



Full wwPDB EM Validation Report ⓘ

Jun 27, 2023 – 02:30 PM JST

PDB ID : 7YC5
EMDB ID : EMD-33734
Title : Cryo-EM structure of SARS-CoV-2 spike in complex with K202.B bispecific antibody
Authors : Yoo, Y.; Cho, H.S.
Deposited on : 2022-06-30
Resolution : 3.10 Å (reported)
Based on initial models : 7D85, 2A9N, 7VXM

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:

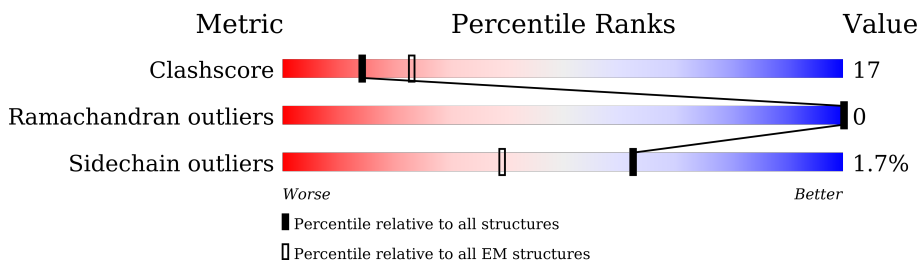
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

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 3.10 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	A	1208	
1	B	1208	
1	C	1208	
2	D	478	
2	E	478	
2	F	478	
3	G	454	
3	H	454	

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Mol	Chain	Length	Quality of chain
3	I	454	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (36%), a green segment (26%), a yellow segment (18%), and a grey segment (56%). The percentages are labeled below the bar.</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 39157 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
			Total	C	N	O	S		
1	A	1037	8094	5170	1343	1545	36	0	0
1	B	1037	8094	5170	1343	1545	36	0	0
1	C	1037	8094	5170	1343	1545	36	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

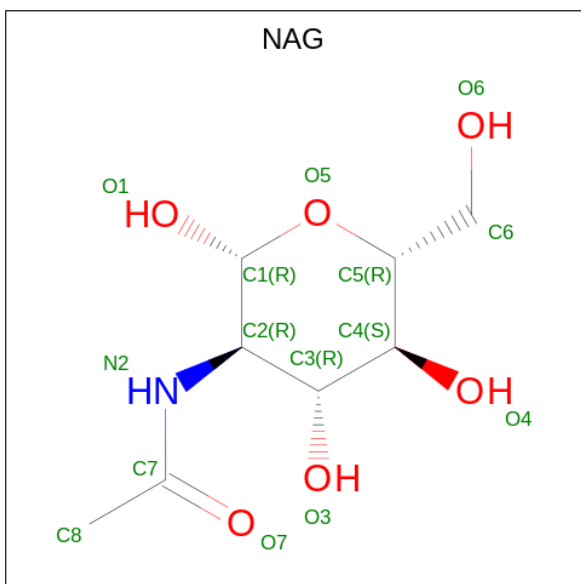
- Molecule 2 is a protein called Light chain from K202.B, bispecific antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		
2	E	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		
2	F	441	Total	C	N	O	S	0	0
			3313	2069	559	675	10		

- Molecule 3 is a protein called Heavy chain from K202.B, bispecific antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		
3	H	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		
3	I	198	Total	C	N	O	S	0	0
			1496	945	252	292	7		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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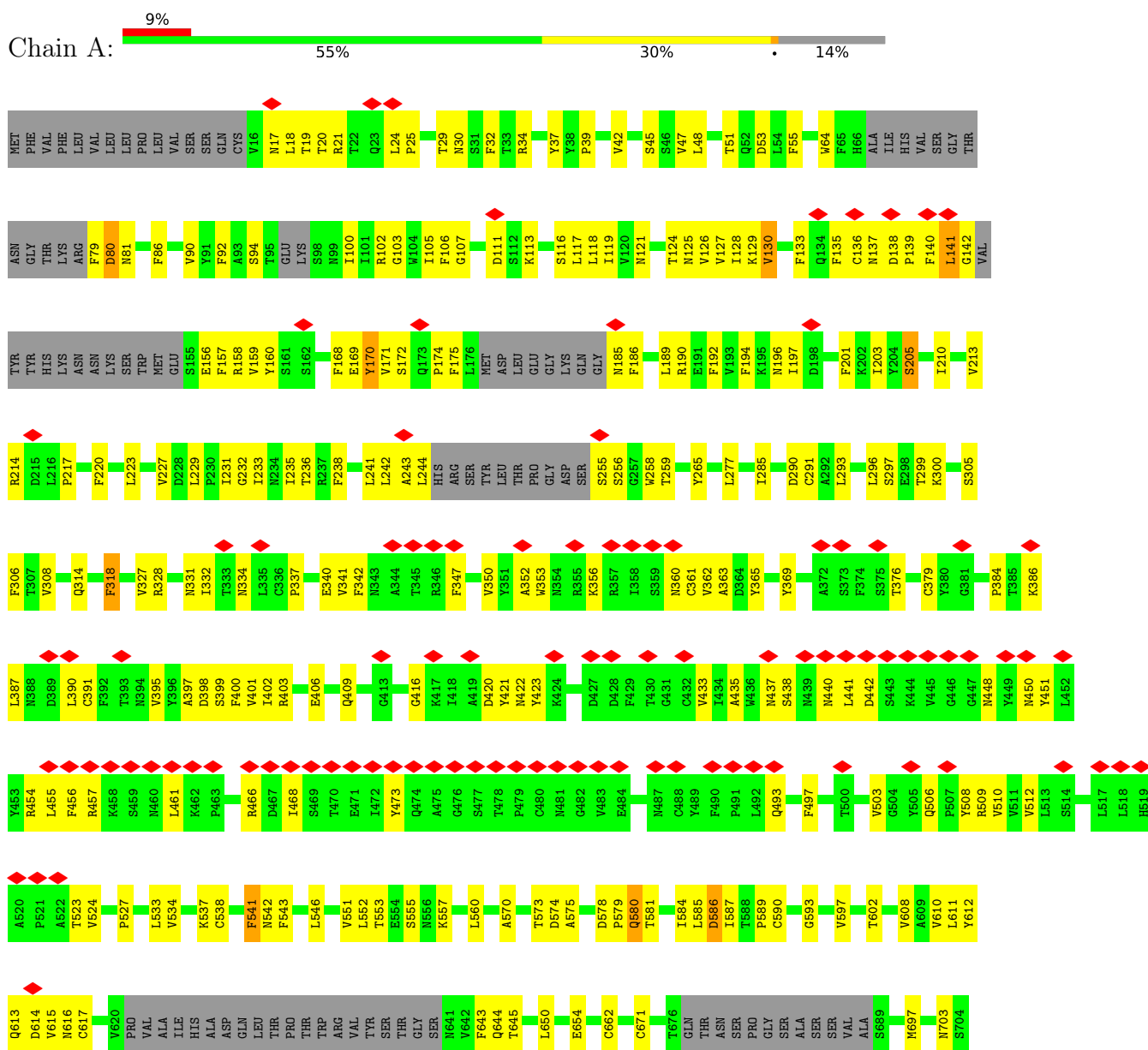
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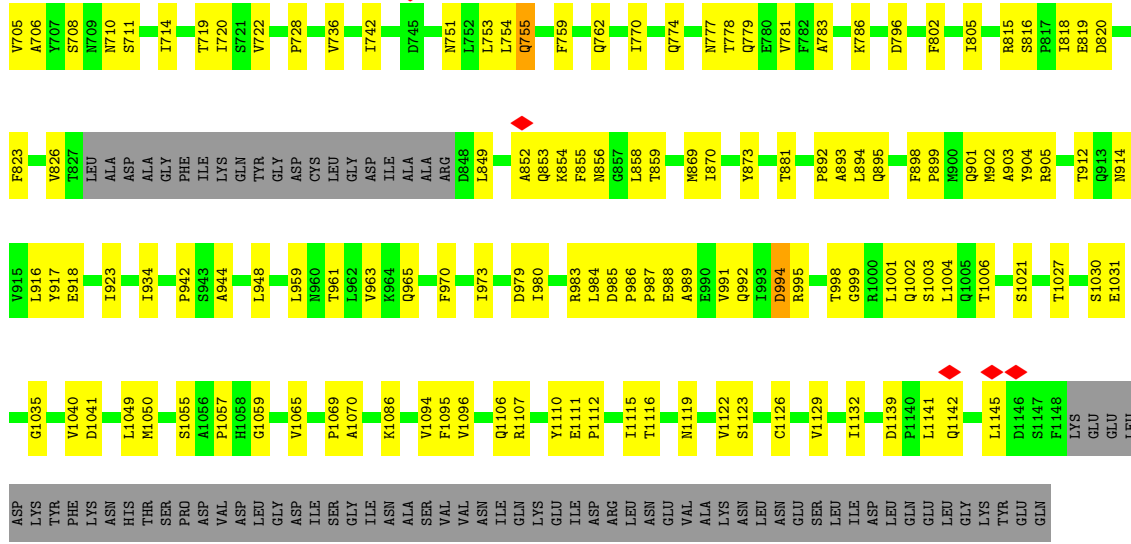
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0
4	C	1	Total 14	8	1	5	0

3 Residue-property plots

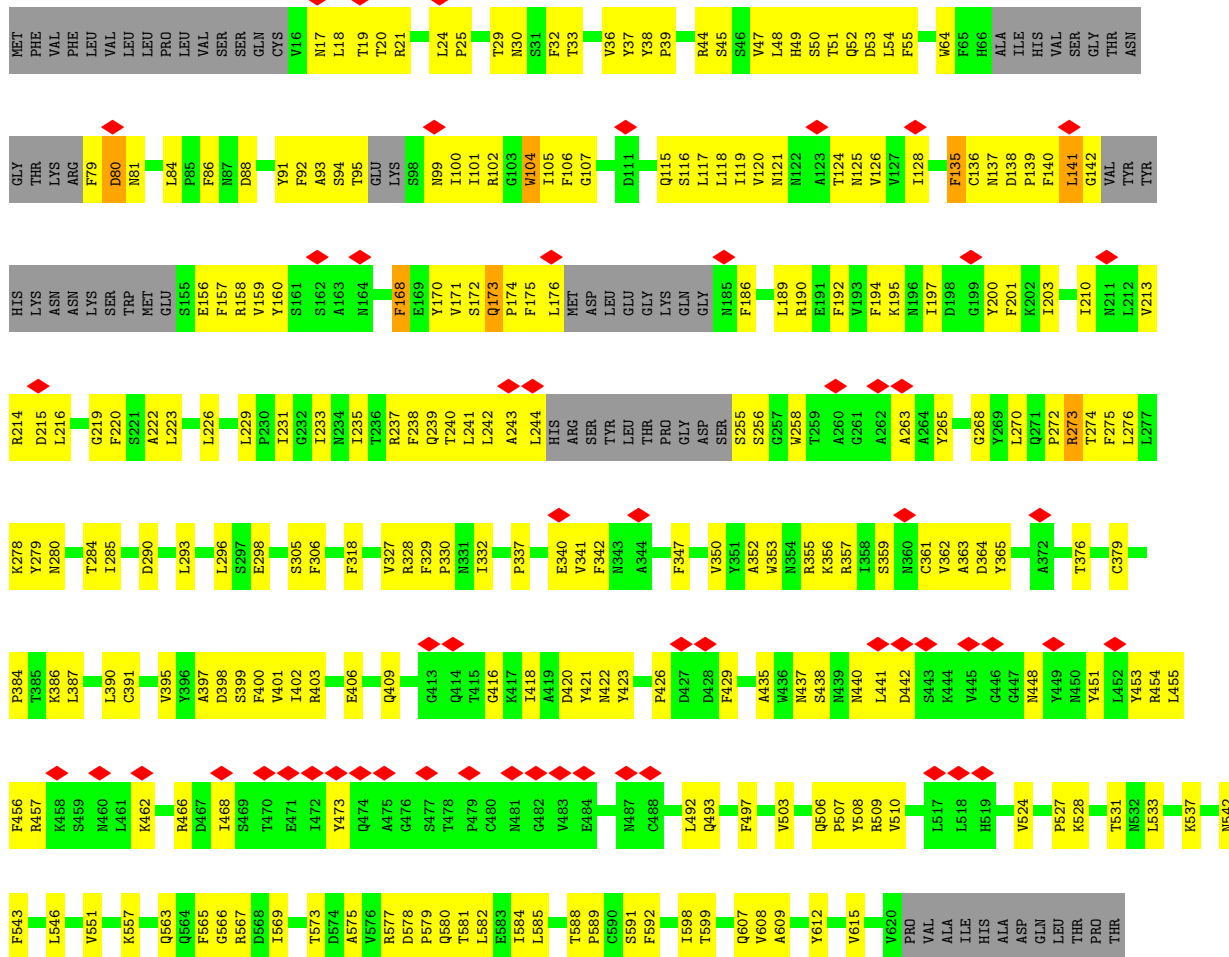
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

