



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:00 AM UTC

PDB ID : 7YC5 / pdb_00007yc5
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:

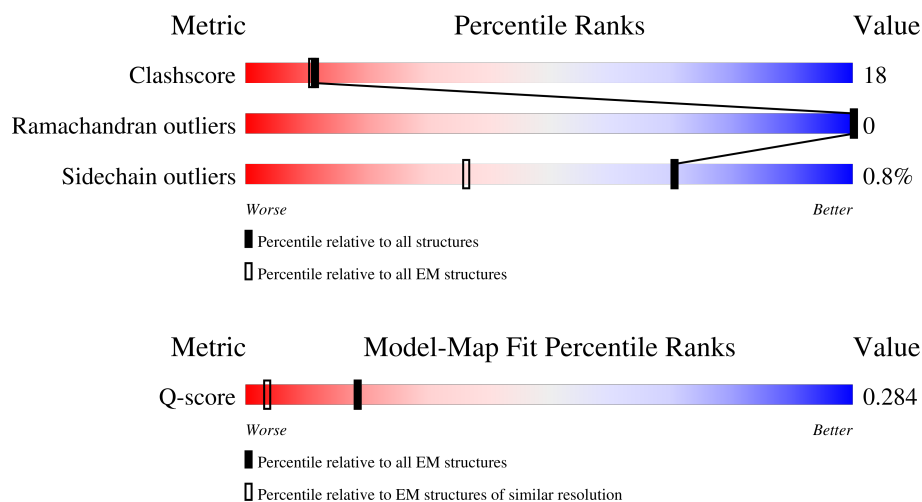
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	9% 56% 29% 14%
1	B	1208	5% 53% 32% 14%
1	C	1208	• 55% 30% 14%
2	D	478	71% 63% 29% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	478	68%65%27%8%
2	F	478	64%64%28%8%
3	G	454	37%26%17%56%
3	H	454	39%27%16%56%
3	I	454	36%25%18%56%



2 Entry composition

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
1	A	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		
1	B	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		
1	C	1037	Total	C	N	O	S	0	0
			8094	5170	1343	1545	36		

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

Continued on next page...

Continued from previous page...

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

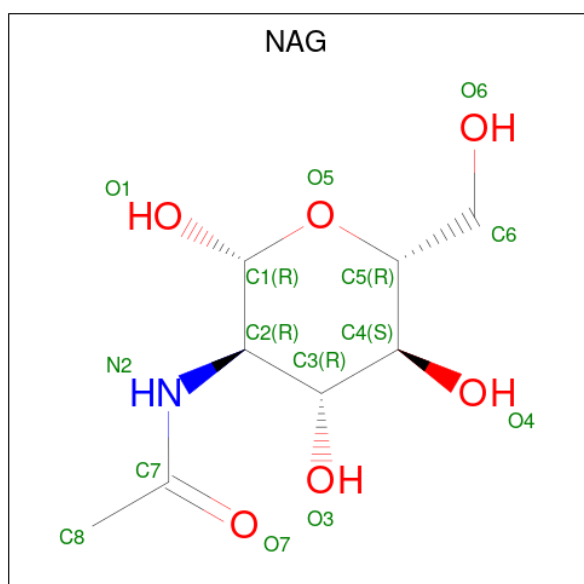
- Molecule 2 is a protein called Bispecific anitybody (scFv and light chain of the antibody).

Mol	Chain	Residues	Atoms					AltConf	Trace
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 antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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	

Continued on next page...

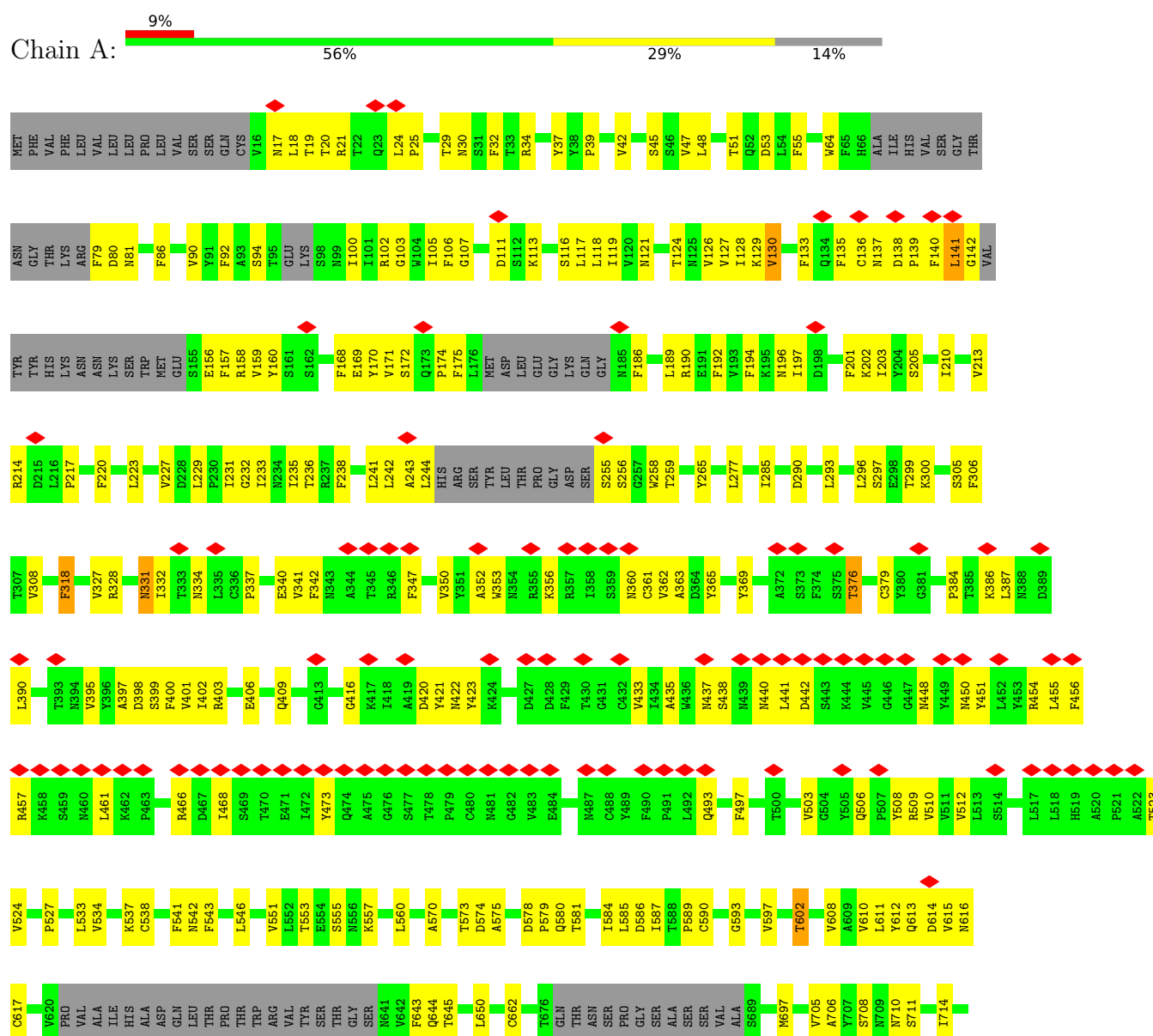
Continued from previous page...

