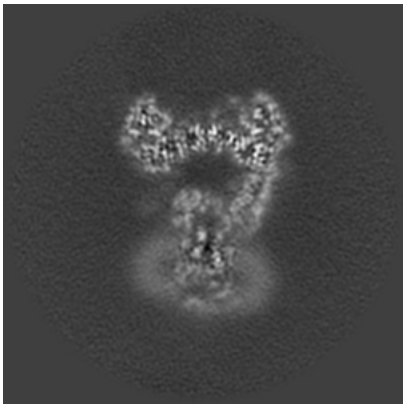


Z

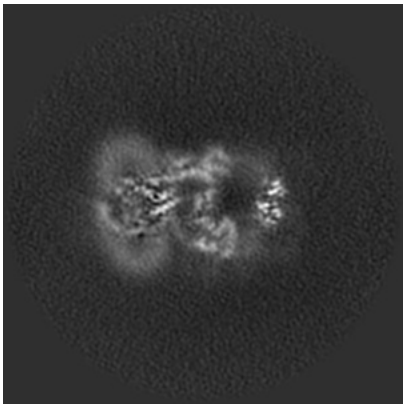
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

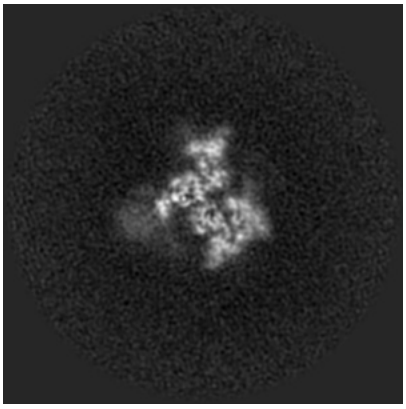
6.2.1 Primary map



X Index: 128



Y Index: 128

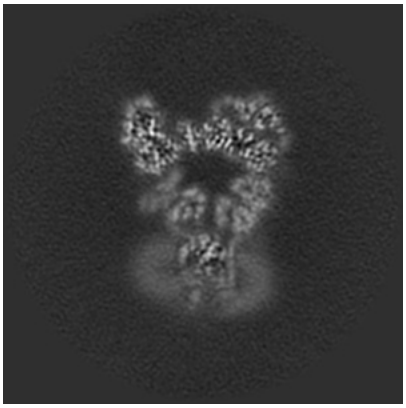


Z Index: 128

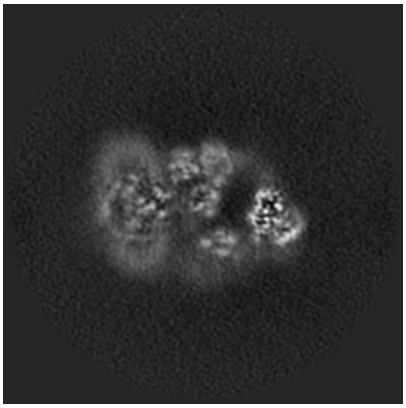
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

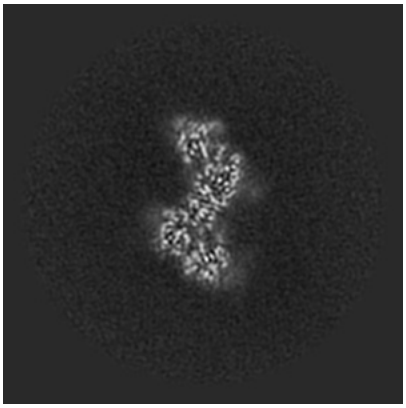
6.3.1 Primary map



X Index: 133



Y Index: 121



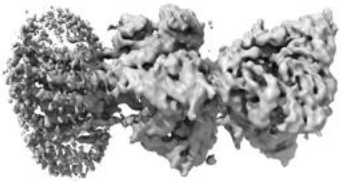
Z Index: 175

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

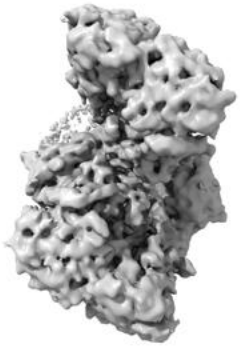
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.455. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