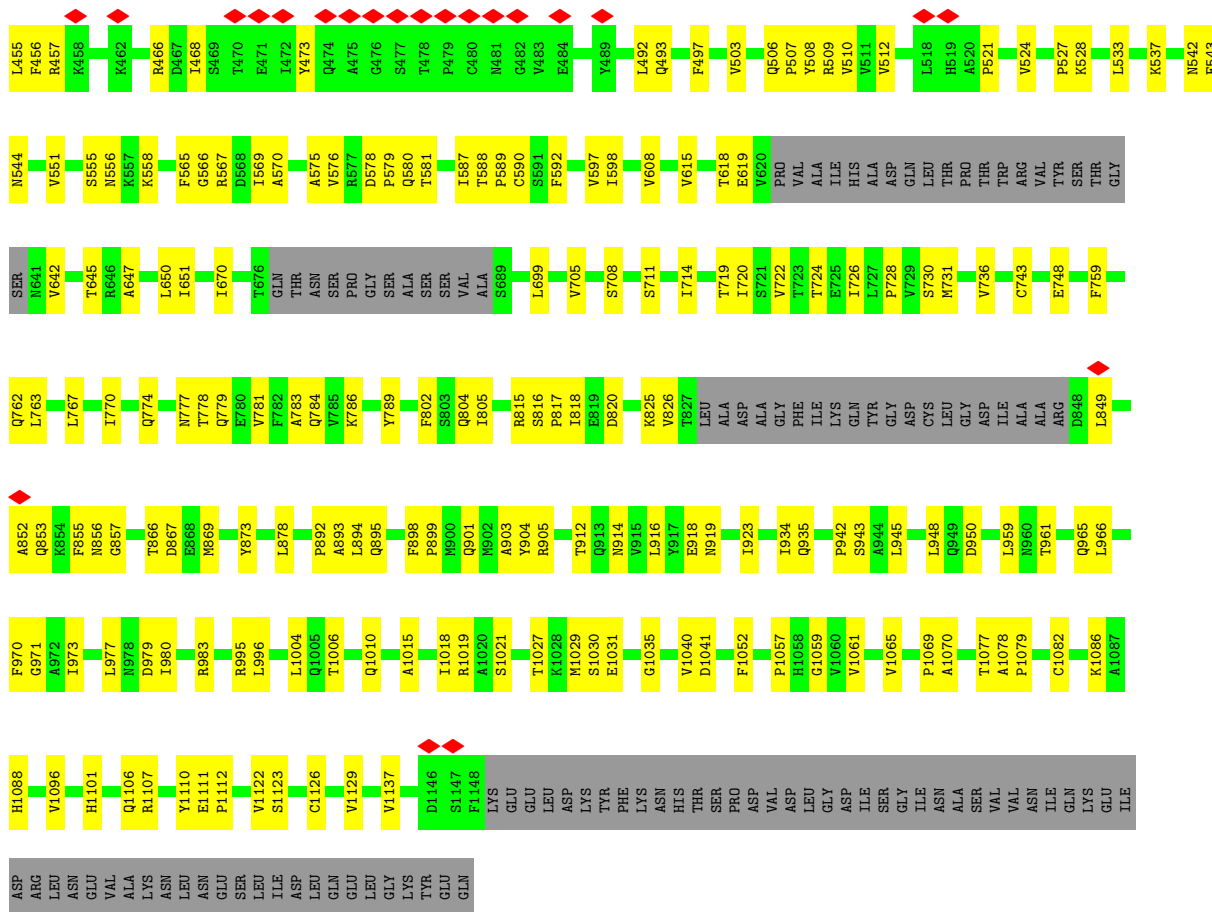
• Molecule 1: Spike glycoprotein



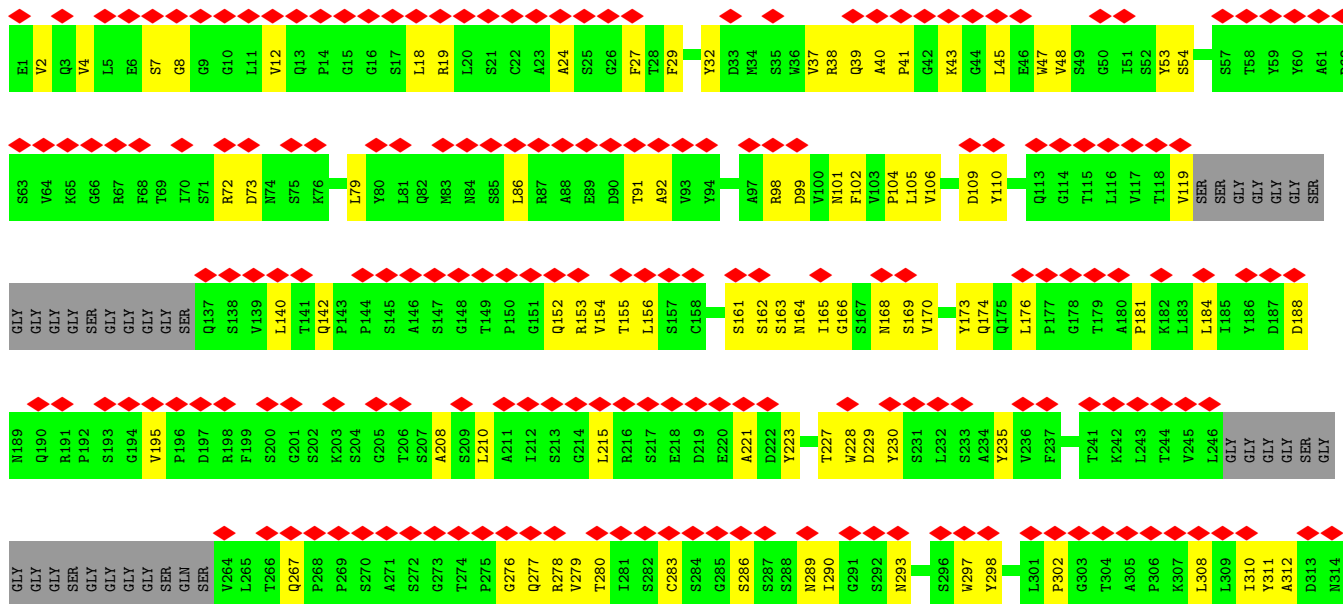


• Molecule 1: Spike glycoprotein



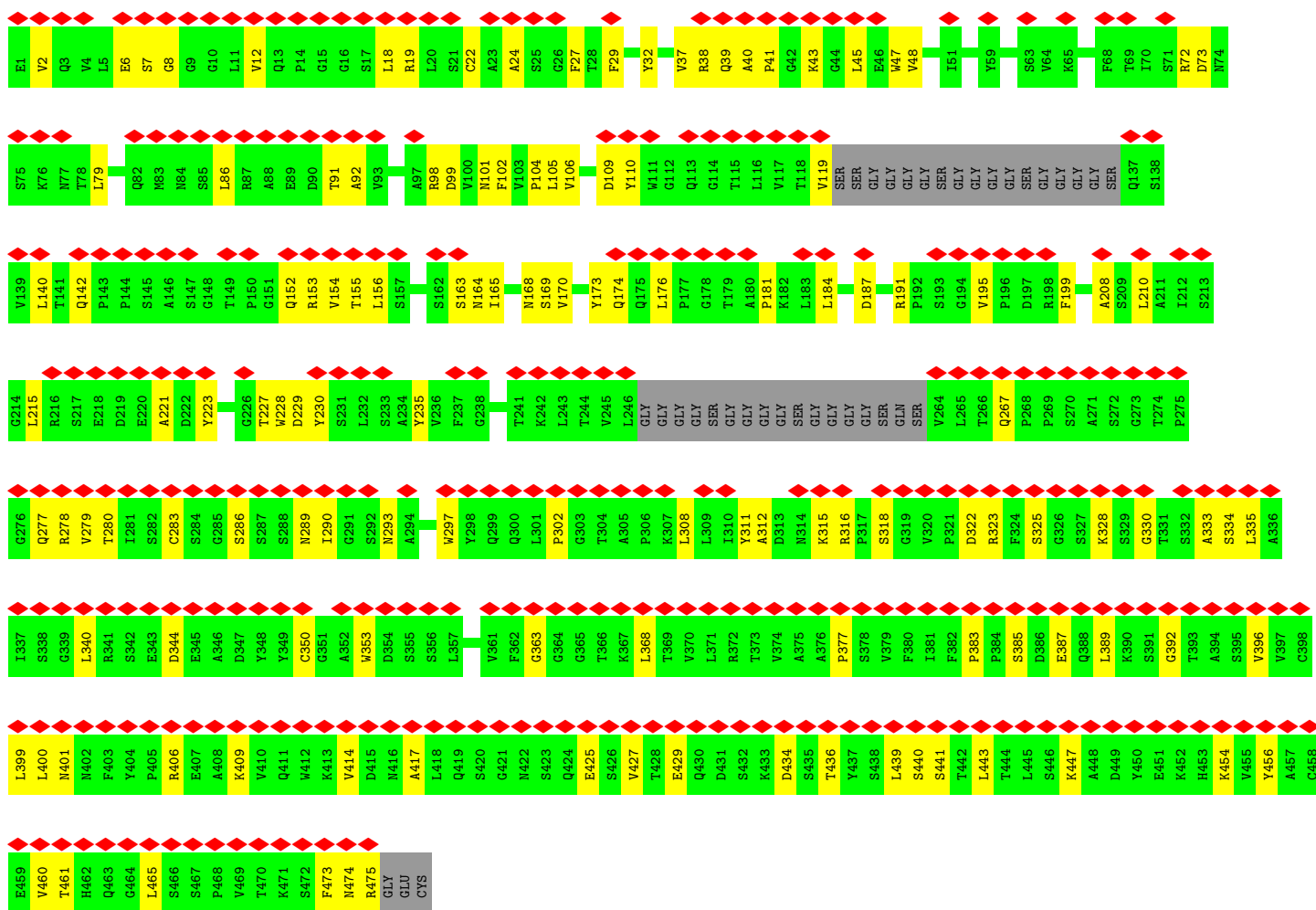


• Molecule 2: Light chain from K202.B, bispecific antibody



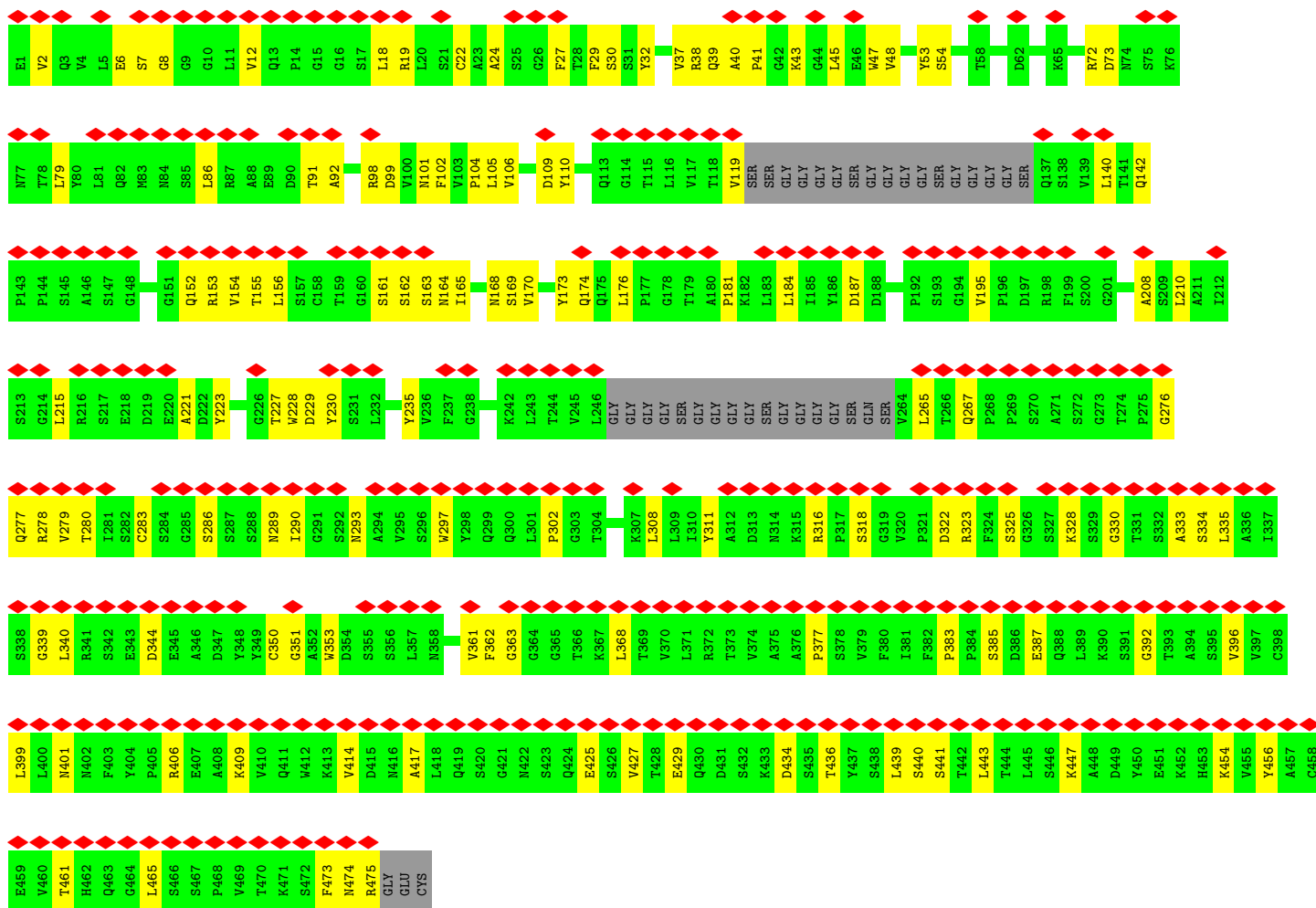


• Molecule 2: Light chain from K202.B, bispecific antibody

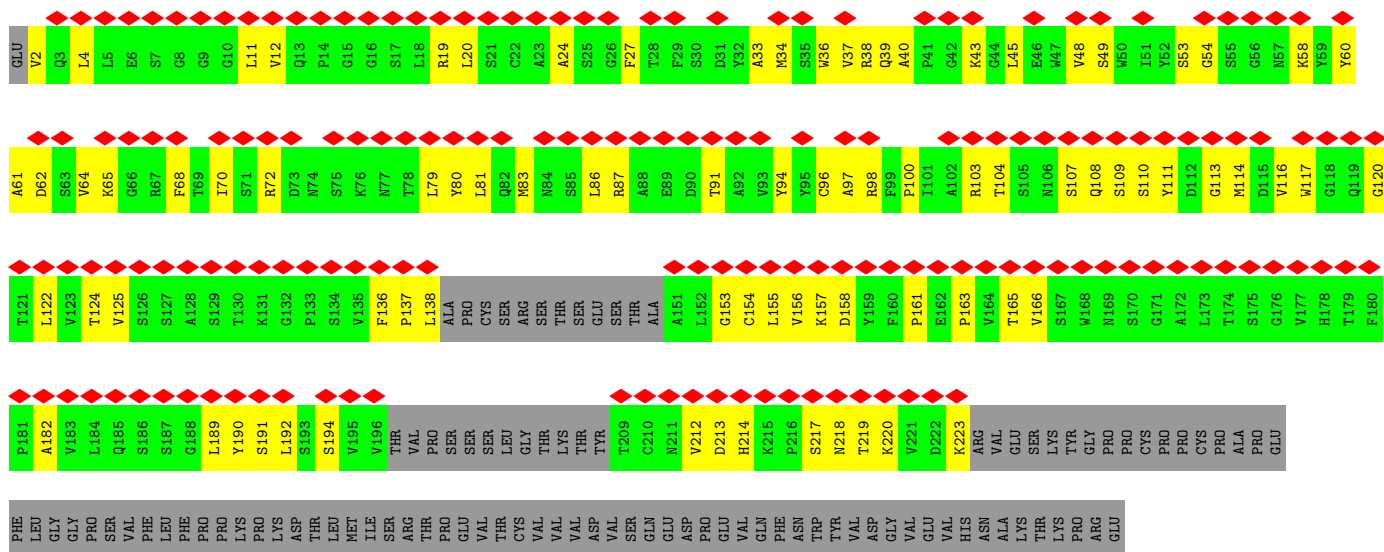


• Molecule 2: Light chain from K202.B, bispecific antibody





● Molecule 3: Heavy chain from K202.B, bispecific antibody



Residue ID	Amino Acid	Validation Metric 1	Validation Metric 2	Validation Metric 3	Validation Metric 4	Validation Metric 5	Validation Metric 6
L184	GLY	ASX	GLU	TRP	GLN	TRP	
Q185	PRO	SER	MET	GLN	GLN	GLY	
S186	VAL	THR	THR	GLY	GLY	GLY	
S187	PHE	ASN	ASN	ASN	VAL	PHE	
G188	LEU	VAL	VAL	GLN	PHE	SER	
L189	PHE	VAL	SER	VAL	SER	CYS	
Y190	PRO	VAL	LEU	LEU	THR	SER	
S191	PRO	THR	THR	CYS	VAL	SER	
L192	LYS	THR	VAL	VAL	VAL	HIS	
S193	LYS	LEU	VAL	VAL	VAL	GLY	
S194	ASP	LEU	LYS	LYS	ALA	LEU	
V195	THR	HIS	GLY	PHE	LEU	ALA	
V196	LEU	ASP	TYR	THR	HIS	HIS	
THR	MET	TRP	TYR	ASP	THR	THR	
VAL	ILE	LEU	PRO	PRO	ASN	HIS	
PRO	SER	ASN	ASP	ASP	THR	TYR	
SER	ARG	GLY	ILE	ILE	THR	THR	
SER	THR	LYS	ALA	VAL	GLN	GLN	
LEU	PRO	TYR	VAL	VAL	LYS	LEU	
GLY	VAL	GLU	GLU	GLU	LEU	SER	
THR	CYS	GLU	TRP	TRP	LEU	LEU	
LYS	VAL	LYS	GLU	GLU	ASP	LEU	
THR	VAL	VAL	SER	ASN	SER	LEU	
TYR	THR	ASN	ASN	GLY	GLY	SER	
T209	VAL	LYS	GLN	PRO	PRO	GLY	
C210	SER	LEU	GLU	ASN	GLU	ASN	
N211	GLN	PRO	ASN	ASN	ASN	ASN	
V212	ASP	SER	TYR	TYR	TYR	TYR	
D213	PRO	SER	LYS	LYS	THR	PRO	
H214	GLU	ILE	THR	THR	THR	PRO	
K215	VAL	GLU	THR	THR	PRO	VAL	
P216	GLN	LYS	THR	THR	PRO	VAL	
S217	PHE	THR	ILE	PRO	VAL	ASP	
N218	ASN	ILE	ILE	VAL	LEU	SER	
T219	TYR	SER	LYS	LEU	ASP	SER	
K220	VAL	ALA	LYS	SER	SER	ASP	
V221	ASP	GLY	GLY	ASP	GLY	GLY	
D222	VAL	GLN	GLN	SER	SER	SER	
K223	VAL	ARG	PHE	LEU	TYR	TYR	
VAL	GLU	ASN	LEU	TYR	SER	SER	
GLU	SER	ALA	GLN	VAL	THR	VAL	
SER	LYS	LYS	VAL	TYR	ARG	ARG	
LYS	TYR	THR	LYS	THR	LEU	LEU	
GLY	PRO	LEU	LEU	THR	THR	THR	
PRO	ARG	PRO	PRO	VAL	ASP	VAL	
CYS	GLU	SER	GLN	ASP	LYS	ASP	
PRO	PRO	ASN	GLN	LYS	SER	LYS	
CYS	PRO	CYS	GLN	ASN	ASN	ASN	
ALA	PRO	ALA	GLN	THR	THR	THR	
PRO	ALA	GLU	TYR	THR	TYR	THR	
PHE	LEU	GLY	TYR	THR	THR	THR	
LEU	GLY	LEU	LEU	THR	THR	THR	
GLY	GLY	LEU	LEU	THR	THR	THR	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.289	Depositor
Minimum map value	-7.992	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.202	Depositor
Recommended contour level	0.55	Depositor
Map size (\AA)	360.52002, 360.52002, 360.52002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.9013001, 0.9013001, 0.9013001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/8280	0.54	3/11274 (0.0%)
1	B	0.38	0/8280	0.53	2/11274 (0.0%)
1	C	0.38	0/8280	0.52	1/11274 (0.0%)
2	D	0.32	0/3386	0.54	0/4606
2	E	0.29	0/3386	0.54	0/4606
2	F	0.30	0/3386	0.54	0/4606
3	G	0.37	0/1531	0.56	0/2080
3	H	0.34	0/1531	0.56	0/2080
3	I	0.38	0/1531	0.57	0/2080
All	All	0.36	0/39591	0.54	6/53880 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	796	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	273	ARG	N-CA-CB	5.57	120.62	110.60
1	A	574	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	80	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	80	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	80	ASP	CB-CG-OD2	5.18	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8094	0	7885	300	0
1	B	8094	0	7883	350	0
1	C	8094	0	7884	322	0
2	D	3313	0	3186	107	0
2	E	3313	0	3186	87	0
2	F	3313	0	3186	99	0
3	G	1496	0	1446	57	0
3	H	1496	0	1446	46	0
3	I	1496	0	1446	53	0
4	A	154	0	143	6	0
4	B	154	0	143	4	0
4	C	140	0	130	2	0
All	All	39157	0	37964	1345	0