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

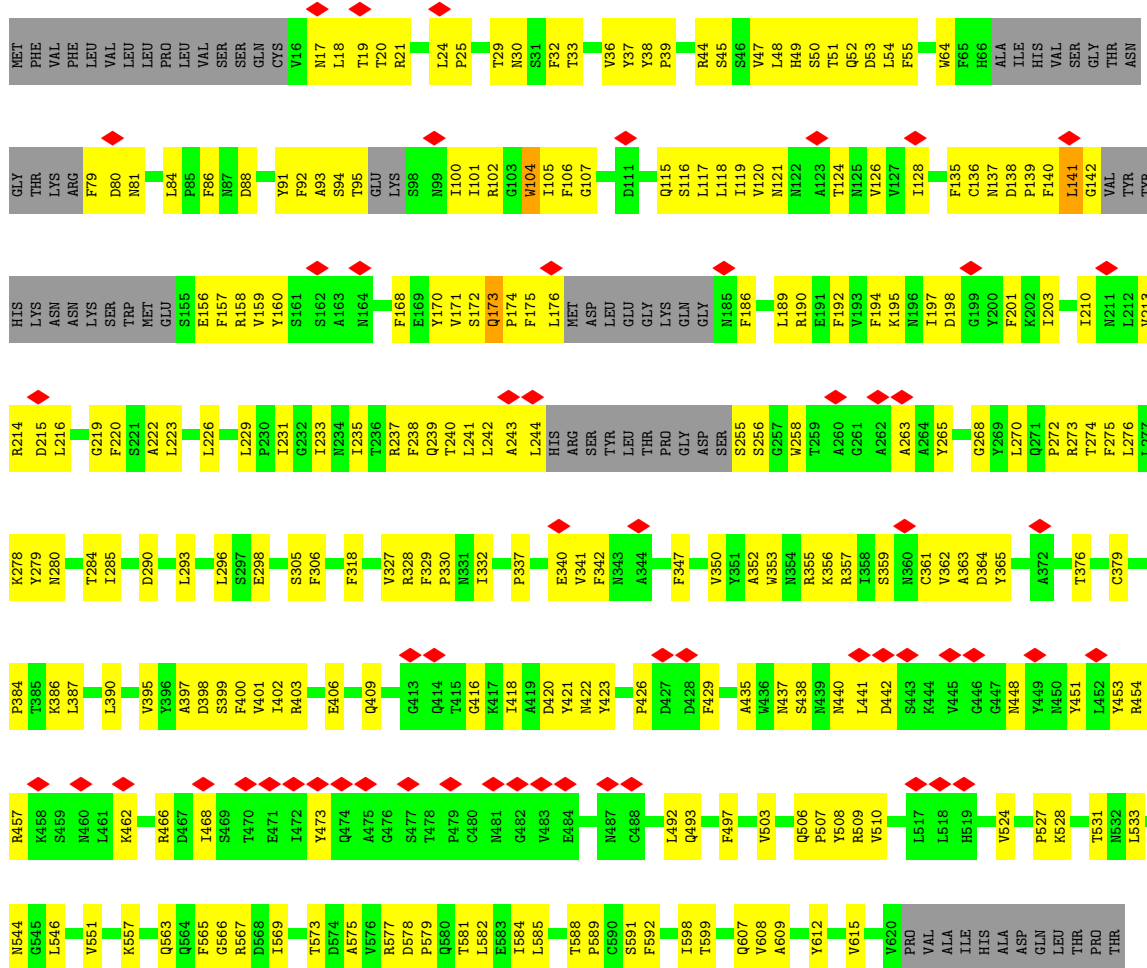
3 Residue-property plots

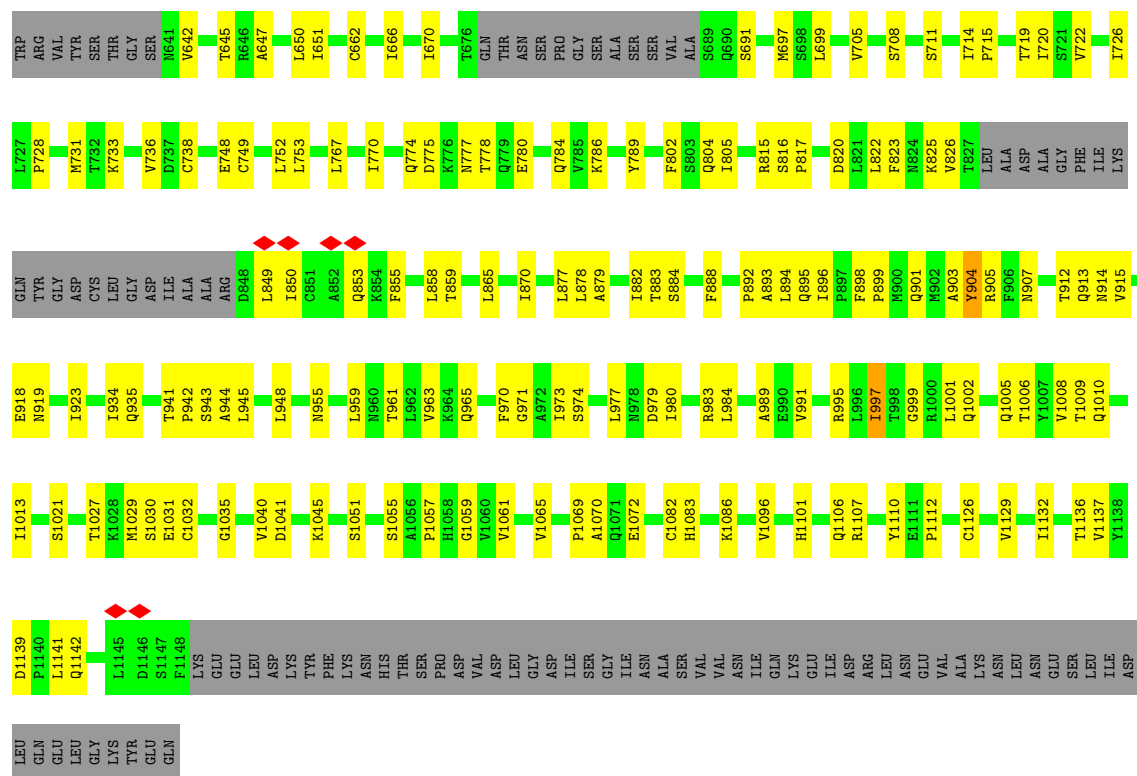
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

