Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 01:10 AM JST

PDB ID	:	7CWL
EMDB ID	:	EMD-30482
Title	:	SARS-CoV-2 spike protein and P17 fab complex with one RBD in close state
Authors	:	Wang, X.; Wang, N.
Deposited on	:	2020-08-29
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

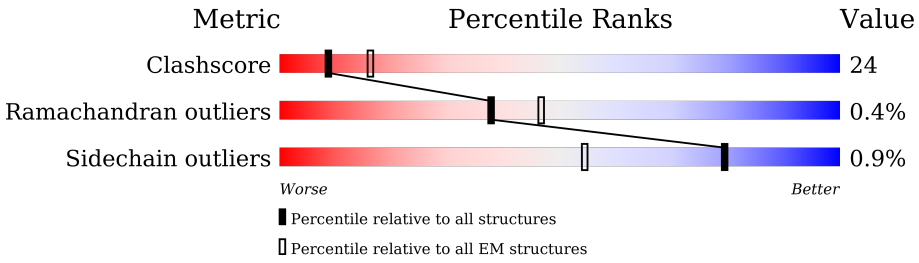
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1273	52% 31% · 16%
1	B	1273	53% 30% · 16%
1	C	1273	55% 29% · 16%
2	G	120	64% 36%
2	H	120	64% 36%
2	I	120	52% 64% 36%
3	J	108	8% 80% 20%
3	K	108	63% 79% 20% ·

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Mol	Chain	Length	Quality of chain
3	L	108	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30638 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1073	Total	C	N	O	S	0	0
			8358	5334	1396	1589	39		
1	B	1070	Total	C	N	O	S	0	0
			8332	5315	1393	1585	39		
1	C	1074	Total	C	N	O	S	0	0
			8372	5342	1399	1592	39		

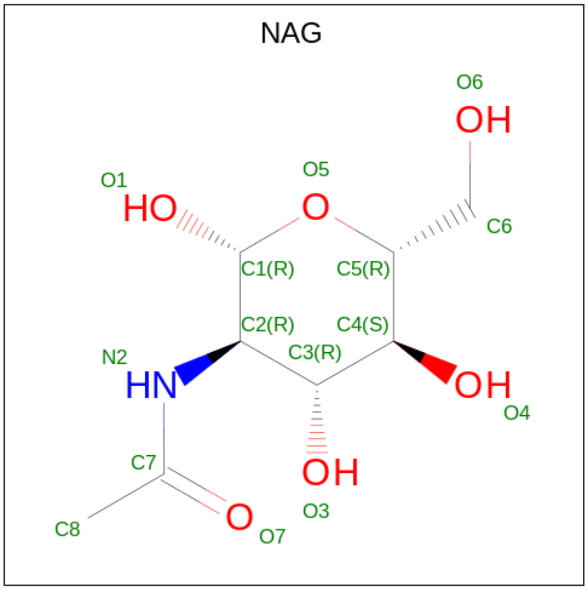
- Molecule 2 is a protein called Fab P17 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	H	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	I	120	Total	C	N	O	S	0	0
			918	574	165	175	4		

- Molecule 3 is a protein called Fab P17 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			814	510	137	165	2		
3	J	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
3	K	107	Total	C	N	O	S	0	0
			813	509	136	166	2		

- 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 C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	A	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0
4	B	1	Total C N O 126 72 9 45	0

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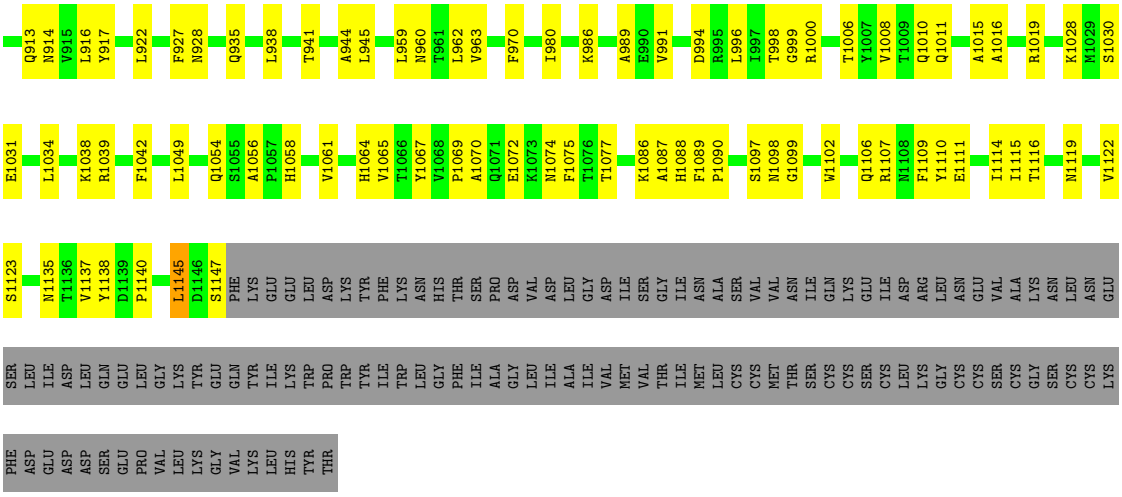
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 126	C 72	N 9	O 45	0
4	B	1	Total 126	C 72	N 9	O 45	0
4	B	1	Total 126	C 72	N 9	O 45	0
4	B	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	0
4	C	1	Total 126	C 72	N 9	O 45	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.

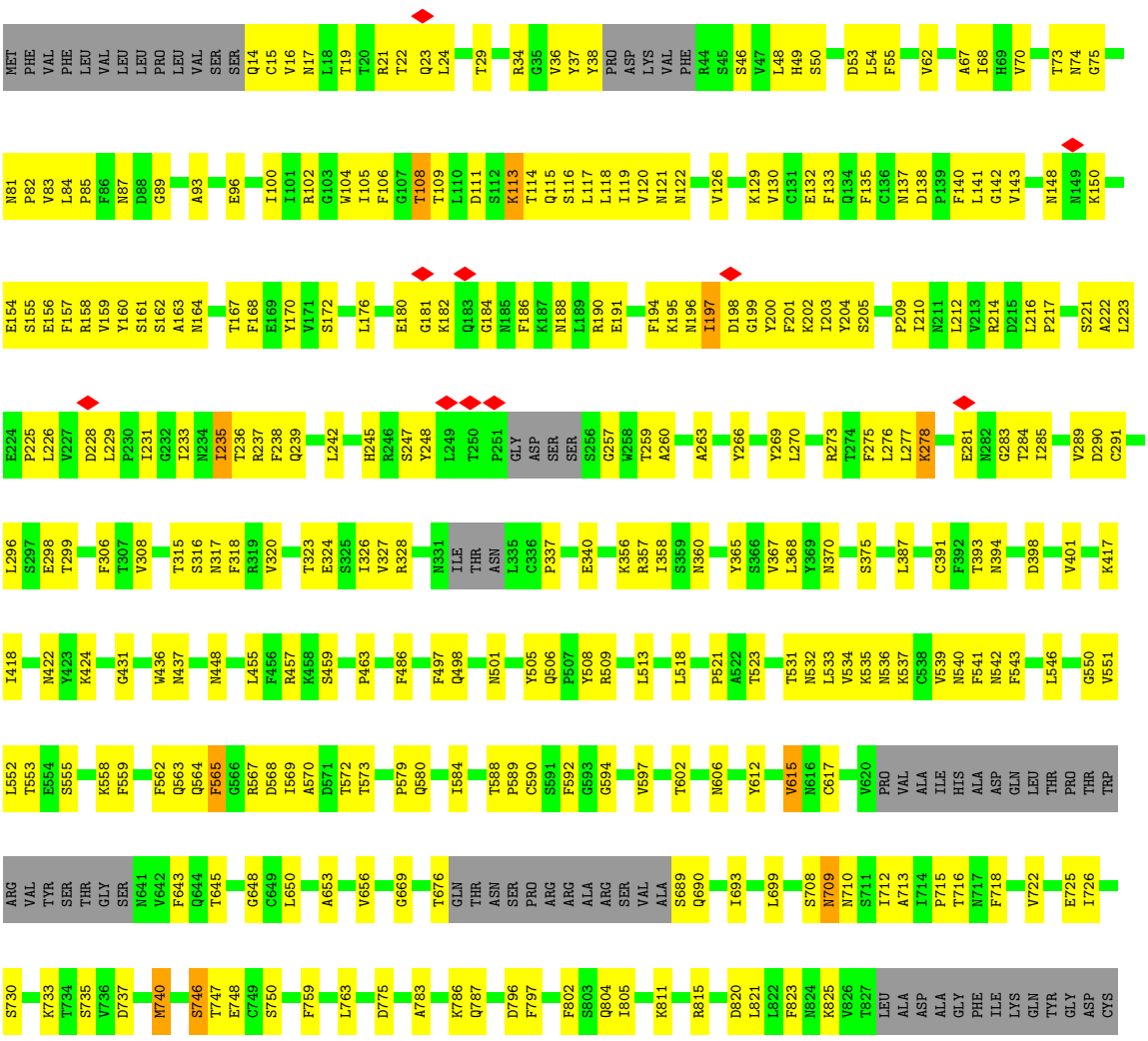
- Molecule 1: Spike glycoprotein

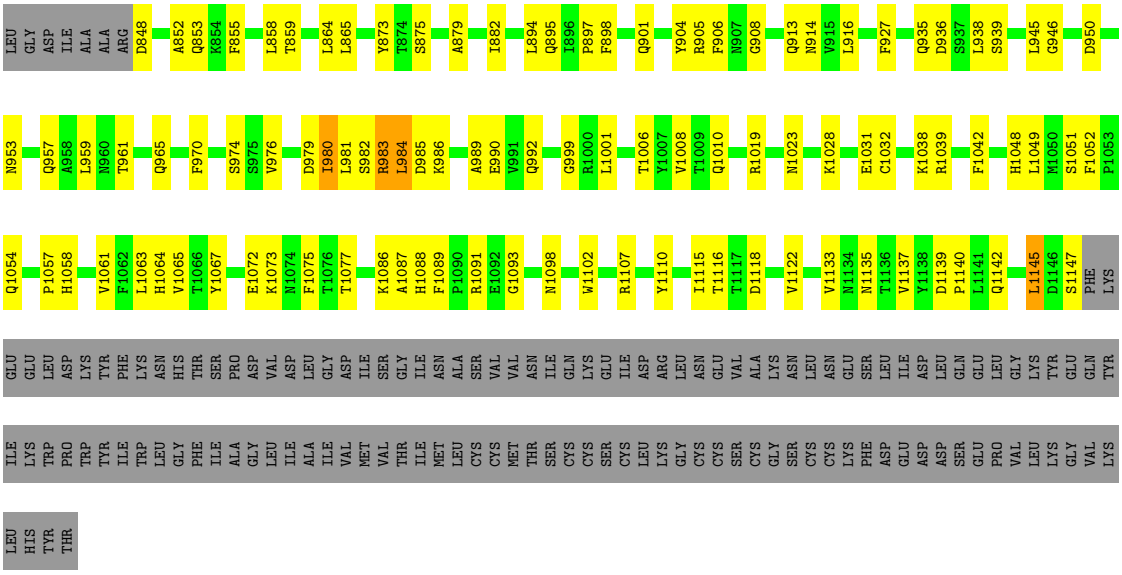
Chain A:



• Molecule 1: Spike glycoprotein

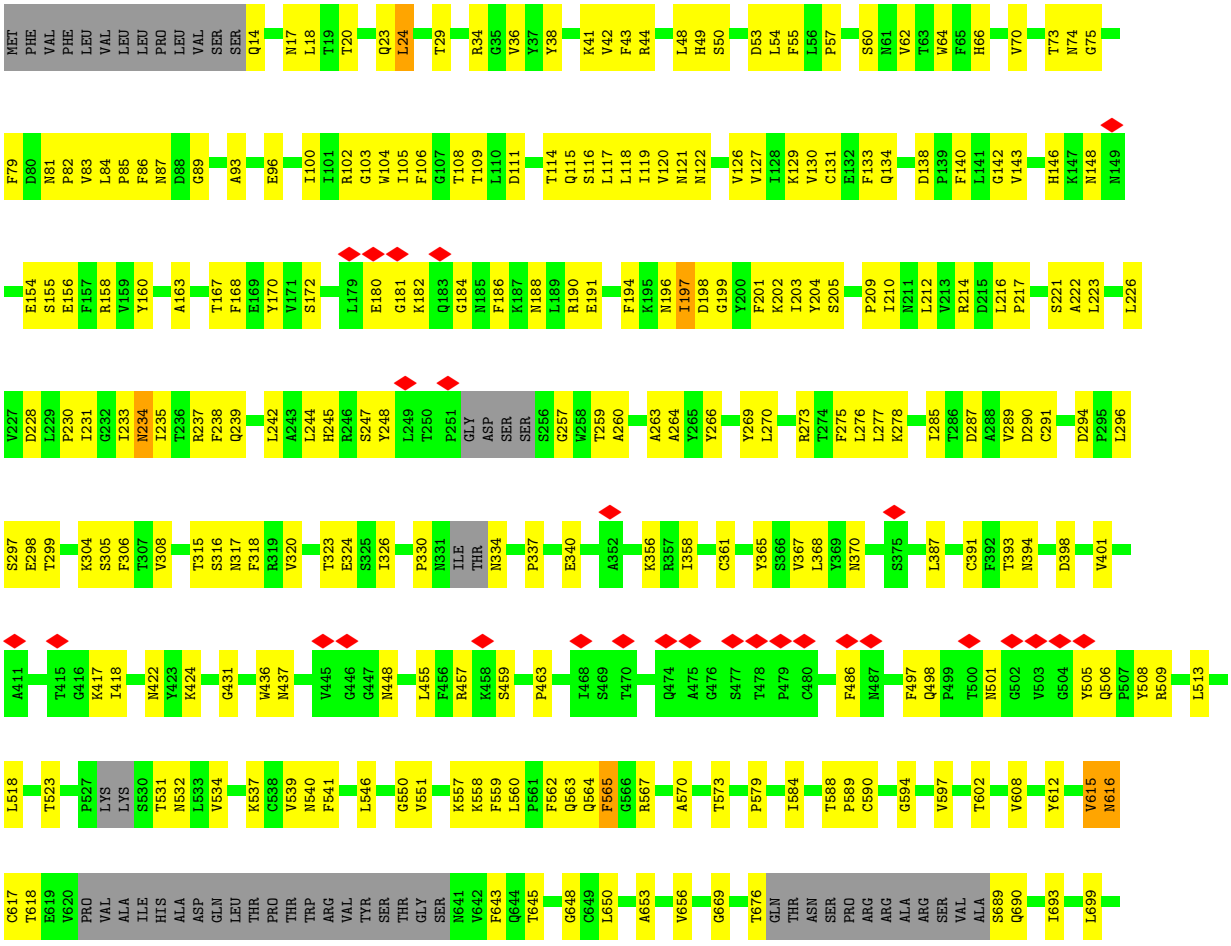
Chain B:

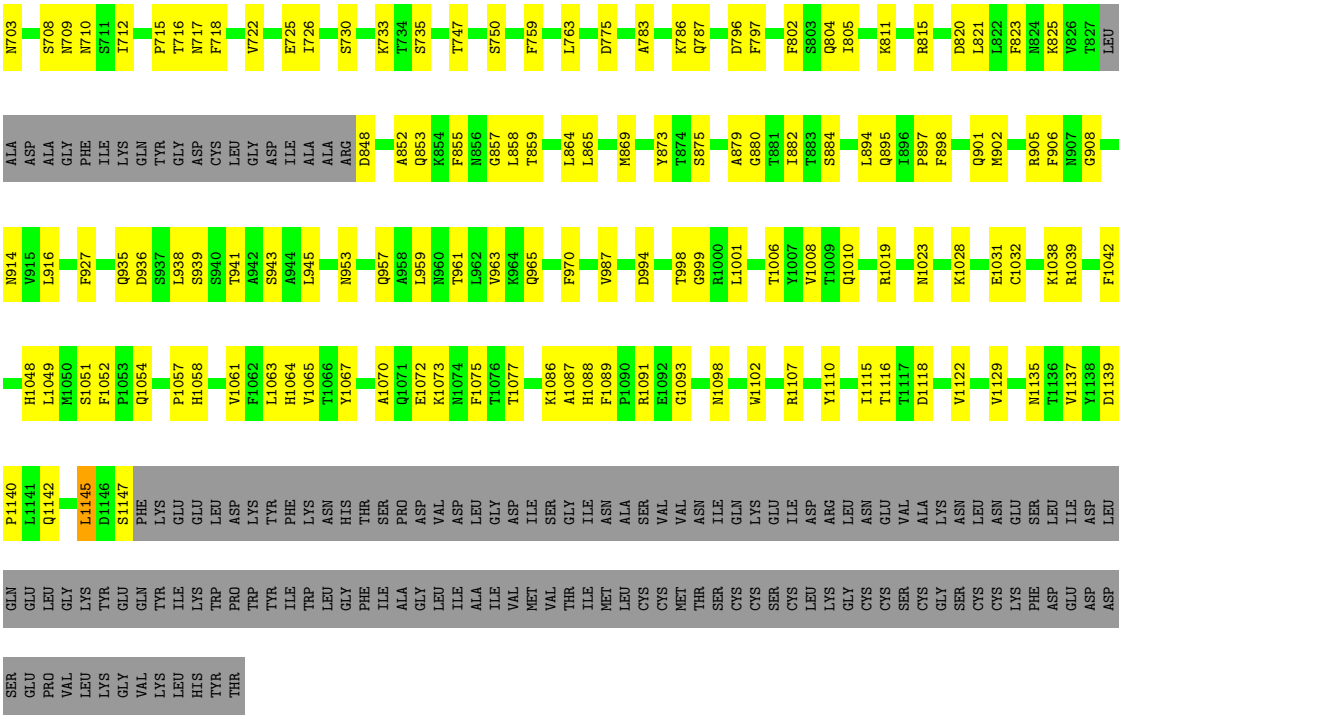




• Molecule 1: Spike glycoprotein

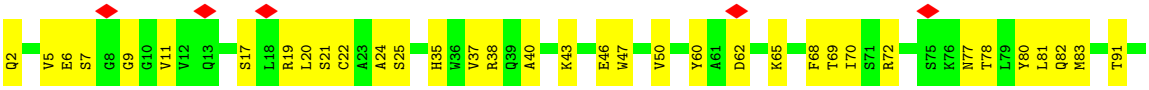
Chain C:





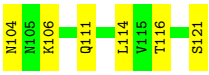
• Molecule 2: Fab P17 heavy chain

Chain G:



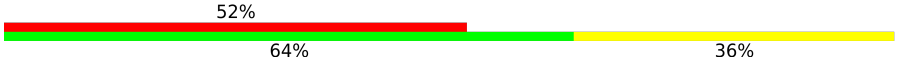
• Molecule 2: Fab P17 heavy chain

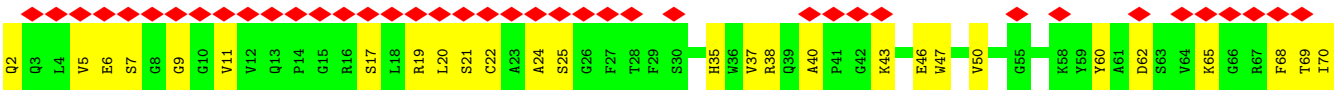
Chain H:

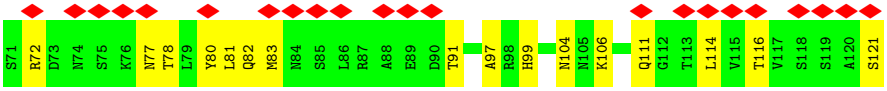


• Molecule 2: Fab P17 heavy chain

Chain I:

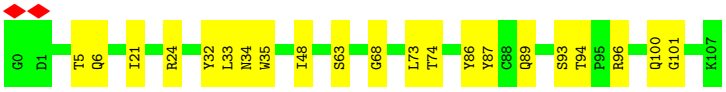






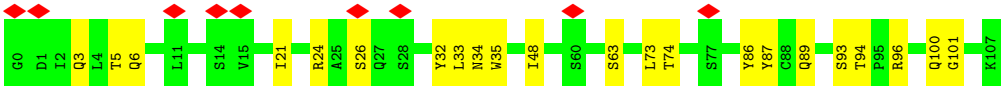
• Molecule 3: Fab P17 light chain

Chain L:



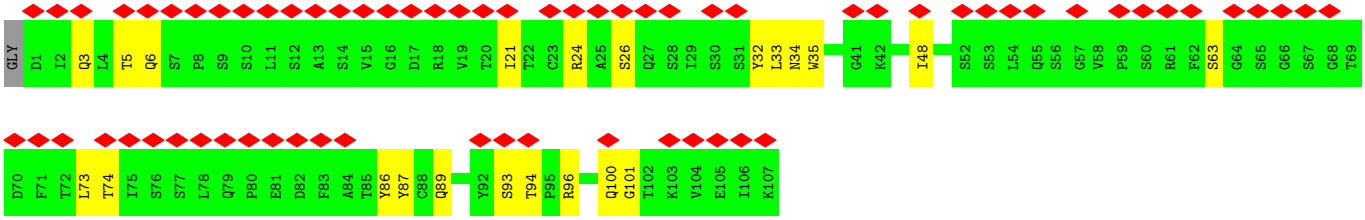
• Molecule 3: Fab P17 light chain

Chain J:



• Molecule 3: Fab P17 light chain

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00502	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	2/8549 (0.0%)	0.59	1/11634 (0.0%)
1	B	0.47	0/8521	0.59	2/11596 (0.0%)
1	C	0.45	0/8563	0.58	2/11653 (0.0%)
2	G	0.37	0/937	0.60	0/1269
2	H	0.37	0/937	0.60	0/1269
2	I	0.37	0/937	0.60	0/1269
3	J	0.38	0/834	0.59	0/1131
3	K	0.38	0/830	0.59	0/1126
3	L	0.38	0/831	0.59	0/1127
All	All	0.46	2/30939 (0.0%)	0.59	5/42074 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	4
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	PRO	N-CA	13.58	1.70	1.47
1	A	588	THR	C-N	6.11	1.45	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	589	PRO	CA-N-CD	-7.64	100.80	111.50
1	C	848	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	848	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	387	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	387	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1145	LEU	Peptide
1	A	248	TYR	Peptide
1	B	1145	LEU	Peptide
1	B	248	TYR	Peptide
1	B	278	LYS	Mainchain
1	B	391	CYS	Peptide
1	B	565	PHE	Peptide
1	C	1145	LEU	Peptide
1	C	248	TYR	Peptide
1	C	391	CYS	Peptide
1	C	565	PHE	Peptide
2	G	72	ARG	Peptide
2	H	72	ARG	Peptide
2	I	72	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8358	0	8130	510	0
1	B	8332	0	8105	478	0
1	C	8372	0	8149	467	0
2	G	918	0	885	26	0
2	H	918	0	885	25	0
2	I	918	0	885	26	0
3	J	817	0	800	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	813	0	797	16	0
3	L	814	0	798	16	0
4	A	126	0	117	7	0
4	B	126	0	117	1	0
4	C	126	0	117	4	0
All	All	30638	0	29785	1433	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 24.