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

All (1345) 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:A:855:PHE:HB3	1:C:589:PRO:HG2	1.31	1.12
1:A:369:TYR:CE2	2:D:53:TYR:CE2	2.56	0.94
1:B:18:LEU:HG	1:B:20:THR:H	1.37	0.88
1:A:105:ILE:HG12	1:A:118:LEU:HD13	1.56	0.87
1:C:17:ASN:HA	1:C:138:ASP:HB2	1.57	0.87
1:A:369:TYR:CD2	2:D:53:TYR:HE2	1.93	0.86
1:A:18:LEU:HG	1:A:20:THR:H	1.39	0.86
1:C:105:ILE:HG12	1:C:118:LEU:HD13	1.58	0.85
3:G:136:PHE:HE1	3:G:157:LYS:HB3	1.43	0.84
1:A:369:TYR:CE2	2:D:53:TYR:CD2	2.66	0.84
1:A:369:TYR:CE2	2:D:53:TYR:HE2	1.96	0.84
1:A:854:LYS:HA	1:A:858:LEU:O	1.82	0.79
1:B:591:SER:HB3	1:B:615:VAL:HG12	1.63	0.79
1:A:141:LEU:HD22	1:A:243:ALA:HA	1.66	0.78
3:G:137:PRO:HA	3:G:154:CYS:HA	1.64	0.78
1:B:332:ILE:HG23	1:B:362:VAL:HG21	1.66	0.75
1:A:129:LYS:HB2	1:A:133:PHE:HZ	1.49	0.75
1:B:318:PHE:CZ	1:B:615:VAL:HG11	2.21	0.75
1:B:104:TRP:HA	1:B:240:THR:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.67	0.75
2:D:165:ILE:HD13	2:D:227:THR:HG21	1.68	0.74
3:I:39:GLN:HB2	3:I:45:LEU:HD23	1.69	0.74
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.67	0.74
3:H:97:ALA:HB1	3:H:114:MET:HG2	1.70	0.74
1:B:1139:ASP:HB3	1:B:1142:GLN:HG2	1.70	0.74
1:A:128:ILE:HG21	1:A:229:LEU:HD13	1.70	0.74
1:A:299:THR:HG21	1:A:308:VAL:HG21	1.71	0.73
1:A:855:PHE:CB	1:C:589:PRO:HG2	2.16	0.73
1:C:124:THR:HB	1:C:174:PRO:HG3	1.71	0.73
1:A:139:PRO:HA	1:A:159:VAL:HA	1.71	0.72
3:I:60:TYR:HB2	3:I:65:LYS:HE2	1.71	0.72
1:B:105:ILE:HG12	1:B:118:LEU:HD13	1.71	0.72
1:A:856:ASN:O	1:A:858:LEU:HG	1.89	0.72
1:A:118:LEU:HD11	1:A:241:LEU:HD11	1.71	0.72
2:E:293:ASN:HD22	2:E:353:TRP:HB3	1.54	0.72
3:G:60:TYR:HB2	3:G:65:LYS:HE2	1.72	0.72
1:A:29:THR:HG22	1:A:30:ASN:H	1.53	0.72
1:B:126:VAL:HG22	1:B:174:PRO:HA	1.71	0.72
2:F:293:ASN:HD22	2:F:353:TRP:HB3	1.54	0.72
1:C:139:PRO:HB3	1:C:159:VAL:HG13	1.71	0.71
2:D:293:ASN:HD22	2:D:353:TRP:HB3	1.54	0.71
1:B:442:ASP:HB3	1:B:451:TYR:HE2	1.56	0.71
3:I:33:ALA:HB2	3:I:101:ILE:HD13	1.73	0.71
1:B:121:ASN:HB2	1:B:126:VAL:HG12	1.71	0.70
1:C:442:ASP:HB3	1:C:451:TYR:HE2	1.56	0.70
1:C:576:VAL:HG22	1:C:587:ILE:HD11	1.73	0.70
3:H:60:TYR:HB2	3:H:65:LYS:HE2	1.72	0.70
1:A:296:LEU:HB2	1:A:608:VAL:HG21	1.72	0.70
1:B:29:THR:HG22	1:B:30:ASN:H	1.57	0.70
3:G:136:PHE:CE1	3:G:157:LYS:HB3	2.27	0.70
1:A:442:ASP:HB3	1:A:451:TYR:HE2	1.56	0.70
2:D:168:ASN:HD22	2:D:228:TRP:HB3	1.55	0.69
1:C:18:LEU:HB3	1:C:21:ARG:HD3	1.73	0.69
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.74	0.69
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.73	0.69
1:B:403:ARG:HB3	1:B:406:GLU:HG3	1.74	0.69
1:C:107:GLY:N	1:C:235:ILE:HD11	2.08	0.69
2:D:279:VAL:HG12	2:D:340:LEU:HD11	1.75	0.69
1:B:102:ARG:HH21	1:B:243:ALA:HB2	1.58	0.68
2:F:279:VAL:HG12	2:F:340:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLY:N	1:B:235:ILE:HD11	2.09	0.68
1:C:190:ARG:HB3	1:C:192:PHE:HE1	1.58	0.68
2:E:279:VAL:HG12	2:E:340:LEU:HD11	1.75	0.68
1:A:105:ILE:HD11	1:A:241:LEU:HD21	1.73	0.68
1:A:403:ARG:HB3	1:A:406:GLU:HG3	1.74	0.68
1:A:1069:PRO:HG2	1:B:892:PRO:HD2	1.75	0.68
1:C:569:ILE:H	1:C:569:ILE:HD12	1.58	0.68
1:C:786:LYS:HE3	1:C:786:LYS:HA	1.73	0.68
1:A:107:GLY:N	1:A:235:ILE:HD11	2.09	0.68
1:C:119:ILE:HA	1:C:127:VAL:O	1.94	0.68
3:I:100:PRO:HD2	3:I:113:GLY:O	1.94	0.67
1:C:403:ARG:HB3	1:C:406:GLU:HG3	1.74	0.67
3:I:97:ALA:HB1	3:I:114:MET:HG2	1.76	0.67
1:C:106:PHE:CD1	1:C:238:PHE:HB3	2.29	0.67
3:G:213:ASP:HB3	3:G:220:LYS:HE3	1.77	0.67
3:I:19:ARG:HE	3:I:80:TYR:HB3	1.60	0.67
3:G:122:LEU:HD13	3:G:163:PRO:HD3	1.76	0.67
1:C:29:THR:HG22	1:C:30:ASN:H	1.59	0.67
3:H:122:LEU:HD13	3:H:163:PRO:HD3	1.76	0.67
3:G:19:ARG:HE	3:G:80:TYR:HB3	1.59	0.67
3:H:213:ASP:HB3	3:H:220:LYS:HE3	1.77	0.66
1:A:121:ASN:HB2	1:A:126:VAL:HG12	1.76	0.66
2:D:308:LEU:HD21	2:D:311:TYR:HB3	1.77	0.66
1:A:92:PHE:HE2	1:A:94:SER:HB3	1.60	0.66
1:C:124:THR:HA	1:C:174:PRO:HB3	1.77	0.66
3:I:122:LEU:HD13	3:I:163:PRO:HD3	1.76	0.66
1:C:92:PHE:HE2	1:C:94:SER:HB3	1.61	0.66
1:B:48:LEU:CD1	1:B:305:SER:HA	2.26	0.66
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.59	0.66
3:I:178:HIS:HD2	3:I:195:VAL:HG23	1.61	0.66
1:A:332:ILE:HG21	1:A:362:VAL:HG21	1.78	0.66
1:B:825:LYS:HD2	1:B:942:PRO:HA	1.78	0.66
1:B:853:GLN:HG2	1:B:959:LEU:HB3	1.78	0.66
1:A:106:PHE:HB3	1:A:235:ILE:HG12	1.78	0.66
1:B:92:PHE:HE2	1:B:94:SER:HB3	1.60	0.66
1:B:328:ARG:NH1	1:B:533:LEU:HB2	2.11	0.66
1:B:543:PHE:HD2	1:B:579:PRO:HD3	1.60	0.66
3:I:213:ASP:HB3	3:I:220:LYS:HE3	1.77	0.65
2:E:165:ILE:HD13	2:E:227:THR:HG21	1.79	0.65
1:C:130:VAL:HG12	1:C:168:PHE:HB3	1.77	0.65
3:H:19:ARG:HE	3:H:80:TYR:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:97:ALA:HB1	3:G:114:MET:HG2	1.78	0.65
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.77	0.65
1:B:135:PHE:HA	1:B:160:TYR:HA	1.78	0.65
1:A:892:PRO:HD2	1:C:1069:PRO:HG2	1.79	0.64
1:C:558:LYS:HE3	1:C:558:LYS:HA	1.78	0.64
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.79	0.64
1:A:751:ASN:HA	1:A:754:LEU:HG	1.78	0.64
1:B:816:SER:HB2	1:B:817:PRO:HD2	1.79	0.64
1:B:1101:HIS:CE1	4:B:1309:NAG:H3	2.33	0.64
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.62	0.64
1:B:786:LYS:HE3	1:B:786:LYS:HA	1.77	0.64
2:F:165:ILE:HD13	2:F:227:THR:HG21	1.79	0.64
1:B:296:LEU:HB2	1:B:608:VAL:HG11	1.80	0.64
1:A:815:ARG:HB2	1:A:820:ASP:OD1	1.98	0.64
1:A:503:VAL:HA	1:A:506:GLN:HG3	1.80	0.64
1:A:369:TYR:CE2	2:D:53:TYR:HD2	2.16	0.64
1:A:870:ILE:HG22	1:A:1055:SER:OG	1.98	0.63
1:B:126:VAL:HG11	1:B:175:PHE:H	1.63	0.63
1:C:140:PHE:HB3	1:C:158:ARG:HB3	1.80	0.63
1:C:503:VAL:HA	1:C:506:GLN:HG3	1.80	0.63
1:A:963:VAL:HG11	1:C:570:ALA:HB1	1.80	0.63
1:B:503:VAL:HA	1:B:506:GLN:HG3	1.80	0.63
1:C:543:PHE:HD2	1:C:579:PRO:HD3	1.63	0.63
1:A:706:ALA:HB2	4:A:1308:NAG:H5	1.81	0.63
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.80	0.63
1:A:662:CYS:HB2	1:A:697:MET:HG2	1.81	0.63
1:C:135:PHE:HE1	1:C:139:PRO:HG3	1.63	0.63
1:B:105:ILE:CG1	1:B:118:LEU:HD13	2.29	0.63
3:I:52:TYR:CD1	3:I:101:ILE:HD11	2.34	0.63
1:C:551:VAL:HG12	1:C:588:THR:O	1.99	0.62
1:C:973:ILE:HD11	1:C:980:ILE:HG23	1.79	0.62
1:B:100:ILE:HD12	1:B:100:ILE:H	1.63	0.62
1:C:64:TRP:CH2	1:C:214:ARG:HB3	2.34	0.62
2:D:286:SER:H	2:D:289:ASN:HB2	1.64	0.62
2:F:173:TYR:HH	2:F:235:TYR:HH	1.44	0.62
1:A:369:TYR:CD2	2:D:53:TYR:CE2	2.81	0.62
1:B:102:ARG:HB2	1:B:241:LEU:HB3	1.81	0.62
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.63	0.62
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.82	0.62
1:A:914:ASN:O	1:A:918:GLU:HG2	2.00	0.62
1:B:107:GLY:O	1:B:237:ARG:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:HB2	1:C:126:VAL:HG12	1.82	0.62
1:A:543:PHE:HD2	1:A:579:PRO:HD3	1.64	0.62
1:C:1101:HIS:CE1	4:C:1408:NAG:H3	2.35	0.62
1:B:36:VAL:HG11	1:B:220:PHE:HZ	1.65	0.61
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.81	0.61
2:E:286:SER:H	2:E:289:ASN:HB2	1.65	0.61
2:E:392:GLY:HA2	2:E:447:LYS:HD3	1.82	0.61
2:F:29:PHE:HZ	2:F:79:LEU:HB2	1.66	0.61
3:G:100:PRO:HD2	3:G:113:GLY:O	1.99	0.61
1:C:91:TYR:N	1:C:268:GLY:O	2.32	0.61
2:E:29:PHE:HZ	2:E:79:LEU:HB2	1.65	0.61
2:F:289:ASN:ND2	2:F:361:VAL:HG21	2.15	0.61
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.18	0.61
1:C:338:PHE:HZ	1:C:363:ALA:HB1	1.65	0.61
1:A:361:CYS:SG	1:A:362:VAL:N	2.73	0.61
1:B:64:TRP:CH2	1:B:214:ARG:HB3	2.36	0.61
2:F:392:GLY:HA2	2:F:447:LYS:HD3	1.82	0.61
1:B:589:PRO:HG2	1:C:855:PHE:HA	1.82	0.61
1:A:898:PHE:N	1:A:899:PRO:HD2	2.16	0.61
1:C:119:ILE:HG13	1:C:128:ILE:HA	1.81	0.61
1:B:327:VAL:HA	1:B:542:ASN:HB3	1.83	0.61
1:A:786:LYS:HE3	1:A:786:LYS:HA	1.81	0.60
2:D:29:PHE:HZ	2:D:79:LEU:HB2	1.66	0.60
1:A:327:VAL:HA	1:A:542:ASN:HB3	1.83	0.60
2:D:392:GLY:HA2	2:D:447:LYS:HD3	1.82	0.60
1:B:945:LEU:HD23	1:B:948:LEU:HD12	1.82	0.60
1:B:231:ILE:HG22	1:B:233:ILE:HG12	1.83	0.60
2:F:286:SER:H	2:F:289:ASN:HB2	1.65	0.60
1:B:1069:PRO:HG2	1:C:892:PRO:HD2	1.83	0.60
1:B:115:GLN:HE21	1:B:233:ILE:HD12	1.67	0.60
1:B:599:THR:HB	1:B:608:VAL:HG12	1.84	0.60
1:C:816:SER:HB2	1:C:817:PRO:HD2	1.84	0.60
1:A:170:TYR:CD1	1:A:172:SER:HB2	2.37	0.59
1:A:299:THR:CG2	1:A:308:VAL:HG21	2.32	0.59
3:I:104:THR:OG1	3:I:107:SER:HB2	2.02	0.59
1:B:91:TYR:N	1:B:268:GLY:O	2.35	0.59
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.83	0.59
2:F:29:PHE:O	2:F:72:ARG:NH2	2.35	0.59
1:B:357:ARG:HG3	4:C:1402:NAG:H81	1.85	0.59
2:E:29:PHE:O	2:E:72:ARG:NH2	2.36	0.59
2:F:45:LEU:HD21	2:F:181:PRO:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.83	0.59
1:A:708:SER:HB3	1:A:711:SER:HB3	1.84	0.59
1:A:905:ARG:HD3	1:A:1050:MET:HB3	1.82	0.59
1:B:92:PHE:CE1	1:B:265:TYR:CD1	2.91	0.59
1:C:130:VAL:HG11	1:C:231:ILE:HG23	1.84	0.59
2:D:45:LEU:HD21	2:D:181:PRO:HG2	1.84	0.59
1:C:24:LEU:HD12	1:C:25:PRO:HD2	1.85	0.59
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.37	0.59
2:D:29:PHE:O	2:D:72:ARG:NH2	2.36	0.59
2:D:174:GLN:HB2	2:D:184:LEU:HD11	1.85	0.59
2:F:174:GLN:HB2	2:F:184:LEU:HD11	1.85	0.59
3:I:166:VAL:HG23	3:I:212:VAL:HG22	1.85	0.59
1:A:231:ILE:HG13	1:A:233:ILE:H	1.67	0.58
1:C:168:PHE:HE1	1:C:170:TYR:HB2	1.66	0.58
1:C:290:ASP:HB3	1:C:293:LEU:HD22	1.85	0.58
2:E:174:GLN:HB2	2:E:184:LEU:HD11	1.85	0.58
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.68	0.58
1:B:577:ARG:HD3	1:B:582:LEU:HD12	1.85	0.58
1:C:369:TYR:OH	2:F:54:SER:HA	2.03	0.58
1:C:708:SER:HB3	1:C:711:SER:HB3	1.84	0.58
3:G:104:THR:OG1	3:G:107:SER:HB2	2.03	0.58
1:A:308:VAL:H	1:A:602:THR:HG1	1.50	0.58
1:C:21:ARG:NH1	1:C:21:ARG:HA	2.18	0.58
1:C:357:ARG:HH21	1:C:359:SER:H	1.52	0.58
1:C:318:PHE:CZ	1:C:615:VAL:HG21	2.39	0.58
3:H:104:THR:OG1	3:H:107:SER:HB2	2.03	0.58
1:B:106:PHE:O	1:B:116:SER:HB2	2.04	0.58
1:B:823:PHE:HD1	1:B:1057:PRO:HG3	1.67	0.58
2:E:45:LEU:HD21	2:E:181:PRO:HG2	1.84	0.58
1:C:369:TYR:CE1	2:F:54:SER:HA	2.38	0.58
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.21	0.58
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.37	0.58
1:B:115:GLN:HE21	1:B:233:ILE:CD1	2.16	0.58
1:C:106:PHE:HA	1:C:238:PHE:HA	1.84	0.58
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.68	0.58
1:C:375:SER:O	2:F:102:PHE:HB3	2.03	0.58
3:I:223:LYS:HA	3:I:223:LYS:HE3	1.86	0.58
1:A:140:PHE:HB3	1:A:158:ARG:HB3	1.86	0.57
1:C:442:ASP:HB3	1:C:451:TYR:CE2	2.39	0.57
3:G:166:VAL:HG23	3:G:212:VAL:HG22	1.85	0.57
1:A:873:TYR:CE1	1:C:699:LEU:HB3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HA	1:B:238:PHE:HA	1.85	0.57
1:B:708:SER:HB3	1:B:711:SER:HB3	1.86	0.57
1:B:731:MET:HG2	1:B:955:ASN:HD21	1.69	0.57
1:C:92:PHE:CE2	1:C:94:SER:HB3	2.39	0.57
3:G:34:MET:HB3	3:G:79:LEU:HD22	1.85	0.57
3:H:68:PHE:CE1	3:H:83:MET:HB3	2.40	0.57
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.69	0.57
3:H:166:VAL:HG23	3:H:212:VAL:HG22	1.85	0.57
1:A:24:LEU:HD12	1:A:25:PRO:HD2	1.86	0.57
1:A:917:TYR:HB3	1:C:1129:VAL:HG23	1.86	0.57
1:C:106:PHE:HB3	1:C:235:ILE:HG12	1.86	0.57
3:H:223:LYS:HE3	3:H:223:LYS:HA	1.86	0.57
1:A:92:PHE:CE2	1:A:94:SER:HB3	2.39	0.57
1:C:212:LEU:HD12	1:C:213:VAL:H	1.69	0.57
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.22	0.57
2:F:377:PRO:HD2	2:F:465:LEU:HG	1.86	0.57
3:G:12:VAL:HG11	3:G:86:LEU:HD12	1.86	0.57
1:A:332:ILE:CG2	1:A:362:VAL:HG21	2.33	0.57
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.53	0.57
1:C:50:SER:HA	1:C:275:PHE:O	2.04	0.57
1:B:106:PHE:CD2	1:B:238:PHE:HB3	2.40	0.57
1:C:369:TYR:OH	2:F:53:TYR:O	2.23	0.57
1:C:898:PHE:N	1:C:899:PRO:HD2	2.19	0.57
3:H:12:VAL:HG11	3:H:86:LEU:HD12	1.86	0.57
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.85	0.57
3:I:34:MET:HB3	3:I:79:LEU:HD22	1.85	0.57
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.87	0.57
1:C:338:PHE:CZ	1:C:363:ALA:HB1	2.40	0.57
3:H:100:PRO:HD2	3:H:113:GLY:O	2.05	0.57
3:I:12:VAL:HG11	3:I:86:LEU:HD12	1.86	0.57
3:I:68:PHE:CE1	3:I:83:MET:HB3	2.40	0.57
1:B:195:LYS:HG2	1:B:197:ILE:HG12	1.87	0.57
1:C:135:PHE:CE1	1:C:139:PRO:HG3	2.40	0.57
2:D:173:TYR:OH	2:D:235:TYR:OH	2.22	0.57
2:D:434:ASP:HB3	2:D:436:THR:HG22	1.87	0.57
2:F:434:ASP:HB3	2:F:436:THR:HG22	1.87	0.57
1:C:320:VAL:HG13	1:C:590:CYS:HB3	1.86	0.56
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.35	0.56
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.86	0.56
1:C:892:PRO:HG2	1:C:894:LEU:HD21	1.85	0.56
2:E:156:LEU:HD23	2:E:156:LEU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:377:PRO:HD2	2:E:465:LEU:HG	1.86	0.56
2:F:39:GLN:HG3	2:F:45:LEU:HD12	1.88	0.56
2:F:351:GLY:HA2	2:F:362:PHE:HA	1.87	0.56
1:A:914:ASN:ND2	1:A:1111:GLU:OE2	2.38	0.56
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.45	0.56
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.88	0.56
2:E:39:GLN:HG3	2:E:45:LEU:HD12	1.88	0.56
1:A:895:GLN:HB3	1:C:705:VAL:HG12	1.86	0.56
1:C:86:PHE:N	1:C:236:THR:O	2.39	0.56
2:D:39:GLN:HG3	2:D:45:LEU:HD12	1.88	0.56
2:D:156:LEU:H	2:D:156:LEU:HD23	1.71	0.56
2:E:350:CYS:O	2:E:363:GLY:N	2.39	0.56
2:F:184:LEU:HA	2:F:195:VAL:HG21	1.88	0.56
3:G:223:LYS:HE3	3:G:223:LYS:HA	1.86	0.56
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.86	0.56
1:B:92:PHE:CE2	1:B:94:SER:HB3	2.39	0.56
1:C:645:THR:HG23	1:C:670:ILE:HG13	1.87	0.56
2:D:377:PRO:HD2	2:D:465:LEU:HG	1.86	0.56
1:A:194:PHE:HD1	1:A:203:ILE:HG12	1.71	0.56
1:A:369:TYR:OH	2:D:54:SER:HA	2.05	0.56
1:B:332:ILE:HG23	1:B:362:VAL:CG2	2.36	0.56
1:C:352:ALA:HB2	1:C:468:ILE:HG13	1.88	0.56
2:D:169:SER:O	2:D:227:THR:HG22	2.06	0.56
2:E:184:LEU:HA	2:E:195:VAL:HG21	1.88	0.56
3:G:68:PHE:CE1	3:G:83:MET:HB3	2.40	0.56
1:C:212:LEU:HD12	1:C:213:VAL:N	2.21	0.56
1:C:566:GLY:N	1:C:575:ALA:O	2.38	0.56
1:C:914:ASN:O	1:C:918:GLU:HG2	2.06	0.56
1:C:18:LEU:HG	1:C:20:THR:H	1.70	0.56
1:C:912:THR:OG1	1:C:1106:GLN:NE2	2.39	0.56
2:D:184:LEU:HA	2:D:195:VAL:HG21	1.88	0.56
1:A:129:LYS:HB2	1:A:133:PHE:CZ	2.38	0.55
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.41	0.55
1:B:645:THR:HG23	1:B:670:ILE:HG13	1.88	0.55
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.39	0.55
1:A:342:PHE:HB2	4:A:1301:NAG:H82	1.86	0.55
1:B:48:LEU:HD13	1:B:305:SER:HA	1.87	0.55
1:C:100:ILE:HD12	1:C:100:ILE:H	1.71	0.55
1:C:141:LEU:HD22	1:C:243:ALA:HA	1.87	0.55
2:D:98:ARG:NH1	2:D:109:ASP:OD2	2.39	0.55
2:F:350:CYS:O	2:F:363:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:399:LEU:HD21	2:F:401:ASN:HB2	1.88	0.55
1:B:352:ALA:HB2	1:B:468:ILE:HG13	1.88	0.55
2:E:91:THR:HB	2:E:119:VAL:H	1.71	0.55
2:E:399:LEU:HD21	2:E:401:ASN:HB2	1.88	0.55
2:E:434:ASP:HB3	2:E:436:THR:HG22	1.87	0.55
2:F:91:THR:HB	2:F:119:VAL:H	1.71	0.55
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.88	0.55
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.87	0.55
1:B:1110:TYR:CZ	1:B:1112:PRO:HG3	2.40	0.55
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.39	0.55
2:D:40:ALA:HB3	2:D:43:LYS:HB3	1.88	0.55
2:D:91:THR:HB	2:D:119:VAL:H	1.71	0.55
2:D:399:LEU:HD21	2:D:401:ASN:HB2	1.88	0.55
1:A:352:ALA:HB2	1:A:468:ILE:HG13	1.88	0.55
1:A:759:PHE:CE2	1:A:1001:LEU:HD21	2.42	0.55
1:B:914:ASN:O	1:B:918:GLU:HG3	2.07	0.55
2:F:156:LEU:H	2:F:156:LEU:HD23	1.71	0.55
1:A:360:ASN:H	1:A:523:THR:HG22	1.72	0.55
1:B:780:GLU:O	1:B:784:GLN:NE2	2.39	0.55
2:D:350:CYS:O	2:D:363:GLY:N	2.39	0.55
2:D:41:PRO:HD3	2:D:92:ALA:HA	1.89	0.55
1:A:142:GLY:HA2	1:A:244:LEU:HD21	1.89	0.55
1:A:124:THR:HA	1:A:174:PRO:HB3	1.88	0.55
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.89	0.55
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.89	0.55
1:B:977:LEU:HD12	1:B:977:LEU:H	1.72	0.55
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.89	0.55
1:A:442:ASP:HB3	1:A:451:TYR:CE2	2.39	0.55
1:A:1030:SER:HB3	1:C:1041:ASP:HB2	1.89	0.55
1:A:1107:ARG:HH12	1:B:896:ILE:HD11	1.71	0.55
2:D:12:VAL:HG11	2:D:18:LEU:HD22	1.89	0.55
2:E:12:VAL:HG11	2:E:18:LEU:HD22	1.89	0.55
2:F:12:VAL:HG11	2:F:18:LEU:HD22	1.89	0.55
1:B:49:HIS:NE2	1:B:51:THR:HB	2.22	0.54
1:B:442:ASP:HB3	1:B:451:TYR:CE2	2.39	0.54
2:F:98:ARG:NH1	2:F:109:ASP:OD2	2.39	0.54
1:A:124:THR:HB	1:A:174:PRO:HG3	1.89	0.54
1:A:597:VAL:HG13	1:A:608:VAL:HG13	1.89	0.54
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.89	0.54
1:B:100:ILE:HD13	1:B:263:ALA:HB2	1.89	0.54
1:B:170:TYR:CE1	1:B:172:SER:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.90	0.54
1:C:1110:TYR:CZ	1:C:1112:PRO:HG3	2.42	0.54
2:E:173:TYR:HH	2:E:235:TYR:HH	1.53	0.54
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.42	0.54
1:C:273:ARG:HH21	1:C:292:ALA:HB3	1.71	0.54
2:E:40:ALA:HB3	2:E:43:LYS:HB3	1.88	0.54
2:F:40:ALA:HB3	2:F:43:LYS:HB3	1.88	0.54
2:F:41:PRO:HD3	2:F:92:ALA:HA	1.89	0.54
1:C:18:LEU:HB3	1:C:21:ARG:CD	2.38	0.54
2:E:102:PHE:CZ	2:E:105:LEU:HD12	2.43	0.54
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.90	0.54
1:A:762:GLN:HE22	1:C:1006:THR:HG21	1.71	0.54
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.89	0.54
1:B:699:LEU:HB3	1:C:873:TYR:CE1	2.43	0.54
1:A:106:PHE:O	1:A:116:SER:HB2	2.07	0.54
1:C:376:THR:OG1	2:F:102:PHE:CD2	2.60	0.54
2:D:109:ASP:OD1	2:D:110:TYR:N	2.40	0.54
2:E:290:ILE:HD11	2:E:333:ALA:HB2	1.90	0.54
2:F:102:PHE:CZ	2:F:105:LEU:HD12	2.43	0.54
3:G:103:ARG:HD3	3:G:111:TYR:CG	2.43	0.54
1:C:142:GLY:HA2	1:C:244:LEU:HD21	1.90	0.54
3:G:38:ARG:HB2	3:G:48:VAL:CG2	2.38	0.54
1:B:804:GLN:OE1	1:B:935:GLN:NE2	2.40	0.54
1:C:341:VAL:HG11	1:C:397:ALA:HB1	1.90	0.54
3:H:38:ARG:HB2	3:H:48:VAL:CG2	2.38	0.54
1:B:318:PHE:CZ	1:B:615:VAL:HG21	2.43	0.53
2:F:308:LEU:HD21	2:F:311:TYR:HB3	1.90	0.53
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.72	0.53
1:B:213:VAL:O	1:B:214:ARG:HG3	2.08	0.53
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.38	0.53
1:A:421:TYR:CD2	1:A:457:ARG:HG2	2.43	0.53
1:B:140:PHE:HB3	1:B:158:ARG:HB3	1.89	0.53
2:D:102:PHE:CZ	2:D:105:LEU:HD12	2.43	0.53
3:H:54:GLY:O	3:H:58:LYS:NZ	2.40	0.53
2:E:308:LEU:HD21	2:E:311:TYR:HB3	1.91	0.53
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.89	0.53
1:C:421:TYR:CD2	1:C:457:ARG:HG2	2.43	0.53
1:A:503:VAL:HA	1:A:506:GLN:HE21	1.74	0.53
1:B:139:PRO:HA	1:B:159:VAL:HA	1.89	0.53
1:B:533:LEU:HD22	1:B:578:ASP:OD2	2.08	0.53
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:THR:HB	1:C:435:ALA:HB3	1.89	0.53
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.89	0.53
2:F:290:ILE:HD11	2:F:333:ALA:HB2	1.90	0.53
1:A:332:ILE:HD13	1:A:362:VAL:HG11	1.90	0.53
1:B:376:THR:HB	1:B:435:ALA:HB3	1.90	0.53
1:C:54:LEU:HD12	1:C:272:PRO:HA	1.91	0.53
2:E:427:VAL:HG23	2:E:439:LEU:HB2	1.91	0.53
1:B:186:PHE:HD2	1:B:213:VAL:HA	1.73	0.53
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.90	0.53
1:C:369:TYR:CZ	2:F:54:SER:HA	2.44	0.53
1:B:330:PRO:HD2	1:B:528:LYS:CE	2.38	0.53
1:C:93:ALA:O	1:C:265:TYR:HA	2.09	0.53
1:C:376:THR:OG1	2:F:102:PHE:HD2	1.90	0.53
2:D:427:VAL:HG23	2:D:439:LEU:HB2	1.91	0.53
1:C:54:LEU:HA	1:C:271:GLN:O	2.09	0.52
1:C:124:THR:HA	1:C:174:PRO:CB	2.40	0.52
2:D:290:ILE:HD11	2:D:333:ALA:HB2	1.90	0.52
2:F:427:VAL:HG23	2:F:439:LEU:HB2	1.91	0.52
1:B:738:CYS:HB3	1:B:753:LEU:HD21	1.90	0.52
1:B:898:PHE:N	1:B:899:PRO:HD2	2.24	0.52
1:C:357:ARG:HH21	1:C:359:SER:N	2.06	0.52
1:C:503:VAL:HA	1:C:506:GLN:HE21	1.74	0.52
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.43	0.52
1:C:124:THR:CA	1:C:174:PRO:HB3	2.39	0.52
1:C:597:VAL:HG13	1:C:608:VAL:HG13	1.92	0.52
1:B:52:GLN:HA	1:B:274:THR:HA	1.91	0.52
1:C:273:ARG:HG3	1:C:290:ASP:OD1	2.09	0.52
1:A:34:ARG:HH21	1:A:217:PRO:HG2	1.75	0.52
1:B:421:TYR:CD2	1:B:457:ARG:HG2	2.43	0.52
1:B:503:VAL:HA	1:B:506:GLN:HE21	1.74	0.52
1:B:850:ILE:HA	1:B:853:GLN:OE1	2.09	0.52
1:C:852:ALA:HA	1:C:855:PHE:CE1	2.44	0.52
2:F:154:VAL:HG12	2:F:215:LEU:HD11	1.92	0.52
3:I:100:PRO:HG2	3:I:110:SER:OG	2.09	0.52
1:A:337:PRO:O	1:A:340:GLU:HG2	2.10	0.52
1:B:201:PHE:O	1:B:229:LEU:N	2.35	0.52
2:F:142:GLN:NE2	2:F:223:TYR:O	2.43	0.52
1:B:329:PHE:HB3	1:B:528:LYS:HE2	1.92	0.52
3:G:54:GLY:O	3:G:58:LYS:NZ	2.40	0.52
1:A:1006:THR:HG21	1:B:1005:GLN:HE21	1.74	0.52
1:B:128:ILE:HD11	1:B:175:PHE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:O	1:B:340:GLU:HG2	2.10	0.52
1:C:139:PRO:HA	1:C:159:VAL:HA	1.91	0.52
1:C:853:GLN:HG2	1:C:959:LEU:HB3	1.90	0.52
2:E:154:VAL:HG12	2:E:215:LEU:HD11	1.92	0.52
2:F:289:ASN:HD22	2:F:361:VAL:HG21	1.74	0.52
1:A:139:PRO:HB3	1:A:159:VAL:HG13	1.92	0.52
1:A:706:ALA:CB	4:A:1308:NAG:H5	2.39	0.52
1:A:759:PHE:CD2	1:A:1001:LEU:HD21	2.45	0.52
2:D:302:PRO:HB3	2:D:429:GLU:HG3	1.92	0.52
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.92	0.51
1:A:81:ASN:HA	1:A:265:TYR:OH	2.10	0.51
1:A:106:PHE:CD2	1:A:238:PHE:HB3	2.45	0.51
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.92	0.51
1:C:328:ARG:NH1	1:C:533:LEU:HB2	2.25	0.51
3:G:136:PHE:N	3:G:155:LEU:O	2.41	0.51
1:A:736:VAL:HG11	1:A:1004:LEU:HD21	1.92	0.51
1:B:36:VAL:HG21	1:B:220:PHE:HE1	1.76	0.51
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.93	0.51
1:B:170:TYR:CD1	1:B:172:SER:HB2	2.45	0.51
1:C:170:TYR:CD1	1:C:172:SER:HB2	2.45	0.51