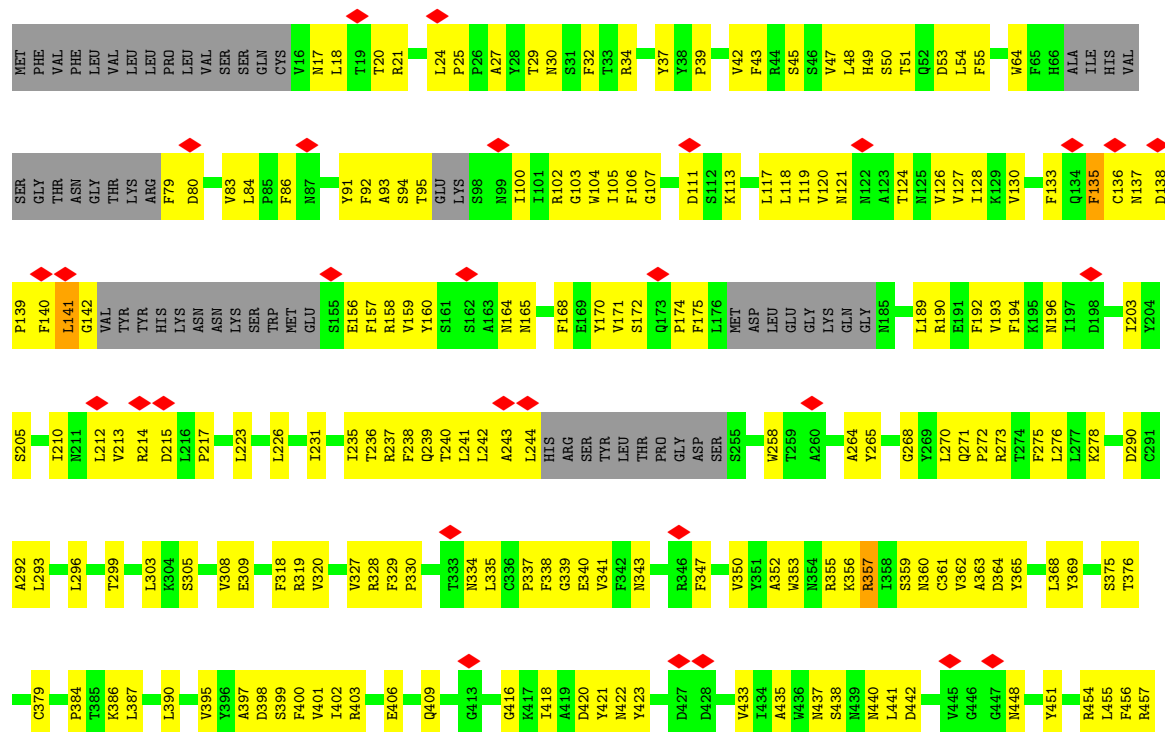


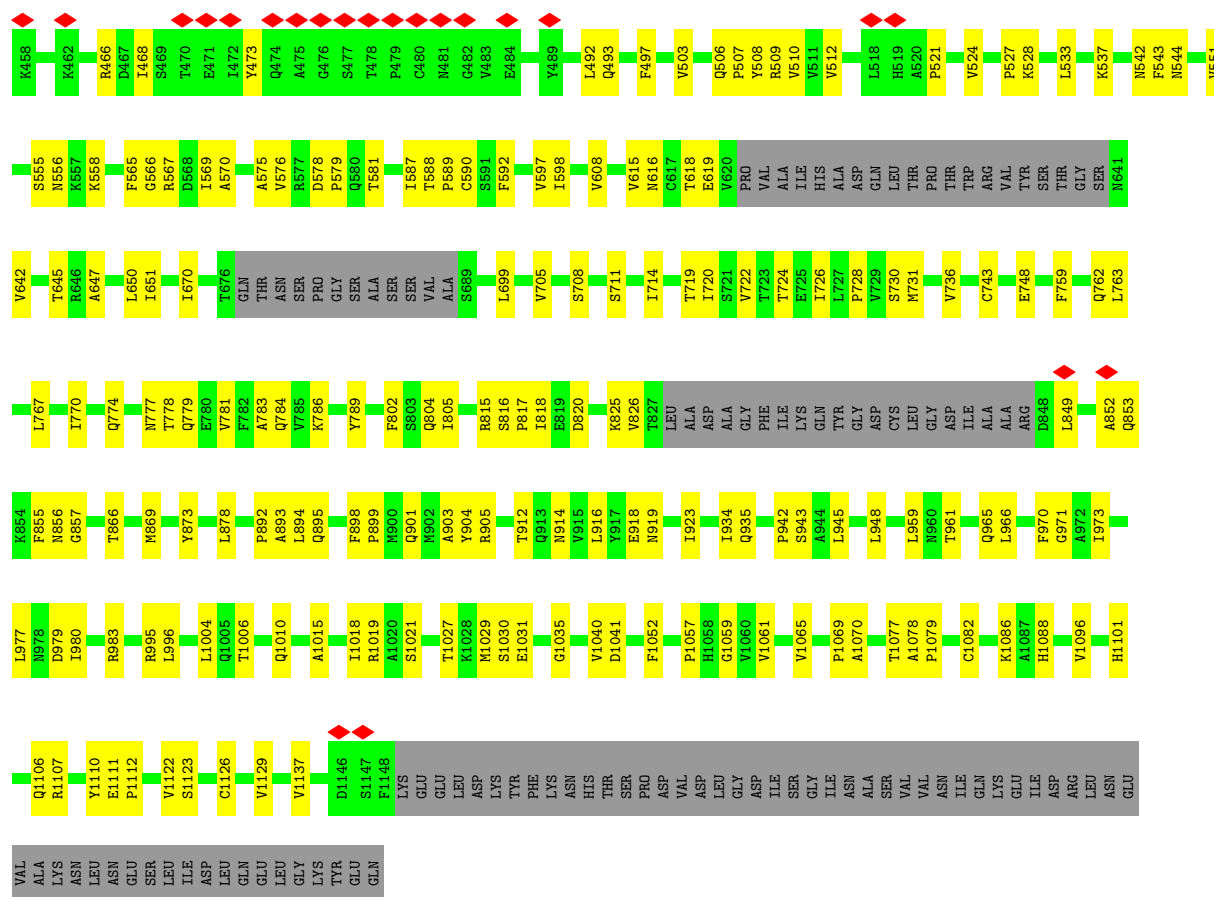
- Molecule 1: Spike glycoprotein



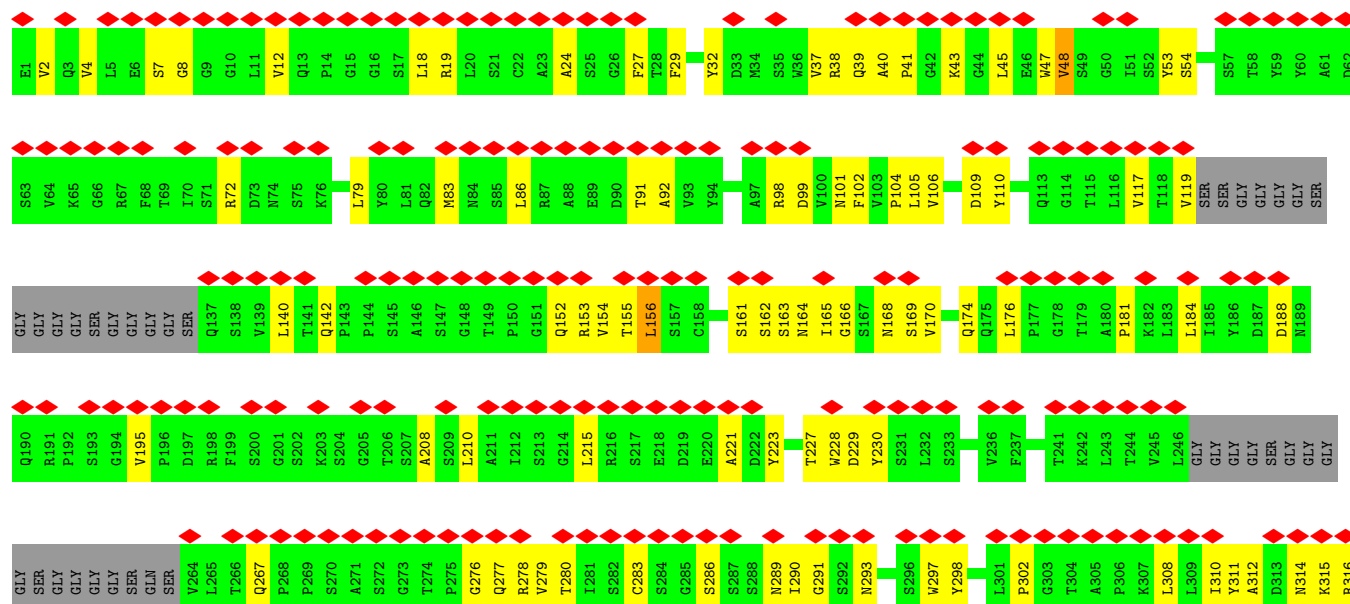


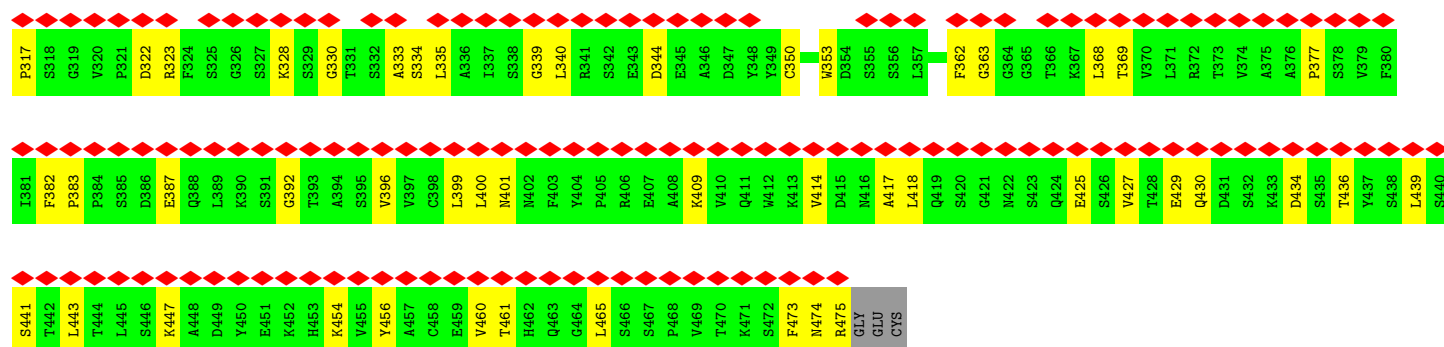
• Molecule 1: Spike glycoprotein



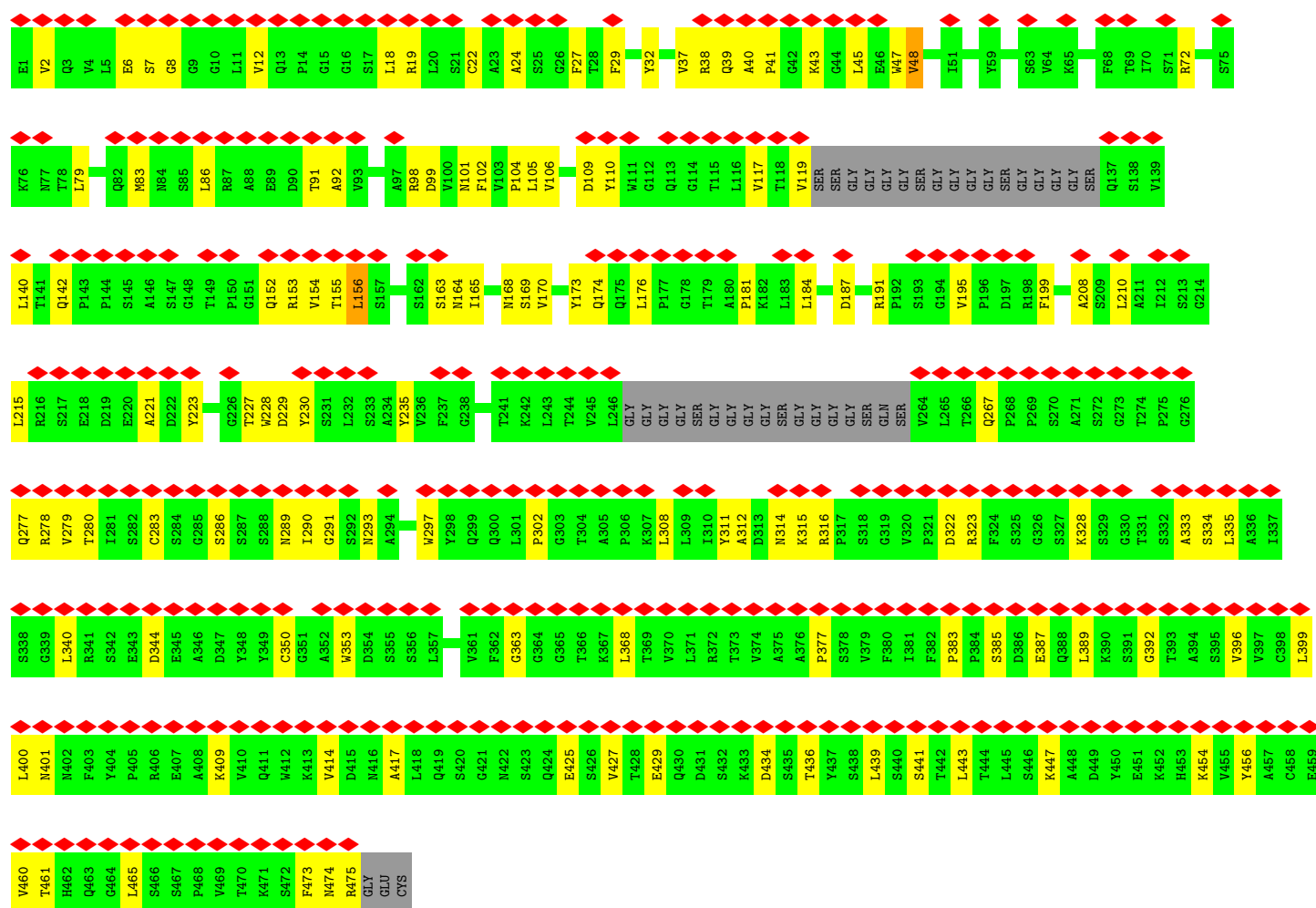


• Molecule 2: Bispecific antibody (scFv and light chain of the antibody)





• Molecule 2: Bispecific anitybody (scFv and light chain of the antibody)

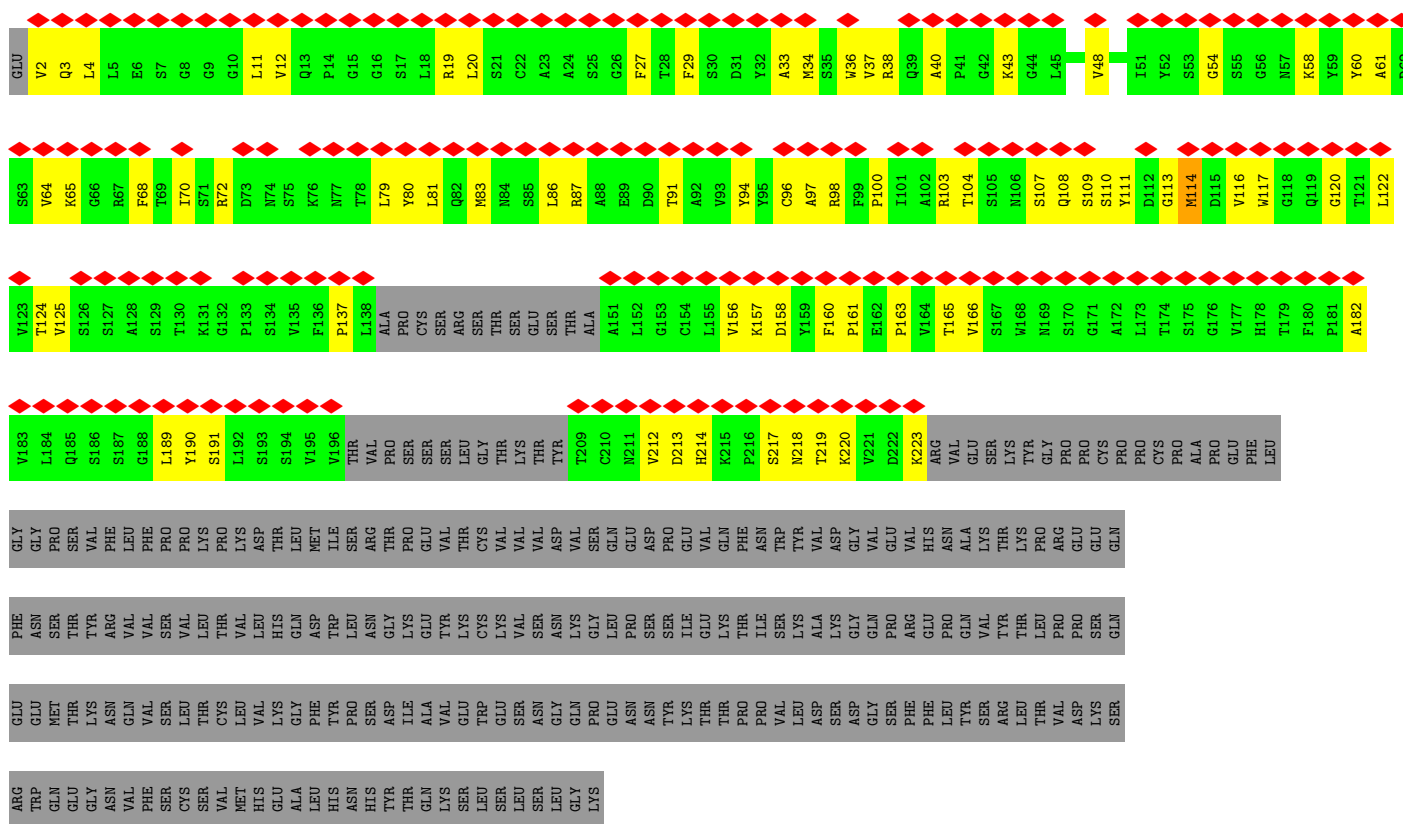


• Molecule 2: Bispecific anitybody (scFv and light chain of the antibody)