All (1433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HD11	1:C:306:PHE:CE1	1.32	1.61
1:A:63:THR:HG21	1:A:65:PHE:CZ	1.36	1.60
1:A:22:THR:CG2	1:A:78:ARG:HD2	1.28	1.54
1:A:63:THR:CG2	1:A:65:PHE:CZ	1.85	1.54
1:C:296:LEU:HD12	1:C:608:VAL:CG1	1.40	1.52
1:C:64:TRP:CZ2	1:C:66:HIS:CE1	1.95	1.51
1:C:276:LEU:CD1	1:C:306:PHE:HE1	1.23	1.50
1:C:64:TRP:CZ2	1:C:66:HIS:HE1	1.28	1.49
1:A:63:THR:HB	1:A:65:PHE:CE2	1.49	1.48
1:A:591:SER:CB	1:A:615:VAL:HG12	1.46	1.45
1:B:360:ASN:ND2	1:C:168:PHE:HD1	1.15	1.44
1:C:296:LEU:CD1	1:C:608:VAL:HG13	1.45	1.43
1:C:296:LEU:CD1	1:C:608:VAL:CG1	1.97	1.42
1:B:115:GLN:NE2	1:B:167:THR:HG21	1.31	1.40
1:A:589:PRO:N	1:A:589:PRO:CA	1.70	1.39
1:A:296:LEU:HD13	1:A:608:VAL:CG1	1.53	1.39
1:B:108:THR:O	1:B:236:THR:HG22	1.23	1.38
1:B:83:VAL:HG23	1:B:237:ARG:NH2	1.36	1.36
1:B:360:ASN:ND2	1:C:168:PHE:CD1	1.92	1.36
1:A:296:LEU:CD1	1:A:608:VAL:HG11	1.55	1.35
1:A:66:HIS:CD2	1:A:69:HIS:HB2	1.59	1.35
1:A:562:PHE:CE2	1:B:225:PRO:HG2	1.59	1.35
1:C:276:LEU:CD1	1:C:306:PHE:CE1	2.00	1.35
1:A:303:LEU:CD2	1:A:305:SER:HB3	1.58	1.32
1:A:196:ASN:HB2	1:A:201:PHE:CD1	1.67	1.27
1:C:48:LEU:CD1	1:C:304:LYS:O	1.80	1.27
1:C:48:LEU:HD13	1:C:304:LYS:O	1.10	1.26
1:C:18:LEU:HD12	1:C:18:LEU:O	1.24	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:CG2	1:B:237:ARG:NH2	2.00	1.25
1:B:83:VAL:CG2	1:B:237:ARG:HH21	1.49	1.24
1:A:591:SER:HB3	1:A:615:VAL:CG1	1.66	1.24
1:C:324:GLU:OE2	1:C:534:VAL:CG2	1.85	1.23
1:B:108:THR:O	1:B:236:THR:CG2	1.87	1.22
1:B:196:ASN:HB2	1:B:201:PHE:CD1	1.74	1.22
1:A:562:PHE:CZ	1:B:225:PRO:HG3	1.75	1.21
1:A:518:LEU:HD22	1:B:200:TYR:CE2	1.74	1.21
1:A:22:THR:CG2	1:A:78:ARG:CD	2.19	1.21
1:C:287:ASP:HB3	1:C:306:PHE:CE2	1.75	1.20
1:C:324:GLU:OE2	1:C:534:VAL:HG21	1.38	1.17
1:A:591:SER:CB	1:A:615:VAL:CG1	2.22	1.17
1:C:64:TRP:CE2	1:C:66:HIS:CE1	2.32	1.17
1:B:748:GLU:HB2	1:B:981:LEU:HD11	1.18	1.16
1:A:63:THR:CB	1:A:65:PHE:CE2	2.27	1.16
1:A:66:HIS:CD2	1:A:69:HIS:CB	2.30	1.15
1:B:565:PHE:HB2	1:C:42:VAL:HG22	1.19	1.15
1:C:296:LEU:HD11	1:C:608:VAL:HG13	1.20	1.15
1:A:42:VAL:HG22	1:C:565:PHE:HB2	1.24	1.15
1:A:562:PHE:CZ	1:B:225:PRO:CG	2.30	1.15
1:A:22:THR:HG21	1:A:78:ARG:HB3	1.20	1.14
1:B:14:GLN:NE2	1:B:157:PHE:HB3	1.61	1.13
1:C:121:ASN:CG	1:C:126:VAL:HG22	1.66	1.13
1:C:797:PHE:CD2	1:C:802:PHE:HD2	1.67	1.13
1:A:379:CYS:SG	1:A:384:PRO:HG3	1.87	1.13
1:A:710:ASN:O	1:A:1077:THR:HG22	1.49	1.12
1:B:104:TRP:CE3	1:B:119:ILE:HD11	1.83	1.11
1:B:104:TRP:HE3	1:B:119:ILE:HD11	0.96	1.11
1:B:85:PRO:HA	1:B:237:ARG:HG2	1.24	1.10
1:B:1075:PHE:CE1	1:B:1098:ASN:HA	1.87	1.10
1:B:797:PHE:CD2	1:B:802:PHE:HD2	1.68	1.09
1:B:118:LEU:HD13	1:B:133:PHE:CD2	1.88	1.09
1:A:63:THR:HG22	1:A:65:PHE:CZ	1.86	1.08
1:C:201:PHE:HB3	1:C:231:ILE:HG13	1.31	1.08
1:B:115:GLN:HE21	1:B:167:THR:CG2	1.68	1.07
1:C:299:THR:HG22	1:C:315:THR:OG1	1.54	1.07
1:A:562:PHE:CE2	1:B:225:PRO:CG	2.38	1.07
1:B:328:ARG:N	1:B:542:ASN:O	1.86	1.07
1:B:85:PRO:CA	1:B:237:ARG:HG2	1.86	1.06
1:B:115:GLN:NE2	1:B:167:THR:CG2	2.18	1.06
1:B:278:LYS:HB2	1:B:306:PHE:CZ	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLN:CD	1:B:157:PHE:HB3	1.75	1.05
1:B:853:GLN:NE2	1:B:959:LEU:HB3	1.70	1.05
1:A:109:THR:HB	1:A:114:THR:OG1	1.57	1.05
1:C:296:LEU:CD1	1:C:608:VAL:HG11	1.83	1.05
1:A:196:ASN:CG	1:A:201:PHE:HB2	1.76	1.05
1:A:369:TYR:OH	1:A:384:PRO:O	1.70	1.05
1:C:853:GLN:NE2	1:C:959:LEU:HB3	1.72	1.05
1:A:18:LEU:O	1:A:18:LEU:HD12	1.56	1.04
1:C:66:HIS:ND1	1:C:264:ALA:HB2	1.72	1.04
1:C:797:PHE:CD2	1:C:802:PHE:CD2	2.44	1.04
1:A:22:THR:HG22	1:A:78:ARG:HD2	1.06	1.04
1:B:797:PHE:CD2	1:B:802:PHE:CD2	2.46	1.03
1:A:22:THR:HG21	1:A:78:ARG:CB	1.89	1.03
1:C:296:LEU:HD12	1:C:608:VAL:CG2	1.89	1.02
1:B:536:ASN:OD1	1:B:553:THR:HG22	1.58	1.02
1:B:853:GLN:NE2	1:B:959:LEU:CB	2.22	1.02
1:C:853:GLN:NE2	1:C:959:LEU:CB	2.23	1.02
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.06	1.02
1:C:1075:PHE:HE1	1:C:1098:ASN:HB3	1.21	1.02
1:B:201:PHE:HB3	1:B:231:ILE:HG13	1.41	1.01
1:A:196:ASN:HB2	1:A:201:PHE:HD1	1.05	1.01
1:A:22:THR:HG23	1:A:78:ARG:HD2	1.41	1.01
1:A:369:TYR:OH	1:A:384:PRO:C	1.97	1.00
1:C:1075:PHE:CE1	1:C:1098:ASN:HB3	1.97	1.00
1:B:567:ARG:HD2	1:C:44:ARG:NH2	1.77	0.99
1:A:413:GLY:CA	1:C:987:VAL:HG21	1.93	0.99
1:C:121:ASN:CG	1:C:126:VAL:CG2	2.30	0.99
1:A:63:THR:CG2	1:A:65:PHE:CE2	2.44	0.98
1:C:287:ASP:CB	1:C:306:PHE:CE2	2.46	0.98
1:C:797:PHE:HD2	1:C:802:PHE:HD2	1.11	0.98
1:C:1075:PHE:HE1	1:C:1098:ASN:CB	1.77	0.98
1:C:296:LEU:HD12	1:C:608:VAL:CB	1.93	0.97
2:H:17:SER:HA	2:H:83:MET:O	1.64	0.97
1:B:797:PHE:HD2	1:B:802:PHE:HD2	1.11	0.97
2:G:17:SER:HA	2:G:83:MET:O	1.65	0.97
1:C:64:TRP:CE2	1:C:66:HIS:HE1	1.76	0.97
1:C:201:PHE:CB	1:C:231:ILE:HG13	1.95	0.96
1:A:365:TYR:CE2	1:A:387:LEU:HD11	1.99	0.96
1:B:328:ARG:CB	1:B:543:PHE:CD1	2.49	0.96
1:C:18:LEU:O	1:C:18:LEU:CD1	2.13	0.96
1:A:63:THR:O	1:A:65:PHE:CD2	2.18	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:GLN:N	1:C:41:LYS:HB3	1.80	0.95
1:A:196:ASN:CB	1:A:201:PHE:HD1	1.79	0.95
2:I:17:SER:HA	2:I:83:MET:O	1.65	0.95
1:B:853:GLN:HE21	1:B:959:LEU:HB3	1.32	0.95
1:A:429:PHE:HZ	1:A:514:SER:HG	1.12	0.94
1:B:85:PRO:HA	1:B:237:ARG:CG	1.95	0.94
1:B:360:ASN:HD22	1:C:168:PHE:HD1	1.09	0.94
1:B:14:GLN:NE2	1:B:157:PHE:CB	2.29	0.94
1:B:1075:PHE:HE1	1:B:1098:ASN:HA	1.24	0.93
1:A:63:THR:CB	1:A:65:PHE:CZ	2.48	0.93
1:B:328:ARG:HB2	1:B:543:PHE:CD1	2.02	0.93
1:A:22:THR:HG21	1:A:78:ARG:HD2	1.49	0.93
1:C:64:TRP:CH2	1:C:66:HIS:NE2	2.37	0.93
1:B:308:VAL:H	1:B:602:THR:CG2	1.82	0.93
1:A:197:ILE:O	1:A:199:GLY:N	2.01	0.92
1:B:197:ILE:O	1:B:199:GLY:N	2.01	0.92
1:B:118:LEU:HD13	1:B:133:PHE:HD2	1.25	0.92
1:C:296:LEU:HD12	1:C:608:VAL:HG11	1.43	0.92
1:C:66:HIS:ND1	1:C:264:ALA:CB	2.32	0.92
1:A:22:THR:HG22	1:A:78:ARG:CD	1.94	0.91
1:B:196:ASN:CB	1:B:201:PHE:HD1	1.81	0.91
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	1.84	0.91
1:A:413:GLY:O	1:C:987:VAL:HG21	1.71	0.91
1:B:196:ASN:HB2	1:B:201:PHE:HD1	1.12	0.91
1:A:41:LYS:HB3	1:C:564:GLN:N	1.85	0.90
1:A:591:SER:HB2	1:A:615:VAL:CG1	1.99	0.90
1:B:1075:PHE:HE1	1:B:1098:ASN:CA	1.83	0.90
1:A:382:VAL:HG13	1:A:430:THR:CG2	2.00	0.90
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.53	0.90
1:A:413:GLY:HA3	1:C:987:VAL:HG21	1.53	0.90
1:B:984:LEU:CD1	1:B:992:GLN:HG3	2.01	0.90
1:B:83:VAL:HG23	1:B:237:ARG:HH21	0.83	0.89
1:C:64:TRP:CH2	1:C:66:HIS:CE1	2.61	0.89
1:C:118:LEU:CD2	1:C:120:VAL:HG23	2.03	0.89
1:C:287:ASP:OD2	1:C:306:PHE:CD2	2.26	0.89
1:B:104:TRP:HE3	1:B:119:ILE:CD1	1.84	0.89
1:C:853:GLN:HE21	1:C:959:LEU:HB3	1.32	0.89
1:B:357:ARG:HH22	1:C:167:THR:HG22	1.37	0.88
1:C:121:ASN:OD1	1:C:126:VAL:HG22	1.71	0.88
3:K:33:LEU:HA	3:K:89:GLN:O	1.74	0.88
1:A:658:ASN:HB3	1:A:660:TYR:CZ	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:HD2	1:A:69:HIS:CB	1.74	0.88
1:A:41:LYS:O	1:C:563:GLN:HB3	1.73	0.88
1:A:196:ASN:CB	1:A:201:PHE:HB2	2.04	0.88
3:J:33:LEU:HA	3:J:89:GLN:O	1.74	0.88
1:A:303:LEU:HD21	1:A:305:SER:HB3	1.52	0.88
1:B:716:THR:HG21	1:B:1073:LYS:HD2	1.55	0.88
1:B:1102:TRP:CD1	1:B:1135:ASN:ND2	2.41	0.88
1:A:109:THR:HG21	1:A:112:SER:O	1.74	0.87
1:A:296:LEU:HD13	1:A:608:VAL:HG11	0.87	0.87
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.57	0.87
1:A:429:PHE:CZ	1:A:514:SER:OG	2.25	0.87
1:A:63:THR:CG2	1:A:65:PHE:CE1	2.58	0.87
3:L:33:LEU:HA	3:L:89:GLN:O	1.74	0.87
1:A:44:ARG:NH2	1:C:567:ARG:HD2	1.90	0.87
1:A:196:ASN:HB2	1:A:201:PHE:CG	2.09	0.87
1:A:22:THR:HG22	1:A:78:ARG:HH11	1.38	0.86
1:A:518:LEU:CD2	1:B:200:TYR:CD2	2.57	0.86
1:B:299:THR:HG21	1:B:597:VAL:HB	1.56	0.86
1:B:357:ARG:NH2	1:C:167:THR:HG22	1.90	0.86
1:B:360:ASN:HD21	1:C:168:PHE:HD1	1.16	0.86
1:C:64:TRP:CZ2	1:C:66:HIS:NE2	2.43	0.86
1:B:853:GLN:HE22	1:B:959:LEU:CD1	1.89	0.86
1:C:196:ASN:HB2	1:C:201:PHE:HD1	1.39	0.86
1:A:365:TYR:CE2	1:A:387:LEU:CD1	2.59	0.86
1:C:853:GLN:HE22	1:C:959:LEU:CD1	1.88	0.85
1:A:303:LEU:HD23	1:A:305:SER:HB3	1.55	0.85
1:B:748:GLU:HB2	1:B:981:LEU:CD1	2.04	0.85
1:A:588:THR:HG23	1:A:589:PRO:HD2	1.58	0.85
1:A:426:PRO:HG2	1:A:429:PHE:HB2	1.59	0.85
1:B:308:VAL:H	1:B:602:THR:HG22	1.39	0.85
1:B:328:ARG:HB3	1:B:543:PHE:CD1	2.12	0.85
1:B:559:PHE:CE1	1:C:43:PHE:HB3	2.11	0.85
1:A:109:THR:O	1:A:111:ASP:N	2.08	0.85
1:B:1075:PHE:HE1	1:B:1098:ASN:CB	1.90	0.84
1:A:303:LEU:HD22	1:A:305:SER:HB3	1.59	0.84
1:B:324:GLU:OE2	1:B:534:VAL:HG21	1.76	0.84
1:C:121:ASN:HA	1:C:126:VAL:HG22	1.59	0.84
1:A:41:LYS:O	1:C:563:GLN:CB	2.26	0.84
1:A:201:PHE:HB3	1:A:231:ILE:HG13	1.57	0.84
1:A:382:VAL:HB	1:B:983:ARG:HB3	1.57	0.84
1:C:299:THR:CG2	1:C:315:THR:OG1	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:HB2	1:B:201:PHE:HB2	1.60	0.83
1:C:534:VAL:HG11	1:C:539:VAL:CG1	2.07	0.83
1:B:196:ASN:HB2	1:B:201:PHE:CB	2.08	0.83
1:A:518:LEU:CD2	1:B:200:TYR:CE2	2.60	0.83
1:A:518:LEU:HD22	1:B:200:TYR:CD2	2.13	0.83
1:C:121:ASN:OD1	1:C:126:VAL:CG2	2.26	0.83
1:A:897:PRO:HB3	1:C:709:ASN:O	1.79	0.82
1:B:106:PHE:CG	1:B:235:ILE:HD13	2.15	0.82
1:B:196:ASN:HB2	1:B:201:PHE:CG	2.13	0.82
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.13	0.82
1:B:328:ARG:CB	1:B:543:PHE:HD1	1.90	0.82
1:A:43:PHE:HB3	1:C:559:PHE:CE1	2.14	0.82
1:C:287:ASP:CG	1:C:306:PHE:CE2	2.53	0.82
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.44	0.82
1:A:196:ASN:HB2	1:A:201:PHE:CB	2.08	0.82
1:B:196:ASN:CG	1:B:201:PHE:HB2	1.99	0.82
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.13	0.82
1:C:296:LEU:CG	1:C:608:VAL:HG11	2.09	0.82
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	1.93	0.81
1:C:115:GLN:HB2	1:C:233:ILE:HD12	1.62	0.81
1:C:716:THR:HG21	1:C:1073:LYS:HD2	1.60	0.81
1:B:986:LYS:O	1:B:990:GLU:HG2	1.79	0.81
1:A:1102:TRP:CD1	1:A:1135:ASN:ND2	2.48	0.81
1:B:984:LEU:HD11	1:B:992:GLN:HG3	1.60	0.81
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.14	0.81
1:B:567:ARG:HG3	1:C:42:VAL:HG11	1.61	0.81
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.14	0.81
1:B:360:ASN:ND2	1:C:168:PHE:CE1	2.48	0.81
1:C:196:ASN:HB2	1:C:201:PHE:CD1	2.14	0.81
1:A:718:PHE:CD1	1:A:1067:TYR:CE1	2.69	0.81
1:A:63:THR:HG22	1:A:65:PHE:CE1	2.17	0.81
1:B:83:VAL:HG21	1:B:237:ARG:NH2	1.96	0.81
1:B:299:THR:CG2	1:B:597:VAL:HB	2.11	0.81
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.14	0.81
1:C:1075:PHE:CD1	1:C:1098:ASN:HA	2.16	0.81
1:A:296:LEU:CD1	1:A:608:VAL:CG1	2.33	0.80
1:B:196:ASN:CB	1:B:201:PHE:HB2	2.11	0.80
1:C:534:VAL:CB	1:C:539:VAL:HG11	2.10	0.80
1:A:518:LEU:HD22	1:B:200:TYR:HE2	1.44	0.80
1:A:369:TYR:HH	1:A:384:PRO:C	1.79	0.80
1:B:563:GLN:HB3	1:C:41:LYS:O	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:CB	1:A:201:PHE:CD1	2.57	0.80
1:A:287:ASP:HB3	1:A:306:PHE:CE2	2.17	0.80
1:B:567:ARG:HD2	1:C:44:ARG:HH21	1.44	0.80
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.64	0.80
1:B:1102:TRP:HD1	1:B:1135:ASN:ND2	1.77	0.80
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.16	0.80
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.17	0.80
1:B:278:LYS:HB2	1:B:306:PHE:HZ	1.44	0.80
1:C:118:LEU:HD23	1:C:120:VAL:HG23	1.63	0.79
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.15	0.79
1:B:716:THR:HG21	1:B:1073:LYS:CD	2.12	0.79
1:A:303:LEU:CD2	1:A:305:SER:CB	2.53	0.79
1:B:564:GLN:H	1:C:41:LYS:HB3	1.45	0.79
1:C:324:GLU:OE2	1:C:534:VAL:HG22	1.83	0.79
1:C:201:PHE:HB3	1:C:231:ILE:CG1	2.11	0.78
1:A:196:ASN:HB2	1:A:201:PHE:HB2	1.64	0.78
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.64	0.78
1:A:109:THR:OG1	1:A:114:THR:CG2	2.31	0.78
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.48	0.78
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.31	0.78
1:A:63:THR:HB	1:A:65:PHE:HE2	1.05	0.78
1:C:853:GLN:HE21	1:C:959:LEU:CB	1.93	0.78
1:A:236:THR:HG23	1:A:237:ARG:HD3	1.66	0.78
1:A:109:THR:OG1	1:A:114:THR:HG23	1.83	0.77
1:A:377:PHE:CE1	1:A:434:ILE:HG12	2.19	0.77
1:B:299:THR:HG21	1:B:597:VAL:CB	2.13	0.77
1:B:1075:PHE:CE1	1:B:1098:ASN:CA	2.61	0.77
1:A:382:VAL:HG13	1:A:430:THR:HG23	1.66	0.77
1:C:534:VAL:HB	1:C:539:VAL:HG11	1.67	0.77
3:L:63:SER:O	3:L:74:THR:HB	1.85	0.77
1:A:66:HIS:HD2	1:A:69:HIS:HB2	1.01	0.77
1:A:413:GLY:C	1:C:987:VAL:HG21	2.05	0.77
3:J:63:SER:O	3:J:74:THR:HB	1.85	0.77
1:A:588:THR:CG2	1:A:589:PRO:HD2	2.15	0.77
1:B:108:THR:O	1:B:236:THR:HG21	1.84	0.77
1:A:303:LEU:HD13	1:A:308:VAL:HG22	1.67	0.76
1:A:429:PHE:HZ	1:A:514:SER:OG	1.66	0.76
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.31	0.76
1:A:231:ILE:HG22	1:A:233:ILE:HG22	1.68	0.76
3:K:63:SER:O	3:K:74:THR:HB	1.85	0.76
1:C:64:TRP:HZ2	1:C:66:HIS:HE1	1.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:853:GLN:NE2	1:C:959:LEU:HD13	2.00	0.76
1:A:118:LEU:HG	1:A:120:VAL:HG23	1.66	0.76
1:B:853:GLN:NE2	1:B:959:LEU:CD1	2.49	0.76
1:C:853:GLN:NE2	1:C:959:LEU:CD1	2.48	0.76
1:A:41:LYS:HB3	1:C:564:GLN:H	1.49	0.76
1:A:914:ASN:ND2	1:A:1111:GLU:OE2	2.19	0.76
1:C:550:GLY:HA2	1:C:589:PRO:HA	1.66	0.75
1:B:550:GLY:HA2	1:B:589:PRO:HA	1.67	0.75
1:B:108:THR:HB	1:B:114:THR:HB	1.66	0.75
1:B:1075:PHE:CD1	1:B:1098:ASN:HA	2.21	0.75
1:C:287:ASP:OD2	1:C:306:PHE:CE2	2.39	0.75
1:C:308:VAL:H	1:C:602:THR:HG22	1.50	0.75
2:I:69:THR:O	2:I:81:LEU:HA	1.86	0.75
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.69	0.75
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.01	0.75
1:B:48:LEU:HD11	1:B:306:PHE:CD2	2.21	0.75
2:H:69:THR:O	2:H:81:LEU:HA	1.86	0.75
1:A:108:THR:HG21	4:A:1301:NAG:H61	1.68	0.74
1:B:710:ASN:O	1:B:1077:THR:HG22	1.86	0.74
2:G:69:THR:O	2:G:81:LEU:HA	1.86	0.74
1:A:276:LEU:HD13	1:A:289:VAL:O	1.86	0.74
1:B:327:VAL:HG12	1:B:542:ASN:CB	2.17	0.74
1:B:106:PHE:CD1	1:B:235:ILE:HD13	2.22	0.74
1:B:853:GLN:NE2	1:B:959:LEU:HD13	2.01	0.74
1:C:115:GLN:HB2	1:C:233:ILE:CD1	2.18	0.74
1:A:658:ASN:HB3	1:A:660:TYR:OH	1.87	0.74
1:B:563:GLN:CB	1:C:41:LYS:O	2.36	0.74
1:C:48:LEU:HD12	1:C:304:LYS:O	1.87	0.74
1:A:718:PHE:CE1	1:A:1067:TYR:HE1	2.06	0.73
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.21	0.73
1:B:748:GLU:CB	1:B:981:LEU:HD11	2.10	0.73
1:C:299:THR:HG21	1:C:597:VAL:HB	1.70	0.73
1:C:534:VAL:CG1	1:C:539:VAL:HG11	2.16	0.73
1:A:365:TYR:CZ	1:A:387:LEU:HD11	2.23	0.73
1:C:276:LEU:CD1	1:C:306:PHE:CZ	2.71	0.73
1:C:797:PHE:HD2	1:C:802:PHE:CD2	1.94	0.73
1:C:1075:PHE:CE1	1:C:1098:ASN:CB	2.64	0.73
4:A:1306:NAG:O7	4:A:1306:NAG:O3	2.05	0.73
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.22	0.73
1:B:797:PHE:HD2	1:B:802:PHE:CD2	1.95	0.73
1:C:317:ASN:HD22	1:C:594:GLY:HA2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ARG:NH1	1:A:571:ASP:O	2.22	0.73
1:B:317:ASN:HD22	1:B:594:GLY:HA2	1.54	0.73
1:C:299:THR:CG2	1:C:597:VAL:HG21	2.19	0.73
1:A:109:THR:CG2	1:A:112:SER:O	2.37	0.72
1:B:709:ASN:O	1:C:897:PRO:HB3	1.89	0.72
1:B:299:THR:HG23	1:B:597:VAL:HG21	1.71	0.72
1:B:328:ARG:HB2	1:B:543:PHE:CE1	2.23	0.72
1:A:22:THR:HG21	1:A:78:ARG:CG	2.18	0.72
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.71	0.72
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.71	0.72
1:A:718:PHE:CE1	1:A:1067:TYR:CE1	2.78	0.72
1:C:296:LEU:HG	1:C:608:VAL:HG11	1.71	0.72
1:A:413:GLY:O	1:C:987:VAL:CG2	2.36	0.72
1:B:100:ILE:HG21	1:B:263:ALA:HB2	1.72	0.72
1:B:559:PHE:CE1	1:C:43:PHE:CB	2.73	0.72
1:C:143:VAL:HG22	1:C:154:GLU:HG2	1.72	0.72
1:C:534:VAL:HG11	1:C:539:VAL:HG11	1.71	0.72
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.53	0.72
1:A:382:VAL:CG1	1:A:430:THR:CG2	2.68	0.71
1:A:109:THR:CB	1:A:114:THR:OG1	2.36	0.71
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.55	0.71
1:A:143:VAL:HG22	1:A:154:GLU:HG2	1.72	0.71
1:B:299:THR:CG2	1:B:597:VAL:CB	2.69	0.71
1:B:737:ASP:OD2	1:B:740:MET:HB3	1.90	0.71
1:A:44:ARG:HH21	1:C:567:ARG:HD2	1.53	0.71
1:C:656:VAL:CG2	1:C:693:ILE:HB	2.21	0.71
1:B:565:PHE:CB	1:C:42:VAL:HG22	2.09	0.71
4:C:1308:NAG:O7	4:C:1308:NAG:O3	2.05	0.71
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.71	0.71
1:B:143:VAL:HG22	1:B:154:GLU:HG2	1.72	0.71
1:B:327:VAL:HA	1:B:542:ASN:HB3	1.72	0.71
1:B:570:ALA:HB1	1:C:963:VAL:HG11	1.73	0.71
1:A:43:PHE:CB	1:C:559:PHE:CD1	2.73	0.71
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.73	0.71
1:A:591:SER:HB2	1:A:615:VAL:HG11	1.73	0.71
1:B:559:PHE:CD1	1:C:43:PHE:CB	2.74	0.71
1:B:196:ASN:CB	1:B:201:PHE:CD1	2.61	0.70
1:B:976:VAL:HG12	1:B:979:ASP:H	1.56	0.70
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.72	0.70
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.71	0.70
1:A:63:THR:O	1:A:65:PHE:CE2	2.44	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:HG22	1:C:315:THR:HG1	1.55	0.70
1:C:815:ARG:HD2	1:C:823:PHE:HE2	1.57	0.70
1:B:83:VAL:CG2	1:B:237:ARG:HH22	2.02	0.70
1:A:63:THR:HG21	1:A:65:PHE:CE1	2.17	0.70
1:A:102:ARG:NH1	1:A:154:GLU:OE2	2.25	0.70
1:A:709:ASN:OD1	1:A:709:ASN:N	2.24	0.70
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.73	0.70
1:B:534:VAL:HG11	1:B:537:LYS:HE2	1.73	0.70
1:C:34:ARG:NH1	1:C:221:SER:OG	2.25	0.70
1:A:121:ASN:HA	1:A:126:VAL:HA	1.74	0.70
1:A:429:PHE:CE1	1:A:514:SER:OG	2.43	0.70
1:A:1102:TRP:HD1	1:A:1135:ASN:ND2	1.90	0.70
1:B:73:THR:HG23	1:B:74:ASN:H	1.57	0.70
1:B:853:GLN:HE21	1:B:959:LEU:CB	1.92	0.70
1:A:34:ARG:NH1	1:A:221:SER:OG	2.25	0.70
1:B:815:ARG:HD2	1:B:823:PHE:HE2	1.57	0.70
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.72	0.69
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.39	0.69
1:B:34:ARG:NH1	1:B:221:SER:OG	2.25	0.69
1:B:536:ASN:HA	1:B:551:VAL:CG1	2.23	0.69
1:C:276:LEU:HD13	1:C:306:PHE:CE1	2.22	0.69
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.73	0.69
1:A:109:THR:C	1:A:111:ASP:H	1.95	0.69
1:B:180:GLU:HG3	1:B:181:GLY:H	1.58	0.69
1:A:321:GLN:HA	1:A:321:GLN:OE1	1.91	0.69
1:B:565:PHE:O	1:C:43:PHE:N	2.25	0.69
1:C:73:THR:HG23	1:C:74:ASN:H	1.57	0.69
1:B:726:ILE:HD13	1:B:945:LEU:HD23	1.73	0.69
1:C:656:VAL:HG23	1:C:693:ILE:HB	1.74	0.69
1:A:180:GLU:HG3	1:A:181:GLY:H	1.58	0.69
1:B:565:PHE:HB2	1:C:42:VAL:CG2	2.11	0.69
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.27	0.69
1:B:104:TRP:CE3	1:B:119:ILE:CD1	2.68	0.69
1:A:426:PRO:CG	1:A:429:PHE:HB2	2.22	0.68
1:C:118:LEU:HD21	1:C:120:VAL:HG23	1.72	0.68
1:A:318:PHE:CE2	1:A:612:TYR:CD1	2.81	0.68
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.57	0.68
1:A:73:THR:HG23	1:A:74:ASN:H	1.57	0.68
1:C:118:LEU:HD21	1:C:120:VAL:CG2	2.22	0.68
1:C:276:LEU:HD12	1:C:306:PHE:CE1	2.25	0.68
1:A:100:ILE:HG21	1:A:263:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:GLN:NE2	1:B:959:LEU:HB2	2.08	0.68
1:C:180:GLU:HG3	1:C:181:GLY:H	1.58	0.68
1:C:308:VAL:H	1:C:602:THR:CG2	2.07	0.68
1:A:63:THR:HG21	1:A:65:PHE:HZ	0.89	0.68
1:B:102:ARG:NH1	1:B:154:GLU:OE2	2.25	0.68
1:B:1075:PHE:CE1	1:B:1098:ASN:CB	2.74	0.68
1:C:1075:PHE:HD1	1:C:1098:ASN:HA	1.57	0.68
1:A:195:LYS:HE2	1:A:204:TYR:OH	1.94	0.68
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.23	0.68
1:B:130:VAL:HG23	1:B:168:PHE:HD2	1.59	0.67
1:B:431:GLY:HA3	1:B:513:LEU:O	1.95	0.67
1:C:296:LEU:HD11	1:C:608:VAL:CG1	1.92	0.67
1:A:379:CYS:CB	1:A:384:PRO:HG3	2.24	0.67
1:B:562:PHE:CZ	1:C:38:TYR:HD2	2.13	0.67
1:C:431:GLY:HA3	1:C:513:LEU:O	1.95	0.67
1:B:327:VAL:CG1	1:B:542:ASN:HB3	2.25	0.67
1:C:320:VAL:HB	1:C:590:CYS:HB2	1.77	0.67
1:A:81:ASN:O	1:A:239:GLN:NE2	2.27	0.67
1:B:299:THR:HG21	1:B:597:VAL:CG1	2.23	0.67
1:C:102:ARG:NH1	1:C:154:GLU:OE2	2.25	0.67
1:C:296:LEU:HD12	1:C:608:VAL:HG22	1.75	0.67
1:B:81:ASN:O	1:B:239:GLN:NE2	2.28	0.67
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.77	0.67
1:A:42:VAL:HG11	1:C:567:ARG:HG3	1.76	0.67
1:B:565:PHE:O	1:C:42:VAL:HA	1.95	0.67
1:C:81:ASN:O	1:C:239:GLN:NE2	2.27	0.67
1:B:656:VAL:CG2	1:B:693:ILE:HB	2.24	0.67
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.77	0.67
1:A:703:ASN:OD1	1:A:704:SER:N	2.28	0.66
1:C:716:THR:HG21	1:C:1073:LYS:CD	2.24	0.66
1:B:645:THR:OG1	1:B:648:GLY:O	2.13	0.66
1:B:748:GLU:CD	1:B:981:LEU:HD13	2.15	0.66
1:C:108:THR:HB	1:C:114:THR:HG21	1.76	0.66
1:A:22:THR:HG22	1:A:78:ARG:NH1	2.10	0.66
1:A:42:VAL:HA	1:C:565:PHE:O	1.95	0.66
1:B:676:THR:H	1:B:690:GLN:HG2	1.60	0.66
4:B:1301:NAG:O7	4:B:1301:NAG:H3	1.93	0.66
1:A:520:ALA:CB	1:B:200:TYR:OH	2.43	0.66
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.76	0.66
1:B:567:ARG:HG3	1:C:42:VAL:CG1	2.26	0.66
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:SER:N	1:C:131:CYS:O	2.28	0.66
1:A:591:SER:HB3	1:A:615:VAL:HG12	0.71	0.66
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.78	0.66
1:B:156:GLU:N	1:B:156:GLU:OE1	2.26	0.66
1:C:676:THR:H	1:C:690:GLN:HG2	1.60	0.66
1:C:710:ASN:O	1:C:1077:THR:HG22	1.96	0.65
1:C:121:ASN:CA	1:C:126:VAL:HG22	2.26	0.65
1:B:1102:TRP:CE2	1:B:1133:VAL:HG21	2.31	0.65
1:B:277:LEU:HD23	1:B:285:ILE:HD11	1.78	0.65
1:B:326:ILE:HA	1:B:531:THR:OG1	1.97	0.65
1:C:234:ASN:ND2	1:C:234:ASN:H	1.93	0.65
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.78	0.65
1:B:68:ILE:HG23	1:B:259:THR:HB	1.78	0.65
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.30	0.65
1:A:746:SER:OG	1:A:748:GLU:OE1	2.14	0.65
1:C:299:THR:HG21	1:C:597:VAL:CB	2.26	0.65
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.29	0.65
1:A:43:PHE:CB	1:C:559:PHE:CE1	2.79	0.65
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.77	0.65
1:A:116:SER:N	1:A:131:CYS:O	2.29	0.65
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.31	0.64
1:A:196:ASN:ND2	1:A:201:PHE:HB2	2.12	0.64
1:A:296:LEU:HD13	1:A:608:VAL:HG13	1.69	0.64
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.29	0.64
1:B:121:ASN:HA	1:B:126:VAL:HA	1.79	0.64
1:B:308:VAL:N	1:B:602:THR:HG22	2.12	0.64
1:B:716:THR:HG22	1:B:1110:TYR:CB	2.27	0.64
1:B:567:ARG:CG	1:C:42:VAL:HG11	2.26	0.64
1:B:656:VAL:HG23	1:B:693:ILE:HB	1.78	0.64
1:C:853:GLN:NE2	1:C:959:LEU:HB2	2.09	0.64
1:A:1031:GLU:OE2	1:C:1039:ARG:NE	2.26	0.64
1:C:121:ASN:CB	1:C:126:VAL:HG22	2.26	0.64
1:C:326:ILE:HD11	1:C:534:VAL:HG23	1.79	0.64
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.30	0.64
2:H:6:GLU:H	2:H:111:GLN:HE22	1.45	0.64
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.30	0.64
1:C:299:THR:HG23	1:C:597:VAL:HG21	1.78	0.64
1:C:716:THR:HG22	1:C:1110:TYR:CB	2.27	0.64
1:A:412:PRO:HD3	1:A:425:LEU:HD13	1.80	0.64
1:B:328:ARG:HB3	1:B:543:PHE:HD1	1.56	0.64
1:B:562:PHE:HZ	1:C:38:TYR:HD2	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:GLU:H	2:I:111:GLN:HE22	1.45	0.64