1:C:369:TYR:CE1	2:F:54:SER:HB3	2.46	0.51
1:C:618:THR:OG1	1:C:619:GLU:OE1	2.23	0.51
1:A:994:ASP:O	1:A:998:THR:HG22	2.10	0.51
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.92	0.51
1:C:64:TRP:HH2	1:C:214:ARG:HB3	1.75	0.51
2:D:154:VAL:HG12	2:D:215:LEU:HD11	1.92	0.51
1:B:39:PRO:HG2	1:B:51:THR:HG21	1.92	0.51
1:B:92:PHE:CZ	1:B:265:TYR:HB2	2.45	0.51
1:B:566:GLY:N	1:B:575:ALA:O	2.43	0.51
1:A:456:PHE:HB3	1:A:473:TYR:CG	2.45	0.51
1:A:578:ASP:HB3	1:A:581:THR:O	2.10	0.51
1:C:456:PHE:HB3	1:C:473:TYR:CG	2.45	0.51
1:A:332:ILE:HG23	1:A:334:ASN:OD1	2.10	0.51
1:A:360:ASN:H	1:A:523:THR:CG2	2.24	0.51
1:B:102:ARG:O	1:B:120:VAL:HA	2.11	0.51
1:A:129:LYS:HG2	1:A:169:GLU:OE1	2.11	0.51
1:B:53:ASP:HB3	1:B:55:PHE:CE1	2.46	0.51
1:B:784:GLN:HG3	1:B:1029:MET:HG2	1.93	0.51
1:C:337:PRO:O	1:C:340:GLU:HG2	2.10	0.51
2:E:18:LEU:HD12	2:E:19:ARG:N	2.26	0.51
2:F:18:LEU:HD12	2:F:19:ARG:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:109:ASP:OD1	2:F:110:TYR:N	2.40	0.51
1:B:330:PRO:HG2	1:B:528:LYS:HE3	1.93	0.51
1:C:770:ILE:O	1:C:774:GLN:HG2	2.11	0.51
2:D:279:VAL:HG11	2:D:368:LEU:HD11	1.93	0.51
2:E:169:SER:HB2	2:E:187:ASP:HA	1.93	0.51
1:A:1041:ASP:HB2	1:B:1030:SER:HB3	1.92	0.50
1:B:102:ARG:HB2	1:B:241:LEU:CB	2.42	0.50
2:D:18:LEU:HD12	2:D:19:ARG:N	2.26	0.50
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.47	0.50
2:F:169:SER:HB2	2:F:187:ASP:HA	1.93	0.50
1:A:103:GLY:HA3	1:A:119:ILE:O	2.12	0.50
1:A:135:PHE:HA	1:A:160:TYR:HA	1.94	0.50
1:B:142:GLY:HA2	1:B:244:LEU:CD2	2.42	0.50
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.75	0.50
1:A:356:LYS:HE2	1:A:356:LYS:HA	1.94	0.50
1:B:106:PHE:C	1:B:235:ILE:HD11	2.31	0.50
2:F:302:PRO:HB3	2:F:429:GLU:HG3	1.92	0.50
3:G:157:LYS:HG3	3:G:191:SER:HB3	1.94	0.50
3:I:38:ARG:HB2	3:I:48:VAL:CG2	2.40	0.50
1:A:869:MET:HB3	1:C:699:LEU:HD21	1.92	0.50
1:B:342:PHE:HB2	4:B:1301:NAG:H82	1.93	0.50
1:B:356:LYS:HA	1:B:356:LYS:HE2	1.94	0.50
1:C:53:ASP:HB3	1:C:55:PHE:CE1	2.46	0.50
1:C:164:ASN:O	1:C:165:ASN:HB3	2.10	0.50
1:C:551:VAL:CG1	1:C:588:THR:HB	2.41	0.50
1:A:170:TYR:HD2	1:C:360:ASN:HD21	1.60	0.50
1:A:369:TYR:CZ	2:D:53:TYR:CD2	2.99	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HG12	1.92	0.50
1:B:748:GLU:O	1:B:752:LEU:HG	2.11	0.50
2:E:142:GLN:NE2	2:E:223:TYR:O	2.43	0.50
2:F:24:ALA:HB1	2:F:27:PHE:CE1	2.47	0.50
2:F:32:TYR:O	2:F:72:ARG:NH2	2.43	0.50
3:H:157:LYS:HG3	3:H:191:SER:HB3	1.93	0.50
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.52	0.50
2:E:109:ASP:OD1	2:E:110:TYR:N	2.40	0.50
1:B:543:PHE:CD2	1:B:579:PRO:HD3	2.45	0.50
1:C:299:THR:HG21	1:C:308:VAL:HG11	1.92	0.50
1:C:384:PRO:HA	1:C:387:LEU:HG	1.94	0.50
1:C:866:THR:OG1	1:C:869:MET:HG3	2.12	0.50
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.47	0.50
2:E:302:PRO:HB3	2:E:429:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:396:VAL:HG13	2:E:443:LEU:HB3	1.94	0.50
1:A:369:TYR:CE1	2:D:54:SER:HB3	2.47	0.50
1:A:961:THR:O	1:A:965:GLN:HG2	2.12	0.50
1:B:171:VAL:HG12	1:B:171:VAL:O	2.12	0.50
1:B:384:PRO:HA	1:B:387:LEU:HG	1.94	0.50
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.93	0.50
1:C:369:TYR:CE1	2:F:54:SER:CB	2.95	0.50
2:E:279:VAL:HG11	2:E:368:LEU:HD11	1.94	0.50
1:A:90:VAL:HG21	1:A:238:PHE:CZ	2.47	0.50
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.47	0.50
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.52	0.50
1:B:173:GLN:H	1:B:173:GLN:NE2	2.10	0.50
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.11	0.50
3:G:100:PRO:HG2	3:G:110:SER:OG	2.12	0.50
1:A:580:GLN:HG3	4:A:1305:NAG:H5	1.94	0.49
1:A:614:ASP:CG	1:B:859:THR:HG23	2.32	0.49
1:B:347:PHE:CE2	1:B:399:SER:HB2	2.47	0.49
1:A:53:ASP:HB3	1:A:55:PHE:CE1	2.46	0.49
1:B:44:ARG:O	1:B:279:TYR:HB3	2.12	0.49
1:B:124:THR:HB	1:B:174:PRO:HG3	1.94	0.49
1:B:290:ASP:HB3	1:B:293:LEU:HD22	1.95	0.49
1:B:363:ALA:O	1:B:527:PRO:HD3	2.12	0.49
1:C:171:VAL:HG12	1:C:171:VAL:O	2.13	0.49
1:C:384:PRO:HD2	2:F:30:SER:OG	2.12	0.49
2:D:32:TYR:O	2:D:72:ARG:NH2	2.43	0.49
2:D:409:LYS:HB2	2:D:461:THR:OG1	2.13	0.49
1:C:353:TRP:CE2	1:C:466:ARG:HB3	2.47	0.49
2:D:98:ARG:HD3	2:D:110:TYR:HD2	1.77	0.49
2:D:298:TYR:CE1	2:D:308:LEU:HD13	2.47	0.49
2:E:98:ARG:HD3	2:E:110:TYR:HD2	1.78	0.49
3:I:91:THR:OG1	3:I:124:THR:HA	2.13	0.49
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.95	0.49
1:B:79:PHE:O	1:B:80:ASP:OD1	2.31	0.49
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.94	0.49
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.61	0.49
1:A:156:GLU:OE1	1:A:158:ARG:HB2	2.11	0.49
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.47	0.49
1:A:384:PRO:HA	1:A:387:LEU:HG	1.94	0.49
1:A:770:ILE:O	1:A:774:GLN:HG2	2.12	0.49
1:C:86:PHE:CE2	1:C:106:PHE:HE1	2.30	0.49
1:C:196:ASN:HD22	1:C:235:ILE:HG22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LYS:HE2	1:C:356:LYS:HA	1.94	0.49
1:A:141:LEU:HD12	1:A:159:VAL:HG23	1.93	0.49
1:A:719:THR:HG23	1:A:1070:ALA:HB2	1.93	0.49
1:A:1139:ASP:OD2	1:A:1141:LEU:HG	2.13	0.49
1:B:128:ILE:HD13	1:B:170:TYR:HB3	1.94	0.49
1:B:353:TRP:CE2	1:B:466:ARG:HB3	2.47	0.49
1:C:79:PHE:O	1:C:80:ASP:OD1	2.31	0.49
2:D:142:GLN:NE2	2:D:223:TYR:O	2.43	0.49
1:A:64:TRP:CH2	1:A:214:ARG:HB3	2.47	0.49
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	1.94	0.49
1:B:49:HIS:HB3	1:B:279:TYR:CE1	2.48	0.49
1:B:95:THR:OG1	1:B:210:ILE:HD11	2.13	0.49
2:E:293:ASN:ND2	2:E:353:TRP:HB3	2.27	0.49
1:B:49:HIS:HB3	1:B:279:TYR:HE1	1.77	0.49
1:B:567:ARG:HD2	1:C:42:VAL:HG11	1.95	0.49
1:C:193:VAL:HG13	1:C:270:LEU:HD11	1.95	0.49
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.47	0.49
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.52	0.49
2:F:279:VAL:HG11	2:F:368:LEU:HD11	1.94	0.49
2:F:454:LYS:HD2	2:F:475:ARG:HB2	1.94	0.49
1:A:341:VAL:HG11	1:A:397:ALA:HB1	1.95	0.49
1:A:779:GLN:O	1:A:783:ALA:HB3	2.12	0.49
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.12	0.49
1:C:39:PRO:HG2	1:C:51:THR:HG21	1.95	0.49
3:H:100:PRO:HG2	3:H:110:SER:OG	2.13	0.49
1:A:39:PRO:HG2	1:A:51:THR:HG21	1.95	0.49
1:A:79:PHE:O	1:A:80:ASP:OD1	2.31	0.49
1:C:29:THR:HG21	1:C:215:ASP:HA	1.95	0.49
1:C:338:PHE:CD1	1:C:368:LEU:HD11	2.47	0.49
1:C:748:GLU:CD	1:C:748:GLU:H	2.15	0.49
1:C:961:THR:O	1:C:965:GLN:HG2	2.13	0.49
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.13	0.49
2:D:396:VAL:HG13	2:D:443:LEU:HB3	1.94	0.49
2:E:454:LYS:HD2	2:E:475:ARG:HB2	1.94	0.49
1:A:170:TYR:CE1	1:A:172:SER:HB2	2.47	0.48
1:A:171:VAL:HG12	1:A:171:VAL:O	2.13	0.48
1:A:555:SER:HB3	1:A:584:ILE:HG22	1.95	0.48
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.46	0.48
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.95	0.48
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.13	0.48
1:C:328:ARG:NH1	1:C:578:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:LYS:HD2	2:D:475:ARG:HB2	1.94	0.48
3:G:155:LEU:HD12	3:G:192:LEU:O	2.12	0.48
3:I:157:LYS:HG3	3:I:191:SER:HB3	1.94	0.48
1:A:854:LYS:O	1:A:854:LYS:HD3	2.13	0.48
1:A:892:PRO:HG2	1:A:894:LEU:HD21	1.95	0.48
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.95	0.48
1:B:128:ILE:HB	1:B:170:TYR:CB	2.44	0.48
1:B:142:GLY:HA2	1:B:244:LEU:HD21	1.96	0.48
2:E:173:TYR:OH	2:E:235:TYR:OH	2.22	0.48
2:F:98:ARG:HD3	2:F:110:TYR:HD2	1.78	0.48
1:A:986:PRO:CB	1:A:987:PRO:HD3	2.42	0.48
1:B:86:PHE:HB2	1:B:238:PHE:CE1	2.49	0.48
1:B:93:ALA:CB	1:B:216:LEU:HD21	2.44	0.48
1:B:778:THR:HG22	1:B:865:LEU:HD12	1.94	0.48
2:F:293:ASN:ND2	2:F:353:TRP:HB3	2.27	0.48
2:F:396:VAL:HG13	2:F:443:LEU:HB3	1.94	0.48
2:F:409:LYS:HB2	2:F:461:THR:OG1	2.13	0.48
3:H:91:THR:OG1	3:H:124:THR:HA	2.13	0.48
1:C:212:LEU:HD22	1:C:217:PRO:HD3	1.95	0.48
1:B:329:PHE:CD1	1:B:528:LYS:HD2	2.48	0.48
1:B:533:LEU:HD11	1:B:585:LEU:CD1	2.43	0.48
1:B:578:ASP:HB3	1:B:581:THR:O	2.14	0.48
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.96	0.48
1:C:118:LEU:HB3	1:C:133:PHE:CE2	2.49	0.48
1:C:170:TYR:CE1	1:C:172:SER:HB2	2.47	0.48
1:C:318:PHE:CZ	1:C:615:VAL:HG11	2.48	0.48
1:C:730:SER:HG	1:C:778:THR:HG1	1.61	0.48
1:C:777:ASN:O	1:C:781:VAL:HG23	2.13	0.48
1:A:86:PHE:N	1:A:236:THR:O	2.45	0.48
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.95	0.48
1:B:973:ILE:HD12	1:B:974:SER:N	2.29	0.48
3:G:91:THR:HB	3:G:125:VAL:HG12	1.96	0.48
3:I:91:THR:HB	3:I:125:VAL:HG12	1.95	0.48
1:A:186:PHE:HD2	1:A:213:VAL:HA	1.78	0.48
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	1.96	0.48
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	1.94	0.48
1:C:142:GLY:HA3	1:C:156:GLU:HB3	1.96	0.48
1:C:320:VAL:CG1	1:C:590:CYS:HB3	2.44	0.48
1:C:334:ASN:O	1:C:362:VAL:HG22	2.13	0.48
2:F:163:SER:HA	2:F:230:TYR:CE1	2.49	0.48
1:A:277:LEU:HG	1:A:285:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:TYR:HB2	1:C:1107:ARG:NH1	2.28	0.48
1:A:1116:THR:H	1:A:1119:ASN:HD22	1.62	0.48
1:B:1107:ARG:CZ	1:C:904:TYR:HB2	2.44	0.48
1:C:327:VAL:HA	1:C:542:ASN:HB3	1.96	0.48
3:I:178:HIS:CD2	3:I:195:VAL:HG23	2.44	0.48
1:A:853:GLN:HG2	1:A:959:LEU:HB3	1.95	0.48
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.95	0.48
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.37	0.48
1:C:587:ILE:N	1:C:587:ILE:HD12	2.28	0.48
1:C:919:ASN:O	1:C:923:ILE:HG13	2.14	0.48
2:D:163:SER:HA	2:D:230:TYR:CE1	2.49	0.48
3:G:20:LEU:HD12	3:G:81:LEU:HD23	1.96	0.48
1:C:135:PHE:HA	1:C:160:TYR:HA	1.95	0.48
3:G:91:THR:OG1	3:G:124:THR:HA	2.13	0.48
1:A:142:GLY:HA3	1:A:156:GLU:HB3	1.96	0.47
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.37	0.47
1:B:88:ASP:O	1:B:270:LEU:HB2	2.14	0.47
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.95	0.47
2:E:409:LYS:HB2	2:E:461:THR:OG1	2.13	0.47
1:A:560:LEU:HD11	1:B:284:THR:HG22	1.96	0.47
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.29	0.47
1:B:941:THR:HG22	1:B:944:ALA:H	1.79	0.47
1:C:157:PHE:CZ	1:C:159:VAL:HB	2.50	0.47
2:D:297:TRP:HB3	2:D:335:LEU:HD22	1.96	0.47
2:E:163:SER:HA	2:E:230:TYR:CE1	2.49	0.47
1:B:105:ILE:HG22	1:B:106:PHE:N	2.29	0.47
1:B:142:GLY:HA3	1:B:156:GLU:HB3	1.96	0.47
1:C:117:LEU:HD12	1:C:117:LEU:H	1.77	0.47
1:C:141:LEU:HG	1:C:157:PHE:HA	1.96	0.47
1:C:779:GLN:O	1:C:783:ALA:HB3	2.14	0.47
2:F:38:ARG:HB2	2:F:48:VAL:HG22	1.96	0.47
3:G:87:ARG:O	3:G:125:VAL:HG11	2.14	0.47
3:I:20:LEU:HD12	3:I:81:LEU:HD23	1.97	0.47
3:I:38:ARG:O	3:I:46:GLU:N	2.32	0.47
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.78	0.47
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.79	0.47
1:A:854:LYS:HE2	1:A:859:THR:HA	1.96	0.47
1:B:50:SER:HA	1:B:276:LEU:HA	1.97	0.47
1:B:551:VAL:HG12	1:B:588:THR:O	2.15	0.47
1:B:778:THR:HG21	1:B:870:ILE:HD11	1.97	0.47
2:D:38:ARG:HB2	2:D:48:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:GLY:O	2:F:18:LEU:HD11	2.15	0.47
3:H:91:THR:HB	3:H:125:VAL:HG12	1.95	0.47
1:A:805:ILE:HG22	1:A:818:ILE:HD12	1.96	0.47
1:B:84:LEU:HB2	1:B:238:PHE:CE2	2.50	0.47
1:B:364:ASP:CG	1:B:527:PRO:HG2	2.35	0.47
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.30	0.47
2:E:32:TYR:O	2:E:72:ARG:NH2	2.43	0.47
2:F:297:TRP:CZ3	2:F:350:CYS:HB3	2.49	0.47
1:A:18:LEU:HB3	1:A:21:ARG:HD3	1.97	0.47
1:B:402:ILE:HD11	1:B:510:VAL:HG21	1.96	0.47
1:B:705:VAL:HG12	1:C:895:GLN:HB3	1.96	0.47
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.96	0.47
1:B:1002:GLN:HG2	1:C:759:PHE:HZ	1.80	0.47
1:B:1129:VAL:HG23	1:B:1132:ILE:HB	1.95	0.47
2:D:8:GLY:O	2:D:18:LEU:HD11	2.15	0.47
2:D:297:TRP:CZ3	2:D:350:CYS:HB3	2.49	0.47
2:E:297:TRP:HB3	2:E:335:LEU:HD22	1.96	0.47
2:E:383:PRO:HB3	2:E:473:PHE:CE1	2.50	0.47
2:F:297:TRP:HB3	2:F:335:LEU:HD22	1.96	0.47
3:H:87:ARG:O	3:H:125:VAL:HG11	2.15	0.47
3:I:87:ARG:O	3:I:125:VAL:HG11	2.14	0.47
1:A:140:PHE:CZ	1:A:255:SER:HB2	2.49	0.47
1:A:168:PHE:CE1	1:A:170:TYR:HB2	2.50	0.47
1:C:168:PHE:CE1	1:C:170:TYR:HB2	2.48	0.47
1:C:402:ILE:HD11	1:C:510:VAL:HG21	1.96	0.47
2:D:382:PHE:CZ	3:G:138:LEU:C	2.88	0.47
1:A:29:THR:HG22	1:A:30:ASN:N	2.26	0.47
1:A:220:PHE:HE2	1:A:285:ILE:HG22	1.79	0.47
1:B:33:THR:OG1	1:B:219:GLY:O	2.32	0.47
1:C:124:THR:C	1:C:174:PRO:HB3	2.35	0.47
2:D:383:PRO:HB3	2:D:473:PHE:CE1	2.50	0.47
2:E:38:ARG:HB2	2:E:48:VAL:HG22	1.96	0.47
1:A:438:SER:HB2	1:A:441:LEU:HD12	1.97	0.47
1:A:440:ASN:OD1	1:A:441:LEU:HG	2.15	0.47
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.96	0.47
1:A:1129:VAL:HG23	1:A:1132:ILE:HB	1.97	0.47
1:B:156:GLU:OE1	1:B:158:ARG:HB2	2.14	0.47
1:B:699:LEU:HD21	1:C:869:MET:HB3	1.96	0.47
1:B:1107:ARG:NH1	1:C:904:TYR:HB2	2.30	0.47
1:C:194:PHE:HD1	1:C:203:ILE:HG12	1.79	0.47
1:C:421:TYR:HD2	1:C:457:ARG:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:VAL:HA	2:E:227:THR:HG22	1.97	0.47
2:E:297:TRP:CZ3	2:E:350:CYS:HB3	2.49	0.47
1:A:290:ASP:O	1:A:297:SER:HB3	2.16	0.46
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.96	0.46
1:B:421:TYR:HD2	1:B:457:ARG:HG2	1.79	0.46
1:B:1139:ASP:OD2	1:B:1141:LEU:HG	2.14	0.46
1:C:107:GLY:O	1:C:237:ARG:HB2	2.15	0.46
1:C:117:LEU:HD12	1:C:117:LEU:N	2.31	0.46
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.97	0.46
1:C:979:ASP:OD1	1:C:983:ARG:NH1	2.48	0.46
2:D:293:ASN:ND2	2:D:353:TRP:HB3	2.27	0.46
1:A:137:ASN:O	1:A:139:PRO:HD3	2.15	0.46
1:B:118:LEU:HD12	1:B:119:ILE:N	2.31	0.46
2:D:170:VAL:HA	2:D:227:THR:HG22	1.97	0.46
2:E:280:THR:HG23	2:E:334:SER:OG	2.16	0.46
1:A:705:VAL:HG12	1:B:895:GLN:HB3	1.98	0.46
1:A:755:GLN:NE2	1:C:970:PHE:HA	2.30	0.46
1:B:438:SER:HB2	1:B:441:LEU:HD12	1.97	0.46
1:B:440:ASN:OD1	1:B:441:LEU:HG	2.15	0.46
1:B:912:THR:OG1	1:B:1106:GLN:NE2	2.48	0.46
1:B:983:ARG:HG3	1:B:984:LEU:HD12	1.96	0.46
1:C:83:VAL:HG23	1:C:239:GLN:NE2	2.30	0.46
1:A:17:ASN:HA	1:A:138:ASP:HB2	1.96	0.46
1:B:29:THR:HG21	1:B:215:ASP:HA	1.96	0.46
1:B:54:LEU:HB3	1:B:270:LEU:HB3	1.96	0.46
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.80	0.46
1:B:815:ARG:HD2	1:B:823:PHE:CE2	2.51	0.46
1:C:825:LYS:HD2	1:C:942:PRO:HA	1.96	0.46
2:E:8:GLY:O	2:E:18:LEU:HD11	2.14	0.46
2:F:383:PRO:HB3	2:F:473:PHE:CE1	2.50	0.46
1:A:777:ASN:O	1:A:781:VAL:HG23	2.16	0.46
1:B:115:GLN:HG2	1:B:233:ILE:HD13	1.96	0.46
1:C:440:ASN:OD1	1:C:441:LEU:HG	2.16	0.46
3:G:39:GLN:HB2	3:G:45:LEU:CD2	2.45	0.46
3:H:61:ALA:HB3	3:H:64:VAL:HG22	1.98	0.46
1:B:100:ILE:HG22	1:B:242:LEU:HD23	1.98	0.46
1:B:330:PRO:HD2	1:B:528:LYS:HE2	1.97	0.46
1:C:103:GLY:HA3	1:C:119:ILE:O	2.15	0.46
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.97	0.46
1:C:815:ARG:HB2	1:C:820:ASP:OD1	2.15	0.46
2:F:170:VAL:HA	2:F:227:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:20:LEU:HD12	3:H:81:LEU:HD23	1.96	0.46
3:H:98:ARG:HE	3:H:116:VAL:HG12	1.81	0.46
1:A:710:ASN:HB3	4:A:1306:NAG:O7	2.16	0.46
1:A:873:TYR:HE1	1:C:699:LEU:HB3	1.78	0.46
1:B:175:PHE:HB3	1:B:226:LEU:HD23	1.97	0.46
1:B:330:PRO:CG	1:B:528:LYS:HE3	2.45	0.46
1:C:92:PHE:CE1	1:C:265:TYR:CD1	3.04	0.46
2:D:165:ILE:HG23	2:D:170:VAL:HG21	1.97	0.46
1:A:119:ILE:HD12	1:A:119:ILE:N	2.31	0.46
1:A:142:GLY:HA2	1:A:244:LEU:CD2	2.45	0.46
1:A:328:ARG:NH1	1:A:533:LEU:HB3	2.31	0.46
1:B:18:LEU:HB3	1:B:21:ARG:HD3	1.98	0.46
1:B:86:PHE:HB2	1:B:238:PHE:CD1	2.51	0.46
1:C:205:SER:HB3	1:C:226:LEU:HD22	1.98	0.46
1:A:852:ALA:HA	1:A:855:PHE:CD2	2.50	0.46
1:B:101:ILE:HD12	1:B:240:THR:OG1	2.16	0.46
1:B:194:PHE:CD1	1:B:203:ILE:HG12	2.51	0.46
1:B:892:PRO:HG2	1:B:894:LEU:HD21	1.97	0.46
1:B:961:THR:O	1:B:965:GLN:HG2	2.16	0.46
1:C:339:GLY:HA2	1:C:343:ASN:H	1.80	0.46
3:G:61:ALA:HB3	3:G:64:VAL:HG22	1.98	0.46
1:A:575:ALA:HA	1:A:586:ASP:HA	1.98	0.46
1:A:774:GLN:OE1	1:A:777:ASN:ND2	2.49	0.46
1:C:104:TRP:HA	1:C:240:THR:HA	1.98	0.46
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.97	0.46
2:E:164:ASN:ND2	2:E:229:ASP:OD1	2.37	0.46
2:E:316:ARG:CZ	2:E:322:ASP:HA	2.46	0.46
2:E:323:ARG:NH1	2:E:344:ASP:OD2	2.49	0.46
3:G:156:VAL:O	3:G:191:SER:HA	2.16	0.46
1:A:363:ALA:O	1:A:527:PRO:HD3	2.16	0.45
1:A:1094:VAL:HG23	1:A:1096:VAL:HG13	1.98	0.45
1:B:330:PRO:HD2	1:B:528:LYS:HE3	1.97	0.45
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.98	0.45
1:C:728:PRO:O	1:C:1021:SER:OG	2.28	0.45
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.49	0.45
2:D:280:THR:HG23	2:D:334:SER:OG	2.16	0.45
2:F:280:THR:HG23	2:F:334:SER:OG	2.16	0.45
1:C:126:VAL:HG21	1:C:175:PHE:CD1	2.51	0.45
2:F:323:ARG:NH1	2:F:344:ASP:OD2	2.49	0.45
3:G:98:ARG:HE	3:G:116:VAL:HG12	1.81	0.45
3:G:213:ASP:OD1	3:G:220:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:ARG:HE	3:I:116:VAL:HG12	1.81	0.45
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.51	0.45
1:A:196:ASN:OD1	1:A:201:PHE:HD1	2.00	0.45
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.99	0.45
1:C:273:ARG:NH2	1:C:292:ALA:HB3	2.31	0.45
1:C:762:GLN:HG2	1:C:763:LEU:HD23	1.98	0.45
2:F:29:PHE:CZ	2:F:79:LEU:HB2	2.50	0.45
1:A:18:LEU:HB3	1:A:21:ARG:CD	2.46	0.45
1:A:130:VAL:CG1	1:A:168:PHE:HB3	2.45	0.45
1:A:917:TYR:HB3	1:C:1129:VAL:CG2	2.45	0.45
1:A:973:ILE:N	1:A:992:GLN:OE1	2.48	0.45
1:B:117:LEU:HD21	1:B:231:ILE:HG13	1.99	0.45
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.75	0.45
1:C:273:ARG:HA	1:C:273:ARG:HD3	1.79	0.45
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.98	0.45
2:D:323:ARG:NH1	2:D:344:ASP:OD2	2.49	0.45
2:E:101:ASN:HB2	2:E:105:LEU:O	2.17	0.45
3:G:37:VAL:HG11	3:G:45:LEU:HD13	1.98	0.45
3:H:213:ASP:OD1	3:H:220:LYS:HG3	2.16	0.45
1:A:854:LYS:HE2	1:A:859:THR:HG22	1.98	0.45
1:B:48:LEU:HD22	1:B:306:PHE:CD1	2.52	0.45
1:B:105:ILE:O	1:B:238:PHE:HB2	2.16	0.45
3:G:98:ARG:O	3:G:100:PRO:HD3	2.17	0.45
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.52	0.45
1:B:168:PHE:HE1	1:B:170:TYR:HD2	1.63	0.45
1:B:879:ALA:O	1:B:883:THR:OG1	2.25	0.45
2:D:316:ARG:CZ	2:D:322:ASP:HA	2.46	0.45
1:A:455:LEU:HD12	1:A:493:GLN:HB2	1.99	0.45
1:A:541:PHE:CZ	1:A:587:ILE:HD13	2.51	0.45
1:A:546:LEU:HD11	1:A:573:THR:HG21	1.99	0.45
1:C:578:ASP:HB3	1:C:581:THR:O	2.17	0.45
3:I:213:ASP:OD1	3:I:220:LYS:HG3	2.16	0.45
1:A:170:TYR:HD1	1:A:172:SER:HB2	1.80	0.45
1:A:232:GLY:HA3	1:C:521:PRO:HD2	1.99	0.45
1:A:386:LYS:O	1:A:386:LYS:HG2	2.17	0.45
1:A:421:TYR:HD2	1:A:457:ARG:HG2	1.79	0.45
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.48	0.45
1:B:45:SER:O	1:B:47:VAL:HG23	2.17	0.45
1:B:598:ILE:HD13	1:B:650:LEU:HD11	1.99	0.45
1:C:435:ALA:HB2	1:C:510:VAL:HG22	1.99	0.45
1:C:438:SER:HB2	1:C:441:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:ARG:NH2	2:D:155:THR:OG1	2.40	0.45
2:D:425:GLU:HB3	2:D:441:SER:HA	1.99	0.45
3:I:165:THR:OG1	3:I:213:ASP:HB2	2.17	0.45
1:A:140:PHE:CE1	1:A:258:TRP:CD1	3.05	0.45
1:A:589:PRO:HG2	1:B:855:PHE:HA	1.99	0.45
1:B:81:ASN:HB2	1:B:240:THR:HG22	1.98	0.45
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.50	0.45
1:B:435:ALA:HB2	1:B:510:VAL:HG22	1.99	0.45
1:B:699:LEU:HB3	1:C:873:TYR:HE1	1.82	0.45
1:C:386:LYS:O	1:C:386:LYS:HG2	2.17	0.45
1:C:503:VAL:HG12	2:F:105:LEU:HD11	1.99	0.45
2:D:152:GLN:HG2	2:D:153:ARG:H	1.82	0.45
2:E:29:PHE:CZ	2:E:79:LEU:HB2	2.50	0.45
1:A:192:PHE:CD2	1:A:205:SER:HB2	2.51	0.45
1:B:970:PHE:O	1:B:995:ARG:NH2	2.46	0.45
1:C:130:VAL:CG1	1:C:168:PHE:HB3	2.46	0.45
1:C:329:PHE:CD2	1:C:528:LYS:HD3	2.51	0.45
1:C:731:MET:HE1	1:C:1015:ALA:HA	1.99	0.45
2:F:101:ASN:HB2	2:F:105:LEU:O	2.17	0.45
2:F:316:ARG:CZ	2:F:322:ASP:HA	2.46	0.45
2:F:425:GLU:HB3	2:F:441:SER:HA	1.99	0.45
3:I:37:VAL:HG11	3:I:117:TRP:HZ3	1.82	0.45
1:A:79:PHE:CD1	1:A:242:LEU:HD13	2.52	0.44
1:A:300:LYS:HE2	1:A:306:PHE:O	2.18	0.44
1:B:731:MET:HB2	1:B:774:GLN:NE2	2.31	0.44
2:E:152:GLN:HG2	2:E:153:ARG:H	1.83	0.44
1:A:100:ILE:HG22	1:A:242:LEU:CD2	2.47	0.44
1:A:881:THR:HG22	1:A:1050:MET:HE1	2.00	0.44
1:B:770:ILE:O	1:B:774:GLN:HG2	2.17	0.44
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.99	0.44
2:D:101:ASN:HB2	2:D:105:LEU:O	2.17	0.44
2:F:456:TYR:HB2	2:F:473:PHE:CE2	2.53	0.44
3:G:153:GLY:HA2	3:G:194:SER:O	2.17	0.44
1:A:105:ILE:O	1:A:238:PHE:HA	2.18	0.44
1:B:81:ASN:CB	1:B:240:THR:HG22	2.47	0.44
1:C:49:HIS:O	1:C:276:LEU:HA	2.18	0.44
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.46	0.44
1:C:598:ILE:HD13	1:C:650:LEU:HD11	1.99	0.44
2:D:369:THR:OG1	2:D:430:GLN:OE1	2.26	0.44
2:F:153:ARG:NH2	2:F:155:THR:OG1	2.40	0.44
3:G:165:THR:OG1	3:G:213:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:VAL:HG11	3:H:117:TRP:HZ3	1.82	0.44
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.30	0.44
1:A:534:VAL:HG21	1:A:537:LYS:HD2	1.99	0.44
1:A:893:ALA:HB1	1:C:705:VAL:HG21	2.00	0.44
1:B:176:LEU:HA	1:B:190:ARG:HD3	1.99	0.44
1:B:327:VAL:O	1:B:531:THR:N	2.50	0.44
1:B:357:ARG:HH21	1:B:359:SER:HB3	1.82	0.44
1:C:48:LEU:HD23	1:C:278:LYS:HA	1.99	0.44
1:C:84:LEU:HB2	1:C:238:PHE:CE1	2.52	0.44
2:D:456:TYR:HB2	2:D:473:PHE:CZ	2.53	0.44
3:H:165:THR:OG1	3:H:213:ASP:HB2	2.17	0.44
1:A:19:THR:HG21	1:A:256:SER:HB2	1.99	0.44
1:A:816:SER:OG	1:A:819:GLU:HG3	2.17	0.44
1:A:984:LEU:HB2	1:A:989:ALA:HB2	1.98	0.44
1:B:93:ALA:HB1	1:B:216:LEU:HD21	1.99	0.44
2:D:277:GLN:HG2	2:D:278:ARG:N	2.33	0.44
2:D:328:LYS:NZ	2:D:330:GLY:O	2.51	0.44
2:E:267:GLN:HG3	2:E:283:CYS:HB3	1.99	0.44