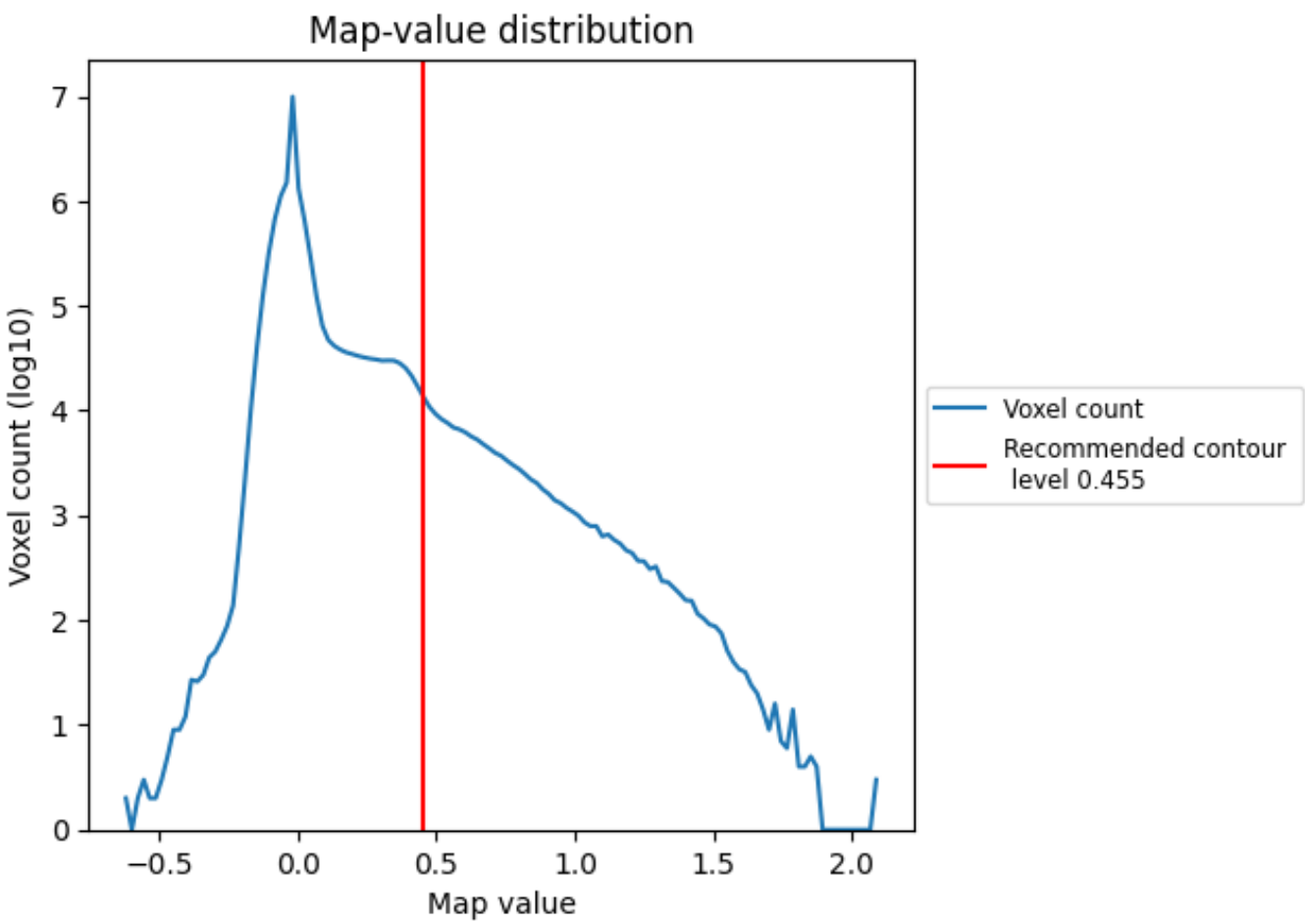
6.5 Mask visualisation (i)