2:G:6:GLU:H	2:G:111:GLN:HE22	1.46	0.63
2:G:20:LEU:O	2:G:80:TYR:HA	1.98	0.63
1:C:1075:PHE:CE1	1:C:1098:ASN:HA	2.34	0.63
1:B:308:VAL:H	1:B:602:THR:HG21	1.59	0.63
1:A:303:LEU:HD13	1:A:308:VAL:HA	1.80	0.63
2:I:20:LEU:O	2:I:80:TYR:HA	1.98	0.63
1:A:22:THR:HG21	1:A:78:ARG:CD	2.08	0.63
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.80	0.63
1:A:963:VAL:HG11	1:C:570:ALA:HB1	1.81	0.63
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.30	0.63
1:A:379:CYS:SG	1:A:384:PRO:CG	2.77	0.63
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.29	0.62
1:A:922:LEU:CD2	4:A:1306:NAG:H3	2.29	0.62
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.63	0.62
1:C:140:PHE:HB2	1:C:242:LEU:HB2	1.81	0.62
2:H:20:LEU:O	2:H:80:TYR:HA	1.98	0.62
1:A:107:GLY:HA2	1:A:235:ILE:HG12	1.80	0.62
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.81	0.62
1:B:106:PHE:CB	1:B:235:ILE:HD13	2.29	0.62
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.82	0.62
1:A:41:LYS:O	1:C:563:GLN:HG2	1.99	0.62
1:B:118:LEU:HD22	1:B:133:PHE:HE2	1.63	0.62
1:A:318:PHE:HE2	1:A:612:TYR:CD1	2.18	0.62
1:B:318:PHE:CZ	1:B:615:VAL:HG11	2.35	0.62
1:A:413:GLY:HA3	1:C:987:VAL:CG2	2.28	0.62
1:B:148:ASN:C	1:B:150:LYS:H	2.02	0.62
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.80	0.62
1:A:429:PHE:HE1	1:A:514:SER:HB3	1.64	0.62
1:B:276:LEU:CD1	1:B:306:PHE:CE1	2.82	0.62
1:A:66:HIS:CD2	1:A:69:HIS:HB3	2.32	0.62
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.32	0.62
1:A:140:PHE:HB2	1:A:242:LEU:HB2	1.81	0.62
1:A:886:TRP:HB2	1:A:1034:LEU:O	1.99	0.62
1:A:1116:THR:HB	1:A:1140:PRO:HD3	1.81	0.62
1:B:1102:TRP:CB	1:B:1135:ASN:HD22	2.12	0.62
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.82	0.62
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.61
1:A:413:GLY:CA	1:C:987:VAL:CG2	2.76	0.61
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.82	0.61
1:B:140:PHE:HB2	1:B:242:LEU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.82	0.61
1:A:797:PHE:CD2	1:A:802:PHE:HD2	2.19	0.61
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.82	0.61
1:B:14:GLN:NE2	1:B:157:PHE:CG	2.68	0.61
1:C:712:ILE:HG22	1:C:1075:PHE:O	2.01	0.61
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.81	0.61
1:B:327:VAL:HA	1:B:542:ASN:O	2.01	0.61
1:A:278:LYS:HD3	1:A:306:PHE:CD2	2.35	0.61
1:A:676:THR:HG23	1:A:690:GLN:HG2	1.82	0.61
1:A:710:ASN:HB2	1:A:1077:THR:O	2.00	0.61
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.29	0.61
1:A:410:ILE:HG22	1:A:410:ILE:O	2.01	0.61
1:A:658:ASN:CB	1:A:660:TYR:OH	2.49	0.61
1:B:559:PHE:CD1	1:C:43:PHE:CG	2.89	0.61
1:B:559:PHE:CD1	1:C:43:PHE:HB2	2.36	0.61
1:C:121:ASN:ND2	1:C:126:VAL:HG21	2.15	0.61
1:A:43:PHE:HB2	1:C:559:PHE:CD1	2.36	0.61
1:C:645:THR:OG1	1:C:648:GLY:O	2.13	0.61
1:A:18:LEU:O	1:A:18:LEU:CD1	2.41	0.60
1:A:410:ILE:HD11	1:A:418:ILE:HG21	1.82	0.60
1:A:853:GLN:NE2	1:A:959:LEU:HB3	2.16	0.60
1:A:922:LEU:HD22	4:A:1306:NAG:H3	1.83	0.60
1:C:299:THR:CG2	1:C:597:VAL:CG2	2.79	0.60
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.82	0.60
1:A:276:LEU:HD12	1:A:276:LEU:N	2.16	0.60
1:B:109:THR:HG22	1:B:109:THR:O	2.02	0.60
1:A:44:ARG:O	1:A:283:GLY:HA2	2.02	0.60
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.28	0.60
1:B:140:PHE:C	1:B:159:VAL:HG22	2.22	0.60
1:A:402:ILE:CD1	1:A:410:ILE:HG13	2.32	0.60
1:B:115:GLN:HE21	1:B:167:THR:HG21	0.71	0.60
1:B:853:GLN:HE22	1:B:959:LEU:HD12	1.65	0.60
1:A:326:ILE:HD11	1:A:534:VAL:HB	1.84	0.60
1:A:41:LYS:O	1:C:563:GLN:CG	2.49	0.59
1:A:276:LEU:HD11	1:A:301:CYS:SG	2.42	0.59
1:A:661:GLU:O	1:A:695:TYR:OH	2.19	0.59
1:B:562:PHE:HZ	1:C:38:TYR:CD2	2.20	0.59
1:B:712:ILE:HG22	1:B:1075:PHE:O	2.01	0.59
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.35	0.59
1:C:299:THR:HG21	1:C:597:VAL:CG2	2.33	0.59
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD12	1:A:670:ILE:HG22	1.83	0.59
1:B:118:LEU:CD1	1:B:133:PHE:HD2	2.09	0.59
1:B:118:LEU:HD13	1:B:133:PHE:CE2	2.36	0.59
1:B:1075:PHE:CE1	1:B:1098:ASN:HB3	2.36	0.59
1:C:326:ILE:HD12	1:C:532:ASN:O	2.02	0.59
1:C:797:PHE:CE2	1:C:802:PHE:CD2	2.90	0.59
2:I:7:SER:HB3	2:I:21:SER:HB3	1.85	0.59
1:C:121:ASN:ND2	1:C:126:VAL:CG2	2.65	0.59
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.35	0.59
2:G:7:SER:HB3	2:G:21:SER:HB3	1.85	0.59
1:A:119:ILE:O	1:A:119:ILE:HG22	2.03	0.59
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.36	0.59
1:A:387:LEU:HD12	1:A:387:LEU:O	2.03	0.58
1:A:1074:ASN:OD1	1:B:895:GLN:NE2	2.36	0.58
1:B:326:ILE:HG22	1:B:326:ILE:O	2.01	0.58
1:A:716:THR:HG22	1:A:1110:TYR:CB	2.33	0.58
1:C:797:PHE:CD2	1:C:802:PHE:CE2	2.90	0.58
1:A:897:PRO:CB	1:C:709:ASN:O	2.51	0.58
1:B:327:VAL:CB	1:B:542:ASN:HB3	2.33	0.58
1:B:853:GLN:HE22	1:B:959:LEU:CB	2.16	0.58
1:C:540:ASN:OD1	1:C:541:PHE:N	2.37	0.58
1:C:853:GLN:HE22	1:C:959:LEU:HD12	1.65	0.58
3:L:86:TYR:O	3:L:101:GLY:HA2	2.04	0.58
2:H:7:SER:HB3	2:H:21:SER:HB3	1.85	0.58
2:I:19:ARG:HA	2:I:82:GLN:HA	1.86	0.58
3:K:86:TYR:O	3:K:101:GLY:HA2	2.04	0.58
1:A:718:PHE:CZ	1:A:1067:TYR:HE1	2.22	0.58
1:A:914:ASN:HA	1:C:1089:PHE:HE2	1.69	0.58
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	1.86	0.58
1:C:1075:PHE:CE1	1:C:1098:ASN:CA	2.87	0.58
3:J:86:TYR:O	3:J:101:GLY:HA2	2.04	0.58
1:A:429:PHE:CE1	1:A:464:PHE:HZ	2.21	0.57
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.37	0.57
1:C:1102:TRP:CD1	1:C:1135:ASN:ND2	2.72	0.57
1:A:43:PHE:CE1	1:C:558:LYS:O	2.57	0.57
1:A:383:SER:HB2	1:B:985:ASP:HB2	1.86	0.57
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.86	0.57
1:A:804:GLN:NE2	4:A:1307:NAG:H61	2.18	0.57
1:B:521:PRO:HG2	1:C:230:PRO:HB3	1.85	0.57
1:B:716:THR:HG21	1:B:1073:LYS:CE	2.34	0.57
1:B:540:ASN:OD1	1:B:541:PHE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:PHE:CE2	1:B:802:PHE:CD2	2.91	0.57
1:C:105:ILE:HG12	1:C:239:GLN:H	1.69	0.57
1:A:303:LEU:CD1	1:A:308:VAL:HG13	2.34	0.57
1:A:429:PHE:HE1	1:A:514:SER:CB	2.17	0.57
1:A:429:PHE:CE1	1:A:514:SER:CB	2.88	0.57
1:A:815:ARG:HD2	1:A:823:PHE:HE2	1.68	0.57
1:C:66:HIS:ND1	1:C:264:ALA:HB1	2.16	0.57
2:H:19:ARG:HA	2:H:82:GLN:HA	1.86	0.57
1:A:41:LYS:HB3	1:C:563:GLN:HA	1.87	0.57
1:A:196:ASN:CB	1:A:201:PHE:CB	2.73	0.57
1:B:212:LEU:HD23	1:B:214:ARG:H	1.70	0.57
1:B:326:ILE:HD12	1:B:532:ASN:O	2.04	0.57
4:C:1308:NAG:HO3	4:C:1308:NAG:C7	2.11	0.57
2:I:2:GLN:N	2:I:25:SER:O	2.38	0.57
1:B:320:VAL:HB	1:B:590:CYS:HB2	1.86	0.57
1:C:212:LEU:HD23	1:C:214:ARG:H	1.70	0.57
1:C:534:VAL:CG1	1:C:539:VAL:CG1	2.78	0.57
1:A:365:TYR:CE2	1:A:387:LEU:HD12	2.40	0.56
1:A:802:PHE:HE1	1:A:927:PHE:CZ	2.22	0.56
1:B:375:SER:O	3:L:68:GLY:HA3	2.05	0.56
1:B:536:ASN:HA	1:B:551:VAL:HG13	1.86	0.56
1:C:57:PRO:O	1:C:60:SER:HB2	2.05	0.56
1:A:195:LYS:O	1:A:195:LYS:HG3	2.05	0.56
1:C:29:THR:HG22	1:C:62:VAL:O	2.05	0.56
1:C:936:ASP:HA	1:C:939:SER:HB2	1.87	0.56
2:G:19:ARG:HA	2:G:82:GLN:HA	1.86	0.56
2:H:104:ASN:HB3	2:H:106:LYS:HG2	1.87	0.56
1:A:66:HIS:HA	1:A:264:ALA:HA	1.88	0.56
1:A:278:LYS:CB	1:A:306:PHE:CE2	2.87	0.56
1:B:118:LEU:HD12	1:B:135:PHE:CE1	2.41	0.56
1:B:936:ASP:HA	1:B:939:SER:HB2	1.88	0.56
1:B:1019:ARG:NH2	1:B:1023:ASN:OD1	2.34	0.56
1:C:534:VAL:HG11	1:C:539:VAL:HG13	1.87	0.56
2:G:2:GLN:N	2:G:25:SER:O	2.38	0.56
1:A:18:LEU:HD11	1:A:79:PHE:CG	2.40	0.56
1:A:212:LEU:HD23	1:A:214:ARG:H	1.70	0.56
1:A:369:TYR:CE2	1:A:385:THR:HA	2.41	0.56
4:C:1301:NAG:H83	4:C:1301:NAG:H3	1.88	0.56
1:A:109:THR:C	1:A:111:ASP:N	2.54	0.56
1:A:709:ASN:O	1:B:897:PRO:HB3	2.05	0.56
1:B:797:PHE:CD2	1:B:802:PHE:CE2	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:O	1:C:24:LEU:HB2	2.06	0.56
1:A:105:ILE:HG12	1:A:239:GLN:H	1.69	0.56
1:A:109:THR:HG22	1:A:111:ASP:HB3	1.87	0.56
1:A:390:LEU:HD11	1:B:982:SER:HB2	1.88	0.56
1:B:115:GLN:NE2	1:B:167:THR:CB	2.67	0.56
1:C:53:ASP:OD1	1:C:54:LEU:N	2.37	0.56
1:C:1102:TRP:HB2	1:C:1135:ASN:HD21	1.64	0.56
1:A:84:LEU:N	1:A:238:PHE:O	2.29	0.56
1:A:86:PHE:N	1:A:236:THR:O	2.29	0.56
2:H:91:THR:HG23	2:H:116:THR:HA	1.88	0.56
1:A:43:PHE:CG	1:C:559:PHE:CD1	2.94	0.56
1:B:106:PHE:O	1:B:235:ILE:HG23	2.06	0.56
1:B:357:ARG:CZ	1:C:167:THR:HG22	2.36	0.56
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.37	0.56
1:C:196:ASN:CB	1:C:201:PHE:HD1	2.15	0.56
2:H:2:GLN:N	2:H:25:SER:O	2.38	0.55
2:I:47:TRP:HZ2	2:I:50:VAL:HG13	1.71	0.55
1:B:853:GLN:CD	1:B:959:LEU:HD13	2.26	0.55
1:C:853:GLN:CD	1:C:959:LEU:HD13	2.26	0.55
2:H:47:TRP:HZ2	2:H:50:VAL:HG13	1.71	0.55
1:A:1075:PHE:CE1	1:A:1098:ASN:HA	2.41	0.55
1:B:650:LEU:HD21	1:B:653:ALA:HB3	1.89	0.55
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.89	0.55
1:A:379:CYS:HB2	1:A:384:PRO:HG3	1.89	0.55
1:A:658:ASN:CB	1:A:660:TYR:CZ	2.86	0.55
1:B:718:PHE:CD1	1:B:1067:TYR:CE1	2.94	0.55
2:G:47:TRP:HZ2	2:G:50:VAL:HG13	1.71	0.55
2:I:91:THR:HG23	2:I:116:THR:HA	1.88	0.55
1:A:109:THR:OG1	1:A:114:THR:HG21	2.06	0.55
1:A:941:THR:HG22	1:A:944:ALA:H	1.72	0.55
1:B:84:LEU:N	1:B:238:PHE:O	2.29	0.55
1:C:367:VAL:HA	1:C:370:ASN:HB2	1.88	0.55
2:G:104:ASN:HB3	2:G:106:LYS:HG2	1.87	0.55
1:B:367:VAL:HA	1:B:370:ASN:HB2	1.88	0.55
1:B:759:PHE:HD2	1:B:1001:LEU:HD21	1.71	0.55
1:C:546:LEU:HD22	1:C:565:PHE:CE1	2.42	0.55
1:C:759:PHE:HD2	1:C:1001:LEU:HD21	1.71	0.55
1:C:853:GLN:HE22	1:C:959:LEU:CB	2.17	0.55
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.40	0.55
1:A:747:THR:HA	1:A:750:SER:HB3	1.88	0.55
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:OD1	1:A:54:LEU:N	2.37	0.55
1:B:417:LYS:HE2	1:B:455:LEU:HD12	1.88	0.55
1:C:318:PHE:CZ	1:C:615:VAL:HG11	2.41	0.55
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.72	0.55
2:I:104:ASN:HB3	2:I:106:LYS:HG2	1.87	0.55
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.87	0.55
1:A:789:TYR:HE1	1:C:703:ASN:HD22	1.55	0.55
1:B:559:PHE:HD1	1:C:43:PHE:CG	2.24	0.55
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.40	0.55
1:A:196:ASN:HA	1:A:201:PHE:HA	1.89	0.54
1:A:303:LEU:HD13	1:A:308:VAL:HG13	1.88	0.54
1:B:19:THR:HG23	1:B:138:ASP:OD2	2.08	0.54
1:B:437:ASN:ND2	1:B:506:GLN:OE1	2.40	0.54
1:B:716:THR:HG22	1:B:1110:TYR:CG	2.42	0.54
1:C:85:PRO:HA	1:C:237:ARG:HA	1.89	0.54
1:A:367:VAL:HA	1:A:370:ASN:HB2	1.88	0.54
1:A:417:LYS:HE2	1:A:455:LEU:HD12	1.88	0.54
1:B:737:ASP:CG	1:B:740:MET:HB3	2.27	0.54
1:A:425:LEU:HD22	1:A:429:PHE:CD2	2.42	0.54
1:A:587:ILE:O	1:A:588:THR:OG1	2.23	0.54
2:G:91:THR:HG23	2:G:116:THR:HA	1.88	0.54
1:A:38:TYR:HD2	1:C:562:PHE:CZ	2.26	0.54
1:A:716:THR:HG22	1:A:1110:TYR:HB3	1.90	0.54
1:C:118:LEU:HD22	1:C:129:LYS:HD2	1.90	0.54
1:C:417:LYS:HE2	1:C:455:LEU:HD12	1.88	0.54
1:A:430:THR:O	1:A:430:THR:HG22	2.06	0.54
1:B:53:ASP:OD1	1:B:54:LEU:N	2.37	0.54
1:C:457:ARG:NH1	1:C:459:SER:OG	2.41	0.54
1:B:457:ARG:NH1	1:B:459:SER:OG	2.41	0.54
1:C:66:HIS:HA	1:C:264:ALA:HA	1.90	0.54
1:A:457:ARG:NH1	1:A:459:SER:OG	2.41	0.54
1:A:904:TYR:O	1:A:907:ASN:N	2.40	0.54
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.90	0.54
1:C:201:PHE:HB2	1:C:231:ILE:HG13	1.88	0.54
1:B:196:ASN:HA	1:B:201:PHE:HA	1.90	0.54
1:A:365:TYR:HA	1:A:368:LEU:HD13	1.90	0.54
1:A:825:LYS:HE3	1:A:938:LEU:O	2.08	0.54
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.42	0.54
1:C:103:GLY:HA3	1:C:119:ILE:O	2.08	0.54
1:C:797:PHE:CE2	1:C:802:PHE:HD2	2.19	0.54
2:I:37:VAL:HG12	2:I:47:TRP:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:CG2	1:A:78:ARG:CG	2.80	0.53
1:A:520:ALA:HB2	1:B:200:TYR:OH	2.08	0.53
1:C:716:THR:HG22	1:C:1110:TYR:CG	2.43	0.53
2:H:62:ASP:HA	2:H:65:LYS:HB2	1.90	0.53
1:A:390:LEU:HD22	1:B:983:ARG:HG3	1.90	0.53
1:B:1087:ALA:HB1	1:B:1089:PHE:HE1	1.72	0.53
1:C:109:THR:O	1:C:109:THR:HG22	2.08	0.53
1:C:1019:ARG:NH2	1:C:1023:ASN:OD1	2.35	0.53
1:A:276:LEU:N	1:A:276:LEU:CD1	2.72	0.53
2:G:62:ASP:HA	2:G:65:LYS:HB2	1.90	0.53
1:A:43:PHE:N	1:C:565:PHE:O	2.37	0.53
1:A:85:PRO:HA	1:A:237:ARG:HA	1.91	0.53
1:A:980:ILE:HD12	1:A:996:LEU:HD11	1.89	0.53
1:B:612:TYR:HB3	1:B:615:VAL:HG21	1.90	0.53
1:A:170:TYR:CE2	1:A:172:SER:HB2	2.44	0.53
1:A:334:ASN:HB2	1:A:361:CYS:HA	1.91	0.53
1:C:34:ARG:NE	1:C:216:LEU:HD23	2.24	0.53
1:C:1087:ALA:HB1	1:C:1089:PHE:HE1	1.72	0.53
1:A:66:HIS:CD2	1:A:69:HIS:CG	2.95	0.53
1:A:303:LEU:HD23	1:A:305:SER:CB	2.28	0.53
2:H:11:VAL:HA	2:H:116:THR:HB	1.91	0.53
1:A:797:PHE:CD2	1:A:802:PHE:CD2	2.97	0.53
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.90	0.53
1:C:365:TYR:HA	1:C:368:LEU:HD13	1.90	0.53
2:G:11:VAL:HA	2:G:116:THR:HB	1.91	0.53
2:H:37:VAL:HG12	2:H:47:TRP:HA	1.90	0.53
1:B:34:ARG:NE	1:B:216:LEU:HD23	2.24	0.53
2:I:11:VAL:HA	2:I:116:THR:HB	1.91	0.53
1:A:316:SER:O	1:A:595:VAL:HB	2.09	0.53
1:B:130:VAL:CG2	1:B:168:PHE:HD2	2.21	0.53
1:A:34:ARG:NE	1:A:216:LEU:HD23	2.24	0.53
1:A:202:LYS:HG2	1:A:228:ASP:HA	1.91	0.53
1:B:85:PRO:N	1:B:237:ARG:HG2	2.22	0.53
1:B:202:LYS:HG2	1:B:228:ASP:HA	1.91	0.53
1:B:558:LYS:O	1:C:43:PHE:CE1	2.62	0.52
1:A:210:ILE:HD12	1:A:217:PRO:HD3	1.92	0.52
1:A:278:LYS:CB	1:A:306:PHE:HE2	2.22	0.52
1:B:106:PHE:CD1	1:B:235:ILE:CD1	2.90	0.52
1:B:299:THR:HG21	1:B:597:VAL:HG11	1.88	0.52
1:C:108:THR:CG2	1:C:114:THR:HG21	2.39	0.52
3:L:63:SER:O	3:L:74:THR:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:ARG:NH2	2:I:46:GLU:OE1	2.38	0.52
1:C:131:CYS:HB2	1:C:133:PHE:CE2	2.44	0.52
1:C:202:LYS:HG2	1:C:228:ASP:HA	1.91	0.52
1:A:426:PRO:CD	1:A:429:PHE:HB2	2.39	0.52
1:B:170:TYR:CE2	1:B:172:SER:HB2	2.44	0.52
1:B:327:VAL:CA	1:B:542:ASN:HB3	2.39	0.52
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.91	0.52
1:B:875:SER:O	1:B:879:ALA:N	2.41	0.52
1:A:555:SER:OG	1:A:584:ILE:O	2.19	0.52
1:A:1089:PHE:HE2	1:B:914:ASN:HA	1.73	0.52
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.39	0.52
1:B:689:SER:OG	1:B:690:GLN:N	2.42	0.52
1:C:170:TYR:CE2	1:C:172:SER:HB2	2.43	0.52
2:I:70:ILE:HB	2:I:81:LEU:HD12	1.91	0.52
1:B:29:THR:HG22	1:B:62:VAL:O	2.10	0.52
1:C:210:ILE:HD12	1:C:217:PRO:HD3	1.92	0.52
1:C:858:LEU:HD23	1:C:959:LEU:HD22	1.90	0.52
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.44	0.52
1:A:718:PHE:CG	1:A:1067:TYR:CE1	2.98	0.52
1:A:1075:PHE:CD1	1:A:1098:ASN:HA	2.45	0.52
1:A:1089:PHE:HB3	1:B:913:GLN:HE21	1.74	0.52
1:B:360:ASN:CG	1:C:168:PHE:CE1	2.82	0.52
1:B:365:TYR:HA	1:B:368:LEU:HD13	1.90	0.52
1:C:689:SER:OG	1:C:690:GLN:N	2.42	0.52
2:I:62:ASP:HA	2:I:65:LYS:HB2	1.90	0.52
3:J:63:SER:O	3:J:74:THR:CB	2.57	0.52
1:A:43:PHE:CG	1:C:559:PHE:HD1	2.26	0.52
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.92	0.52
1:A:914:ASN:HA	1:C:1089:PHE:CE2	2.44	0.52
2:G:70:ILE:HB	2:G:81:LEU:HD12	1.91	0.52
1:B:15:CYS:SG	1:B:161:SER:HB3	2.50	0.52
1:B:186:PHE:CD1	1:B:209:PRO:HB3	2.45	0.52
1:B:328:ARG:HB3	1:B:543:PHE:HA	1.92	0.52
1:B:1102:TRP:CB	1:B:1135:ASN:ND2	2.69	0.52
1:C:244:LEU:HD22	1:C:259:THR:HA	1.92	0.52
1:A:712:ILE:HG22	1:A:1075:PHE:O	2.08	0.51
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.93	0.51
2:G:37:VAL:HG12	2:G:47:TRP:HA	1.90	0.51
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.43	0.51
1:B:551:VAL:N	1:B:588:THR:O	2.42	0.51
1:C:186:PHE:CD1	1:C:209:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASN:HB2	1:C:361:CYS:HA	1.91	0.51
1:C:875:SER:O	1:C:879:ALA:N	2.41	0.51
2:H:70:ILE:HB	2:H:81:LEU:HD12	1.91	0.51
1:B:210:ILE:HD12	1:B:217:PRO:HD3	1.92	0.51
1:A:29:THR:CG2	1:A:62:VAL:HB	2.41	0.51
1:A:41:LYS:HB3	1:C:563:GLN:C	2.30	0.51
1:A:186:PHE:CD1	1:A:209:PRO:HB3	2.45	0.51
1:B:38:TYR:OH	1:B:284:THR:HA	2.11	0.51
1:C:276:LEU:HD12	1:C:306:PHE:CZ	2.43	0.51
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.91	0.51
1:C:953:ASN:O	1:C:957:GLN:N	2.39	0.51
3:K:63:SER:O	3:K:74:THR:CB	2.57	0.51
1:C:122:ASN:ND2	1:C:127:VAL:HG12	2.25	0.51
3:L:94:THR:OG1	3:L:96:ARG:NH1	2.44	0.51
1:A:63:THR:HG22	1:A:65:PHE:CE2	2.33	0.51
1:C:276:LEU:HD11	1:C:306:PHE:HE1	0.40	0.51
1:B:296:LEU:HD11	1:B:606:ASN:O	2.11	0.51
3:J:94:THR:OG1	3:J:96:ARG:NH1	2.44	0.51
1:B:643:PHE:CE2	1:B:645:THR:HG22	2.45	0.51
1:A:1102:TRP:HB2	1:A:1135:ASN:HD22	1.74	0.51
1:B:328:ARG:HG3	1:B:579:PRO:HG2	1.92	0.51
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.93	0.51
1:B:974:SER:H	1:B:980:ILE:HD11	1.75	0.51
2:G:11:VAL:HG11	2:G:121:SER:HA	1.93	0.51
2:I:11:VAL:HG11	2:I:121:SER:HA	1.93	0.51
1:A:42:VAL:HG11	1:C:567:ARG:CG	2.40	0.50
1:C:299:THR:HG21	1:C:597:VAL:HG21	1.90	0.50
1:C:718:PHE:CD1	1:C:1067:TYR:CE1	2.98	0.50
1:A:42:VAL:CG1	1:C:567:ARG:HG3	2.41	0.50
1:B:46:SER:HB3	1:B:281:GLU:HA	1.93	0.50
1:B:572:THR:HG21	1:C:855:PHE:HD2	1.76	0.50
1:B:148:ASN:C	1:B:150:LYS:N	2.64	0.50
1:B:1102:TRP:CG	1:B:1135:ASN:ND2	2.80	0.50
1:C:245:HIS:CD2	1:C:260:ALA:HB2	2.46	0.50
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.45	0.50
2:I:35:HIS:HB2	2:I:97:ALA:HB3	1.94	0.50
1:A:41:LYS:CB	1:C:564:GLN:H	2.21	0.50
1:A:1107:ARG:HD3	1:B:904:TYR:CE1	2.45	0.50
1:A:328:ARG:CZ	1:A:533:LEU:HB2	2.42	0.50
1:A:1089:PHE:CE2	1:B:914:ASN:HA	2.47	0.50
1:B:118:LEU:HD12	1:B:135:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.93	0.50
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.94	0.50
1:A:115:GLN:HE21	1:A:167:THR:HG21	1.77	0.50
1:B:17:ASN:HD22	1:B:137:ASN:HD21	1.60	0.50
1:B:106:PHE:CB	1:B:235:ILE:HG21	2.42	0.50
2:H:11:VAL:HG11	2:H:121:SER:HA	1.93	0.50
3:J:5:THR:HB	3:J:24:ARG:HB2	1.94	0.50
1:A:234:ASN:H	1:A:234:ASN:HD22	1.59	0.50
1:B:19:THR:CG2	1:B:138:ASP:OD2	2.60	0.50
1:B:201:PHE:CB	1:B:231:ILE:HG13	2.29	0.50
1:B:656:VAL:HG21	1:B:693:ILE:HB	1.94	0.50
1:C:122:ASN:HD21	1:C:127:VAL:HG12	1.76	0.50
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.40	0.50
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.94	0.50
1:A:276:LEU:O	1:A:288:ALA:HA	2.12	0.50
1:A:379:CYS:HB2	1:A:384:PRO:HD3	1.93	0.50
1:B:119:ILE:HG13	1:B:119:ILE:O	2.12	0.50
1:B:564:GLN:H	1:C:41:LYS:CB	2.19	0.50
2:H:35:HIS:HB2	2:H:97:ALA:HB3	1.94	0.50
3:K:5:THR:HB	3:K:24:ARG:HB2	1.94	0.50
3:K:94:THR:OG1	3:K:96:ARG:NH1	2.44	0.50
1:A:786:LYS:NZ	1:A:892:ALA:HA	2.26	0.50
1:B:326:ILE:CA	1:B:531:THR:OG1	2.60	0.50
2:G:35:HIS:HB2	2:G:97:ALA:HB3	1.93	0.50
1:B:67:ALA:O	1:B:68:ILE:C	2.50	0.49
1:B:118:LEU:HD22	1:B:129:LYS:HD2	1.93	0.49
1:C:84:LEU:N	1:C:238:PHE:O	2.29	0.49
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.93	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.49
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.93	0.49
1:B:1089:PHE:HE2	1:C:914:ASN:HA	1.76	0.49
1:C:337:PRO:HB2	1:C:340:GLU:HB2	1.93	0.49
1:A:29:THR:HG23	1:A:62:VAL:HB	1.94	0.49
2:G:40:ALA:HB3	2:G:43:LYS:HB2	1.94	0.49
1:A:382:VAL:CG1	1:A:430:THR:HG21	2.42	0.49
1:A:1145:LEU:O	1:A:1147:SER:N	2.46	0.49
1:B:935:GLN:O	1:B:939:SER:N	2.39	0.49
1:C:290:ASP:O	1:C:297:SER:HB3	2.12	0.49
2:G:24:ALA:HB3	2:G:77:ASN:HB3	1.95	0.49
1:B:521:PRO:CG	1:C:230:PRO:HB3	2.42	0.49
1:A:46:SER:HA	1:A:279:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:PHE:CD2	1:B:1001:LEU:HD21	2.47	0.49
1:C:115:GLN:HE21	1:C:167:THR:HG21	1.76	0.49
2:I:24:ALA:HB3	2:I:77:ASN:HB3	1.95	0.49
3:L:5:THR:HB	3:L:24:ARG:HB2	1.94	0.49
1:A:38:TYR:HD2	1:C:562:PHE:HZ	1.61	0.49
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.95	0.49
1:C:180:GLU:HG3	1:C:181:GLY:N	2.27	0.49
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.94	0.49
1:A:612:TYR:HB3	1:A:615:VAL:HG21	1.94	0.49
1:B:245:HIS:CD2	1:B:260:ALA:HB2	2.47	0.49
1:C:656:VAL:HG21	1:C:693:ILE:HB	1.92	0.49
1:A:182:LYS:HG3	1:A:186:PHE:CD2	2.48	0.49
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.95	0.49
1:B:536:ASN:N	1:B:552:LEU:O	2.39	0.49
1:A:1072:GLU:HG2	1:B:894:LEU:CD2	2.42	0.49
1:B:48:LEU:CD1	1:B:306:PHE:CD2	2.93	0.49
1:B:276:LEU:HG	1:B:289:VAL:HB	1.95	0.49
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.94	0.49
1:A:303:LEU:HD13	1:A:308:VAL:CG2	2.41	0.48
1:B:796:ASP:OD1	1:B:796:ASP:N	2.46	0.48
1:C:276:LEU:HG	1:C:289:VAL:HB	1.95	0.48
1:C:759:PHE:CD2	1:C:1001:LEU:HD21	2.47	0.48
1:B:130:VAL:O	1:B:167:THR:OG1	2.31	0.48
1:B:984:LEU:HD13	1:B:992:GLN:HG3	1.90	0.48
1:C:182:LYS:HG3	1:C:186:PHE:CD2	2.48	0.48
1:C:716:THR:HG22	1:C:1110:TYR:HB3	1.95	0.48
1:C:1102:TRP:CB	1:C:1135:ASN:ND2	2.68	0.48
1:A:303:LEU:CD1	1:A:308:VAL:HA	2.42	0.48
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.44	0.48
1:B:113:LYS:HE2	1:B:113:LYS:HB2	1.40	0.48
1:B:182:LYS:HG3	1:B:186:PHE:CD2	2.48	0.48
1:B:718:PHE:CG	1:B:1067:TYR:CE1	3.01	0.48
1:C:718:PHE:CG	1:C:1067:TYR:CE1	3.02	0.48
2:I:68:PHE:HB3	2:I:81:LEU:HD21	1.96	0.48
1:A:42:VAL:HG22	1:C:565:PHE:CB	2.17	0.48
1:A:897:PRO:CG	1:C:709:ASN:O	2.62	0.48
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.95	0.48
1:C:551:VAL:N	1:C:588:THR:O	2.43	0.48
1:C:935:GLN:O	1:C:939:SER:N	2.40	0.48
1:A:1054:GLN:N	1:A:1061:VAL:O	2.45	0.48
1:B:120:VAL:HG13	1:B:141:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:93:SER:OG	3:L:94:THR:N	2.46	0.48
1:A:1114:ILE:O	1:A:1119:ASN:ND2	2.46	0.48
1:B:299:THR:CG2	1:B:597:VAL:CG2	2.91	0.48
1:B:1032:CYS:SG	1:B:1048:HIS:NE2	2.87	0.48
1:C:20:THR:OG1	1:C:79:PHE:HB3	2.13	0.48
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.49	0.48
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.95	0.48
2:G:38:ARG:NH2	2:G:46:GLU:OE1	2.38	0.48
3:J:93:SER:OG	3:J:94:THR:N	2.46	0.48
1:A:89:GLY:HA3	1:A:270:LEU:HD12	1.95	0.48
1:B:535:LYS:HA	1:B:552:LEU:O	2.13	0.48
1:C:1102:TRP:CB	1:C:1135:ASN:HD22	2.24	0.48
3:K:93:SER:OG	3:K:94:THR:N	2.46	0.48
1:A:180:GLU:HG3	1:A:181:GLY:N	2.27	0.48
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.49	0.48
1:A:319:ARG:NH1	1:B:740:MET:SD	2.87	0.48
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.96	0.48
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.96	0.48
1:C:1032:CYS:SG	1:C:1048:HIS:NE2	2.87	0.48
1:A:201:PHE:CB	1:A:231:ILE:HG13	2.37	0.48
1:A:808:ASP:OD2	1:A:811:LYS:HG2	2.13	0.48
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.95	0.48
1:C:296:LEU:CD1	1:C:608:VAL:CG2	2.79	0.48
2:H:24:ALA:HB3	2:H:77:ASN:HB3	1.95	0.48
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.96	0.47
1:C:14:GLN:HB3	1:C:158:ARG:HD3	1.96	0.47
1:C:156:GLU:OE1	1:C:156:GLU:N	2.44	0.47
1:A:287:ASP:CB	1:A:306:PHE:CE2	2.96	0.47
1:A:873:TYR:CZ	1:C:699:LEU:HD23	2.50	0.47
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.95	0.47
1:A:897:PRO:HG3	1:C:709:ASN:O	2.13	0.47
1:B:283:GLY:O	1:B:284:THR:HB	2.14	0.47
1:A:278:LYS:HE3	1:A:287:ASP:HB3	1.95	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.49	0.47