3:I:51:ILE:HG13	3:I:58:LYS:HG3	2.00	0.44
1:A:232:GLY:CA	1:C:521:PRO:HD2	2.48	0.44
1:C:743:CYS:HB2	1:C:977:LEU:HD12	2.00	0.44
1:C:825:LYS:HD2	1:C:942:PRO:HB3	1.99	0.44
2:E:2:VAL:HG12	2:E:2:VAL:O	2.18	0.44
2:F:7:SER:OG	2:F:8:GLY:N	2.51	0.44
3:I:61:ALA:HB3	3:I:64:VAL:HG22	1.98	0.44
1:A:102:ARG:HH21	1:A:243:ALA:HB2	1.83	0.44
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.99	0.44
1:C:455:LEU:HD12	1:C:493:GLN:HB2	1.99	0.44
1:C:565:PHE:N	1:C:565:PHE:CD1	2.84	0.44
3:H:98:ARG:O	3:H:100:PRO:HD3	2.17	0.44
3:I:98:ARG:O	3:I:100:PRO:HD3	2.18	0.44
1:A:48:LEU:HD13	1:A:305:SER:HA	2.00	0.44
1:A:244:LEU:HB3	1:A:259:THR:O	2.18	0.44
1:A:643:PHE:CE2	1:A:645:THR:HG22	2.53	0.44
1:A:904:TYR:HB2	1:C:1107:ARG:CZ	2.48	0.44
1:B:79:PHE:CD1	1:B:242:LEU:HD13	2.52	0.44
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.53	0.44
1:B:815:ARG:HB2	1:B:820:ASP:OD1	2.18	0.44
1:C:212:LEU:CD2	1:C:217:PRO:HD3	2.48	0.44
1:C:226:LEU:HD12	1:C:226:LEU:HA	1.77	0.44
2:D:456:TYR:HB2	2:D:473:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:425:GLU:HB3	2:E:441:SER:HA	1.99	0.44
3:H:33:ALA:HA	3:H:72:ARG:HH12	1.83	0.44
3:H:182:ALA:HB1	3:H:190:TYR:HB3	2.00	0.44
2:D:297:TRP:CD2	2:D:335:LEU:HB2	2.53	0.44
2:D:311:TYR:CE1	2:D:315:LYS:HB2	2.52	0.44
2:E:387:GLU:OE2	3:H:137:PRO:HD2	2.18	0.44
2:F:297:TRP:CD2	2:F:335:LEU:HB2	2.53	0.44
1:A:124:THR:CA	1:A:174:PRO:HB3	2.48	0.43
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.53	0.43
1:B:19:THR:HG21	1:B:256:SER:HB2	2.00	0.43
1:B:126:VAL:CG2	1:B:174:PRO:HA	2.45	0.43
1:B:126:VAL:HG21	1:B:175:PHE:CD2	2.53	0.43
1:B:455:LEU:HD12	1:B:493:GLN:HB2	1.99	0.43
1:B:557:LYS:HB2	1:B:584:ILE:HG21	2.00	0.43
1:C:805:ILE:HG22	1:C:818:ILE:HD12	2.00	0.43
2:E:456:TYR:HB2	2:E:473:PHE:CE2	2.53	0.43
2:F:267:GLN:HG3	2:F:283:CYS:HB3	1.99	0.43
2:F:456:TYR:HB2	2:F:473:PHE:CZ	2.53	0.43
3:G:182:ALA:HB1	3:G:190:TYR:HB3	2.00	0.43
3:I:33:ALA:HA	3:I:72:ARG:HH12	1.83	0.43
1:A:42:VAL:HG11	1:C:567:ARG:HD2	2.00	0.43
1:A:141:LEU:HG	1:A:157:PHE:HA	1.99	0.43
1:A:853:GLN:O	1:A:858:LEU:HB2	2.18	0.43
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.00	0.43
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.49	0.43
1:C:95:THR:HG22	1:C:264:ALA:O	2.19	0.43
1:C:555:SER:OG	1:C:556:ASN:N	2.51	0.43
1:C:590:CYS:O	1:C:592:PHE:HD1	2.01	0.43
2:E:456:TYR:HB2	2:E:473:PHE:CZ	2.53	0.43
2:F:37:VAL:HG22	2:F:47:TRP:HD1	1.83	0.43
3:G:39:GLN:HB2	3:G:45:LEU:HD23	2.00	0.43
1:A:133:PHE:HD1	1:A:160:TYR:CD2	2.37	0.43
1:A:350:VAL:HA	1:A:400:PHE:HB2	2.00	0.43
1:A:980:ILE:HG23	1:A:984:LEU:HD12	2.01	0.43
1:B:86:PHE:HD2	1:B:238:PHE:CE1	2.36	0.43
1:B:119:ILE:N	1:B:119:ILE:HD12	2.34	0.43
1:B:213:VAL:O	1:B:214:ARG:CG	2.65	0.43
2:D:267:GLN:HG3	2:D:283:CYS:HB3	1.99	0.43
2:E:37:VAL:HG22	2:E:47:TRP:HD1	1.84	0.43
2:E:140:LEU:HD21	2:E:164:ASN:HB3	2.00	0.43
2:E:168:ASN:ND2	2:E:228:TRP:O	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:LYS:NZ	2:F:330:GLY:O	2.51	0.43
3:H:103:ARG:HD3	3:H:111:TYR:CG	2.53	0.43
3:I:214:HIS:O	3:I:218:ASN:N	2.51	0.43
1:A:448:ASN:OD1	1:A:450:ASN:ND2	2.51	0.43
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.88	0.43
1:B:37:TYR:CB	1:B:223:LEU:HB2	2.46	0.43
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.37	0.43
1:B:870:ILE:HG22	1:B:1055:SER:HB2	2.00	0.43
1:C:48:LEU:HD13	1:C:305:SER:HA	2.01	0.43
1:C:731:MET:HE2	1:C:1018:ILE:HG13	2.00	0.43
2:D:37:VAL:HG22	2:D:47:TRP:HD1	1.84	0.43
2:D:140:LEU:HD21	2:D:164:ASN:HB3	2.00	0.43
2:F:2:VAL:HG12	2:F:2:VAL:O	2.18	0.43
3:H:103:ARG:HH11	3:H:111:TYR:HB2	1.82	0.43
3:I:217:SER:OG	3:I:219:THR:HG23	2.19	0.43
1:A:614:ASP:OD2	1:B:859:THR:HG23	2.19	0.43
1:A:728:PRO:O	1:A:1021:SER:OG	2.26	0.43
1:A:902:MET:HG3	1:A:916:LEU:CD1	2.48	0.43
1:B:126:VAL:CG1	1:B:175:PHE:H	2.29	0.43
1:B:386:LYS:O	1:B:386:LYS:HG2	2.17	0.43
1:B:421:TYR:HE2	1:B:457:ARG:H	1.66	0.43
1:B:980:ILE:O	1:B:984:LEU:HB2	2.18	0.43
1:C:165:ASN:ND2	1:C:165:ASN:O	2.51	0.43
1:C:619:GLU:OE1	1:C:619:GLU:N	2.48	0.43
1:C:736:VAL:HG22	1:C:767:LEU:HD12	2.01	0.43
1:C:1082:CYS:HB2	1:C:1126:CYS:HB2	1.72	0.43
2:E:297:TRP:CD2	2:E:335:LEU:HB2	2.53	0.43
2:F:265:LEU:HB2	2:F:362:PHE:O	2.18	0.43
3:G:33:ALA:HA	3:G:72:ARG:HH12	1.83	0.43
1:A:360:ASN:N	1:A:523:THR:HG22	2.33	0.43
1:A:826:VAL:HB	1:A:1057:PRO:HG2	2.00	0.43
2:F:152:GLN:HG2	2:F:153:ARG:H	1.83	0.43
3:G:214:HIS:O	3:G:218:ASN:N	2.51	0.43
3:H:125:VAL:HG13	3:H:125:VAL:O	2.19	0.43
3:H:217:SER:OG	3:H:219:THR:HG23	2.19	0.43
3:I:182:ALA:HB1	3:I:190:TYR:HB3	2.00	0.43
1:B:878:LEU:O	1:B:882:ILE:HG13	2.19	0.43
1:B:903:ALA:HB1	1:B:913:GLN:CB	2.46	0.43
1:C:119:ILE:HD12	1:C:119:ILE:N	2.34	0.43
1:C:784:GLN:HG3	1:C:1029:MET:HG2	2.00	0.43
2:D:162:SER:HA	2:D:166:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:VAL:N	2:D:188:ASP:OD1	2.49	0.43
2:E:153:ARG:NH2	2:E:155:THR:OG1	2.40	0.43
2:E:328:LYS:NZ	2:E:330:GLY:O	2.51	0.43
3:G:2:VAL:HG23	3:G:27:PHE:CD1	2.54	0.43
3:G:37:VAL:HG11	3:G:117:TRP:HZ3	1.82	0.43
1:B:44:ARG:HB2	1:B:279:TYR:CG	2.54	0.43
1:B:64:TRP:HH2	1:B:214:ARG:HB3	1.81	0.43
1:B:136:CYS:O	1:B:138:ASP:N	2.52	0.43
1:B:941:THR:HG22	1:B:944:ALA:N	2.33	0.43
1:C:364:ASP:CG	1:C:527:PRO:HG2	2.39	0.43
3:I:4:LEU:HD23	3:I:96:CYS:SG	2.59	0.43
1:A:175:PHE:CZ	1:A:227:VAL:HG11	2.54	0.43
1:A:537:LYS:N	1:A:551:VAL:HG23	2.33	0.43
1:A:720:ILE:HG13	1:A:923:ILE:HG23	2.00	0.43
1:A:736:VAL:HG21	1:A:1004:LEU:HD11	2.01	0.43
1:A:902:MET:SD	1:A:1049:LEU:HD13	2.59	0.43
1:B:17:ASN:HA	1:B:138:ASP:HB2	2.01	0.43
1:B:128:ILE:HD12	1:B:128:ILE:N	2.34	0.43
1:B:416:GLY:O	1:B:420:ASP:HB2	2.19	0.43
1:C:20:THR:O	1:C:21:ARG:HD2	2.18	0.43
1:C:102:ARG:HB2	1:C:241:LEU:HB2	2.01	0.43
1:C:106:PHE:HB3	1:C:235:ILE:CG1	2.48	0.43
1:C:136:CYS:O	1:C:137:ASN:C	2.57	0.43
1:C:543:PHE:CD2	1:C:579:PRO:HD3	2.49	0.43
2:E:7:SER:OG	2:E:8:GLY:N	2.51	0.43
2:F:140:LEU:HD21	2:F:164:ASN:HB3	2.01	0.43
3:G:94:TYR:O	3:G:120:GLY:HA2	2.19	0.43
1:A:849:LEU:HD23	1:A:849:LEU:H	1.84	0.43
1:B:18:LEU:HB3	1:B:21:ARG:CD	2.48	0.43
1:B:54:LEU:HD12	1:B:272:PRO:HA	2.00	0.43
1:B:592:PHE:CE2	1:C:857:GLY:HA2	2.53	0.43
2:D:2:VAL:HG12	2:D:2:VAL:O	2.18	0.43
2:E:99:ASP:OD2	2:E:106:VAL:HG13	2.19	0.43
3:I:103:ARG:HD3	3:I:111:TYR:CG	2.54	0.43
1:B:350:VAL:HA	1:B:400:PHE:HB2	2.01	0.42
1:B:537:LYS:N	1:B:551:VAL:HG23	2.34	0.42
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.36	0.42
2:D:176:LEU:HD23	2:D:221:ALA:HB2	2.01	0.42
1:B:121:ASN:HD22	1:B:176:LEU:HB2	1.84	0.42
1:B:731:MET:HG2	1:B:955:ASN:ND2	2.34	0.42
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HB2	1:C:238:PHE:CZ	2.54	0.42
1:C:126:VAL:CG1	1:C:175:PHE:H	2.32	0.42
1:C:849:LEU:HD23	1:C:849:LEU:H	1.83	0.42
1:C:856:ASN:ND2	1:C:966:LEU:HD12	2.34	0.42
2:D:7:SER:OG	2:D:8:GLY:N	2.51	0.42
2:D:105:LEU:HD22	2:D:169:SER:HB3	2.00	0.42
2:F:454:LYS:NZ	2:F:474:ASN:HB3	2.35	0.42
3:H:214:HIS:O	3:H:218:ASN:N	2.51	0.42
1:A:331:ASN:HB3	1:A:580:GLN:HB2	2.01	0.42
1:A:942:PRO:C	1:A:944:ALA:N	2.71	0.42
1:B:175:PHE:CD1	1:B:226:LEU:HG	2.54	0.42
1:B:662:CYS:HB2	1:B:697:MET:HG2	2.00	0.42
1:C:126:VAL:HG11	1:C:175:PHE:H	1.84	0.42
1:C:128:ILE:HD12	1:C:128:ILE:N	2.34	0.42
1:C:303:LEU:HD12	1:C:308:VAL:HG22	2.01	0.42
1:C:335:LEU:H	1:C:335:LEU:HD23	1.84	0.42
1:C:437:ASN:HB2	1:C:508:TYR:CZ	2.55	0.42
1:C:720:ILE:HG13	1:C:923:ILE:HG23	2.01	0.42
1:B:329:PHE:CG	1:B:528:LYS:HB3	2.54	0.42
1:B:736:VAL:H	1:B:767:LEU:HD12	1.83	0.42
1:C:903:ALA:HB2	1:C:916:LEU:HD22	2.01	0.42
2:D:86:LEU:HB3	2:D:119:VAL:HG21	2.01	0.42
2:E:176:LEU:HD23	2:E:221:ALA:HB2	2.01	0.42
2:E:414:VAL:HG13	2:E:417:ALA:HB3	2.02	0.42
2:F:99:ASP:OD2	2:F:106:VAL:HG13	2.19	0.42
3:G:109:SER:O	3:G:110:SER:C	2.58	0.42
3:I:2:VAL:HG23	3:I:27:PHE:CD1	2.54	0.42
1:A:136:CYS:O	1:A:138:ASP:N	2.53	0.42
1:A:168:PHE:HE1	1:A:170:TYR:HB2	1.84	0.42
1:B:565:PHE:O	1:C:43:PHE:HB3	2.20	0.42
1:B:1106:GLN:H	1:B:1106:GLN:HG3	1.67	0.42
1:C:329:PHE:CE2	1:C:544:ASN:HA	2.55	0.42
2:D:102:PHE:CE1	2:D:105:LEU:HD12	2.55	0.42
2:D:164:ASN:ND2	2:D:229:ASP:OD1	2.37	0.42
3:G:125:VAL:HG13	3:G:125:VAL:O	2.19	0.42
3:G:217:SER:OG	3:G:219:THR:HG23	2.19	0.42
3:I:99:PHE:CE1	3:I:112:ASP:HA	2.54	0.42
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.55	0.42
1:A:369:TYR:CZ	2:D:53:TYR:CE2	3.03	0.42
1:A:742:ILE:HG21	1:A:753:LEU:HD21	2.02	0.42
1:A:869:MET:HB3	1:C:699:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PRO:CD	1:A:987:PRO:HD3	2.49	0.42
1:A:991:VAL:O	1:A:995:ARG:HG3	2.19	0.42
1:B:93:ALA:O	1:B:265:TYR:HA	2.20	0.42
1:B:728:PRO:O	1:B:1021:SER:OG	2.24	0.42
1:B:731:MET:HB2	1:B:774:GLN:HE21	1.85	0.42
1:C:996:LEU:HA	1:C:996:LEU:HD23	1.74	0.42
2:D:156:LEU:HD23	2:D:210:LEU:O	2.20	0.42
2:D:311:TYR:CD1	2:D:312:ALA:N	2.88	0.42
2:E:102:PHE:CE1	2:E:105:LEU:HD12	2.55	0.42
2:F:164:ASN:ND2	2:F:229:ASP:OD1	2.37	0.42
3:H:4:LEU:HD23	3:H:96:CYS:SG	2.59	0.42
3:I:99:PHE:CZ	3:I:112:ASP:O	2.72	0.42
3:I:109:SER:O	3:I:110:SER:C	2.57	0.42
1:A:139:PRO:CA	1:A:159:VAL:HA	2.45	0.42
1:B:140:PHE:CZ	1:B:255:SER:HB2	2.55	0.42
1:B:231:ILE:CG2	1:B:233:ILE:HG12	2.49	0.42
1:B:645:THR:HG22	1:B:647:ALA:H	1.85	0.42
2:F:414:VAL:HG13	2:F:417:ALA:HB3	2.02	0.42
3:H:2:VAL:HG23	3:H:27:PHE:CD1	2.54	0.42
3:I:47:TRP:HH2	3:I:59:TYR:HB3	1.84	0.42
1:A:119:ILE:HA	1:A:127:VAL:O	2.20	0.42
1:A:327:VAL:HG12	1:A:542:ASN:HB3	2.02	0.42
1:A:553:THR:O	1:A:585:LEU:HA	2.18	0.42
1:B:53:ASP:O	1:B:273:ARG:O	2.38	0.42
1:B:105:ILE:CG2	1:B:106:PHE:N	2.83	0.42
1:B:140:PHE:HE1	1:B:258:TRP:CD1	2.38	0.42
1:B:141:LEU:HD22	1:B:243:ALA:HA	2.00	0.42
1:B:365:TYR:CD2	1:B:387:LEU:HB3	2.55	0.42
1:C:79:PHE:CD1	1:C:242:LEU:HD13	2.55	0.42
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.01	0.42
1:C:970:PHE:O	1:C:995:ARG:NH2	2.53	0.42
2:E:277:GLN:HG2	2:E:278:ARG:N	2.35	0.42
3:I:94:TYR:O	3:I:120:GLY:HA2	2.20	0.42
1:A:129:LYS:O	1:A:133:PHE:HE2	2.01	0.42
1:A:610:VAL:O	1:A:650:LEU:HD12	2.19	0.42
1:B:546:LEU:HD11	1:B:573:THR:HG21	2.01	0.42
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	2.01	0.42
1:B:970:PHE:CG	1:B:999:GLY:HA3	2.54	0.42
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.55	0.42
1:C:361:CYS:SG	1:C:362:VAL:N	2.93	0.42
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ARG:CZ	1:C:492:LEU:HD21	2.50	0.42
2:E:86:LEU:HB3	2:E:119:VAL:HG21	2.01	0.42
2:F:156:LEU:HD23	2:F:210:LEU:O	2.20	0.42
3:G:4:LEU:HD23	3:G:96:CYS:SG	2.59	0.42
3:H:160:PHE:HA	3:H:161:PRO:HA	1.84	0.42
1:A:100:ILE:HG22	1:A:242:LEU:HD22	2.02	0.42
1:B:137:ASN:O	1:B:139:PRO:HD3	2.20	0.42
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.89	0.42
1:B:361:CYS:SG	1:B:362:VAL:N	2.93	0.42
1:B:849:LEU:H	1:B:849:LEU:HD23	1.85	0.42
1:B:997:ILE:HD13	1:B:997:ILE:HA	1.81	0.42
1:C:416:GLY:O	1:C:420:ASP:HB2	2.19	0.42
1:C:418:ILE:HA	1:C:422:ASN:HB2	2.02	0.42
1:C:789:TYR:CE1	1:C:893:ALA:HB2	2.55	0.42
2:D:454:LYS:NZ	2:D:474:ASN:HB3	2.35	0.42
3:I:47:TRP:CH2	3:I:59:TYR:HB3	2.54	0.42
1:A:117:LEU:HD21	1:A:231:ILE:HD13	2.02	0.41
1:A:290:ASP:OD1	1:A:293:LEU:HB3	2.20	0.41
1:A:386:LYS:HD2	1:A:390:LEU:HD21	2.02	0.41
1:A:611:LEU:HD23	1:A:613:GLN:NE2	2.35	0.41
1:A:778:THR:HG21	1:A:870:ILE:HD11	2.02	0.41
1:B:94:SER:O	1:B:189:LEU:HA	2.20	0.41
1:B:157:PHE:CZ	1:B:159:VAL:HB	2.54	0.41
1:B:418:ILE:HA	1:B:422:ASN:HB2	2.02	0.41
1:B:1045:LYS:HE3	1:B:1045:LYS:HB3	1.87	0.41
1:B:1083:HIS:HB2	1:B:1137:VAL:HG23	2.02	0.41
1:C:350:VAL:HA	1:C:400:PHE:HB2	2.00	0.41
1:C:409:GLN:OE1	1:C:416:GLY:HA3	2.20	0.41
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.19	0.41
2:D:276:GLY:HA2	2:D:339:GLY:HA2	2.02	0.41
2:E:6:GLU:HB3	2:E:22:CYS:HB2	2.02	0.41
2:F:277:GLN:HG2	2:F:278:ARG:N	2.35	0.41
1:A:24:LEU:HD23	1:A:80:ASP:OD2	2.19	0.41
1:A:118:LEU:HD23	1:A:133:PHE:CE1	2.55	0.41
1:A:386:LYS:HE2	1:A:386:LYS:HB3	1.75	0.41
1:A:416:GLY:O	1:A:420:ASP:HB2	2.19	0.41
1:B:280:ASN:HD22	4:B:1304:NAG:H83	1.84	0.41
1:B:599:THR:CB	1:B:608:VAL:HG12	2.49	0.41
1:B:877:LEU:HD13	1:B:1029:MET:SD	2.59	0.41
1:B:904:TYR:HA	1:B:907:ASN:HB2	2.02	0.41
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:PHE:HB3	1:C:473:TYR:CD2	2.55	0.41
1:C:537:LYS:N	1:C:551:VAL:HG23	2.34	0.41
1:C:714:ILE:HD12	1:C:1096:VAL:HG11	2.01	0.41
2:D:99:ASP:OD2	2:D:106:VAL:HG13	2.19	0.41
2:F:104:PRO:O	2:F:106:VAL:N	2.51	0.41
2:F:176:LEU:HD23	2:F:221:ALA:HB2	2.01	0.41
3:G:11:LEU:HD13	3:G:11:LEU:HA	1.92	0.41
3:H:109:SER:O	3:H:110:SER:C	2.58	0.41
3:I:125:VAL:HG13	3:I:125:VAL:O	2.19	0.41
1:A:409:GLN:OE1	1:A:416:GLY:HA3	2.20	0.41
1:A:437:ASN:HB2	1:A:508:TYR:CZ	2.55	0.41
1:B:437:ASN:HB2	1:B:508:TYR:CZ	2.55	0.41
1:B:612:TYR:HB3	1:B:615:VAL:HG21	2.02	0.41
1:B:991:VAL:O	1:B:995:ARG:HG3	2.20	0.41
1:C:120:VAL:O	1:C:127:VAL:HG22	2.20	0.41
1:C:137:ASN:O	1:C:139:PRO:HD3	2.20	0.41
1:C:165:ASN:O	1:C:165:ASN:CG	2.59	0.41
1:C:448:ASN:HB3	1:C:497:PHE:HB2	2.02	0.41
2:D:170:VAL:HG21	2:D:208:ALA:HB2	2.01	0.41
2:E:104:PRO:O	2:E:106:VAL:N	2.51	0.41
2:F:102:PHE:CE1	2:F:105:LEU:HD12	2.55	0.41
2:F:168:ASN:ND2	2:F:228:TRP:O	2.42	0.41
3:I:47:TRP:HZ2	3:I:50:TRP:HB3	1.85	0.41
1:A:461:LEU:HD12	1:A:461:LEU:HA	1.91	0.41
1:A:1095:PHE:CE1	1:A:1115:ILE:HG12	2.55	0.41
1:B:448:ASN:HB3	1:B:497:PHE:HB2	2.02	0.41
1:B:815:ARG:HD2	1:B:823:PHE:CD2	2.55	0.41
1:B:979:ASP:O	1:B:983:ARG:HG2	2.20	0.41
1:C:54:LEU:HD12	1:C:272:PRO:CA	2.50	0.41
1:C:139:PRO:CB	1:C:159:VAL:HG22	2.51	0.41
2:D:18:LEU:HD12	2:D:19:ARG:H	1.86	0.41
2:D:104:PRO:O	2:D:106:VAL:N	2.51	0.41
2:E:454:LYS:NZ	2:E:474:ASN:HB3	2.35	0.41
2:F:86:LEU:HB3	2:F:119:VAL:HG21	2.01	0.41
3:I:70:ILE:HD11	3:I:79:LEU:HD11	2.03	0.41
1:A:985:ASP:HB2	1:A:988:GLU:HB3	2.02	0.41
1:A:1106:GLN:H	1:A:1106:GLN:HG3	1.71	0.41
1:B:30:ASN:HB3	1:B:32:PHE:HE1	1.86	0.41
1:B:241:LEU:HD12	1:B:241:LEU:N	2.35	0.41
1:C:497:PHE:CD2	1:C:507:PRO:HB3	2.56	0.41
3:H:70:ILE:HD11	3:H:79:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:94:TYR:O	3:H:120:GLY:HA2	2.20	0.41
1:A:189:LEU:HB2	1:A:210:ILE:HD13	2.03	0.41
1:A:612:TYR:HB3	1:A:615:VAL:HG11	2.02	0.41
1:A:616:ASN:CG	1:A:617:CYS:H	2.23	0.41
1:B:454:ARG:CZ	1:B:492:LEU:HD21	2.50	0.41
1:B:774:GLN:OE1	1:B:777:ASN:ND2	2.54	0.41
1:C:30:ASN:HB3	1:C:32:PHE:HE1	1.86	0.41
1:C:111:ASP:HB2	1:C:113:LYS:HG2	2.03	0.41
1:C:1088:HIS:CG	1:C:1137:VAL:HG21	2.55	0.41
2:F:276:GLY:HA2	2:F:339:GLY:HA2	2.02	0.41
3:G:70:ILE:HD11	3:G:79:LEU:HD11	2.03	0.41
3:H:11:LEU:HD13	3:H:124:THR:OG1	2.20	0.41
1:A:136:CYS:O	1:A:137:ASN:C	2.58	0.41
1:A:538:CYS:HB2	1:A:590:CYS:HB2	1.95	0.41
1:A:979:ASP:O	1:A:983:ARG:HG2	2.21	0.41
1:B:92:PHE:HB3	1:B:192:PHE:HB2	2.02	0.41
1:B:409:GLN:OE1	1:B:416:GLY:HA3	2.20	0.41
1:C:120:VAL:HG22	1:C:241:LEU:CD1	2.51	0.41
1:C:309:GLU:HA	1:C:309:GLU:OE2	2.21	0.41
2:D:311:TYR:HE2	2:D:317:PRO:HA	1.84	0.41
2:F:6:GLU:HB3	2:F:22:CYS:HB2	2.03	0.41
2:F:161:SER:OG	2:F:162:SER:N	2.54	0.41
3:G:86:LEU:HD23	3:G:86:LEU:HA	1.89	0.41
3:I:11:LEU:HD21	3:I:161:PRO:HD3	2.03	0.41
1:A:555:SER:HB2	1:A:586:ASP:CG	2.41	0.41
1:A:644:GLN:HG2	4:A:1311:NAG:H61	2.02	0.41
1:A:895:GLN:HB3	1:C:705:VAL:CG1	2.51	0.41
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.20	0.41
1:B:462:LYS:HE2	1:B:462:LYS:HB2	1.83	0.41
1:C:34:ARG:NH2	1:C:217:PRO:HG2	2.35	0.41
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.86	0.41
1:C:375:SER:O	2:F:102:PHE:CB	2.68	0.41
2:D:161:SER:OG	2:D:162:SER:N	2.54	0.41
2:E:385:SER:HB3	2:E:387:GLU:OE1	2.21	0.41
2:E:400:LEU:HD11	2:E:460:VAL:HG12	2.03	0.41
2:E:414:VAL:HG13	2:E:414:VAL:O	2.21	0.41
1:A:111:ASP:HB2	1:A:113:LYS:HG2	2.02	0.41
1:A:433:VAL:HG22	1:A:512:VAL:HG13	2.02	0.41
1:A:570:ALA:HB1	1:B:963:VAL:HG11	2.02	0.41
1:B:48:LEU:CD2	1:B:278:LYS:HG3	2.51	0.41
1:B:55:PHE:HB2	1:B:275:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ILE:HG12	1:B:666:ILE:CD1	2.50	0.41
1:B:1009:THR:O	1:B:1013:ILE:HG12	2.20	0.41
1:C:45:SER:O	1:C:47:VAL:HG23	2.21	0.41
1:C:86:PHE:CD2	1:C:106:PHE:HE1	2.38	0.41
1:C:422:ASN:HD21	1:C:454:ARG:H	1.69	0.41
1:C:645:THR:HG22	1:C:647:ALA:H	1.86	0.41
1:C:724:THR:HB	1:C:934:ILE:HD12	2.03	0.41
2:D:29:PHE:CZ	2:D:79:LEU:HB2	2.50	0.41
2:D:38:ARG:HB2	2:D:48:VAL:CG2	2.51	0.41
2:D:312:ALA:HB3	2:D:315:LYS:H	1.86	0.41
2:D:400:LEU:HD11	2:D:460:VAL:HG12	2.03	0.41
2:E:156:LEU:HD23	2:E:210:LEU:O	2.20	0.41
2:E:170:VAL:HG21	2:E:208:ALA:HB2	2.01	0.41
2:F:18:LEU:HD12	2:F:19:ARG:H	1.85	0.41
2:F:170:VAL:HG21	2:F:208:ALA:HB2	2.01	0.41
3:G:11:LEU:HD13	3:G:124:THR:OG1	2.20	0.41
3:H:98:ARG:HB3	3:H:116:VAL:HG12	2.03	0.41
3:I:11:LEU:HD13	3:I:124:THR:OG1	2.20	0.41
1:A:376:THR:HB	1:A:435:ALA:HB3	2.03	0.41
1:A:448:ASN:HB3	1:A:497:PHE:HB2	2.02	0.41
1:A:456:PHE:HB3	1:A:473:TYR:CD2	2.55	0.41
1:B:238:PHE:C	1:B:239:GLN:HG3	2.41	0.41
1:B:353:TRP:HZ3	1:B:355:ARG:HB2	1.86	0.41
1:C:386:LYS:HD2	1:C:390:LEU:HD21	2.02	0.41
3:H:19:ARG:NE	3:H:80:TYR:HB3	2.33	0.41
1:A:30:ASN:HB3	1:A:32:PHE:HE1	1.86	0.40
1:A:45:SER:O	1:A:47:VAL:HG23	2.21	0.40
1:A:328:ARG:HH22	1:A:533:LEU:HD23	1.86	0.40
1:B:789:TYR:CE1	1:B:893:ALA:HB2	2.56	0.40
1:B:934:ILE:HA	1:B:934:ILE:HD13	1.85	0.40
1:C:943:SER:C	1:C:945:LEU:N	2.73	0.40
2:D:4:VAL:HG23	2:D:4:VAL:O	2.21	0.40
2:E:312:ALA:HB3	2:E:315:LYS:H	1.86	0.40
2:F:38:ARG:HB2	2:F:48:VAL:CG2	2.51	0.40
3:G:19:ARG:NE	3:G:80:TYR:HB3	2.33	0.40
3:G:40:ALA:HB3	3:G:43:LYS:HB2	2.04	0.40
3:H:158:ASP:C	3:H:189:LEU:HD12	2.42	0.40
1:A:140:PHE:HE1	1:A:258:TRP:CD1	2.39	0.40
1:A:318:PHE:HD1	1:A:593:GLY:O	2.05	0.40
1:A:422:ASN:HD21	1:A:454:ARG:H	1.68	0.40
1:B:497:PHE:CD2	1:B:507:PRO:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:H	1:B:569:ILE:HG12	1.65	0.40
1:B:607:GLN:OE1	1:B:691:SER:HA	2.21	0.40
1:B:715:PRO:HD3	1:C:894:LEU:HD13	2.02	0.40
1:B:1032:CYS:HB3	1:B:1051:SER:OG	2.22	0.40
1:B:1101:HIS:HE1	4:B:1309:NAG:H3	1.80	0.40
1:C:244:LEU:HD22	1:C:258:TRP:CD2	2.56	0.40
1:C:340:GLU:HG3	1:C:341:VAL:HG23	2.01	0.40
1:C:386:LYS:HB3	1:C:386:LYS:HE2	1.74	0.40
2:D:308:LEU:HD11	2:D:310:ILE:O	2.21	0.40
3:I:24:ALA:HB1	3:I:27:PHE:CZ	2.56	0.40
1:A:196:ASN:C	1:A:197:ILE:HD13	2.41	0.40
1:A:986:PRO:HD2	1:A:987:PRO:HD3	2.02	0.40
1:A:1142:GLN:O	1:A:1145:LEU:HB2	2.21	0.40
1:B:36:VAL:O	1:B:222:ALA:HA	2.21	0.40
1:B:386:LYS:HD2	1:B:390:LEU:HD21	2.03	0.40
1:B:426:PRO:O	1:B:429:PHE:HB2	2.21	0.40
1:B:767:LEU:HD21	1:B:1008:VAL:HG22	2.03	0.40
1:B:997:ILE:O	1:B:1001:LEU:HB2	2.22	0.40
1:C:433:VAL:HG22	1:C:512:VAL:HG13	2.03	0.40
2:D:24:ALA:HB3	2:D:29:PHE:CD1	2.57	0.40
2:E:24:ALA:HB3	2:E:29:PHE:CD1	2.57	0.40
2:E:191:ARG:HD3	2:E:199:PHE:O	2.21	0.40
2:E:389:LEU:HD13	2:E:447:LYS:HG3	2.04	0.40
2:F:385:SER:HB3	2:F:387:GLU:OE1	2.21	0.40
3:H:40:ALA:HB3	3:H:43:LYS:HB2	2.03	0.40
3:I:160:PHE:HA	3:I:161:PRO:HA	1.84	0.40
1:A:128:ILE:N	1:A:128:ILE:HD12	2.37	0.40
1:A:360:ASN:OD1	1:A:523:THR:HG21	2.22	0.40
1:B:30:ASN:HB3	1:B:32:PHE:CE1	2.56	0.40
1:B:422:ASN:HD21	1:B:453:TYR:HB2	1.87	0.40
1:B:884:SER:OG	1:B:888:PHE:HB3	2.22	0.40
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.84	0.40
1:C:25:PRO:O	1:C:27:ALA:N	2.53	0.40
1:C:37:TYR:HB3	1:C:223:LEU:HB2	2.03	0.40
1:C:855:PHE:H	1:C:855:PHE:HD1	1.70	0.40
2:D:414:VAL:HG13	2:D:417:ALA:HB3	2.02	0.40
2:E:38:ARG:HB2	2:E:48:VAL:CG2	2.51	0.40
2:F:414:VAL:HG13	2:F:414:VAL:O	2.21	0.40
3:G:24:ALA:HB1	3:G:27:PHE:CZ	2.57	0.40
3:G:158:ASP:C	3:G:189:LEU:HD12	2.42	0.40
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:36:TRP:NE1	3:I:81:LEU:HB2	2.37	0.40
1:A:130:VAL:O	1:A:130:VAL:HG22	2.20	0.40
1:B:140:PHE:CE1	1:B:258:TRP:CD1	3.10	0.40
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.54	0.40
1:B:563:GLN:NE2	1:C:43:PHE:HA	2.36	0.40
1:B:915:VAL:O	1:B:919:ASN:ND2	2.35	0.40
1:B:1001:LEU:HD12	1:B:1001:LEU:HA	1.96	0.40
1:B:1086:LYS:HB2	1:B:1086:LYS:HE2	1.92	0.40
1:C:30:ASN:HB3	1:C:32:PHE:CE1	2.57	0.40
1:C:135:PHE:HE1	1:C:139:PRO:CG	2.32	0.40
2:D:414:VAL:HG13	2:D:414:VAL:O	2.21	0.40
2:D:418:LEU:H	2:D:418:LEU:HD23	1.87	0.40
3:G:11:LEU:HD21	3:G:161:PRO:HD3	2.03	0.40
3:G:36:TRP:CD1	3:G:81:LEU:HD13	2.57	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	1019/1208 (84%)	954 (94%)	65 (6%)	0	100	100
1	B	1019/1208 (84%)	960 (94%)	59 (6%)	0	100	100
1	C	1019/1208 (84%)	954 (94%)	65 (6%)	0	100	100
2	D	435/478 (91%)	411 (94%)	24 (6%)	0	100	100
2	E	435/478 (91%)	412 (95%)	23 (5%)	0	100	100
2	F	435/478 (91%)	409 (94%)	26 (6%)	0	100	100
3	G	192/454 (42%)	184 (96%)	8 (4%)	0	100	100
3	H	192/454 (42%)	185 (96%)	7 (4%)	0	100	100
3	I	192/454 (42%)	182 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4938/6420 (77%)	4651 (94%)	287 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	909/1056 (86%)	887 (98%)	22 (2%)	49	76
1	B	909/1056 (86%)	894 (98%)	15 (2%)	60	83
1	C	909/1056 (86%)	900 (99%)	9 (1%)	76	90
2	D	369/381 (97%)	363 (98%)	6 (2%)	62	84
2	E	369/381 (97%)	364 (99%)	5 (1%)	67	86
2	F	369/381 (97%)	364 (99%)	5 (1%)	67	86
3	G	166/402 (41%)	162 (98%)	4 (2%)	49	76
3	H	166/402 (41%)	162 (98%)	4 (2%)	49	76
3	I	166/402 (41%)	162 (98%)	4 (2%)	49	76
All	All	4332/5517 (78%)	4258 (98%)	74 (2%)	62	83