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

7 Map analysis (i)

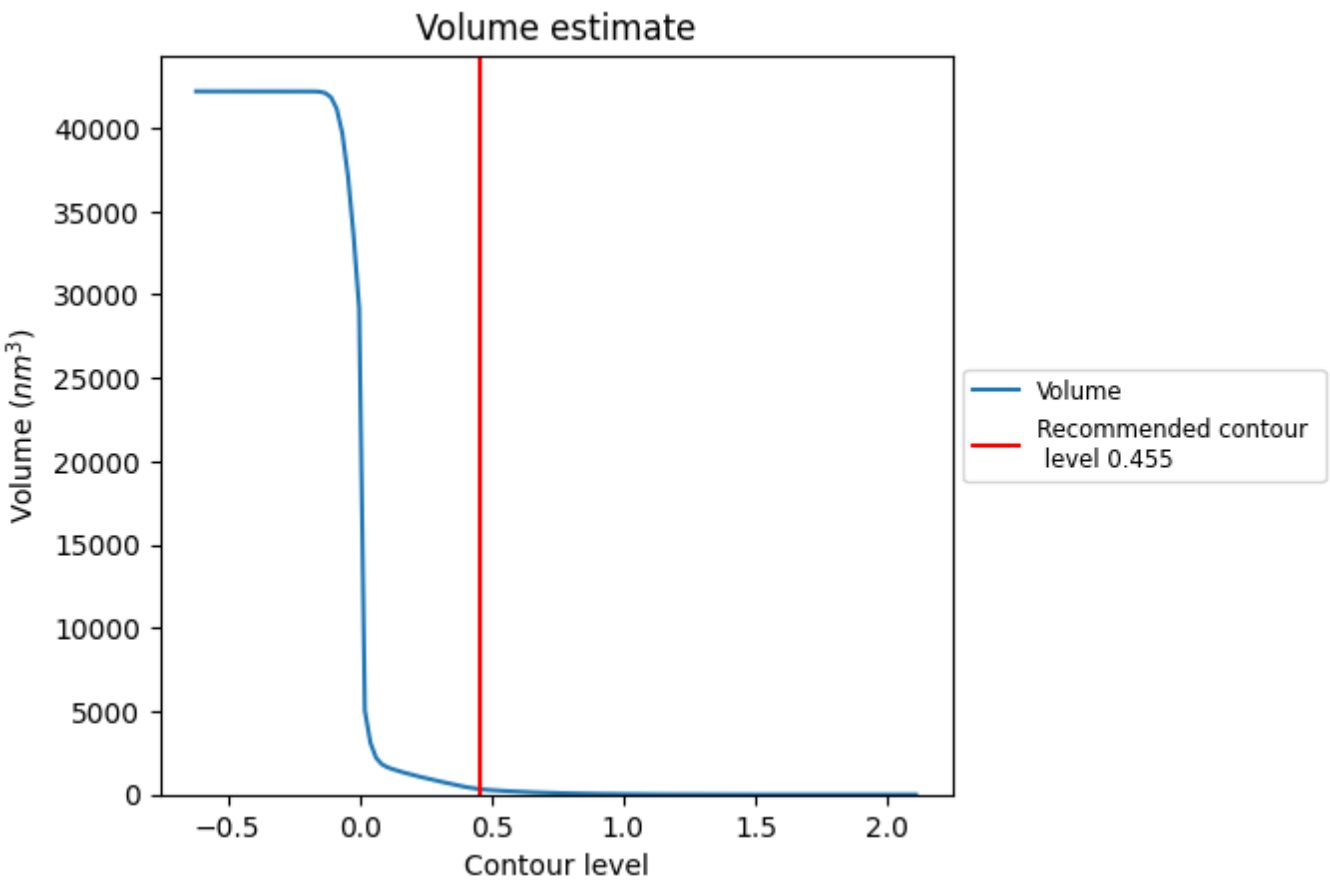
This section contains the results of statistical analysis of the map.

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.