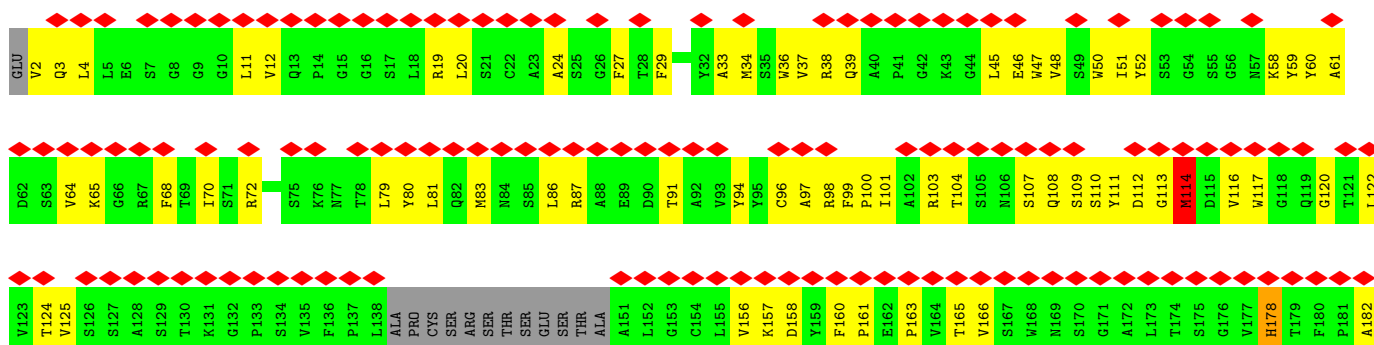




- Molecule 3: Heavy chain from K202.B antibody



- Molecule 3: Heavy chain from K202.B antibody



[illegible]

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 ($\text{\AA}$)	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 ($\text{\AA}$)	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	0.42	0/8280	0.57	1/11274 (0.0%)
1	B	0.43	0/8280	0.57	2/11274 (0.0%)
1	C	0.42	0/8280	0.55	0/11274
2	D	0.26	0/3386	0.41	0/4606
2	E	0.18	0/3386	0.37	0/4606
2	F	0.20	0/3386	0.37	0/4606
3	G	0.42	0/1531	0.59	1/2080 (0.0%)
3	H	0.34	0/1531	0.54	1/2080 (0.0%)
3	I	0.44	0/1531	0.61	1/2080 (0.0%)
All	All	0.38	0/39591	0.53	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	B	544	ASN	CB-CA-C	-5.84	109.82	116.54
1	A	331	ASN	CB-CA-C	5.63	118.28	109.84
3	G	114	MET	N-CA-C	-5.18	101.69	109.15
1	B	456	PHE	N-CA-C	5.16	117.05	108.02
3	H	114	MET	N-CA-C	-5.09	101.82	109.15
3	I	114	MET	N-CA-C	-5.08	101.84	109.15

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	314	0
1	B	8094	0	7883	358	0
1	C	8094	0	7884	325	0
2	D	3313	0	3186	111	0
2	E	3313	0	3186	88	0
2	F	3313	0	3186	102	0
3	G	1496	0	1446	59	0
3	H	1496	0	1446	47	0
3	I	1496	0	1446	56	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	1380	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 18.

All (1380) 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:308:VAL:H	1:A:602:THR:HG1	1.46	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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:731:MET:HE2	1:A:774:GLN:NE2	2.17	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: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

Continued on next page...

Continued from previous page...

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
1:A:731:MET:HE2	1:A:774:GLN:HE21	1.69	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:C:618:THR:OG1	1:C:619:GLU:OE1	2.23	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:LEU:HD23	2:E:156:LEU:H	1.71	0.56
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:83:MET:HE1	2:D:117:VAL:HG11	1.88	0.56
2:D:184:LEU:HA	2:D:195:VAL:HG21	1.88	0.56
2:F:362:PHE:HZ	3:I:114:MET:HE1	1.70	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:PHE:C	1:B:235:ILE:HD11	2.31	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:E:83:MET:HE1	2:E:117:VAL:HG11	1.88	0.55
2:F:83:MET:HE1	2:F:117:VAL:HG11	1.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:614:ASP:CG	1:B:859:THR:HG23	2.32	0.54
1:A:1050:MET:HE2	1:A:1052:PHE:CZ	2.42	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
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
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:A:740:MET:HE2	1:C:319:ARG:HE	1.73	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:748:GLU:CD	1:C:748:GLU:H	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:G:29:PHE:HE1	3:G:34:MET:HE2	1.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:364:ASP:CG	1:B:527:PRO:HG2	2.35	0.52
1:B:748:GLU:H	1:B:748:GLU:CD	2.16	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
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
2:D:382:PHE:CZ	3:G:138:LEU:C	2.88	0.51
3:G:136:PHE:N	3:G:155:LEU:O	2.41	0.51
1:C:124:THR:C	1:C:174:PRO:HB3	2.35	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:109:ASP:OD1	2:F:110:TYR:N	2.40	0.51
3:H:29:PHE:HE1	3:H:34:MET:HE2	1.75	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:733:LYS:NZ	1:B:775:ASP:OD2	2.36	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PHE:CD1	1:C:368:LEU:HD11	2.47	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
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: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:C:731:MET:HE2	1:C:1018:ILE:HG13	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:777:ASN:O	1:C:781:VAL:HG23	2.13	0.48
2:F:291:GLY:HA2	2:F:328:LYS:HZ3	1.79	0.48
1:A:86:PHE:N	1:A:236:THR:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:364:ASP:CG	1:C:527:PRO:HG2	2.39	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:A:898:PHE:HE1	1:A:1050:MET:HE1	1.78	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:136:CYS:O	1:C:137:ASN:C	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:109:SER:O	3:G:110:SER:C	2.58	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:A:942:PRO:C	1:A:944:ALA:N	2.71	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:109:SER:O	3:I:110:SER:C	2.57	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
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
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:291:GLY:HA2	2:D:328:LYS:HZ3	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:109:SER:O	3:H:110:SER:C	2.58	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
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:A:616:ASN:CG	1:A:617:CYS:H	2.23	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:136:CYS:O	1:A:137:ASN:C	2.58	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
2:E:291:GLY:HA2	2:E:328:LYS:HZ3	1.80	0.46
3:G:61:ALA:HB3	3:G:64:VAL:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:O	2:D:53:TYR:OH	2.28	0.46
1:A:555:SER:HB2	1:A:586:ASP:CG	2.41	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
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:B:238:PHE:C	1:B:239:GLN:HG3	2.41	0.45
1:C:165:ASN:CG	1:C:165:ASN:O	2.59	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
3:H:158:ASP:C	3:H:189:LEU:HD12	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:196:ASN:C	1:A:197:ILE:HD13	2.41	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
1:C:943:SER:C	1:C:945:LEU:N	2.73	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
3:G:158:ASP:C	3:G:189:LEU:HD12	2.42	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:I:158:ASP:C	3:I:189:LEU:HD12	2.42	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: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:A:386:LYS:O	1:A:386:LYS:HG2	2.17	0.44
1:B:81:ASN:CB	1:B:240:THR:HG22	2.47	0.44
1:B:943:SER:C	1:B:945:LEU:N	2.75	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
3:H:37:VAL:HG11	3:H:117:TRP:HZ3	1.82	0.44
1:A:124:THR:C	1:A:174:PRO:HB3	2.42	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:A:942:PRO:C	1:A:944:ALA:H	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLN:H	1:B:173:GLN:CD	2.26	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:PHE:C	1:A:235:ILE:HD11	2.42	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:O	1:C:165:ASN:ND2	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:E:173:TYR:OH	2:E:235:TYR:OH	2.22	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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:136:CYS:C	1:B:138:ASP:N	2.75	0.42
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
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
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:D:362:PHE:HZ	3:G:114:MET:HE1	1.85	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:CYS:O	1:B:137:ASN:C	2.62	0.42
1:B:213:VAL:C	1:B:214:ARG:HG3	2.44	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: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:290:ASP:C	1:A:290:ASP:OD1	2.62	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:725:GLU:CD	1:A:1028:LYS:HZ2	2.26	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
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:730:SER:HG	1:C:778:THR:HG1	1.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:106:PHE:C	1:C:235:ILE:HD11	2.45	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: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:B:662:CYS:HB2	1:B:697:MET:HE3	2.02	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:125:VAL:HG13	3:I:125:VAL:O	2.19	0.41
1:A:136:CYS:C	1:A:138:ASP:N	2.76	0.41
1:A:409:GLN:OE1	1:A:416:GLY:HA3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:197:ILE:HG22	1:B:198:ASP:CG	2.46	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
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:B:105:ILE:CG2	1:B:106:PHE:N	2.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:ILE:HB	1:A:202:LYS:HZ3	1.84	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
3:I:29:PHE:HE1	3:I:34:MET:HE2	1.85	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:64:TRP:CD1	1:A:64:TRP:C	2.99	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:A:574:ASP:OD1	1:A:574:ASP:C	2.63	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:328:LYS:NZ	2:D:330:GLY:O	2.51	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: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
2:D:314:ASN:C	2:D:314:ASN:OD1	2.64	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
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:E:314:ASN:OD1	2:E:314:ASN:C	2.64	0.40
2:F:29:PHE:HE1	2:F:34:MET:HE2	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:1029:MET:HE2	1:C:1029:MET:HB2	1.94	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:H:36:TRP:NE1	3:H:81:LEU:HB2	2.36	0.40
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:731:MET:HE1	1:C:1015:ALA:HA	2.04	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
2:F:173:TYR:OH	2:F:235:TYR:OH	2.22	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

5.3.1 Protein backbone

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
All	All	4938/6420 (77%)	4651 (94%)	287 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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%)	904 (99%)	5 (1%)	78	83
1	B	909/1056 (86%)	903 (99%)	6 (1%)	76	82
1	C	909/1056 (86%)	905 (100%)	4 (0%)	84	86
2	D	369/381 (97%)	366 (99%)	3 (1%)	73	81
2	E	369/381 (97%)	367 (100%)	2 (0%)	81	85
2	F	369/381 (97%)	367 (100%)	2 (0%)	81	85
3	G	166/402 (41%)	162 (98%)	4 (2%)	43	69
3	H	166/402 (41%)	163 (98%)	3 (2%)	51	73
3	I	166/402 (41%)	161 (97%)	5 (3%)	36	65
All	All	4332/5517 (78%)	4298 (99%)	34 (1%)	70	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	141	LEU
1	A	318	PHE
1	A	376	THR
1	A	602	THR
1	B	104	TRP
1	B	141	LEU
1	B	173	GLN
1	B	298	GLU
1	B	904	TYR
1	B	997	ILE
1	C	135	PHE
1	C	141	LEU
1	C	357	ARG
1	C	616	ASN
2	D	48	VAL
2	D	156	LEU
2	D	387	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	48	VAL
2	E	156	LEU
2	F	48	VAL
2	F	156	LEU
3	G	108	GLN
3	G	114	MET
3	G	155	LEU
3	G	156	VAL
3	H	3	GLN
3	H	108	GLN
3	H	156	VAL
3	I	3	GLN
3	I	108	GLN
3	I	114	MET
3	I	156	VAL
3	I	178	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	354	ASN
1	A	613	GLN
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	134	GLN
1	B	173	GLN
1	B	185	ASN
1	B	354	ASN
1	B	606	ASN
1	B	613	GLN
1	B	856	ASN
1	B	872	GLN
1	B	901	GLN
1	B	955	ASN
1	B	965	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1054	GLN
1	B	1058	HIS
1	B	1083	HIS
1	B	1106	GLN
1	B	1135	ASN
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	690	GLN
1	C	856	ASN
1	C	901	GLN
1	C	907	ASN
1	C	957	GLN
1	C	1002	GLN
1	C	1106	GLN
2	D	168	ASN
2	D	174	GLN
2	D	289	ASN
2	D	388	GLN
2	D	474	ASN
2	E	174	GLN
2	E	289	ASN
2	E	474	ASN
2	F	174	GLN
2	F	289	ASN
2	F	474	ASN
3	G	108	GLN
3	H	108	GLN
3	I	108	GLN
3	I	178	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides 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	1305	1	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	C	1407	1	14,14,15	1.01	1 (7%)	17,19,21	1.11	1 (5%)
4	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.60	0
4	NAG	A	1308	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
4	NAG	B	1308	1	14,14,15	0.90	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	C	1404	1	14,14,15	0.36	0	17,19,21	0.69	0
4	NAG	A	1307	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	C	1402	1	14,14,15	0.96	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	C	1401	1	14,14,15	0.39	0	17,19,21	0.56	0
4	NAG	C	1409	1	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	C	1405	1	14,14,15	0.72	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	C	1406	1	14,14,15	0.33	0	17,19,21	0.54	0
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.64	0
4	NAG	A	1301	1	14,14,15	0.35	0	17,19,21	0.61	0
4	NAG	B	1311	-	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	C	1410	-	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	B	1309	1	14,14,15	0.30	0	17,19,21	0.77	0
4	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	A	1311	-	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	B	1310	1	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1307	1	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.62	0
4	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.77	0
4	NAG	C	1403	1	14,14,15	0.27	0	17,19,21	0.62	0
4	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	C	1408	1	14,14,15	0.73	1 (7%)	17,19,21	0.98	1 (5%)