1:C:278:LYS:HE3	1:C:287:ASP:HB3	1.95	0.47
1:C:1088:HIS:CE1	1:C:1122:VAL:HG22	2.50	0.47
1:A:23:GLN:O	1:A:23:GLN:HG2	2.15	0.47
1:A:797:PHE:HD2	1:A:802:PHE:CD2	2.33	0.47
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG11	2.49	0.47
2:G:68:PHE:HB3	2:G:81:LEU:HD21	1.95	0.47
2:H:60:TYR:HE1	2:H:70:ILE:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:TRP:HA	3:L:87:TYR:O	2.15	0.47
1:A:716:THR:HG22	1:A:1110:TYR:CD2	2.49	0.47
1:B:121:ASN:HD22	1:B:176:LEU:HB2	1.78	0.47
3:J:35:TRP:HA	3:J:87:TYR:O	2.15	0.47
1:A:85:PRO:HA	1:A:237:ARG:HG3	1.95	0.47
1:A:620:VAL:HG11	1:A:651:ILE:HD11	1.96	0.47
1:A:797:PHE:HD2	1:A:802:PHE:HD2	1.62	0.47
1:A:815:ARG:HD2	1:A:823:PHE:CE2	2.49	0.47
1:B:23:GLN:O	1:B:24:LEU:HB2	2.15	0.47
1:B:168:PHE:CZ	1:B:170:TYR:HB2	2.50	0.47
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.97	0.47
1:B:716:THR:HG22	1:B:1110:TYR:HB3	1.95	0.47
1:B:716:THR:HA	1:B:1110:TYR:HB3	1.97	0.47
1:B:953:ASN:O	1:B:957:GLN:N	2.39	0.47
1:B:1145:LEU:O	1:B:1147:SER:N	2.48	0.47
1:C:1145:LEU:O	1:C:1147:SER:N	2.47	0.47
2:H:68:PHE:HB3	2:H:81:LEU:HD21	1.96	0.47
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.50	0.47
1:B:486:PHE:HA	3:J:32:TYR:HE2	1.80	0.47
1:A:180:GLU:O	1:A:182:LYS:HG2	2.15	0.47
1:A:287:ASP:OD2	1:A:306:PHE:CD2	2.67	0.47
1:A:786:LYS:HZ1	1:A:892:ALA:HA	1.79	0.47
1:B:328:ARG:HD2	1:B:580:GLN:HG3	1.97	0.47
1:C:38:TYR:CD1	1:C:285:ILE:HD12	2.50	0.47
1:A:14:GLN:HB3	1:A:158:ARG:HD3	1.96	0.47
1:A:486:PHE:HA	3:L:32:TYR:HE2	1.80	0.47
1:B:783:ALA:HB2	1:B:873:TYR:CZ	2.50	0.47
1:B:797:PHE:CE2	1:B:802:PHE:HD2	2.22	0.47
1:A:393:THR:O	1:A:523:THR:OG1	2.31	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.46
1:B:16:VAL:HG22	1:B:158:ARG:HD3	1.96	0.46
1:B:180:GLU:HG3	1:B:181:GLY:N	2.27	0.46
1:B:748:GLU:OE1	1:B:981:LEU:CD1	2.63	0.46
1:C:17:ASN:HB2	1:C:138:ASP:OD2	2.15	0.46
1:C:486:PHE:HA	3:K:32:TYR:HE2	1.80	0.46
1:C:961:THR:O	1:C:965:GLN:HG2	2.15	0.46
1:C:1116:THR:HB	1:C:1140:PRO:HD3	1.97	0.46
1:A:710:ASN:ND2	4:A:1305:NAG:H81	2.31	0.46
1:A:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.46
1:B:180:GLU:O	1:B:182:LYS:HG2	2.15	0.46
1:B:188:ASN:O	1:B:190:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:C	1:C:41:LYS:HB3	2.34	0.46
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.96	0.46
1:C:906:PHE:CE2	1:C:916:LEU:HB2	2.50	0.46
1:A:718:PHE:CB	1:A:1069:PRO:HA	2.45	0.46
1:B:328:ARG:HA	1:B:328:ARG:HD3	1.71	0.46
3:K:35:TRP:HA	3:K:87:TYR:O	2.15	0.46
1:A:106:PHE:CB	1:A:235:ILE:HD13	2.44	0.46
1:A:188:ASN:O	1:A:190:ARG:HG3	2.16	0.46
1:A:412:PRO:HA	1:A:425:LEU:HB2	1.98	0.46
1:A:518:LEU:HD21	1:B:200:TYR:CD2	2.45	0.46
1:A:1016:ALA:HA	1:A:1019:ARG:HB3	1.97	0.46
1:B:83:VAL:CB	1:B:237:ARG:HH21	2.20	0.46
1:B:393:THR:HG21	1:B:518:LEU:H	1.81	0.46
1:B:1088:HIS:CE1	1:B:1122:VAL:HG22	2.50	0.46
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.50	0.46
1:C:783:ALA:HB2	1:C:873:TYR:CZ	2.50	0.46
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.97	0.46
1:B:21:ARG:HG3	1:B:22:THR:N	2.31	0.46
1:B:735:SER:O	1:B:859:THR:OG1	2.27	0.46
2:H:38:ARG:NH2	2:H:46:GLU:OE1	2.38	0.46
2:I:60:TYR:HE1	2:I:70:ILE:HG22	1.80	0.46
1:A:402:ILE:HD11	1:A:410:ILE:HG13	1.97	0.46
1:A:520:ALA:HB2	1:B:200:TYR:CZ	2.51	0.46
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.15	0.46
1:B:23:GLN:HG2	1:B:24:LEU:N	2.30	0.46
1:B:141:LEU:HD23	1:B:159:VAL:HG21	1.98	0.46
1:C:796:ASP:OD1	1:C:796:ASP:N	2.46	0.46
2:G:60:TYR:HE1	2:G:70:ILE:HG22	1.80	0.46
1:A:390:LEU:HD22	1:B:983:ARG:CG	2.46	0.46
1:A:600:PRO:HG3	1:A:674:TYR:CD1	2.51	0.46
1:A:676:THR:HG23	1:A:690:GLN:CG	2.46	0.46
1:B:906:PHE:CE2	1:B:916:LEU:HB2	2.51	0.46
1:B:961:THR:O	1:B:965:GLN:HG2	2.15	0.46
1:C:66:HIS:CE1	1:C:264:ALA:CB	2.98	0.46
1:A:38:TYR:CD2	1:C:562:PHE:HZ	2.34	0.46
1:A:369:TYR:OH	1:A:384:PRO:CA	2.62	0.46
1:B:984:LEU:HD22	1:B:989:ALA:N	2.31	0.46
1:C:104:TRP:HB2	1:C:106:PHE:CE2	2.51	0.46
1:C:180:GLU:O	1:C:182:LYS:HG2	2.15	0.46
2:G:5:VAL:O	2:G:22:CYS:HA	2.16	0.46
1:A:87:ASN:HB2	1:A:269:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG13	1:A:141:LEU:HD11	1.96	0.46
1:A:393:THR:HG21	1:A:518:LEU:H	1.81	0.46
1:A:429:PHE:CZ	1:A:431:GLY:HA3	2.51	0.46
1:A:850:ILE:HB	1:A:854:LYS:HE3	1.97	0.46
1:B:748:GLU:CB	1:B:981:LEU:CD1	2.85	0.46
1:B:901:GLN:NE2	1:B:905:ARG:HE	2.08	0.46
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.97	0.46
1:A:104:TRP:HB2	1:A:106:PHE:CE2	2.51	0.46
1:A:107:GLY:CA	1:A:235:ILE:HG12	2.46	0.46
1:A:913:GLN:HE21	1:C:1089:PHE:HB3	1.81	0.46
1:B:748:GLU:OE1	1:B:981:LEU:HD13	2.15	0.46
1:B:1116:THR:HB	1:B:1140:PRO:HD3	1.97	0.46
1:C:48:LEU:CD1	1:C:305:SER:HA	2.46	0.46
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.98	0.46
1:C:393:THR:HG21	1:C:518:LEU:H	1.81	0.46
2:H:5:VAL:O	2:H:22:CYS:HA	2.16	0.46
3:L:35:TRP:HD1	3:L:48:ILE:HB	1.81	0.46
1:A:380:TYR:CZ	1:A:412:PRO:HD2	2.50	0.45
1:A:816:SER:OG	1:A:819:GLU:HG3	2.16	0.45
1:A:1102:TRP:HB2	1:A:1135:ASN:HD21	1.75	0.45
1:A:86:PHE:H	1:A:236:THR:C	2.14	0.45
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.51	0.45
1:B:197:ILE:C	1:B:199:GLY:N	2.70	0.45
1:A:41:LYS:CB	1:C:563:GLN:HA	2.47	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HD23	1.99	0.45
1:A:156:GLU:OE1	1:A:156:GLU:N	2.44	0.45
1:A:197:ILE:C	1:A:199:GLY:N	2.69	0.45
1:A:716:THR:HG22	1:A:1110:TYR:CG	2.51	0.45
1:A:1115:ILE:HA	1:A:1119:ASN:HD22	1.81	0.45
1:B:709:ASN:O	1:C:897:PRO:CB	2.63	0.45
1:C:87:ASN:HB2	1:C:269:TYR:CD1	2.51	0.45
1:C:108:THR:CB	1:C:114:THR:HG21	2.44	0.45
1:C:197:ILE:O	1:C:199:GLY:N	2.50	0.45
1:C:326:ILE:HA	1:C:531:THR:OG1	2.16	0.45
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.50	0.45
3:J:34:ASN:HB2	3:J:89:GLN:HB3	1.98	0.45
1:A:599:THR:OG1	1:A:600:PRO:O	2.25	0.45
1:B:327:VAL:CA	1:B:542:ASN:O	2.63	0.45
1:C:108:THR:HB	1:C:114:THR:CG2	2.45	0.45
1:C:188:ASN:O	1:C:190:ARG:HG3	2.16	0.45
1:A:145:TYR:CE2	1:A:147:LYS:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:CB	1:B:168:PHE:HB3	2.35	0.45
1:B:247:SER:H	1:B:257:GLY:HA3	1.81	0.45
1:B:882:ILE:O	1:B:898:PHE:HD1	2.00	0.45
1:B:1093:GLY:HA2	1:B:1107:ARG:HG3	1.99	0.45
1:C:64:TRP:HZ2	1:C:66:HIS:CE1	2.06	0.45
1:C:201:PHE:H	1:C:231:ILE:HG12	1.81	0.45
1:A:43:PHE:CD1	1:C:559:PHE:HA	2.51	0.45
1:A:591:SER:CB	1:A:615:VAL:HG11	2.30	0.45
1:C:747:THR:HA	1:C:750:SER:HB3	1.99	0.45
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.52	0.45
1:A:83:VAL:HA	1:A:239:GLN:HB2	1.99	0.45
1:A:145:TYR:HE1	1:A:150:LYS:HA	1.80	0.45
1:B:117:LEU:HD11	1:B:119:ILE:CG2	2.47	0.45
1:B:356:LYS:HE3	1:B:358:ILE:HD11	1.99	0.45
1:B:563:GLN:HG2	1:C:41:LYS:O	2.17	0.45
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.50	0.45
1:C:324:GLU:CD	1:C:534:VAL:HG21	2.27	0.45
1:C:393:THR:O	1:C:523:THR:OG1	2.31	0.45
3:L:34:ASN:HB2	3:L:89:GLN:HB3	1.98	0.45
3:K:34:ASN:HB2	3:K:89:GLN:HB3	1.98	0.45
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.98	0.45
1:A:142:GLY:O	1:A:155:SER:N	2.50	0.45
1:B:559:PHE:HA	1:C:43:PHE:CD1	2.52	0.45
1:C:142:GLY:O	1:C:155:SER:N	2.50	0.45
1:A:318:PHE:CE2	1:A:612:TYR:CG	3.05	0.45
1:A:797:PHE:O	1:A:800:PHE:HD2	2.00	0.45
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.82	0.45
1:B:83:VAL:HG23	1:B:237:ARG:HH22	1.56	0.45
1:B:327:VAL:HA	1:B:542:ASN:CB	2.45	0.45
1:B:864:LEU:HG	1:B:865:LEU:HD12	1.99	0.45
1:B:1054:GLN:N	1:B:1061:VAL:O	2.50	0.45
1:C:287:ASP:OD2	1:C:306:PHE:CG	2.68	0.45
3:J:35:TRP:HD1	3:J:48:ILE:HB	1.81	0.45
1:A:497:PHE:HA	1:A:501:ASN:HD21	1.82	0.45
1:A:877:LEU:HD22	1:A:1034:LEU:HD11	1.98	0.45
1:C:100:ILE:HD13	1:C:263:ALA:HB2	1.98	0.45
1:C:864:LEU:HG	1:C:865:LEU:HD12	1.99	0.45
2:I:5:VAL:O	2:I:22:CYS:HA	2.16	0.45
1:A:41:LYS:HB3	1:C:563:GLN:CA	2.46	0.44
1:B:299:THR:CG2	1:B:597:VAL:HG11	2.47	0.44
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:THR:HA	1:B:750:SER:HB3	1.99	0.44
1:C:356:LYS:HE3	1:C:358:ILE:HD11	1.99	0.44
1:C:716:THR:HA	1:C:1110:TYR:HB3	1.98	0.44
1:A:326:ILE:O	1:A:542:ASN:N	2.26	0.44
1:A:578:ASP:HB3	1:A:583:GLU:HG2	1.99	0.44
1:C:83:VAL:HA	1:C:239:GLN:HB2	1.99	0.44
1:C:106:PHE:HB2	1:C:117:LEU:HD23	1.99	0.44
1:C:970:PHE:CD2	1:C:999:GLY:HA3	2.53	0.44
1:A:18:LEU:HD12	1:A:18:LEU:C	2.32	0.44
1:A:429:PHE:CE1	1:A:514:SER:HB3	2.47	0.44
1:B:142:GLY:O	1:B:155:SER:N	2.50	0.44
1:B:497:PHE:HA	1:B:501:ASN:HD21	1.83	0.44
3:K:35:TRP:HD1	3:K:48:ILE:HB	1.81	0.44
1:A:29:THR:HG22	1:A:62:VAL:O	2.18	0.44
1:A:276:LEU:HD22	1:A:289:VAL:HB	1.98	0.44
1:A:384:PRO:HA	1:A:387:LEU:HD23	1.99	0.44
1:A:398:ASP:N	1:A:398:ASP:OD1	2.51	0.44
1:A:590:CYS:HB2	1:A:592:PHE:CE1	2.52	0.44
1:B:83:VAL:HA	1:B:239:GLN:HB2	1.99	0.44
1:B:393:THR:O	1:B:523:THR:OG1	2.31	0.44
1:C:115:GLN:HB2	1:C:233:ILE:HD13	1.99	0.44
1:C:315:THR:HG22	1:C:316:SER:N	2.33	0.44
1:A:425:LEU:HD22	1:A:429:PHE:CE2	2.52	0.44
1:A:802:PHE:CE1	1:A:927:PHE:CZ	3.05	0.44
1:B:100:ILE:HD13	1:B:263:ALA:HB2	1.99	0.44
1:B:164:ASN:OD1	1:B:164:ASN:N	2.51	0.44
1:C:323:THR:OG1	1:C:537:LYS:HE3	2.18	0.44
1:C:497:PHE:HA	1:C:501:ASN:HD21	1.83	0.44
3:K:6:GLN:O	3:K:100:GLN:NE2	2.51	0.44
1:A:1016:ALA:O	1:A:1019:ARG:HB3	2.17	0.44
1:B:70:VAL:HG23	1:B:75:GLY:O	2.18	0.44
1:B:87:ASN:HB2	1:B:269:TYR:CD1	2.51	0.44
1:C:184:GLY:C	1:C:186:PHE:H	2.21	0.44
1:C:296:LEU:HD12	1:C:608:VAL:HG13	1.19	0.44
2:H:99:HIS:CG	3:L:89:GLN:HE22	2.36	0.44
3:L:6:GLN:O	3:L:100:GLN:NE2	2.51	0.44
1:A:356:LYS:HE3	1:A:358:ILE:HD11	1.99	0.44
1:A:518:LEU:HD21	1:B:200:TYR:HD2	1.83	0.44
1:A:853:GLN:HE21	1:A:959:LEU:HB3	1.82	0.44
1:A:869:MET:CE	1:C:669:GLY:HA3	2.48	0.44
1:B:398:ASP:OD1	1:B:398:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:TYR:HB3	1:C:615:VAL:HG21	1.99	0.44
2:G:99:HIS:CG	3:J:89:GLN:HE22	2.36	0.44
1:A:67:ALA:O	1:A:79:PHE:HA	2.18	0.44
1:A:70:VAL:HG23	1:A:75:GLY:O	2.18	0.44
1:A:184:GLY:C	1:A:186:PHE:H	2.21	0.44
1:A:319:ARG:HB3	1:A:590:CYS:SG	2.58	0.44
1:A:379:CYS:HB2	1:A:384:PRO:CD	2.48	0.44
1:A:386:LYS:HZ1	1:B:986:LYS:HG2	1.82	0.44
1:A:850:ILE:O	1:A:854:LYS:HG3	2.17	0.44
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.18	0.44
1:B:357:ARG:NH1	1:C:167:THR:HG22	2.32	0.44
1:B:709:ASN:OD1	1:B:709:ASN:N	2.47	0.44
1:C:70:VAL:HG23	1:C:75:GLY:O	2.18	0.44
1:C:398:ASP:OD1	1:C:398:ASP:N	2.51	0.44
1:A:318:PHE:O	1:A:318:PHE:CD1	2.70	0.44
1:A:436:TRP:O	1:A:508:TYR:HA	2.18	0.44
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.00	0.44
1:B:436:TRP:O	1:B:508:TYR:HA	2.18	0.44
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.99	0.44
1:B:759:PHE:O	1:B:763:LEU:HG	2.18	0.44
1:B:1139:ASP:CG	1:B:1142:GLN:H	2.21	0.44
1:C:143:VAL:O	1:C:245:HIS:HA	2.18	0.44
1:A:143:VAL:O	1:A:245:HIS:HA	2.18	0.43
1:A:277:LEU:HD23	1:A:285:ILE:HD11	2.00	0.43
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.99	0.43
1:A:564:GLN:HG3	1:A:565:PHE:CD1	2.53	0.43
1:A:1102:TRP:CG	1:A:1135:ASN:ND2	2.85	0.43
1:B:96:GLU:HB2	1:B:190:ARG:NH1	2.33	0.43
1:B:970:PHE:CD2	1:B:999:GLY:HA3	2.53	0.43
1:C:882:ILE:O	1:C:898:PHE:HD1	2.00	0.43
1:C:1093:GLY:HA2	1:C:1107:ARG:HG3	1.99	0.43
3:L:21:ILE:HD12	3:L:73:LEU:HD23	2.00	0.43
3:J:21:ILE:HD12	3:J:73:LEU:HD23	2.00	0.43
1:A:205:SER:HB3	1:A:226:LEU:HD11	1.99	0.43
1:A:986:LYS:O	1:A:989:ALA:N	2.50	0.43
1:B:205:SER:HB3	1:B:226:LEU:HD11	1.99	0.43
1:B:315:THR:HG22	1:B:316:SER:N	2.33	0.43
1:B:713:ALA:HB2	1:C:895:GLN:NE2	2.33	0.43
2:I:99:HIS:CG	3:K:89:GLN:HE22	2.36	0.43
3:J:6:GLN:O	3:J:100:GLN:NE2	2.51	0.43
3:K:21:ILE:HD12	3:K:73:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASN:HB3	1:A:505:TYR:HB2	2.00	0.43
1:A:822:LEU:HD13	1:A:1056:ALA:HB2	1.99	0.43
1:A:922:LEU:HD21	4:A:1306:NAG:H3	1.97	0.43
1:A:1102:TRP:CB	1:A:1135:ASN:ND2	2.77	0.43
1:B:669:GLY:N	1:C:864:LEU:O	2.51	0.43
1:B:815:ARG:HD2	1:B:823:PHE:CE2	2.45	0.43
1:B:1089:PHE:CE2	1:C:914:ASN:HA	2.53	0.43
1:C:205:SER:HB3	1:C:226:LEU:HD11	1.99	0.43
1:C:234:ASN:ND2	1:C:234:ASN:N	2.64	0.43
1:C:436:TRP:O	1:C:508:TYR:HA	2.18	0.43
1:A:200:TYR:HA	1:A:229:LEU:O	2.18	0.43
1:A:562:PHE:HZ	1:B:225:PRO:HG3	1.65	0.43
1:A:802:PHE:CE1	1:A:927:PHE:CE2	3.06	0.43
1:B:143:VAL:O	1:B:245:HIS:HA	2.18	0.43
1:C:902:MET:HE1	1:C:1049:LEU:HD13	2.01	0.43
1:B:276:LEU:HD11	1:B:306:PHE:CE1	2.53	0.43
1:B:563:GLN:CG	1:C:41:LYS:O	2.66	0.43
1:A:96:GLU:HB2	1:A:190:ARG:NH1	2.34	0.43
1:A:234:ASN:H	1:A:234:ASN:ND2	2.16	0.43
1:A:542:ASN:HA	1:A:546:LEU:O	2.18	0.43
1:C:1032:CYS:SG	1:C:1051:SER:OG	2.77	0.43
1:C:1054:GLN:N	1:C:1061:VAL:O	2.50	0.43
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.85	0.43
1:A:1088:HIS:CE1	1:A:1122:VAL:HG22	2.53	0.43
1:B:100:ILE:HG21	1:B:263:ALA:CB	2.46	0.43
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.40	0.43
1:C:330:PRO:HA	1:C:579:PRO:HB2	2.01	0.43
1:C:735:SER:O	1:C:859:THR:OG1	2.27	0.43
1:C:821:LEU:O	1:C:825:LYS:HG2	2.19	0.43
1:A:753:LEU:HD21	1:A:760:CYS:SG	2.59	0.43
1:B:106:PHE:CD1	1:B:235:ILE:HG21	2.54	0.43
1:B:106:PHE:HD1	1:B:235:ILE:HG21	1.83	0.43
1:C:34:ARG:HD2	1:C:191:GLU:OE2	2.19	0.43
1:C:1139:ASP:CG	1:C:1142:GLN:H	2.21	0.43
1:A:145:TYR:CE1	1:A:150:LYS:HA	2.53	0.43
1:A:328:ARG:HD3	1:A:530:SER:HB2	2.00	0.43
1:B:120:VAL:HG12	1:B:122:ASN:N	2.34	0.43
1:B:184:GLY:C	1:B:186:PHE:H	2.21	0.43
1:B:716:THR:HG22	1:B:1110:TYR:CD2	2.54	0.43
1:B:748:GLU:HB3	1:B:981:LEU:HD21	2.00	0.43
1:B:821:LEU:O	1:B:825:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:CA	1:A:513:LEU:O	2.67	0.43
1:A:599:THR:HB	1:A:608:VAL:HG12	2.01	0.43
1:A:960:ASN:O	1:A:963:VAL:N	2.52	0.43
1:B:34:ARG:HE	1:B:216:LEU:HD23	1.83	0.43
1:B:291:CYS:O	1:B:298:GLU:HG3	2.19	0.43
1:B:699:LEU:HD21	1:C:869:MET:HB3	2.01	0.43
1:C:34:ARG:HE	1:C:216:LEU:HD23	1.83	0.43
1:C:115:GLN:OE1	1:C:233:ILE:CG2	2.67	0.43
1:C:287:ASP:CG	1:C:306:PHE:CZ	2.91	0.43
1:C:294:ASP:OD1	1:C:297:SER:N	2.45	0.43
1:C:656:VAL:HG21	1:C:693:ILE:CD1	2.49	0.43
1:A:328:ARG:HD3	1:A:328:ARG:HA	1.78	0.42
1:C:108:THR:HB	1:C:114:THR:CB	2.49	0.42
1:C:115:GLN:NE2	1:C:167:THR:HG21	2.34	0.42
1:C:146:HIS:C	1:C:148:ASN:H	2.22	0.42
1:C:759:PHE:O	1:C:763:LEU:HG	2.19	0.42
1:A:18:LEU:CD1	1:A:79:PHE:CD2	3.01	0.42
1:A:391:CYS:HB3	1:A:525:CYS:HA	2.01	0.42
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.52	0.42
1:B:34:ARG:HD2	1:B:191:GLU:OE2	2.19	0.42
1:B:568:ASP:OD1	1:B:569:ILE:N	2.45	0.42
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.19	0.42
1:B:1032:CYS:SG	1:B:1051:SER:OG	2.77	0.42
1:C:121:ASN:HA	1:C:126:VAL:CG2	2.39	0.42
1:A:412:PRO:HB3	1:A:425:LEU:HB3	2.00	0.42
1:A:869:MET:HB3	1:C:699:LEU:HD21	2.01	0.42
1:A:1116:THR:HA	1:A:1138:TYR:O	2.19	0.42
1:C:96:GLU:HB2	1:C:190:ARG:NH1	2.34	0.42
1:C:296:LEU:CD1	1:C:608:VAL:HG22	2.46	0.42
1:A:186:PHE:C	1:A:188:ASN:H	2.22	0.42
1:B:676:THR:HG23	1:B:690:GLN:HG2	2.01	0.42
1:C:994:ASP:O	1:C:998:THR:N	2.46	0.42
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.55	0.42
1:B:200:TYR:HA	1:B:229:LEU:O	2.20	0.42
1:B:501:ASN:HB3	1:B:505:TYR:HB2	2.00	0.42
1:C:86:PHE:HB3	1:C:235:ILE:O	2.20	0.42
1:A:369:TYR:OH	1:A:384:PRO:CB	2.67	0.42
1:B:117:LEU:CD1	1:B:119:ILE:HG23	2.49	0.42
2:H:22:CYS:O	2:H:78:THR:HA	2.19	0.42
1:A:43:PHE:CZ	1:C:558:LYS:O	2.73	0.42
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ASN:HB3	1:C:505:TYR:HB2	2.00	0.42
1:C:825:LYS:HE3	1:C:938:LEU:O	2.19	0.42
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.19	0.42
1:C:1102:TRP:HD1	1:C:1135:ASN:ND2	2.17	0.42
2:G:22:CYS:O	2:G:78:THR:HA	2.19	0.42
1:A:34:ARG:HD2	1:A:191:GLU:OE2	2.19	0.42
1:B:186:PHE:C	1:B:188:ASN:H	2.22	0.42
1:B:327:VAL:C	1:B:542:ASN:O	2.53	0.42
1:C:115:GLN:CB	1:C:233:ILE:HD12	2.39	0.42
1:C:394:ASN:N	1:C:394:ASN:OD1	2.52	0.42
1:A:106:PHE:HB3	1:A:235:ILE:HG21	2.02	0.42
1:A:394:ASN:OD1	1:A:394:ASN:N	2.52	0.42
1:A:407:VAL:O	1:A:410:ILE:HB	2.20	0.42
1:B:115:GLN:HB2	1:B:233:ILE:HG21	2.01	0.42
1:B:852:ALA:HA	1:B:855:PHE:CE2	2.54	0.42
1:B:1088:HIS:C	1:B:1089:PHE:HD1	2.23	0.42
1:C:64:TRP:CE2	1:C:66:HIS:NE2	2.78	0.42
1:C:186:PHE:C	1:C:188:ASN:H	2.22	0.42
1:C:656:VAL:HG21	1:C:693:ILE:CB	2.49	0.42
1:A:75:GLY:O	1:A:76:THR:OG1	2.35	0.42
1:A:994:ASP:O	1:A:998:THR:N	2.44	0.42
1:B:323:THR:OG1	1:B:539:VAL:HG12	2.20	0.42
1:B:327:VAL:HG12	1:B:542:ASN:HB2	1.99	0.42
1:B:592:PHE:CE1	1:C:857:GLY:HA2	2.55	0.42
1:C:717:ASN:O	1:C:1070:ALA:N	2.43	0.42
1:A:160:TYR:HE1	1:A:163:ALA:HB2	1.85	0.41
1:C:1088:HIS:C	1:C:1089:PHE:HD1	2.23	0.41
2:G:68:PHE:HD1	2:G:83:MET:HA	1.85	0.41
2:I:22:CYS:O	2:I:78:THR:HA	2.19	0.41
1:A:115:GLN:NE2	1:A:167:THR:HG21	2.34	0.41
1:A:308:VAL:HB	1:A:602:THR:HG23	2.01	0.41
1:A:386:LYS:C	1:A:388:ASN:H	2.24	0.41
1:B:203:ILE:HG22	1:B:226:LEU:HD12	2.03	0.41
1:B:825:LYS:HE3	1:B:938:LEU:O	2.19	0.41
1:B:1145:LEU:O	1:B:1147:SER:O	2.38	0.41
1:C:49:HIS:O	1:C:277:LEU:N	2.43	0.41
1:C:560:LEU:N	1:C:563:GLN:OE1	2.43	0.41
1:C:852:ALA:HA	1:C:855:PHE:CE2	2.54	0.41
2:I:68:PHE:HD1	2:I:83:MET:HA	1.86	0.41
1:A:34:ARG:HE	1:A:216:LEU:HD23	1.83	0.41
1:A:275:PHE:C	1:A:276:LEU:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ALA:HB2	1:B:895:GLN:NE2	2.35	0.41
1:B:555:SER:OG	1:B:584:ILE:O	2.34	0.41
1:B:36:VAL:O	1:B:222:ALA:HA	2.21	0.41
1:C:203:ILE:HG22	1:C:226:LEU:HD12	2.03	0.41
1:C:656:VAL:HG21	1:C:693:ILE:HD12	2.01	0.41
1:A:1087:ALA:HB3	1:A:1123:SER:O	2.21	0.41
1:B:130:VAL:CG2	1:B:168:PHE:CD2	3.01	0.41
1:C:36:VAL:O	1:C:222:ALA:HA	2.21	0.41
1:C:82:PRO:HG2	1:C:84:LEU:HD21	2.03	0.41
1:C:237:ARG:HB2	1:C:237:ARG:NH1	2.35	0.41
1:C:247:SER:HB3	1:C:257:GLY:HA3	2.02	0.41
3:J:21:ILE:HB	3:J:73:LEU:HB3	2.03	0.41
1:A:424:LYS:HB3	1:A:463:PRO:HA	2.03	0.41
1:A:801:ASN:N	1:A:928:ASN:OD1	2.51	0.41
1:A:861:LEU:H	1:A:861:LEU:HG	1.68	0.41
1:B:105:ILE:O	1:B:105:ILE:HG13	2.21	0.41
1:B:424:LYS:HB3	1:B:463:PRO:HA	2.03	0.41
1:B:730:SER:O	1:B:1058:HIS:HB3	2.20	0.41
1:C:498:GLN:H	1:C:501:ASN:ND2	2.19	0.41
1:C:676:THR:HG23	1:C:690:GLN:HG2	2.01	0.41
1:A:308:VAL:H	1:A:602:THR:CG2	2.34	0.41
1:A:770:ILE:O	1:A:774:GLN:HG2	2.20	0.41
1:B:118:LEU:CD2	1:B:129:LYS:HD2	2.51	0.41
1:B:160:TYR:CE1	1:B:163:ALA:HB2	2.55	0.41
1:B:572:THR:HG21	1:C:855:PHE:CD2	2.54	0.41
1:C:880:GLY:O	1:C:884:SER:OG	2.31	0.41
2:H:9:GLY:HA3	2:H:114:LEU:O	2.21	0.41
1:A:82:PRO:HG2	1:A:84:LEU:HD21	2.03	0.41
1:A:643:PHE:CE2	1:A:645:THR:HG22	2.56	0.41
1:B:82:PRO:HG2	1:B:84:LEU:HD21	2.03	0.41
1:B:656:VAL:HG21	1:B:693:ILE:CB	2.51	0.41
1:B:746:SER:OG	1:B:981:LEU:CD1	2.69	0.41
1:B:927:PHE:HE1	1:B:1065:VAL:HG21	1.86	0.41
1:C:205:SER:O	1:C:223:LEU:HG	2.21	0.41
1:C:424:LYS:HB3	1:C:463:PRO:HA	2.03	0.41
3:K:21:ILE:HB	3:K:73:LEU:HB3	2.03	0.41
1:A:205:SER:O	1:A:223:LEU:HG	2.21	0.41
1:A:234:ASN:HD22	1:A:234:ASN:N	2.17	0.41
1:A:278:LYS:HD3	1:A:306:PHE:CE2	2.55	0.41
1:A:498:GLN:H	1:A:501:ASN:ND2	2.19	0.41
1:A:796:ASP:OD1	1:A:796:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLN:O	1:A:1015:ALA:N	2.38	0.41
1:A:1030:SER:O	1:A:1034:LEU:HB2	2.21	0.41
1:B:19:THR:HG22	1:B:138:ASP:OD1	2.21	0.41
1:C:716:THR:HG22	1:C:1110:TYR:CD2	2.56	0.41
1:C:730:SER:O	1:C:1058:HIS:HB3	2.20	0.41
1:C:927:PHE:HE1	1:C:1065:VAL:HG21	1.86	0.41
3:J:3:GLN:HB2	3:J:26:SER:HB3	2.03	0.41
1:A:190:ARG:HG2	1:A:207:HIS:ND1	2.36	0.41
1:A:762:GLN:HE22	1:C:1006:THR:HG21	1.84	0.41
1:A:991:VAL:O	1:A:994:ASP:HB2	2.21	0.41
1:B:563:GLN:HA	1:C:41:LYS:HB3	2.03	0.41
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.57	0.41
1:C:64:TRP:CZ2	1:C:214:ARG:HD2	2.56	0.41
1:C:557:LYS:O	1:C:584:ILE:HG13	2.21	0.41
1:C:616:ASN:C	1:C:618:THR:H	2.23	0.41
3:L:21:ILE:HB	3:L:73:LEU:HB3	2.03	0.41
1:A:23:GLN:N	1:A:23:GLN:OE1	2.54	0.40
1:A:42:VAL:CG2	1:C:565:PHE:HB2	2.18	0.40
1:A:203:ILE:HG22	1:A:226:LEU:HD12	2.03	0.40
1:A:873:TYR:O	1:A:876:ALA:N	2.54	0.40
1:B:50:SER:HA	1:B:275:PHE:O	2.20	0.40
1:B:106:PHE:HB2	1:B:117:LEU:H	1.86	0.40
1:C:50:SER:HA	1:C:275:PHE:O	2.21	0.40
2:I:9:GLY:HA3	2:I:114:LEU:O	2.21	0.40
1:A:671:CYS:SG	1:A:697:MET:HB3	2.61	0.40
1:A:730:SER:O	1:A:1058:HIS:HB3	2.21	0.40
1:B:49:HIS:O	1:B:277:LEU:N	2.43	0.40
1:B:290:ASP:OD1	1:B:291:CYS:N	2.54	0.40
1:B:725:GLU:OE2	1:B:1028:LYS:HE3	2.22	0.40
1:B:946:GLY:O	1:B:950:ASP:N	2.44	0.40
1:C:298:GLU:OE2	1:C:316:SER:OG	2.21	0.40
1:A:1090:PRO:HD2	1:B:913:GLN:HE22	1.86	0.40
1:B:498:GLN:H	1:B:501:ASN:ND2	2.19	0.40
1:B:592:PHE:HE1	1:C:857:GLY:HA2	1.86	0.40
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	2.03	0.40
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.56	0.40
1:C:618:THR:HG23	4:C:1303:NAG:H82	2.03	0.40
1:C:941:THR:HG22	1:C:943:SER:H	1.87	0.40
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	2.03	0.40
1:C:1089:PHE:N	1:C:1089:PHE:CD1	2.89	0.40
3:K:3:GLN:HB2	3:K:26:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:O	1:A:409:GLN:HB2	2.21	0.40
1:B:205:SER:O	1:B:223:LEU:HG	2.21	0.40
1:C:290:ASP:OD1	1:C:291:CYS:N	2.55	0.40
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.57	0.40
1:A:102:ARG:NH1	1:A:123:ALA:HB2	2.36	0.40
1:A:365:TYR:HE2	1:A:387:LEU:HD12	1.87	0.40
1:A:717:ASN:O	1:A:1070:ALA:N	2.49	0.40
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.56	0.40
1:B:394:ASN:OD1	1:B:394:ASN:N	2.52	0.40
1:C:160:TYR:HE1	1:C:163:ALA:HB2	1.85	0.40
2:G:9:GLY:HA3	2:G:114:LEU:O	2.21	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	1059/1273 (83%)	971 (92%)	79 (8%)	9 (1%)	19 57
1	B	1056/1273 (83%)	977 (92%)	76 (7%)	3 (0%)	41 74
1	C	1060/1273 (83%)	984 (93%)	72 (7%)	4 (0%)	34 70
2	G	118/120 (98%)	105 (89%)	13 (11%)	0	100 100
2	H	118/120 (98%)	106 (90%)	12 (10%)	0	100 100
2	I	118/120 (98%)	105 (89%)	13 (11%)	0	100 100
3	J	106/108 (98%)	97 (92%)	9 (8%)	0	100 100
3	K	105/108 (97%)	96 (91%)	9 (9%)	0	100 100
3	L	106/108 (98%)	97 (92%)	9 (8%)	0	100 100
All	All	3846/4503 (85%)	3538 (92%)	292 (8%)	16 (0%)	38 70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	197	ILE
1	A	198	ASP
1	B	197	ILE
1	B	198	ASP
1	C	198	ASP
1	A	387	LEU
1	A	410	ILE
1	A	617	CYS
1	A	1099	GLY
1	B	617	CYS
1	A	381	GLY
1	C	617	CYS
1	A	593	GLY
1	C	24	LEU
1	C	197	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	929/1112 (84%)	919 (99%)	10 (1%)	73 85
1	B	926/1112 (83%)	911 (98%)	15 (2%)	62 79
1	C	932/1112 (84%)	928 (100%)	4 (0%)	91 95
2	G	96/98 (98%)	96 (100%)	0	100 100
2	H	96/98 (98%)	96 (100%)	0	100 100
2	I	96/98 (98%)	96 (100%)	0	100 100
3	J	93/93 (100%)	93 (100%)	0	100 100
3	K	93/93 (100%)	93 (100%)	0	100 100
3	L	92/93 (99%)	92 (100%)	0	100 100
All	All	3353/3909 (86%)	3324 (99%)	29 (1%)	79 88