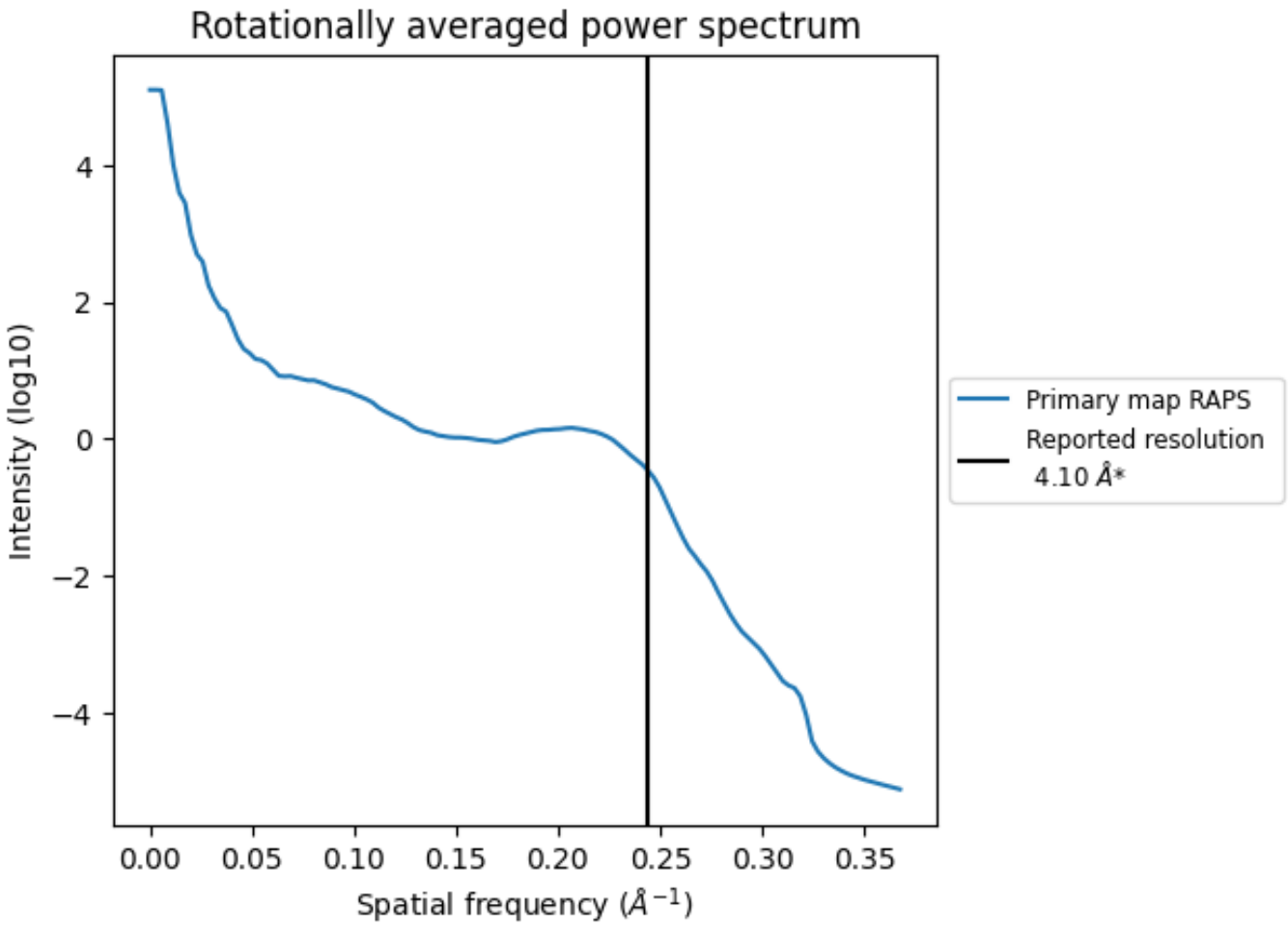
7.2 Volume estimate (i)



The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 298 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 0.244 Å^{-1}

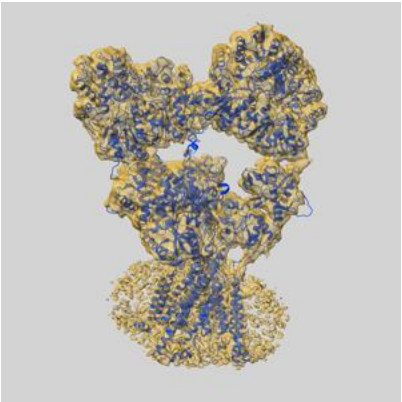
8 Fourier-Shell correlation (i)

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

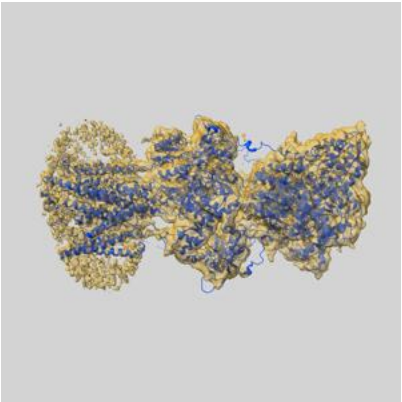
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31459 and PDB model 7F56. Per-residue inclusion information can be found in section 3 on page 7.