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	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1407	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	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1311	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1410	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1311	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1407	NAG	C1-C2	3.60	1.57	1.52
4	C	1402	NAG	C1-C2	3.31	1.56	1.52
4	B	1308	NAG	C1-C2	3.19	1.56	1.52
4	C	1408	NAG	C1-C2	2.51	1.55	1.52
4	C	1405	NAG	C1-C2	2.16	1.55	1.52

All (6) 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	-2.33	107.68	111.29
4	C	1405	NAG	C4-C3-C2	-2.25	107.72	111.02
4	C	1402	NAG	C2-N2-C7	-2.21	119.94	122.90
4	C	1408	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C1-C2-N2-C7
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	C1-C2-N2-C7
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	C1-C2-N2-C7
4	A	1310	NAG	C8-C7-N2-C2
4	A	1310	NAG	O7-C7-N2-C2
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	1302	NAG	C1-C2-N2-C7
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	C1-C2-N2-C7
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	C1-C2-N2-C7
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	A	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
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	B	1308	NAG	O7-C7-N2-C2
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	B	1305	NAG	C3-C2-N2-C7
4	A	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
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	B	1301	NAG	1	0
4	A	1308	NAG	2	0
4	C	1402	NAG	1	0
4	B	1304	NAG	1	0
4	A	1301	NAG	1	0
4	B	1309	NAG	2	0
4	A	1311	NAG	1	0
4	A	1306	NAG	1	0
4	A	1305	NAG	1	0
4	C	1408	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.

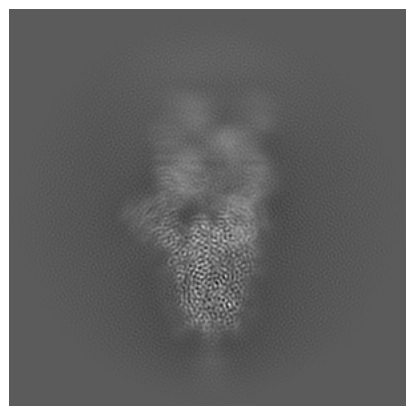
6 Map visualisation [i](#)

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.

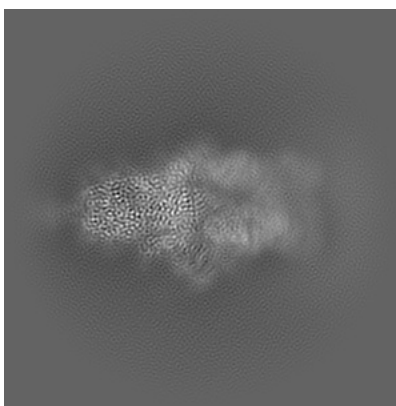
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

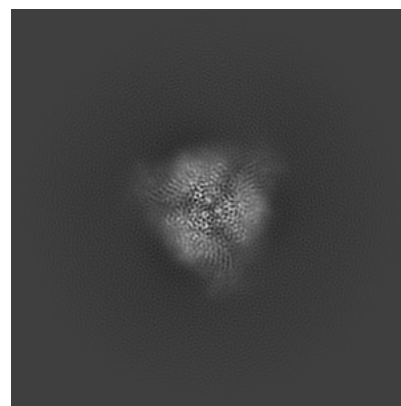
6.1.1 Primary map



X

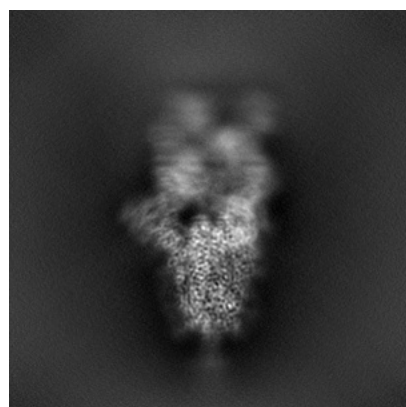


Y

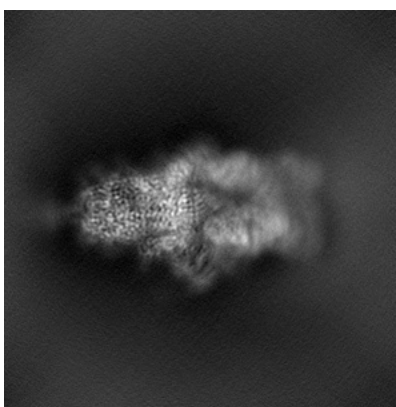


Z

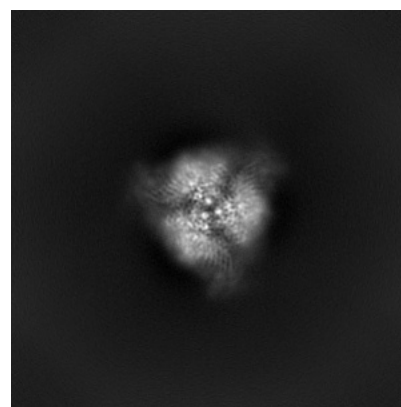
6.1.2 Raw map



X



Y

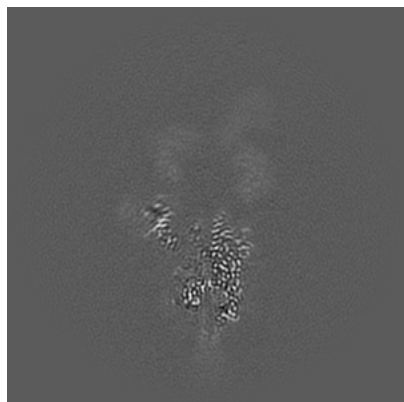


Z

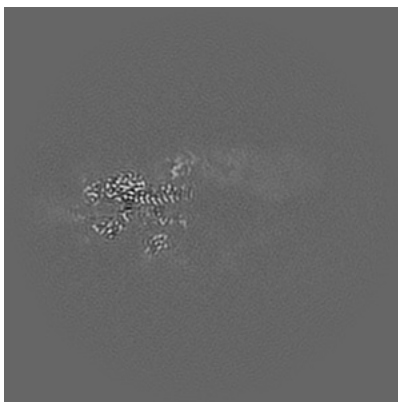
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

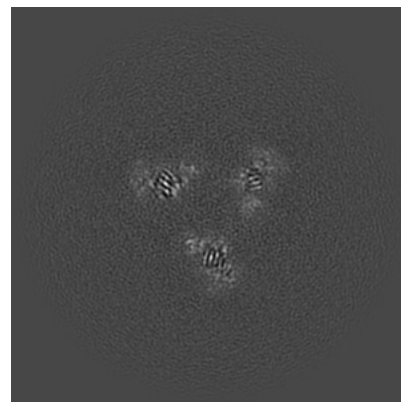
6.2.1 Primary map



X Index: 200

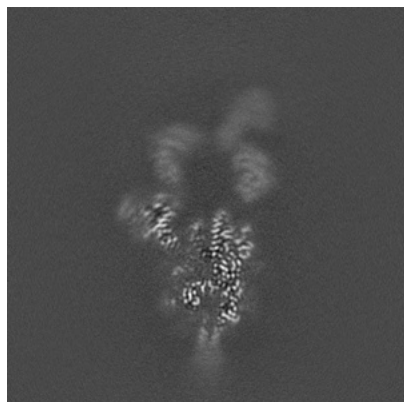


Y Index: 200

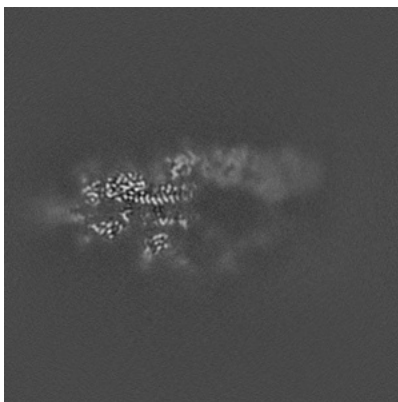


Z Index: 200

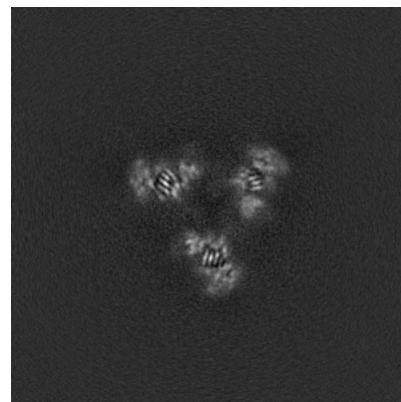
6.2.2 Raw map



X Index: 200



Y Index: 200

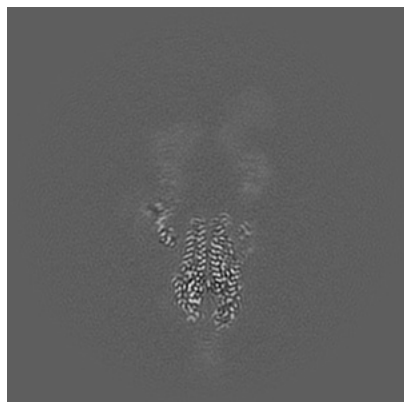


Z Index: 200

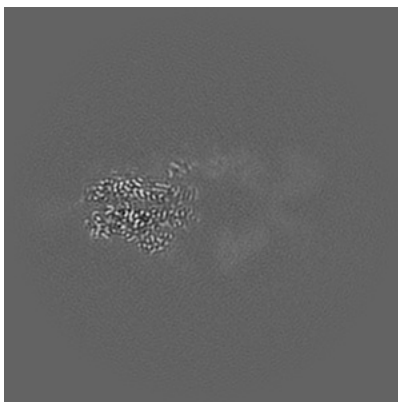
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