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	130	VAL
1	A	141	LEU
1	A	170	TYR
1	A	185	ASN
1	A	205	SER
1	A	291	CYS
1	A	314	GLN
1	A	318	PHE
1	A	391	CYS

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Mol	Chain	Res	Type
1	A	541	PHE
1	A	552	LEU
1	A	580	GLN
1	A	586	ASP
1	A	654	GLU
1	A	671	CYS
1	A	703	ASN
1	A	755	GLN
1	A	823	PHE
1	A	994	ASP
1	A	1003	SER
1	A	1123	SER
1	B	99	ASN
1	B	104	TRP
1	B	125	ASN
1	B	135	PHE
1	B	141	LEU
1	B	168	PHE
1	B	173	GLN
1	B	200	TYR
1	B	298	GLU
1	B	391	CYS
1	B	580	GLN
1	B	737	ASP
1	B	904	TYR
1	B	1055	SER
1	B	1123	SER
1	C	125	ASN
1	C	135	PHE
1	C	141	LEU
1	C	200	TYR
1	C	357	ARG
1	C	391	CYS
1	C	580	GLN
1	C	867	ASP
1	C	950	ASP
2	D	73	ASP
2	D	318	SER
2	D	325	SER
2	D	387	GLU
2	D	406	ARG
2	D	440	SER

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Mol	Chain	Res	Type
2	E	73	ASP
2	E	318	SER
2	E	325	SER
2	E	406	ARG
2	E	440	SER
2	F	73	ASP
2	F	318	SER
2	F	325	SER
2	F	406	ARG
2	F	440	SER
3	G	49	SER
3	G	53	SER
3	G	62	ASP
3	G	108	GLN
3	H	49	SER
3	H	53	SER
3	H	62	ASP
3	H	108	GLN
3	I	49	SER
3	I	53	SER
3	I	62	ASP
3	I	108	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	354	ASN
1	A	616	ASN
1	A	762	GLN
1	A	901	GLN
1	A	955	ASN
1	A	1106	GLN
1	A	1108	ASN
1	A	1119	ASN
1	B	125	ASN
1	B	173	GLN
1	B	354	ASN
1	B	606	ASN
1	B	613	GLN
1	B	616	ASN
1	B	955	ASN