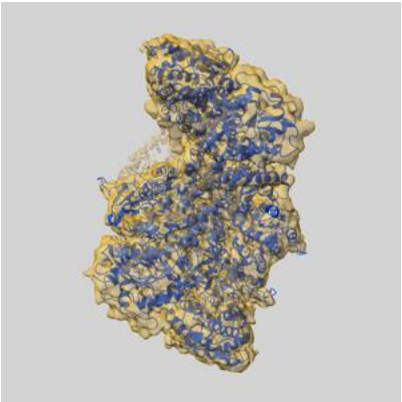
9.1 Map-model overlay (i)



X



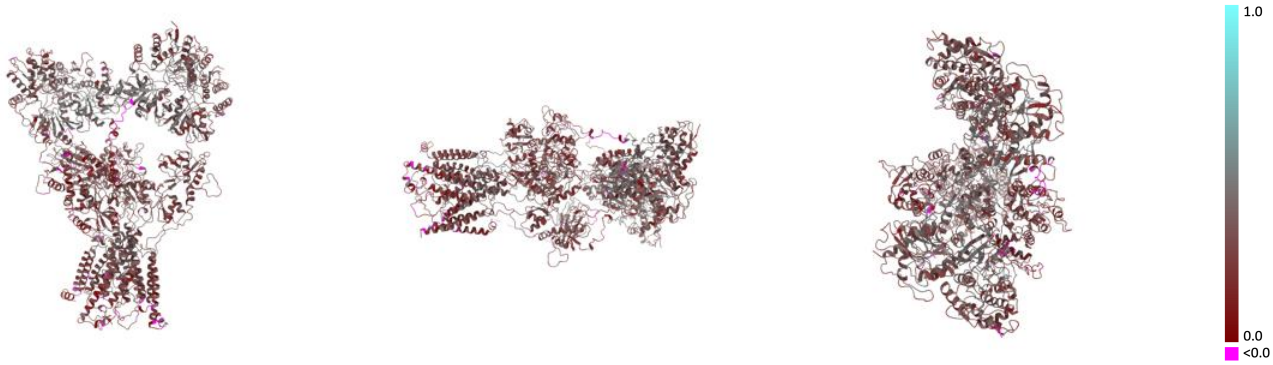
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.455 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

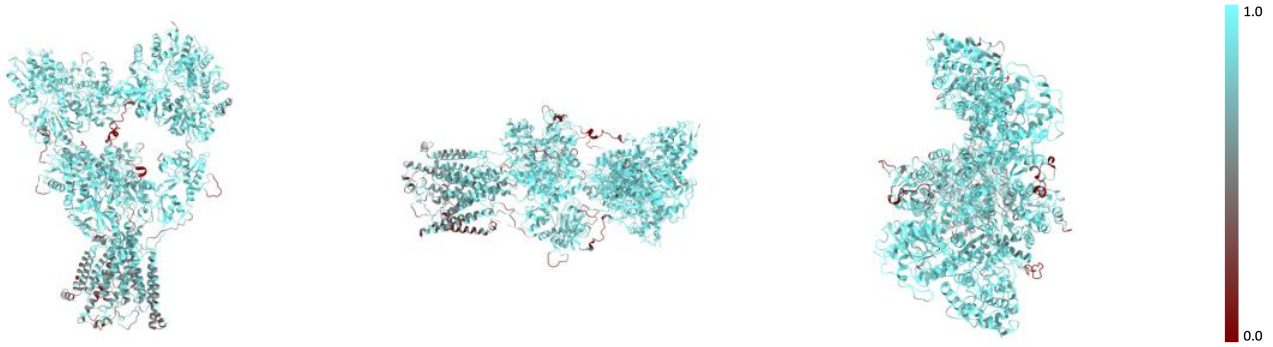
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