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	A	234	ASN
1	A	237	ARG
1	A	317	ASN
1	A	319	ARG
1	A	387	LEU
1	A	390	LEU
1	A	591	SER
1	A	708	SER
1	A	709	ASN
1	B	108	THR
1	B	111	ASP
1	B	113	LYS
1	B	116	SER
1	B	162	SER
1	B	235	ILE
1	B	533	LEU
1	B	615	VAL
1	B	708	SER
1	B	709	ASN
1	B	740	MET
1	B	746	SER
1	B	980	ILE
1	B	983	ARG
1	B	984	LEU
1	C	234	ASN
1	C	615	VAL
1	C	616	ASN
1	C	708	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	HIS
1	A	146	HIS
1	A	148	ASN
1	A	239	GLN
1	A	282	ASN
1	A	317	ASN
1	A	501	ASN
1	A	804	GLN
1	A	853	GLN

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Mol	Chain	Res	Type
1	A	901	GLN
1	A	913	GLN
1	A	935	GLN
1	A	1119	ASN
1	A	1135	ASN
1	B	115	GLN
1	B	121	ASN
1	B	239	GLN
1	B	317	ASN
1	B	501	ASN
1	B	779	GLN
1	B	804	GLN
1	B	853	GLN
1	B	901	GLN
1	B	913	GLN
1	B	935	GLN
1	B	1011	GLN
1	B	1135	ASN
1	C	122	ASN
1	C	239	GLN
1	C	317	ASN
1	C	501	ASN
1	C	779	GLN
1	C	804	GLN
1	C	853	GLN
1	C	901	GLN
1	C	935	GLN
1	C	1011	GLN
1	C	1135	ASN
2	G	84	ASN
2	G	104	ASN
2	H	84	ASN
2	H	104	ASN
2	I	84	ASN
2	I	104	ASN
3	L	38	GLN
3	L	90	GLN
3	J	38	GLN
3	J	90	GLN
3	K	38	GLN
3	K	90	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