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Mol	Chain	Res	Type
1	B	965	GLN
1	B	1054	GLN
1	B	1106	GLN
1	C	99	ASN
1	C	125	ASN
1	C	134	GLN
1	C	196	ASN
1	C	354	ASN
1	C	544	ASN
1	C	613	GLN
1	C	901	GLN
1	C	1106	GLN
2	D	168	ASN
2	D	289	ASN
2	D	358	ASN
2	D	388	GLN
2	E	289	ASN
2	E	358	ASN
2	E	388	GLN
2	F	289	ASN
2	F	358	ASN
2	F	388	GLN
3	G	108	GLN
3	H	108	GLN
3	I	108	GLN
3	I	178	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

32 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	B	1311	-	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	C	1408	1	14,14,15	0.67	1 (7%)	17,19,21	1.03	2 (11%)
4	NAG	A	1308	1	14,14,15	0.46	0	17,19,21	0.95	1 (5%)
4	NAG	C	1401	1	14,14,15	0.38	0	17,19,21	0.60	0
4	NAG	B	1303	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.74	0
4	NAG	C	1404	1	14,14,15	0.34	0	17,19,21	0.73	0
4	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.64	0
4	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	C	1409	1	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	B	1307	1	14,14,15	0.30	0	17,19,21	0.66	0
4	NAG	B	1301	1	14,14,15	0.36	0	17,19,21	0.64	0
4	NAG	A	1307	1	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	C	1407	1	14,14,15	0.93	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	C	1406	1	14,14,15	0.33	0	17,19,21	0.61	0
4	NAG	B	1309	1	14,14,15	0.29	0	17,19,21	0.82	0
4	NAG	C	1403	1	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	B	1308	1	14,14,15	0.83	1 (7%)	17,19,21	1.13	1 (5%)
4	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	A	1311	-	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.63	0
4	NAG	C	1405	1	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
4	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.71	0
4	NAG	C	1410	-	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	A	1310	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	C	1402	1	14,14,15	0.89	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.77	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	B	1311	-	-	5/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1410	-	-	5/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1407	NAG	C1-C2	3.29	1.57	1.52
4	C	1402	NAG	C1-C2	3.02	1.56	1.52
4	B	1308	NAG	C1-C2	2.91	1.56	1.52
4	C	1408	NAG	C1-C2	2.29	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1308	NAG	C4-C3-C2	-3.49	105.91	111.02
4	C	1407	NAG	C4-C3-C2	-3.31	106.17	111.02
4	A	1308	NAG	O5-C1-C2	-2.28	107.68	111.29
4	C	1405	NAG	C4-C3-C2	-2.25	107.72	111.02
4	C	1402	NAG	C2-N2-C7	-2.08	119.94	122.90
4	C	1408	NAG	C6-C5-C4	-2.08	108.13	113.00
4	C	1408	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C3-C2-N2-C7
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	A	1306	NAG	C8-C7-N2-C2
4	A	1306	NAG	O7-C7-N2-C2
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	A	1309	NAG	C8-C7-N2-C2
4	A	1309	NAG	O7-C7-N2-C2
4	A	1310	NAG	C8-C7-N2-C2
4	A	1310	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1311	NAG	C3-C2-N2-C7
4	A	1311	NAG	C8-C7-N2-C2
4	A	1311	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	B	1310	NAG	C8-C7-N2-C2
4	B	1310	NAG	O7-C7-N2-C2
4	B	1311	NAG	C3-C2-N2-C7
4	B	1311	NAG	C8-C7-N2-C2
4	B	1311	NAG	O7-C7-N2-C2
4	C	1402	NAG	C3-C2-N2-C7
4	C	1402	NAG	C8-C7-N2-C2
4	C	1402	NAG	O7-C7-N2-C2
4	C	1403	NAG	C3-C2-N2-C7
4	C	1403	NAG	C8-C7-N2-C2
4	C	1403	NAG	O7-C7-N2-C2
4	C	1404	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	C	1406	NAG	O7-C7-N2-C2
4	C	1408	NAG	C8-C7-N2-C2
4	C	1408	NAG	O7-C7-N2-C2
4	C	1409	NAG	C8-C7-N2-C2
4	C	1409	NAG	O7-C7-N2-C2
4	C	1410	NAG	C3-C2-N2-C7
4	C	1410	NAG	C8-C7-N2-C2
4	C	1410	NAG	O7-C7-N2-C2
4	C	1404	NAG	C8-C7-N2-C2
4	C	1406	NAG	C8-C7-N2-C2
4	B	1310	NAG	C1-C2-N2-C7
4	C	1409	NAG	C1-C2-N2-C7
4	A	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	C1-C2-N2-C7
4	A	1310	NAG	C1-C2-N2-C7
4	B	1302	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	O7-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	A	1305	NAG	C1-C2-N2-C7
4	B	1304	NAG	C1-C2-N2-C7
4	B	1308	NAG	O7-C7-N2-C2
4	B	1305	NAG	C1-C2-N2-C7
4	A	1311	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	C	1410	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	A	1303	NAG	C8-C7-N2-C2
4	B	1305	NAG	C3-C2-N2-C7
4	B	1311	NAG	C1-C2-N2-C7
4	B	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	A	1311	NAG	C1-C2-N2-C7
4	C	1410	NAG	C1-C2-N2-C7
4	B	1303	NAG	O7-C7-N2-C2
4	C	1403	NAG	C1-C2-N2-C7
4	A	1304	NAG	C1-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1408	NAG	1	0
4	A	1308	NAG	2	0
4	A	1306	NAG	1	0
4	B	1301	NAG	1	0
4	B	1309	NAG	2	0
4	A	1311	NAG	1	0
4	A	1301	NAG	1	0
4	B	1304	NAG	1	0
4	C	1402	NAG	1	0
4	A	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

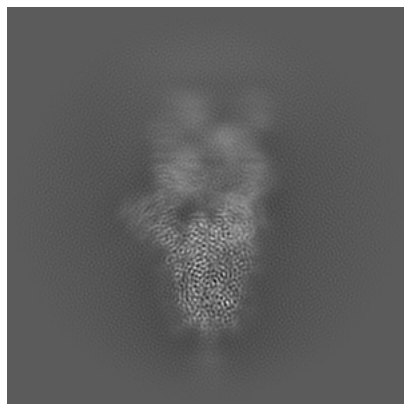
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33734. These allow visual inspection of the internal detail of the map and identification of artifacts.

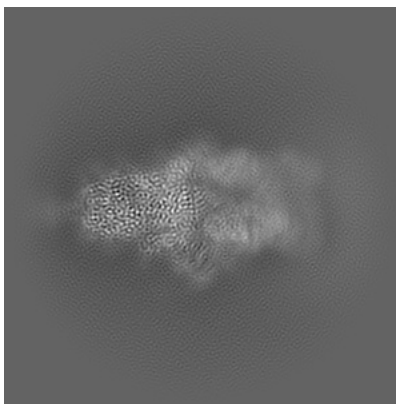
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

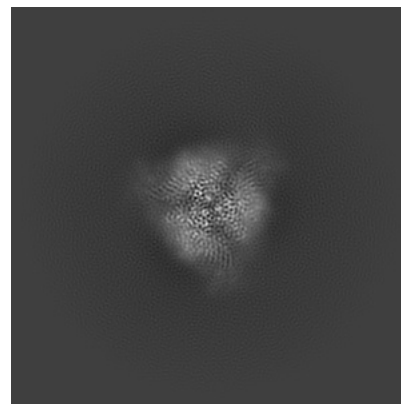
6.1.1 Primary map



X

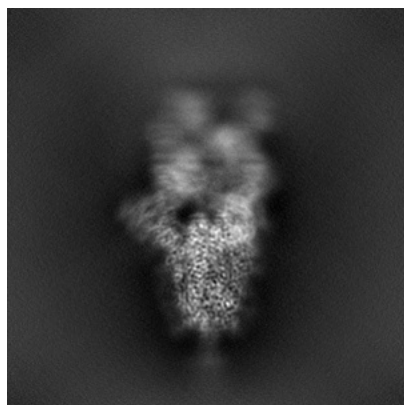


Y

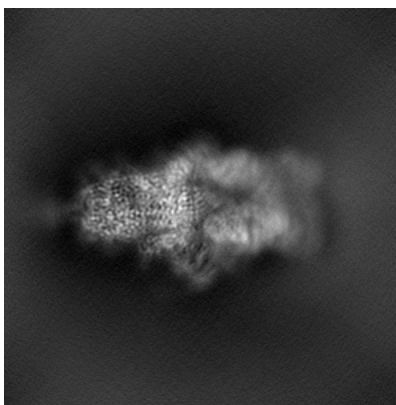


Z

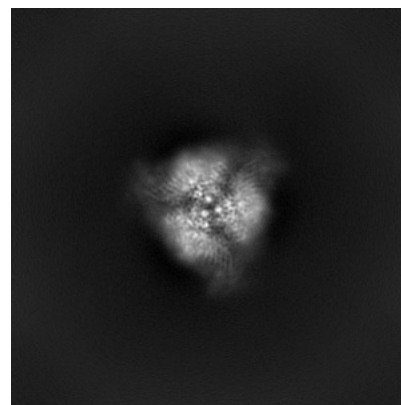
6.1.2 Raw map



X



Y

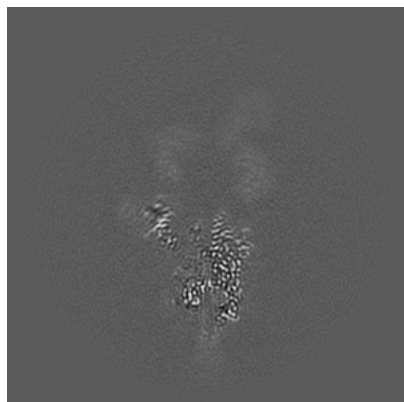


Z

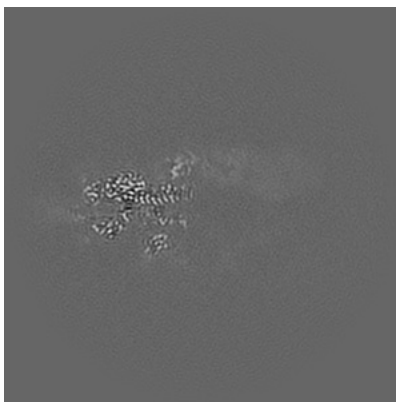
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

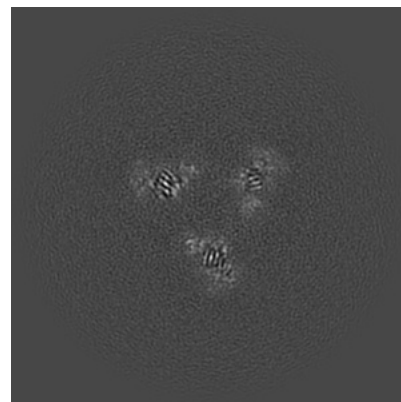
6.2.1 Primary map



X Index: 200

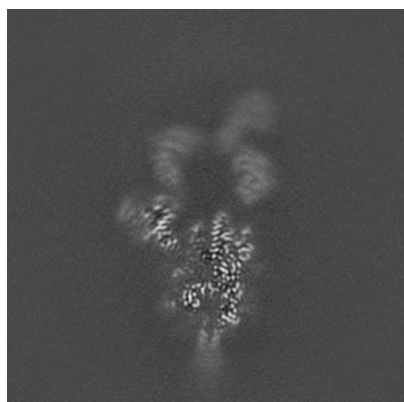


Y Index: 200

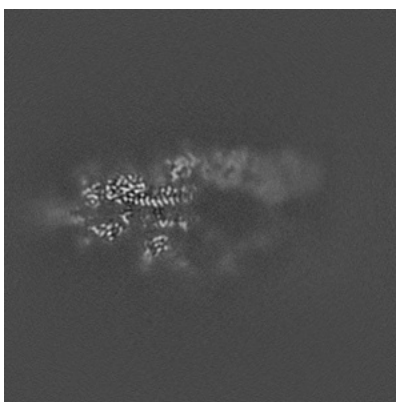


Z Index: 200

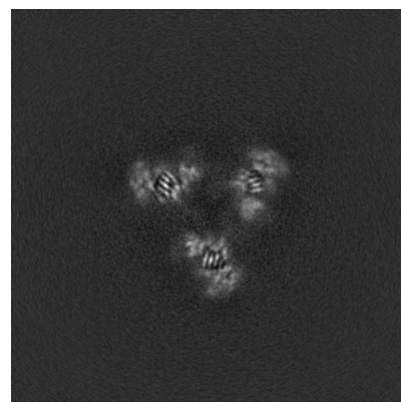
6.2.2 Raw map



X Index: 200



Y Index: 200

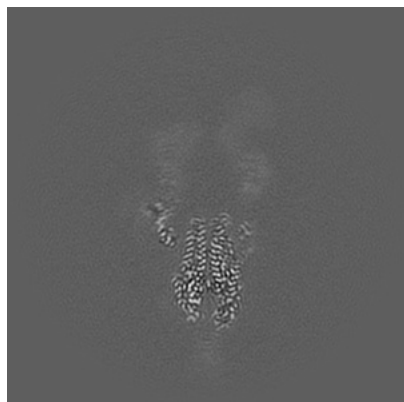


Z Index: 200

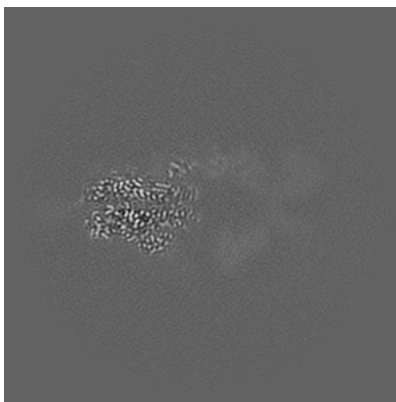
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

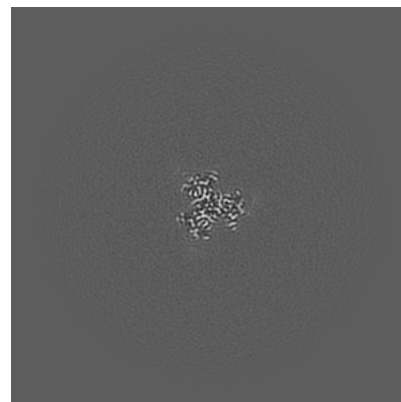
6.3.1 Primary map



X Index: 195

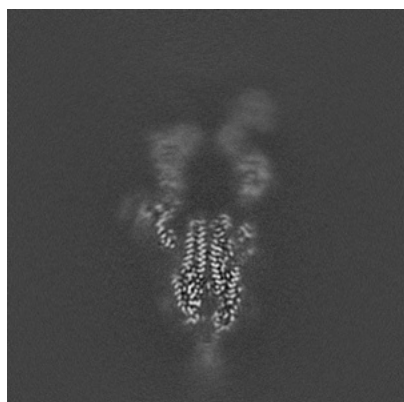


Y Index: 191

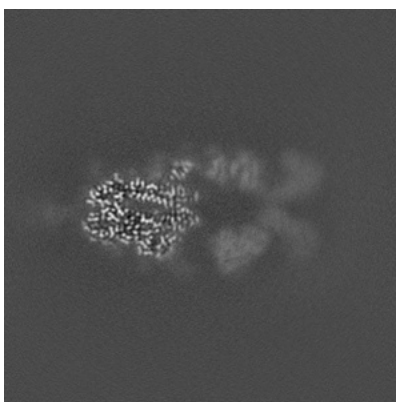


Z Index: 122

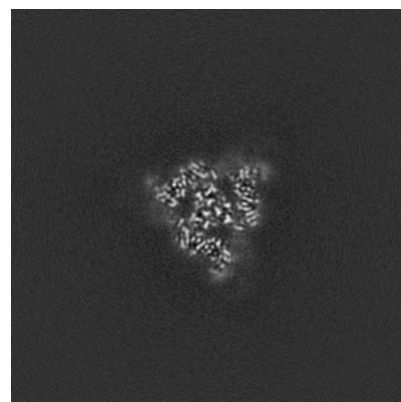
6.3.2 Raw map



X Index: 195



Y Index: 188

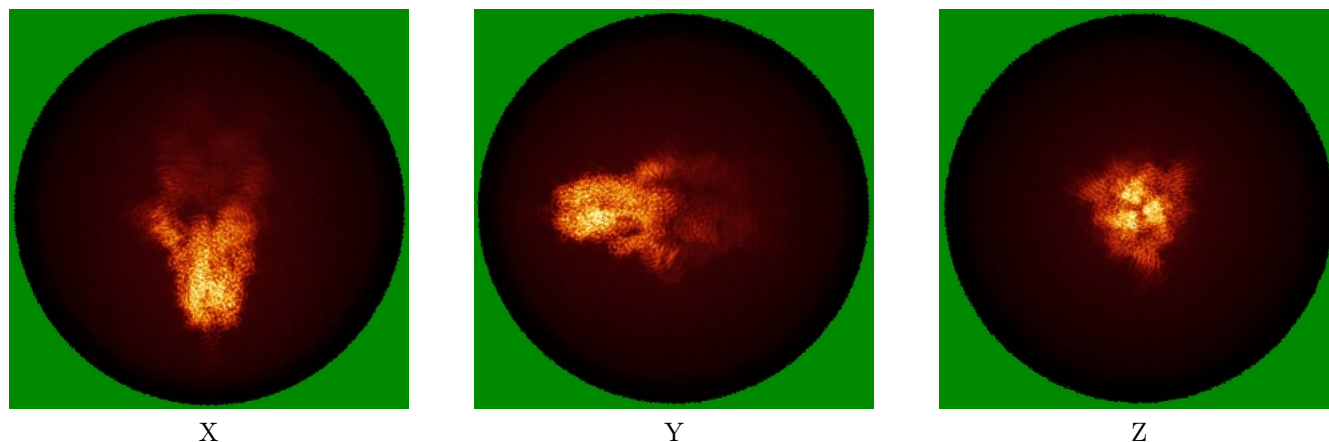


Z Index: 169

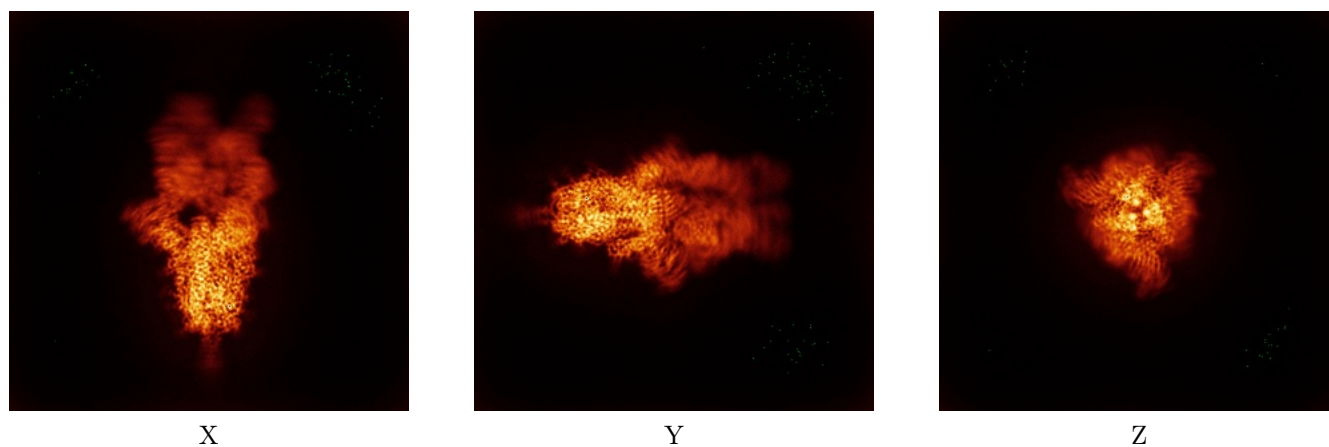
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



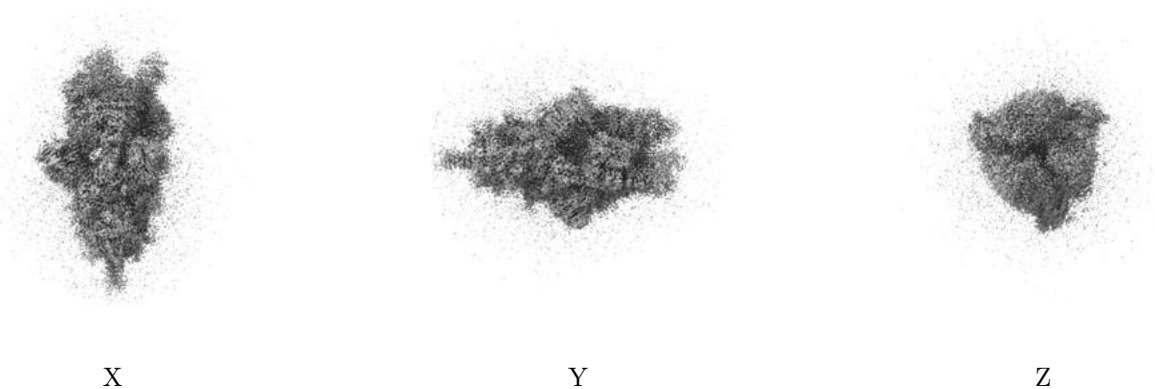
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

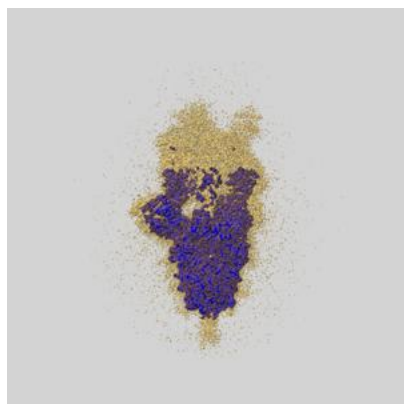
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

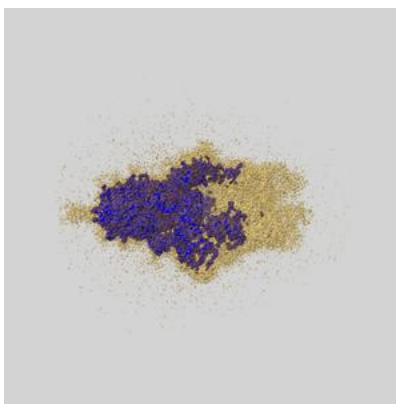
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

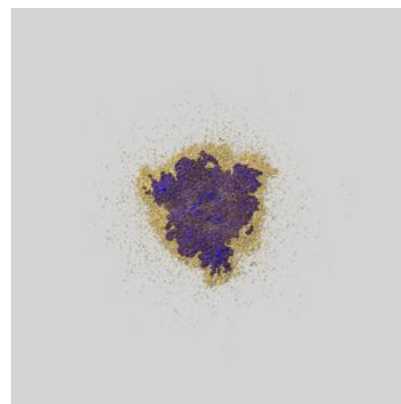
6.6.1 emd_33734_msk_1.map [i](#)