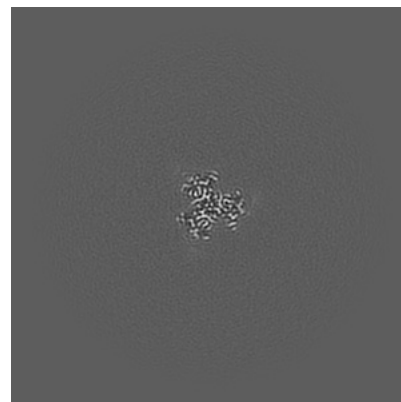
6.3.1 Primary map



X Index: 195

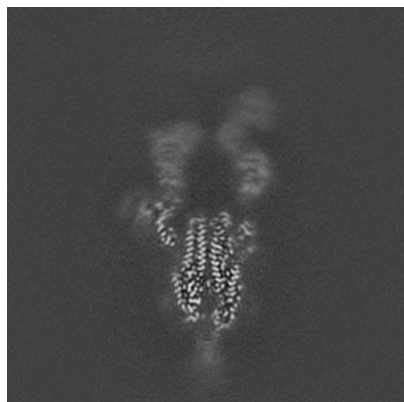


Y Index: 191

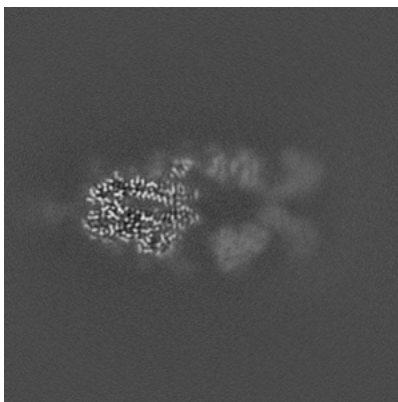


Z Index: 122

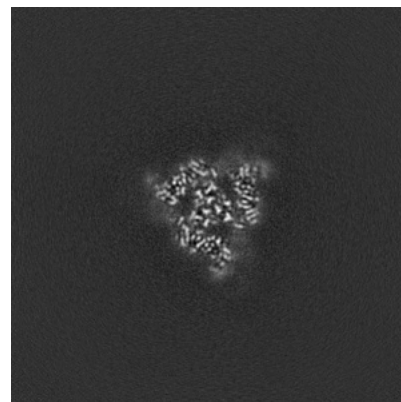
6.3.2 Raw map



X Index: 195



Y Index: 188

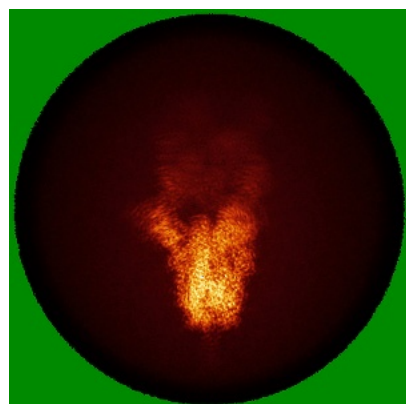


Z Index: 169

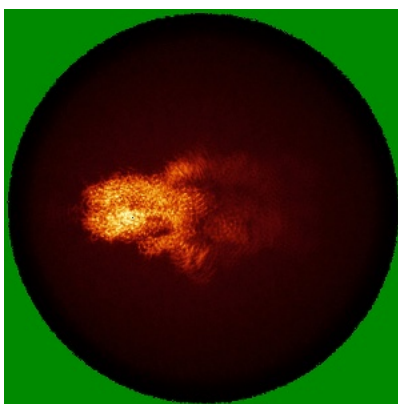
The images above show the largest variance slices of the map in three orthogonal directions.

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

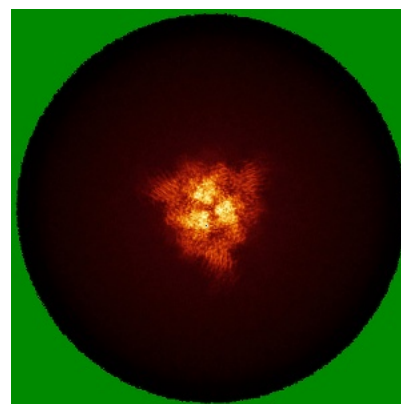
6.4.1 Primary map



X

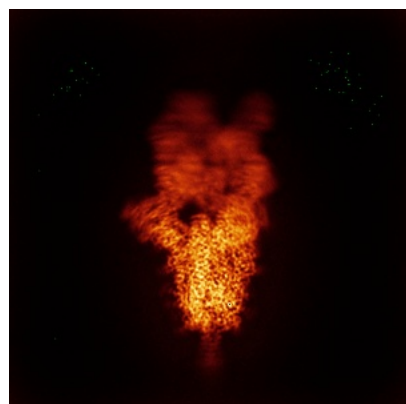


Y

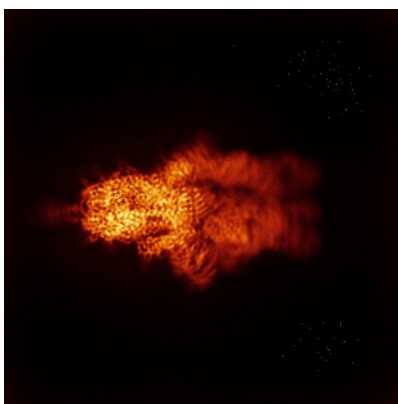


Z

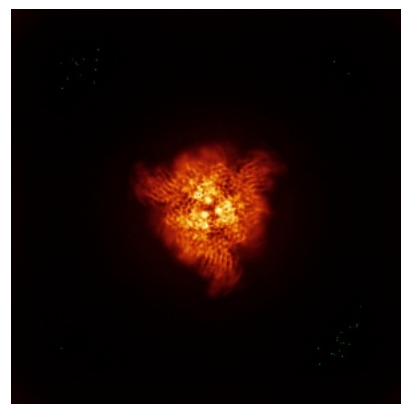
6.4.2 Raw map



X



Y



Z

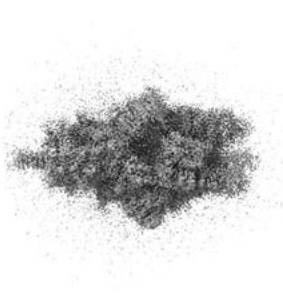
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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.

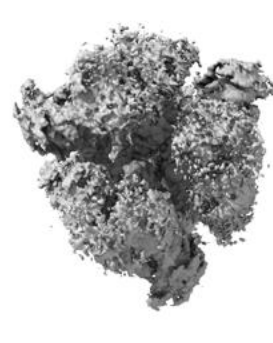
6.5.2 Raw map



X



Y



Z

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.

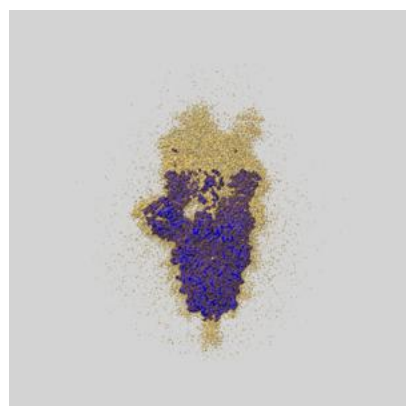
6.6 Mask visualisation [i](#)

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

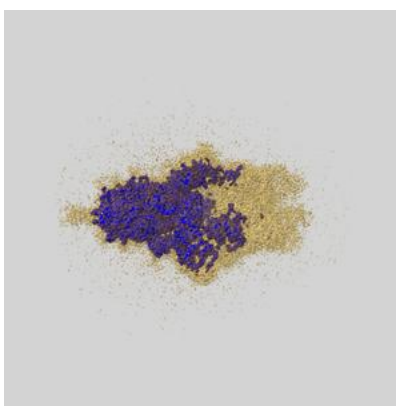
A mask typically either:

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

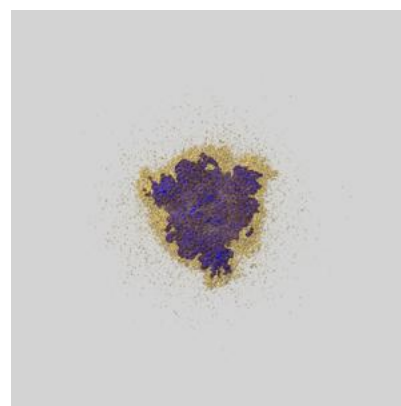
6.6.1 emd_33734_msk_1.map [i](#)