27 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	C	1302	1	14,14,15	0.27	0	17,19,21	0.68	0
4	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	B	1304	1	14,14,15	0.27	0	17,19,21	0.68	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.68	0
4	NAG	B	1307	1	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	1308	1	14,14,15	0.30	0	17,19,21	0.71	0
4	NAG	A	1309	1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.71	0
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.80	0
4	NAG	C	1304	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.72	0
4	NAG	C	1309	1	14,14,15	0.26	0	17,19,21	0.61	0
4	NAG	A	1307	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	A	1308	1	14,14,15	0.29	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1305	1	14,14,15	0.26	0	17,19,21	0.73	0
4	NAG	A	1305	1	14,14,15	0.27	0	17,19,21	0.74	0
4	NAG	B	1306	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.70	0
4	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.65	0
4	NAG	C	1303	1	14,14,15	0.29	0	17,19,21	0.69	0
4	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.58	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	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	C	1301	NAG	C3-C2-N2-C7
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1308	NAG	C3-C2-N2-C7
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	A	1307	NAG	C8-C7-N2-C2
4	A	1309	NAG	C8-C7-N2-C2
4	A	1309	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	B	1301	NAG	O5-C5-C6-O6
4	A	1306	NAG	C1-C2-N2-C7
4	A	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	A	1303	NAG	C1-C2-N2-C7
4	C	1306	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	B	1305	NAG	C1-C2-N2-C7
4	A	1306	NAG	C3-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	C	1303	NAG	C8-C7-N2-C2
4	C	1308	NAG	C1-C2-N2-C7
4	B	1302	NAG	C4-C5-C6-O6
4	A	1305	NAG	O7-C7-N2-C2
4	B	1302	NAG	O5-C5-C6-O6
4	A	1309	NAG	C1-C2-N2-C7
4	C	1303	NAG	O7-C7-N2-C2
4	A	1309	NAG	C3-C2-N2-C7
4	B	1308	NAG	C8-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	A	1303	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	A	1302	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	NAG	1	0
4	C	1308	NAG	2	0
4	C	1301	NAG	1	0
4	B	1301	NAG	1	0
4	A	1307	NAG	1	0
4	A	1305	NAG	1	0
4	A	1306	NAG	4	0
4	C	1303	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