X



Y

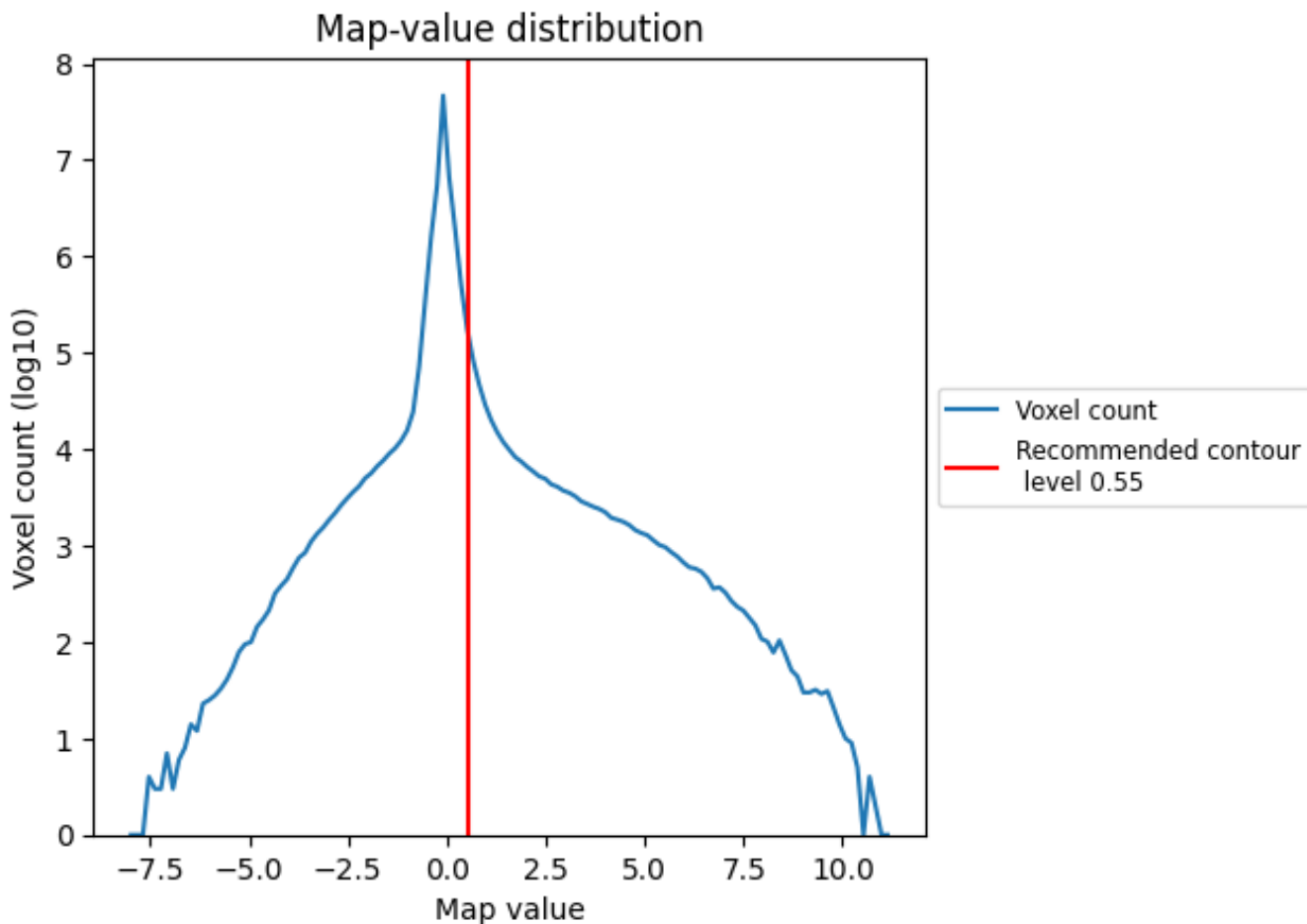


Z

7 Map analysis [i](#)

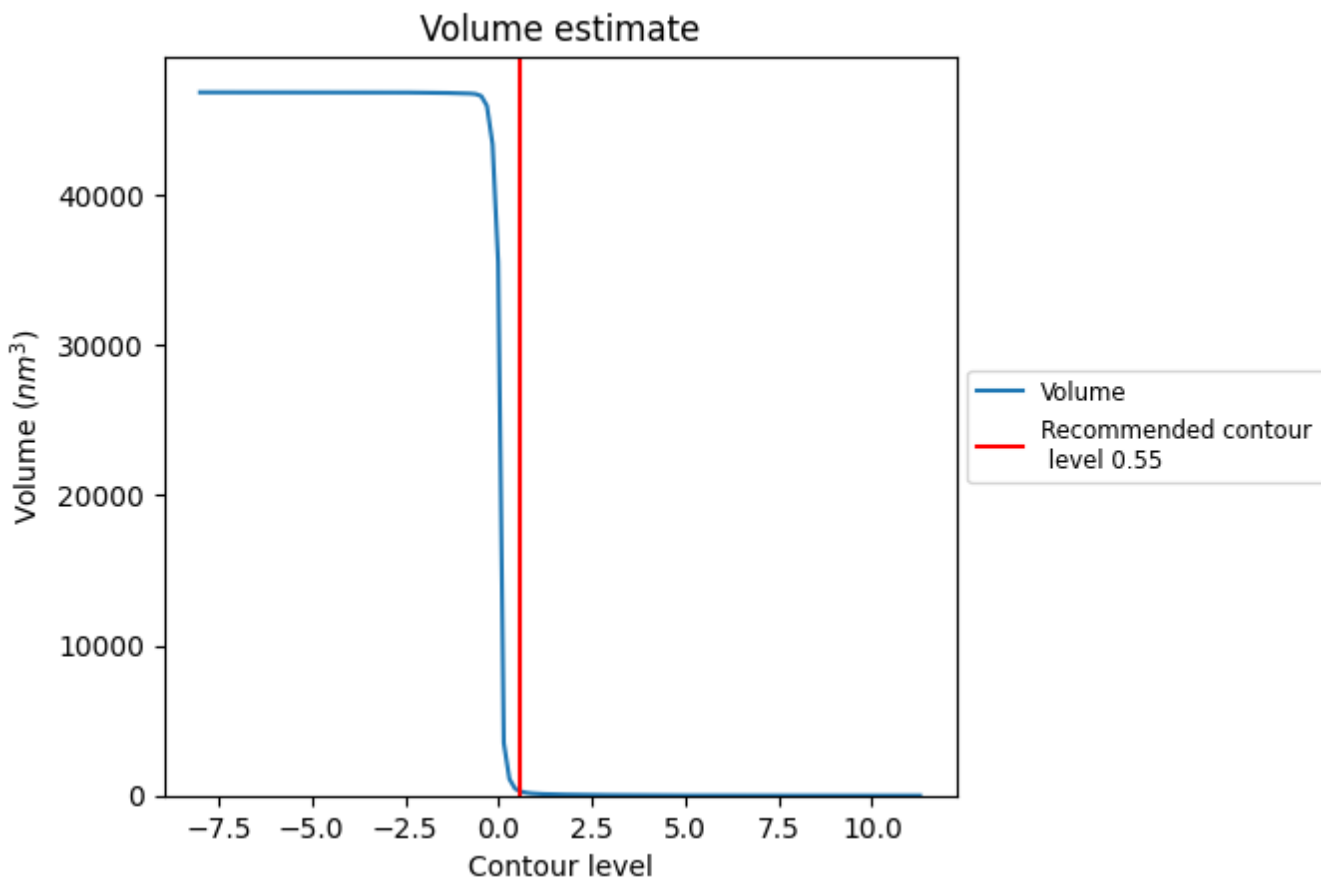
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

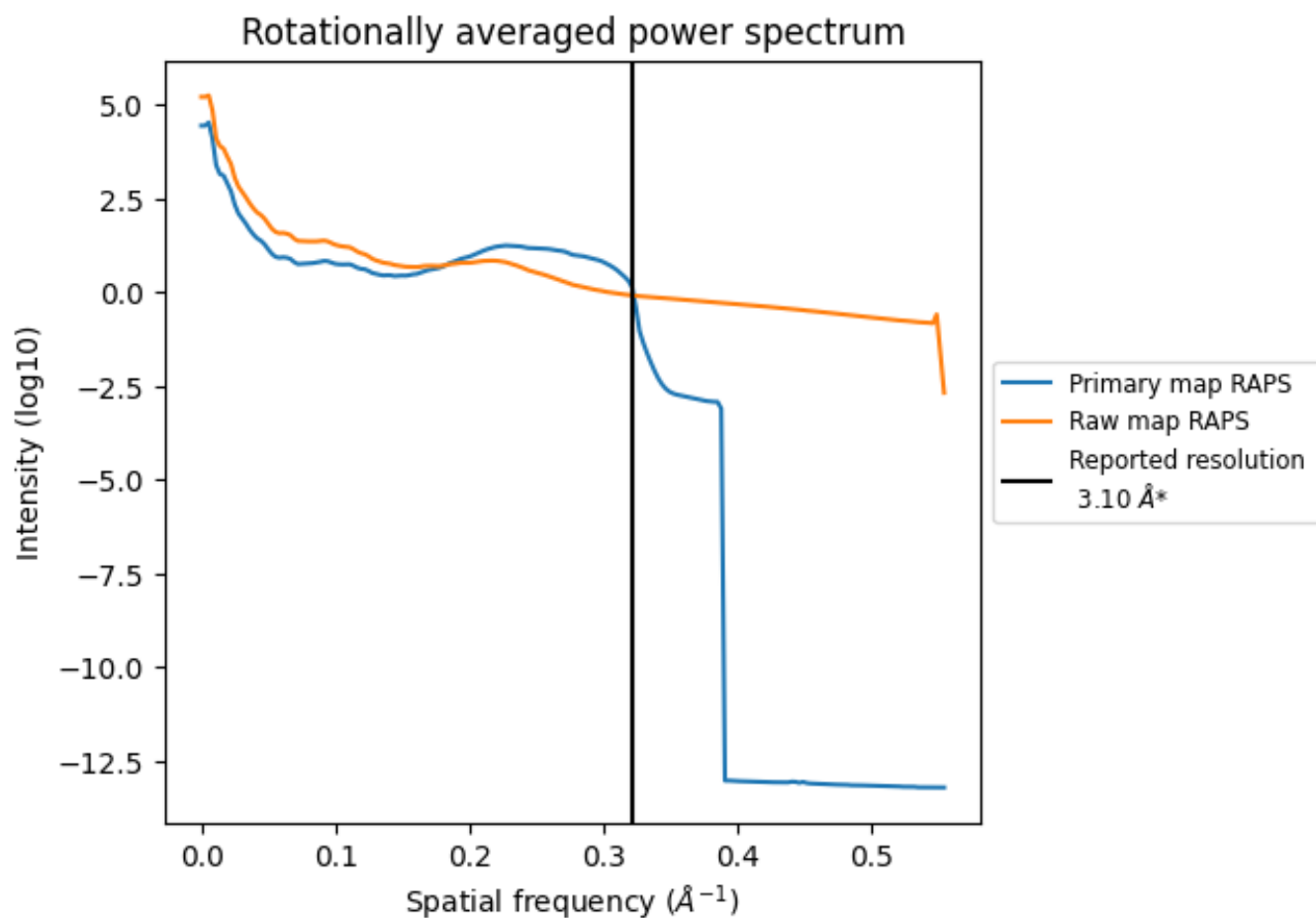
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm^3 ; this corresponds to an approximate mass of 295 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](#)

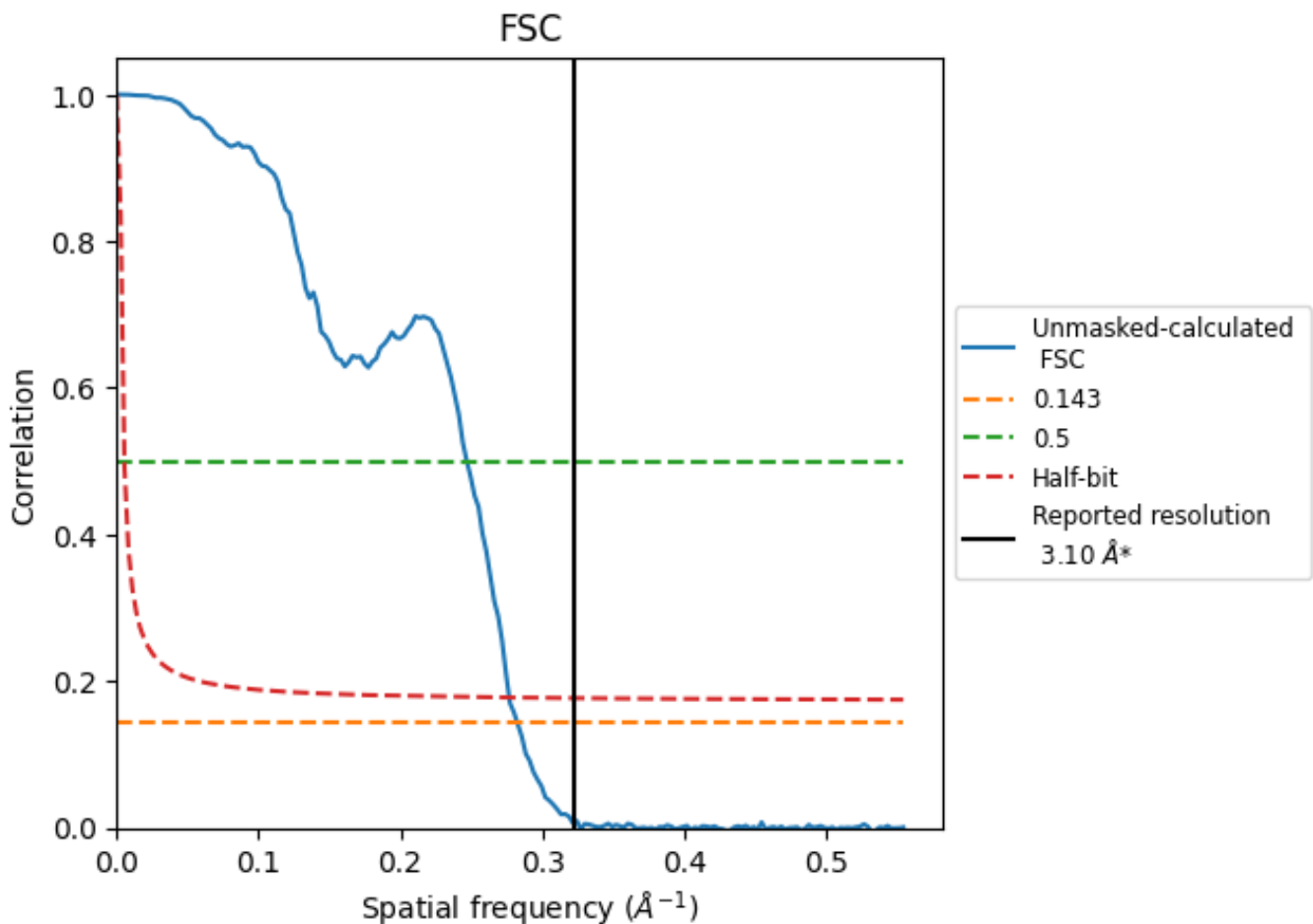


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

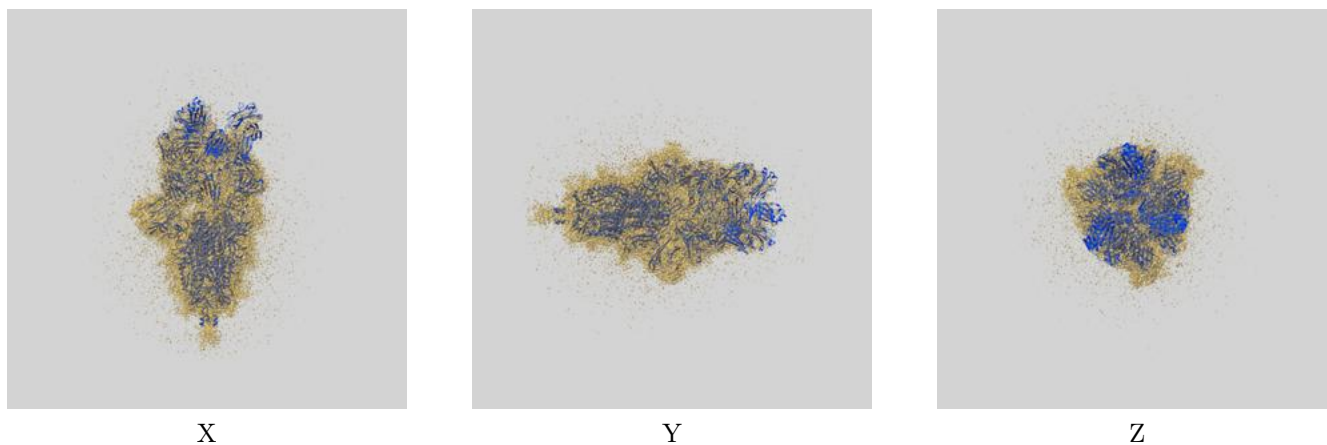
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.05	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

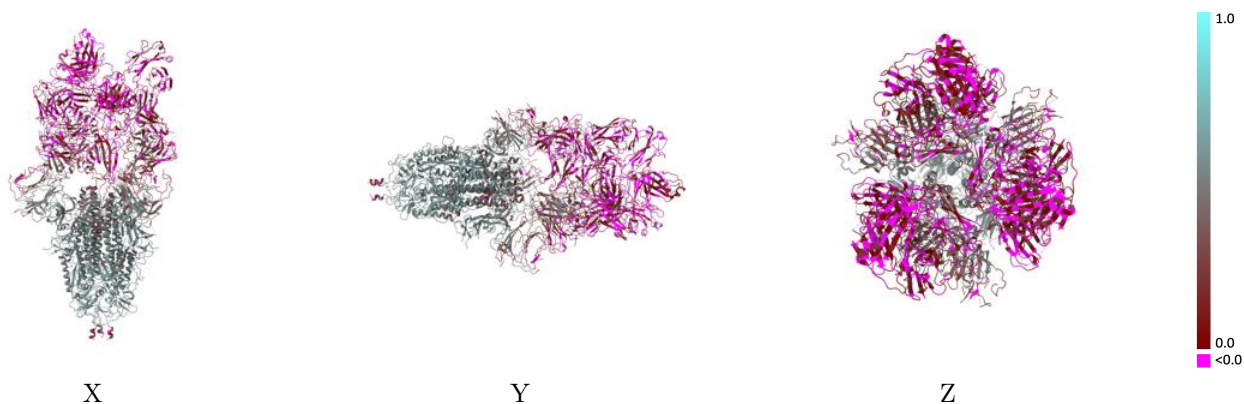
This section contains information regarding the fit between EMDB map EMD-33734 and PDB model 7YC5. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



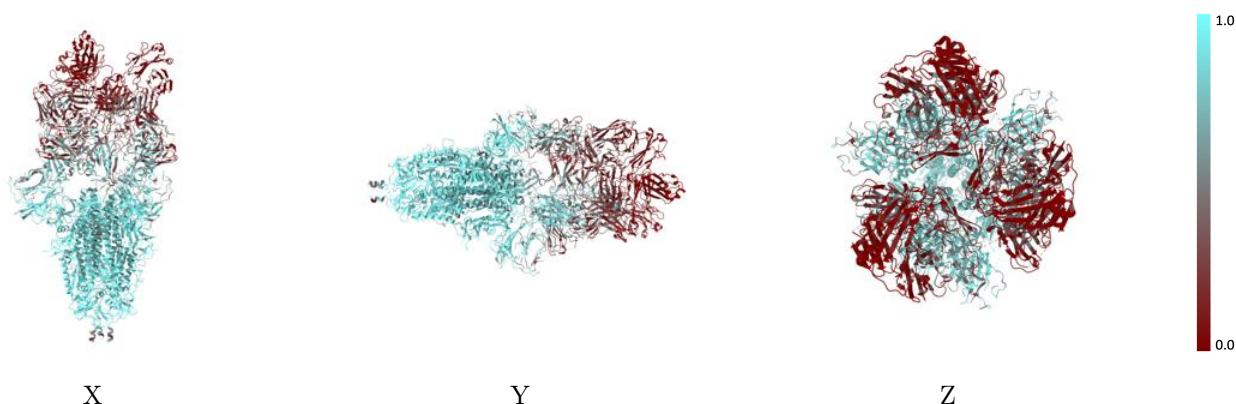
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



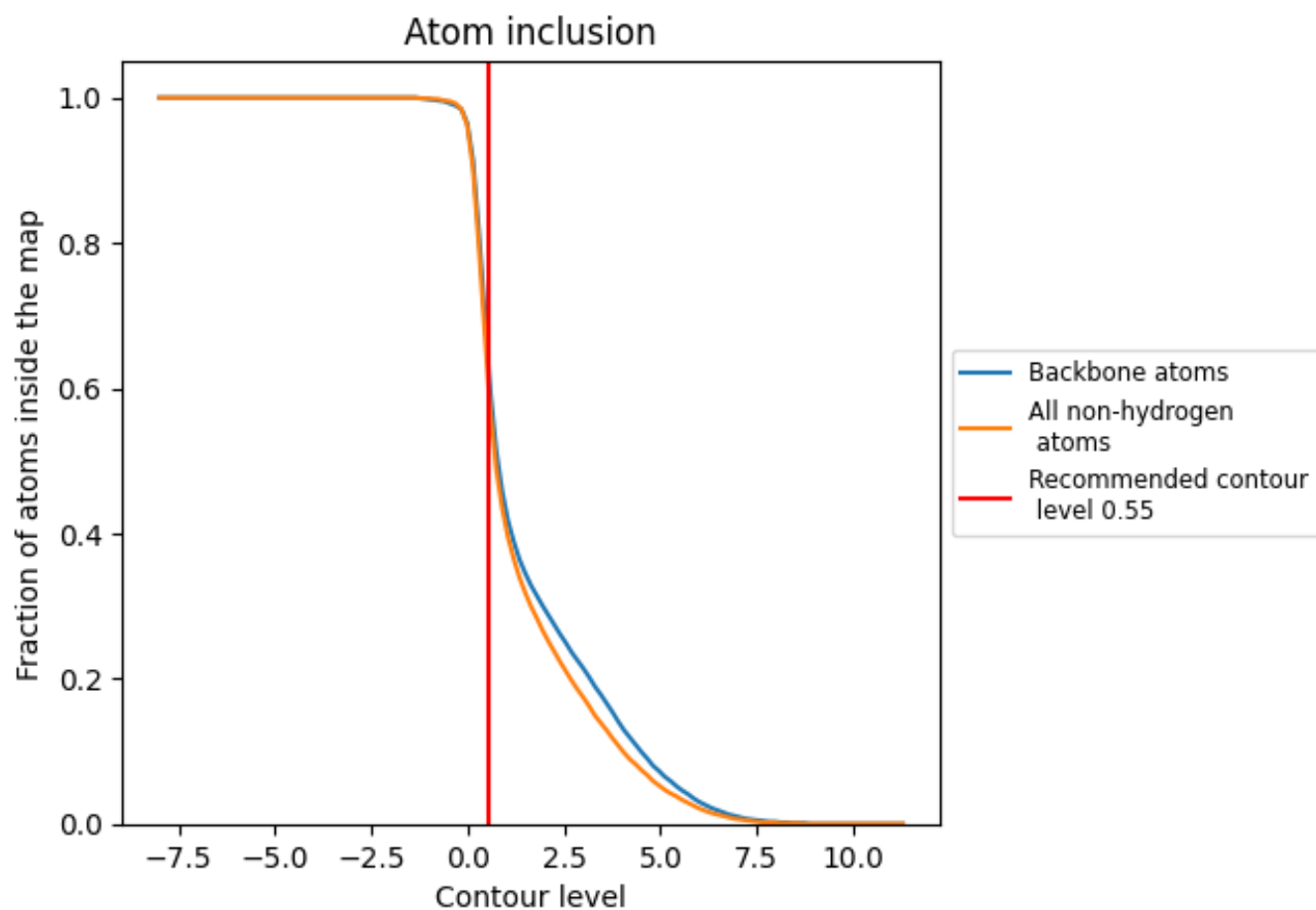
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.2840
A	 0.7820	 0.3930
B	 0.8100	 0.4220
C	 0.8270	 0.4380
D	 0.2330	 0.0450
E	 0.2560	 0.0680
F	 0.2830	 0.0680
G	 0.1730	 0.0320
H	 0.1460	 0.0350
I	 0.2060	 0.0580