X



Y

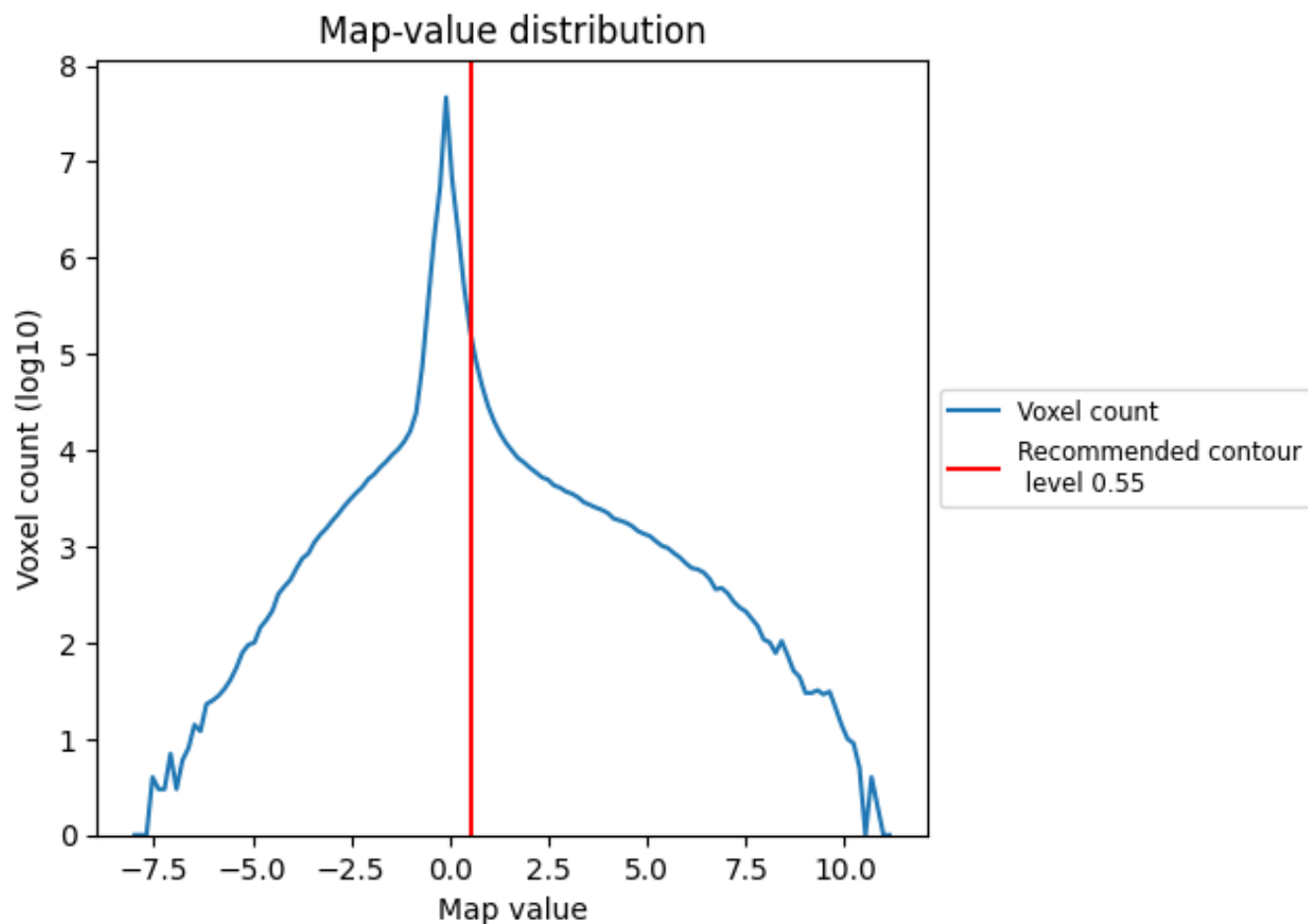


Z

7 Map analysis [i](#)

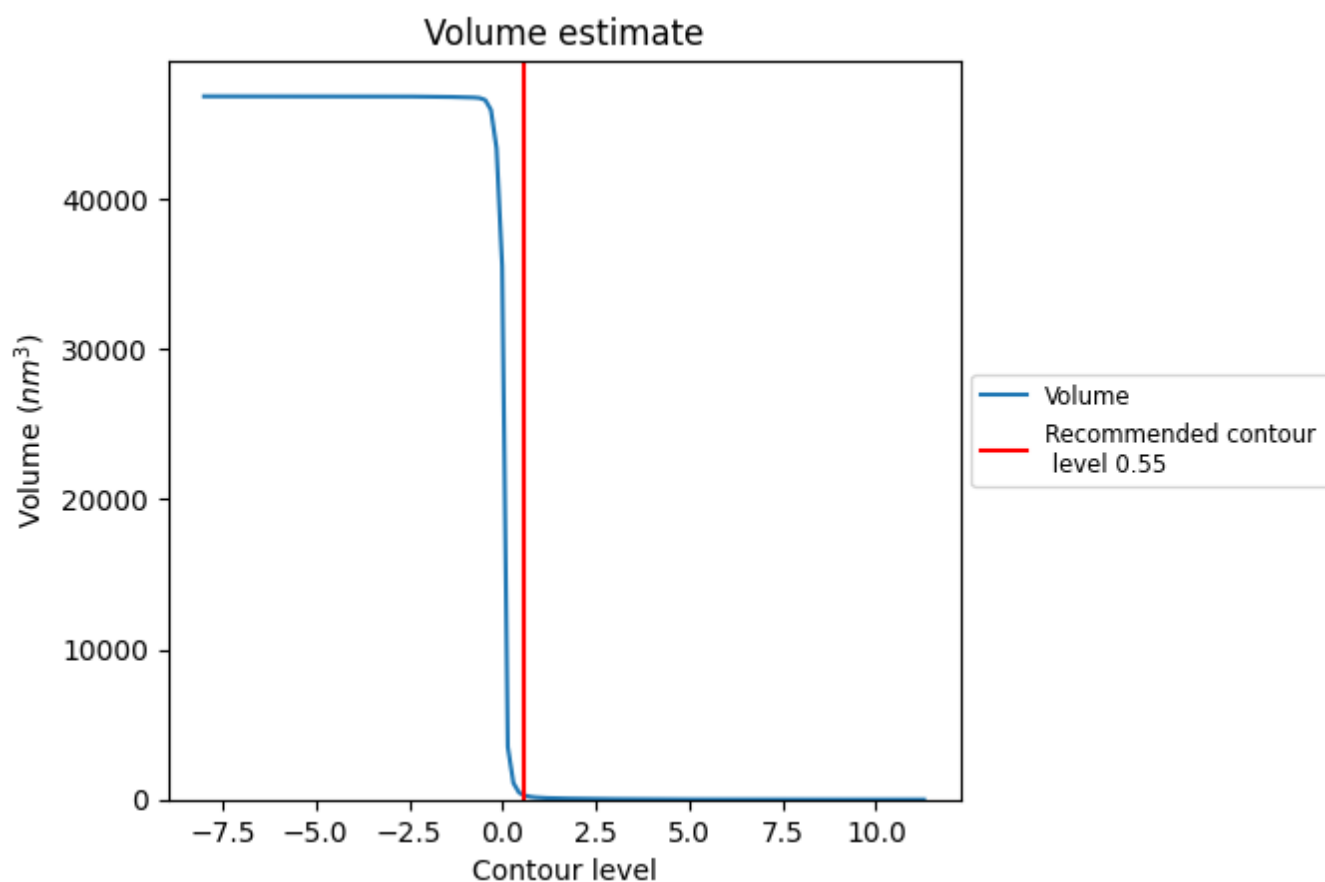
This section contains the results of statistical analysis of the map.

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.

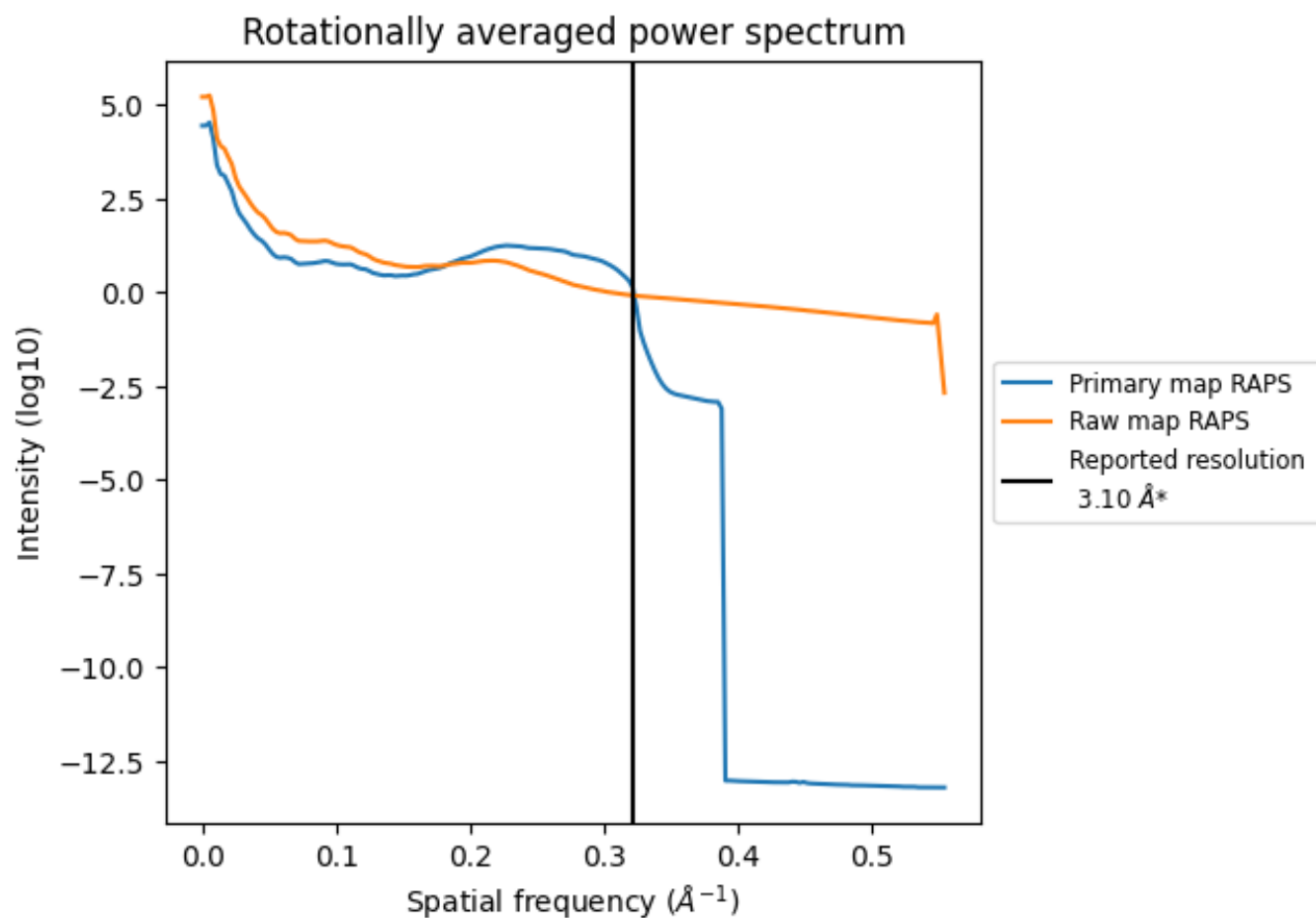
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; 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 ⓘ