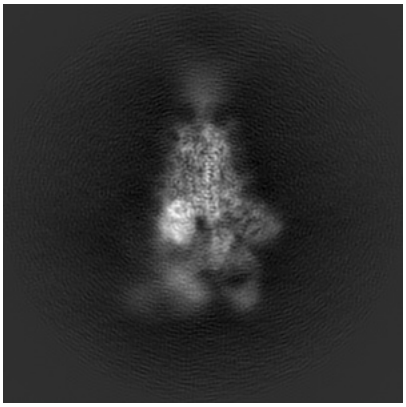
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30482. These allow visual inspection of the internal detail of the map and identification of artifacts.

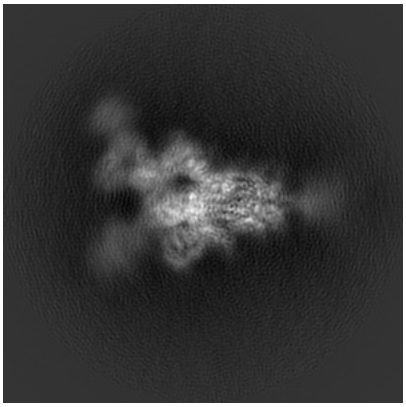
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

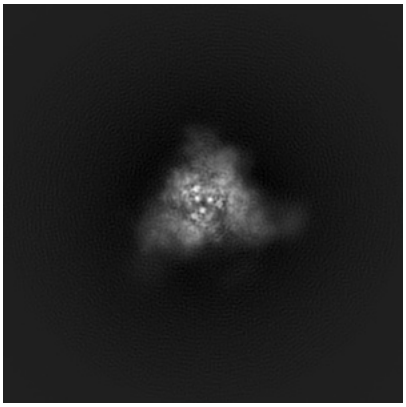
6.1.1 Primary map



X



Y

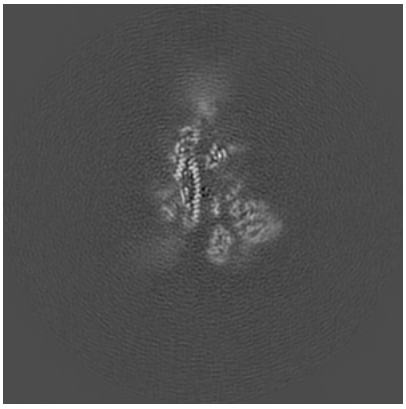


Z

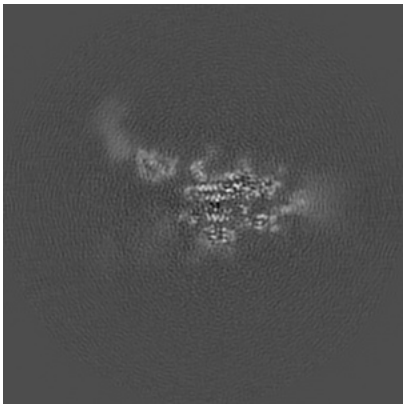
The images above show the map projected in three orthogonal directions.