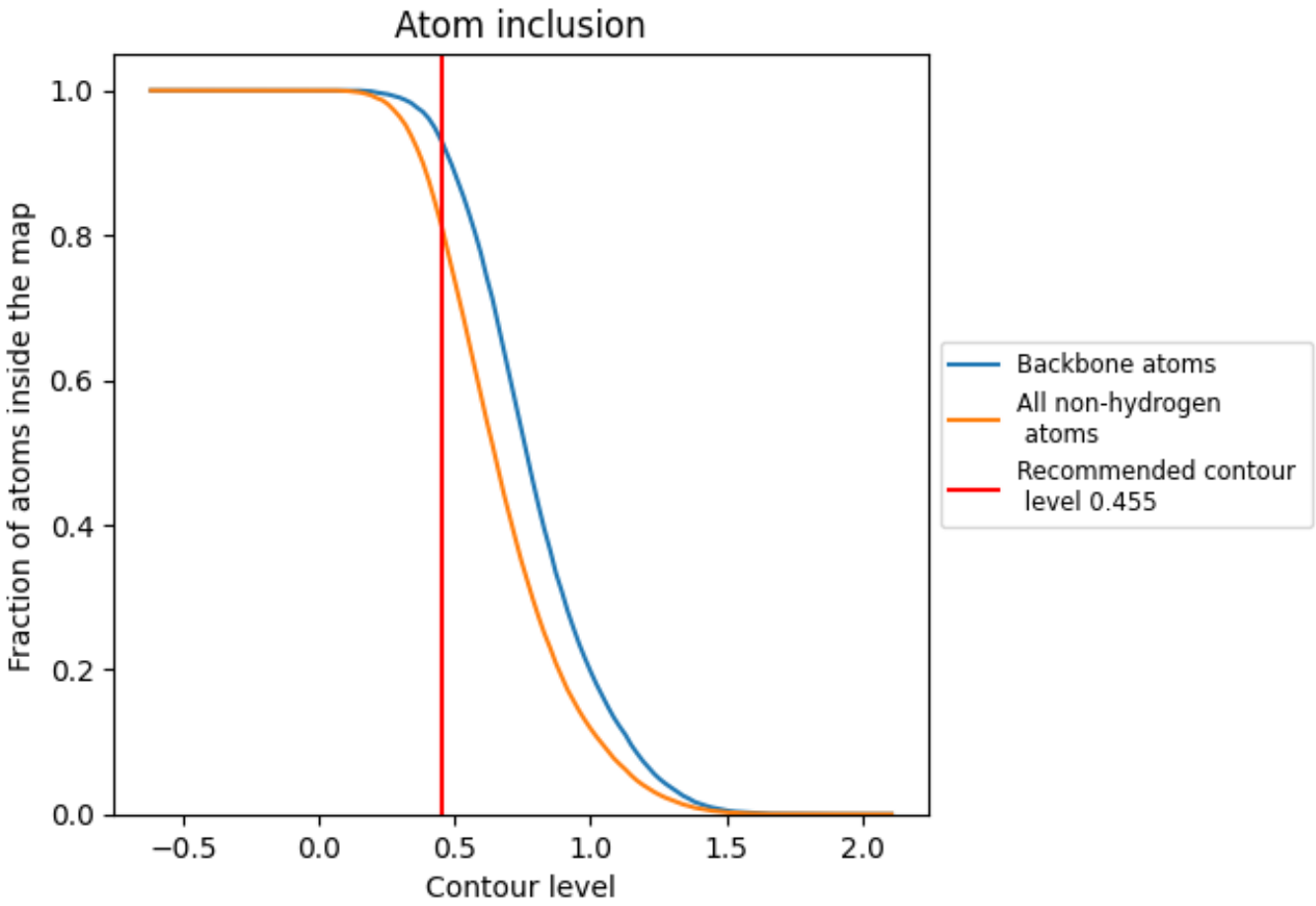
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.455).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 81% 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 (0.455) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8069	0.3090
A	0.8249	0.3060
B	0.8130	0.3060
C	0.8011	0.3000
D	0.8147	0.3300
E	0.6544	0.2680
F	0.8205	0.4550
G	0.9231	0.4210
H	0.8718	0.4230
I	0.9487	0.4250