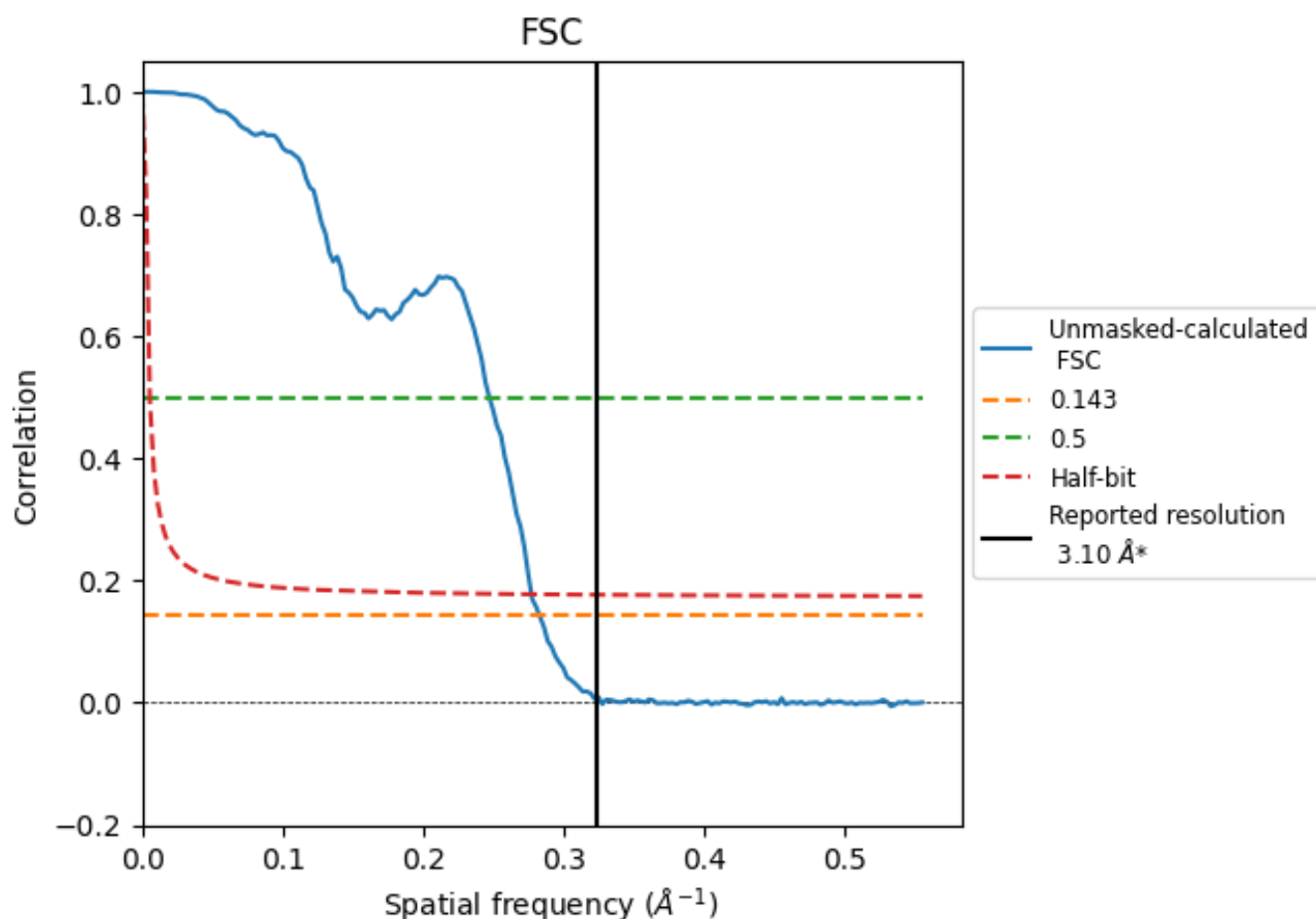


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

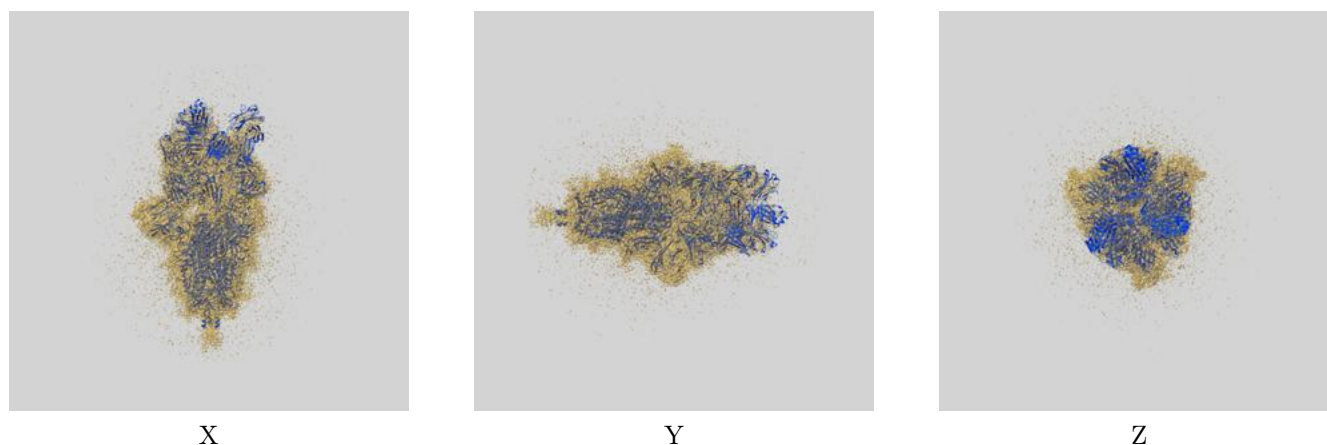
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.05	3.61

*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](#)

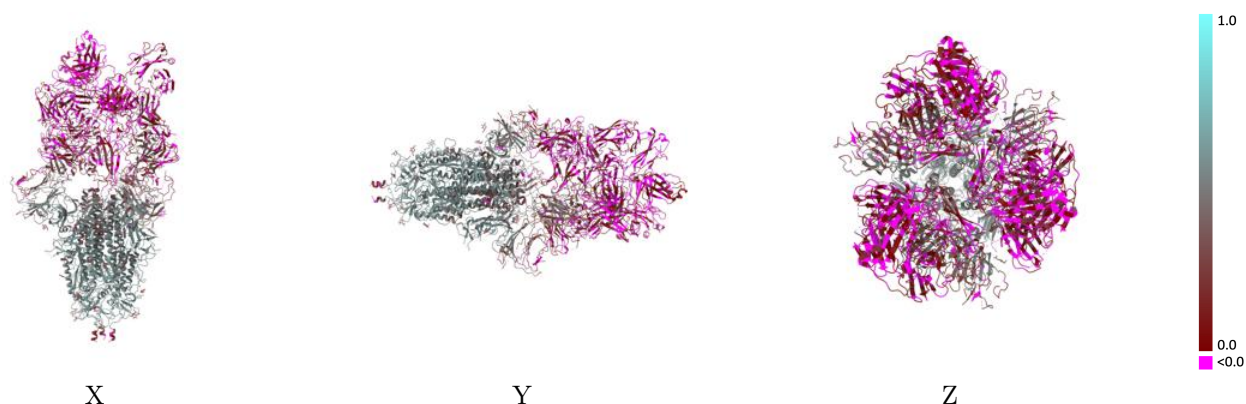
This section contains information regarding the fit between EMDB map EMD-33734 and PDB model 7YC5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



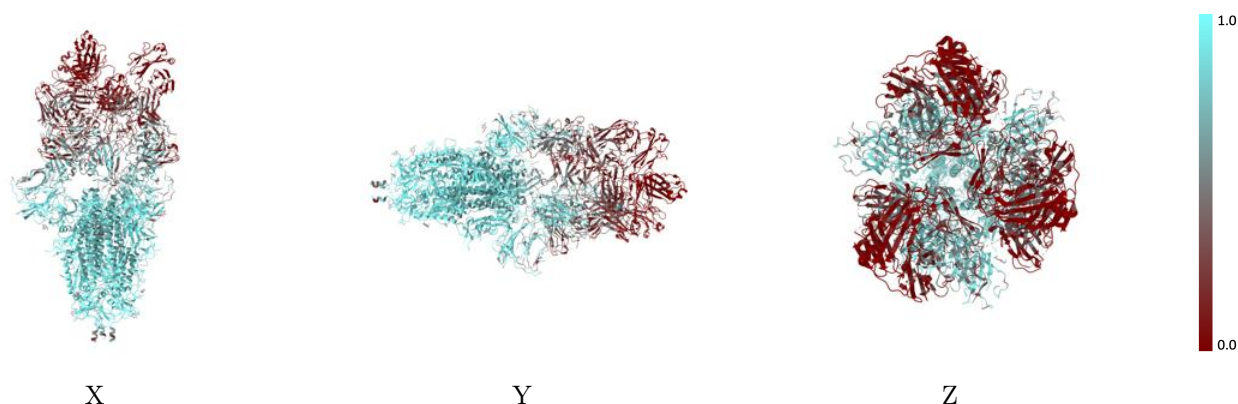
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



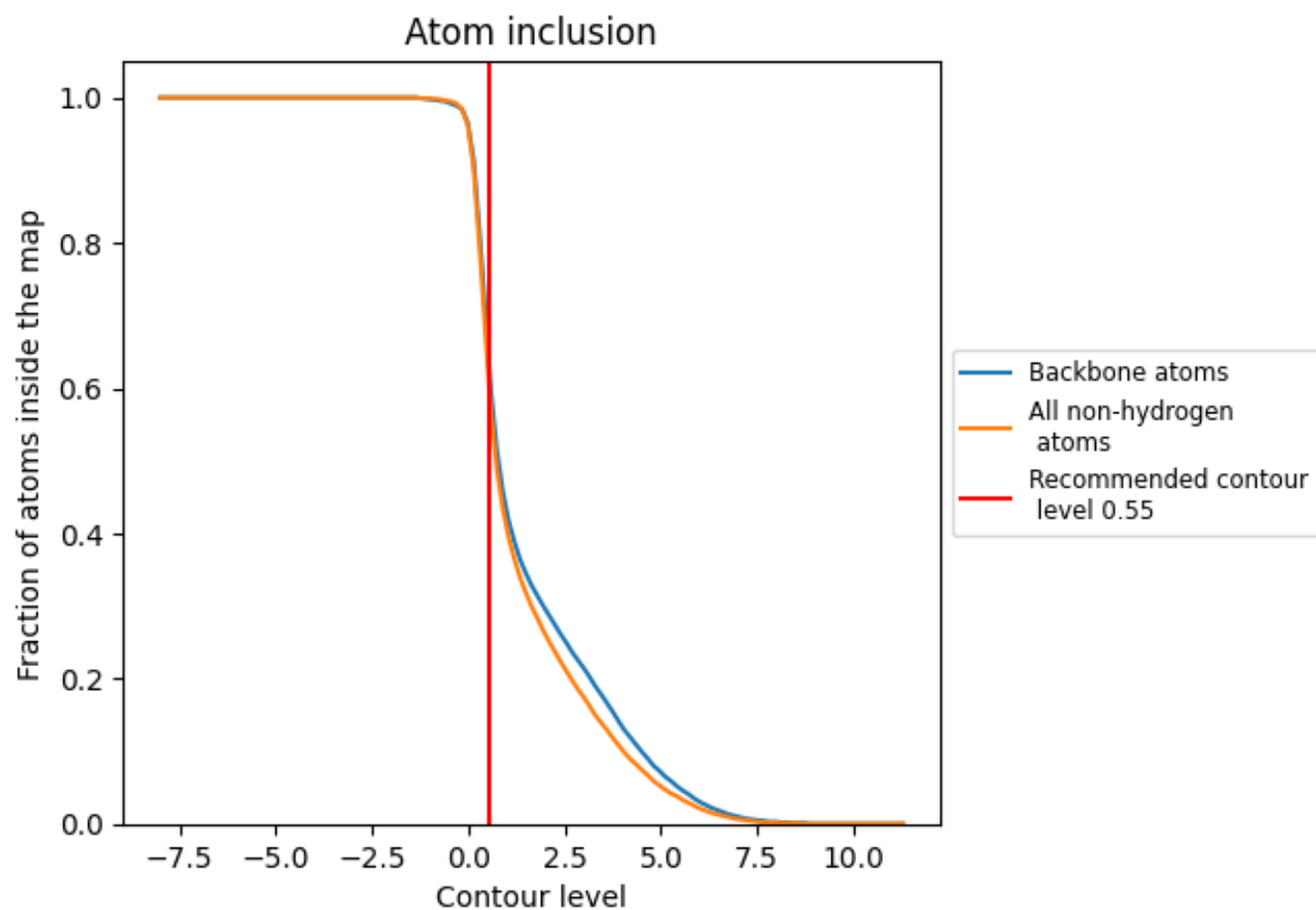
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

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

1.0

0.0

<0.0