6.2 Central slices

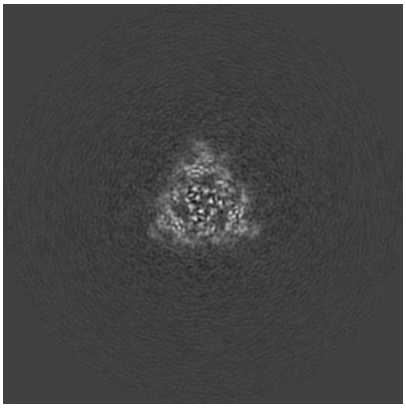
6.2.1 Primary map



X Index: 200



Y Index: 200



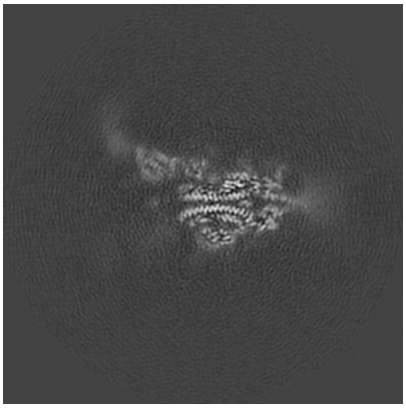
Z Index: 200

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

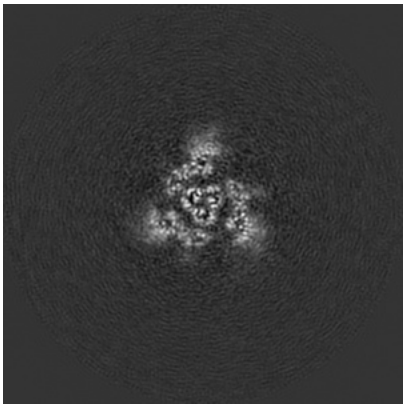
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 193



Y Index: 204



Z Index: 189

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 0.00502. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

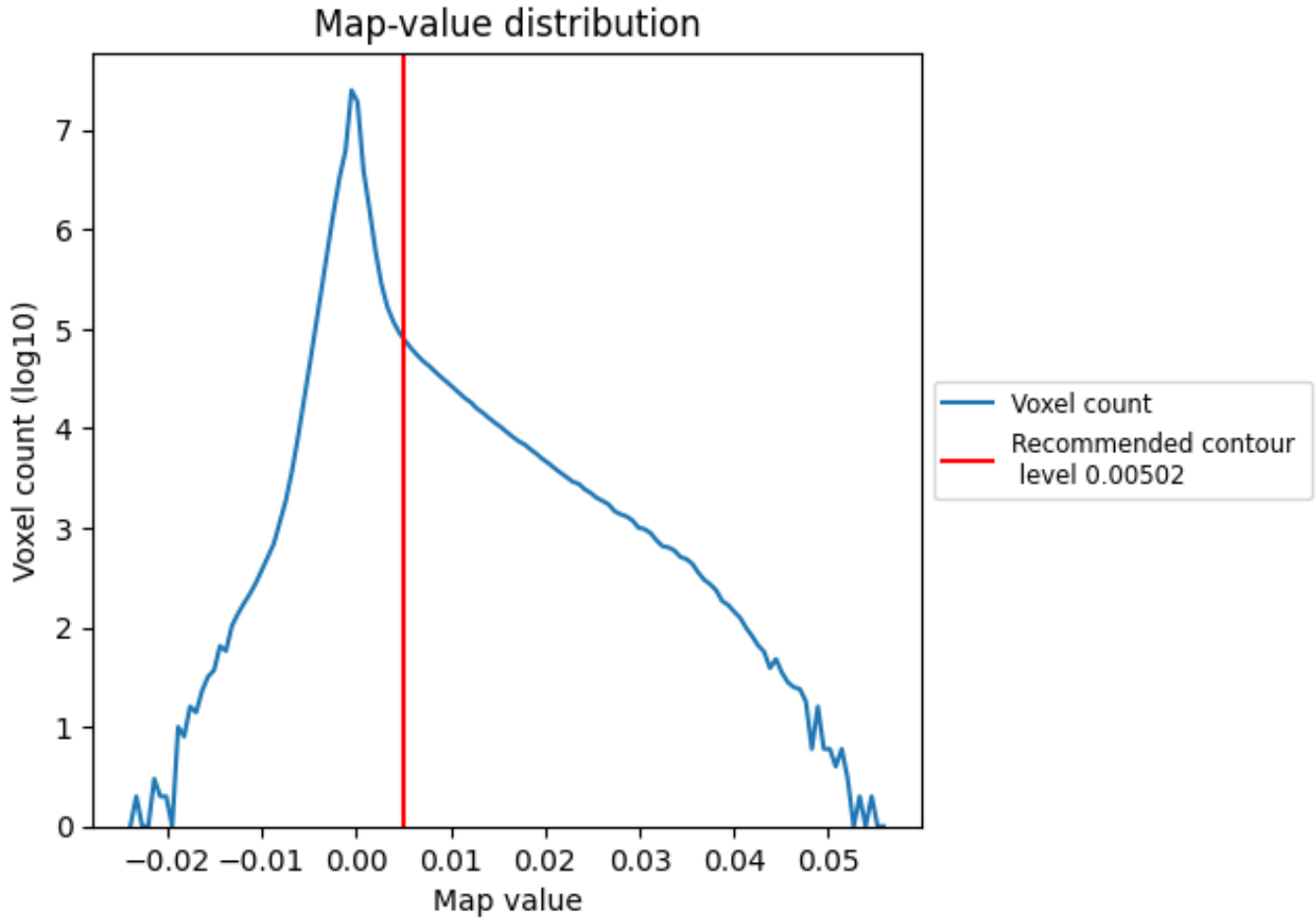
6.5 Mask visualisation (i)

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

7 Map analysis

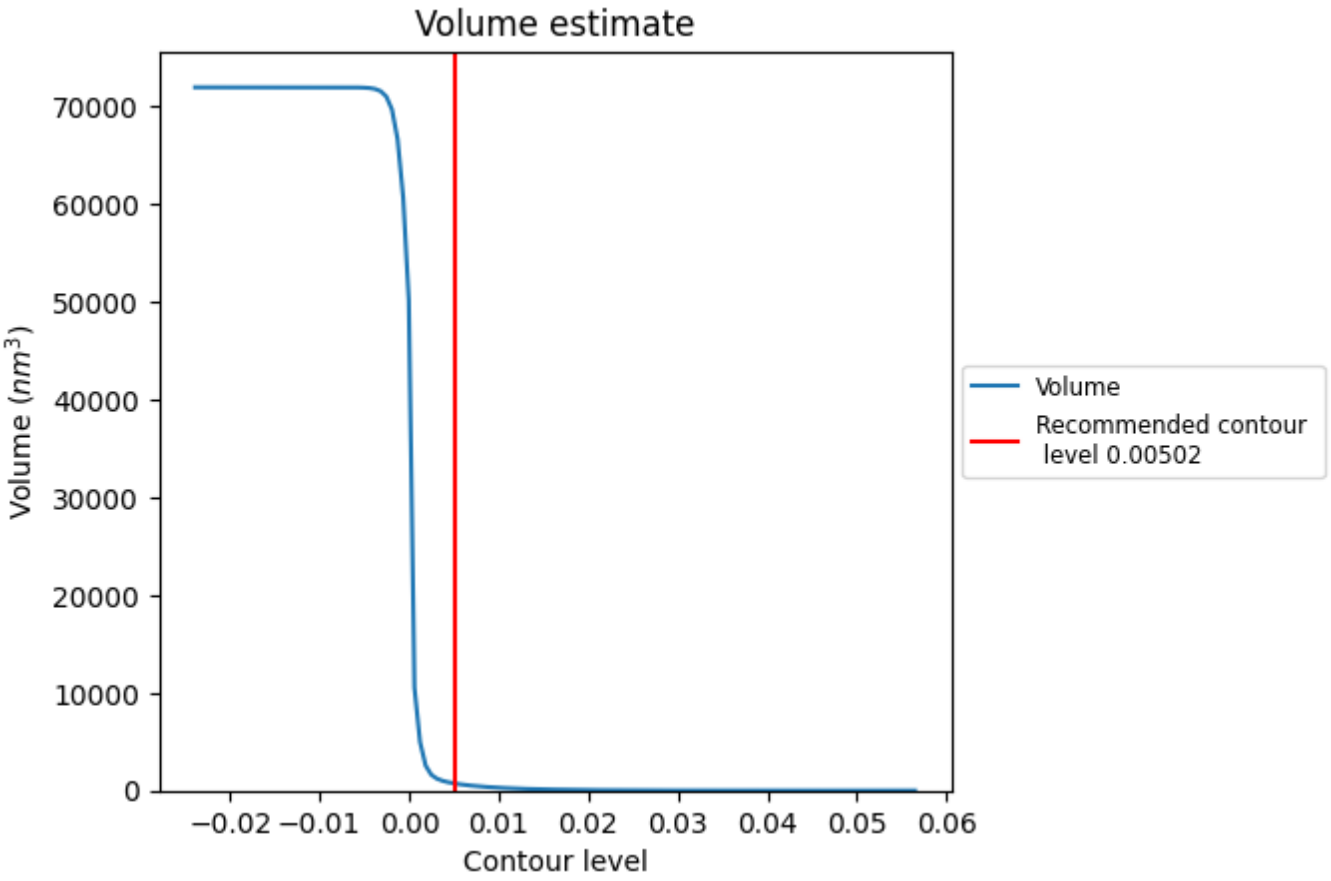
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

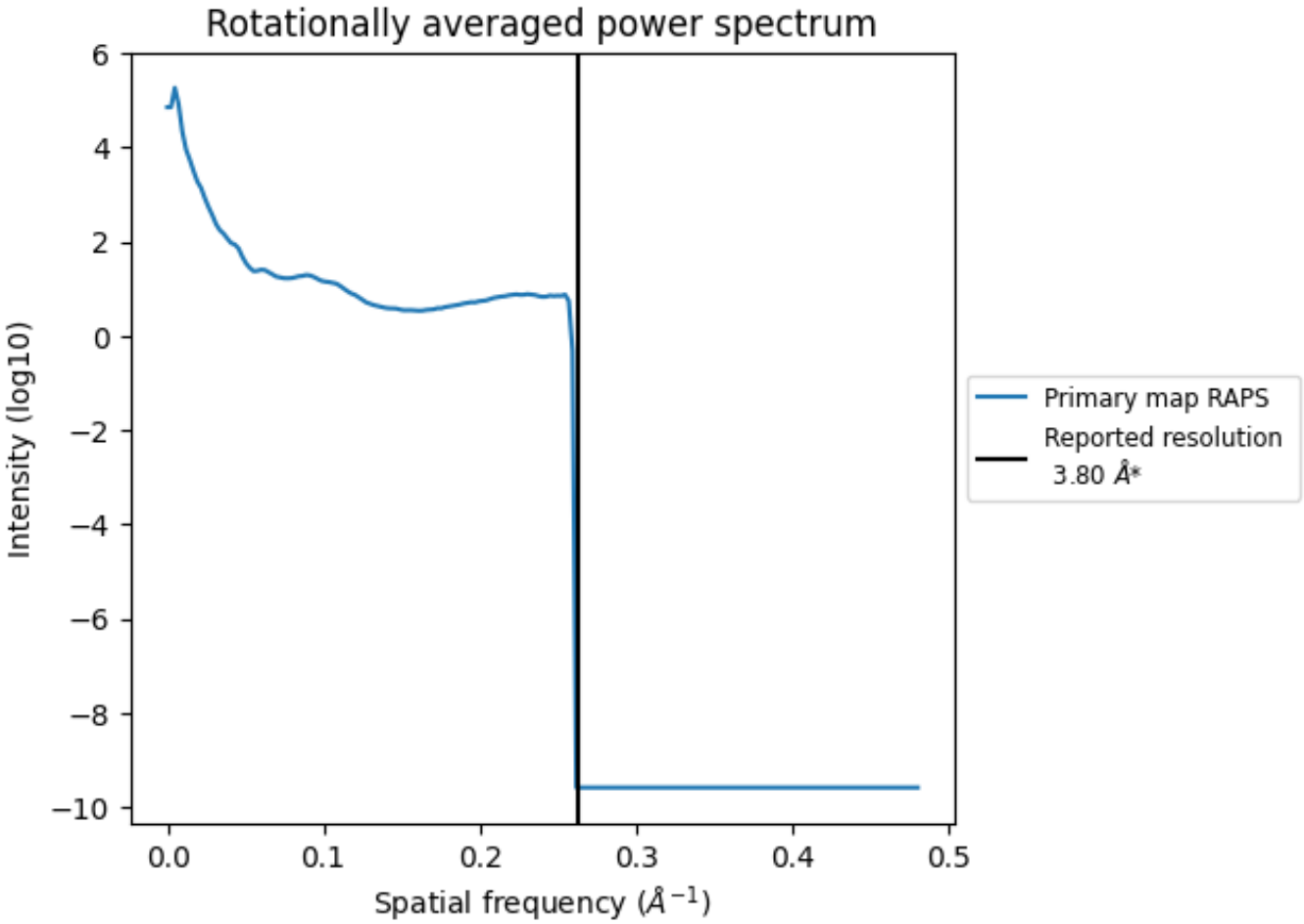
7.2 Volume estimate



The volume at the recommended contour level is 737 nm^3; this corresponds to an approximate mass of 666 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

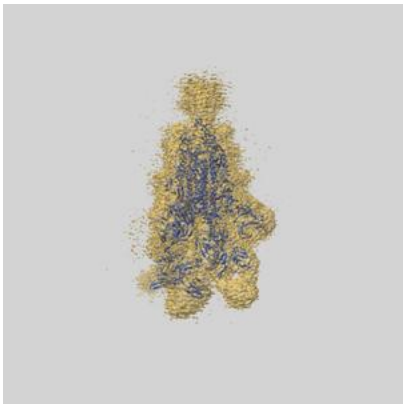
8 Fourier-Shell correlation (i)

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

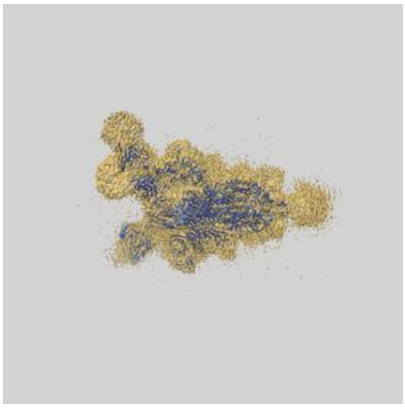
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30482 and PDB model 7CWL. Per-residue inclusion information can be found in section 3 on page 7.

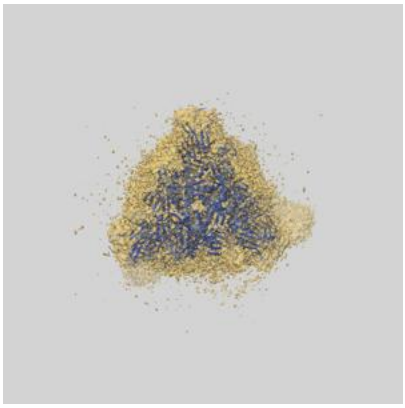
9.1 Map-model overlay



X



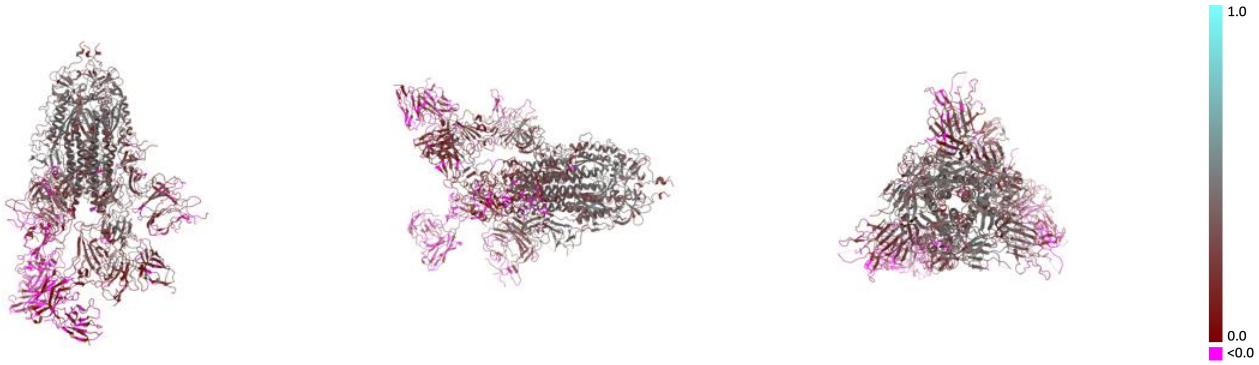
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00502 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.

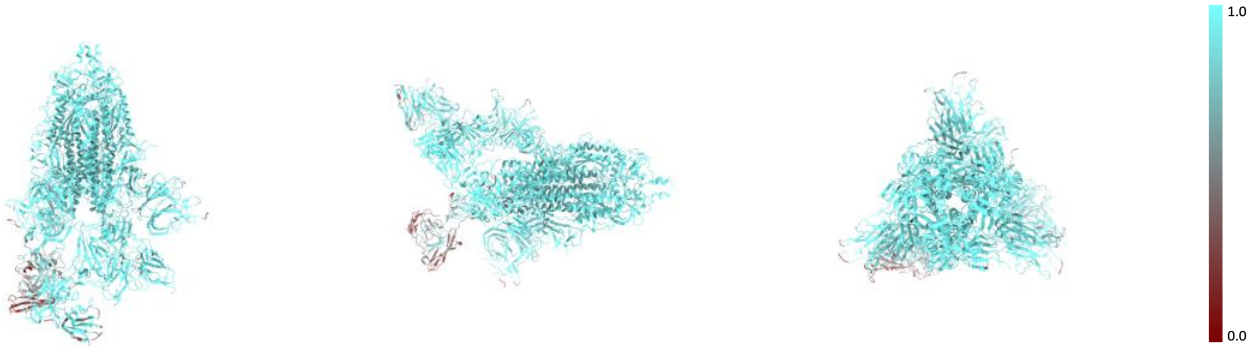
9.2 Q-score mapped to coordinate model (i)



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.

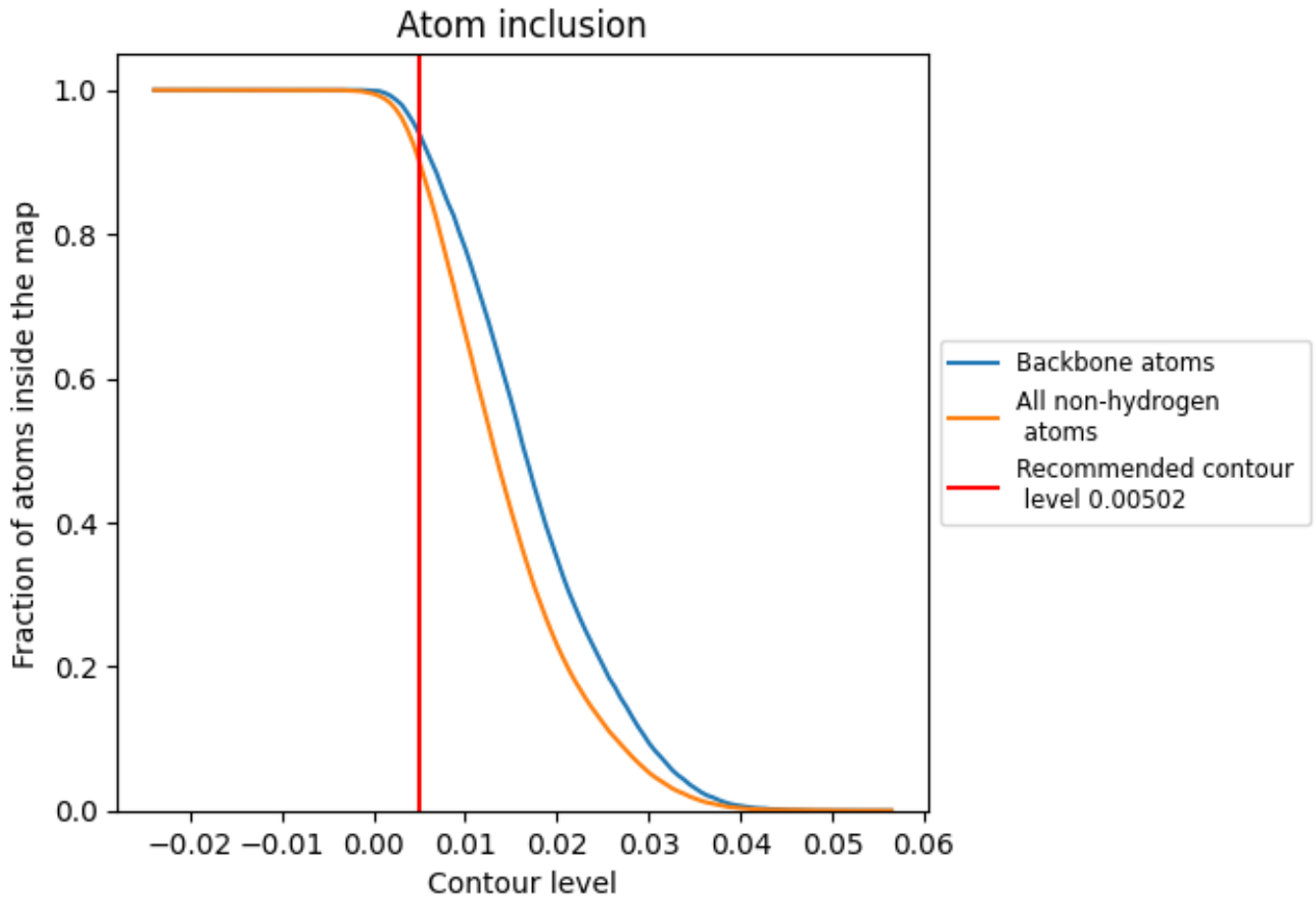
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00502).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00502) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9004	0.2570
A	0.9448	0.3080
B	0.9383	0.2800
C	0.9189	0.2780
G	0.8814	0.0550
H	0.9676	0.2230
I	0.4407	0.0100
J	0.8242	0.0490
K	0.3446	0.0600
L	0.9362	0.2280