



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 10:46 AM JST

PDB ID : 5X59
EMDB ID : EMD-6704
Title : Prefusion structure of MERS-CoV spike glycoprotein, three-fold symmetry
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

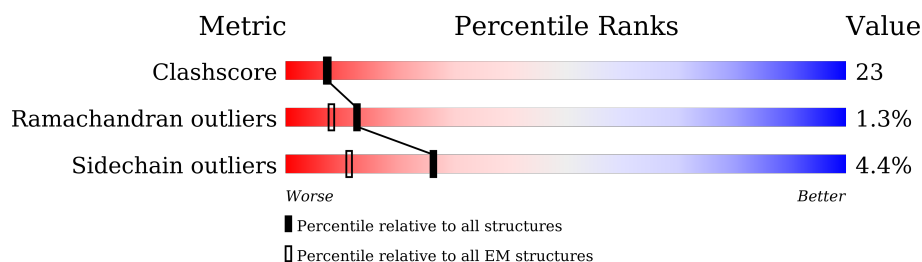
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1323	<div> <div>44%</div> <div>59% 23% • 14%</div> </div>
1	B	1323	<div> <div>42%</div> <div>59% 23% • • 14%</div> </div>
1	C	1323	<div> <div>56%</div> <div>60% 23% • 14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1402	-	-	X	-
2	NAG	A	1409	-	-	X	-
2	NAG	B	1402	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1409	-	-	X	-
2	NAG	C	1402	-	-	X	-
2	NAG	C	1409	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27258 atoms, of which 420 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 S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
B	1305	GLY	-	expression tag	UNP W6A028
B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

Continued on next page...

Continued from previous page...

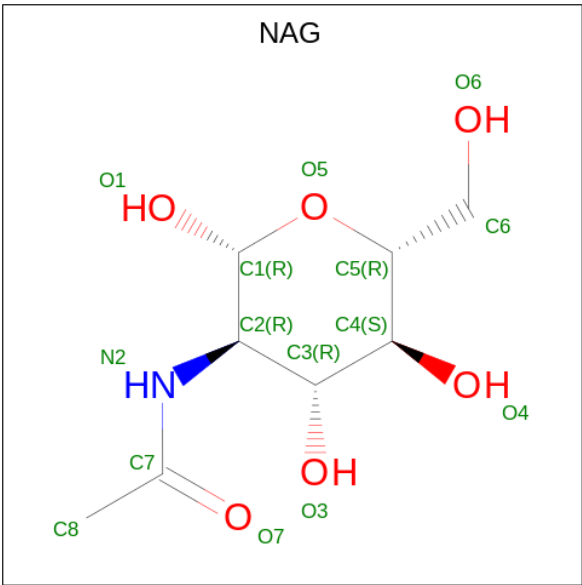
Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	

Continued on next page...

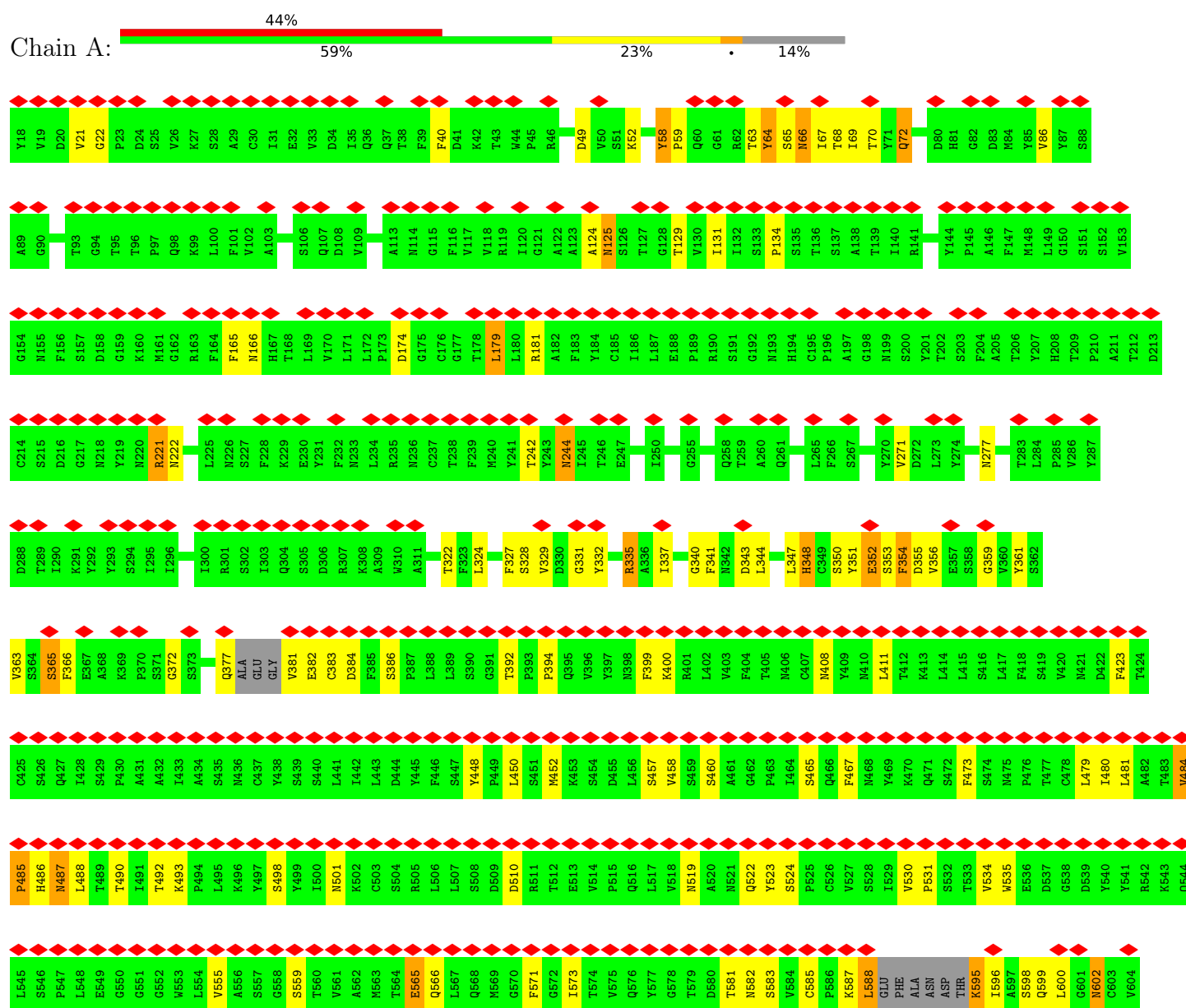
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
2	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

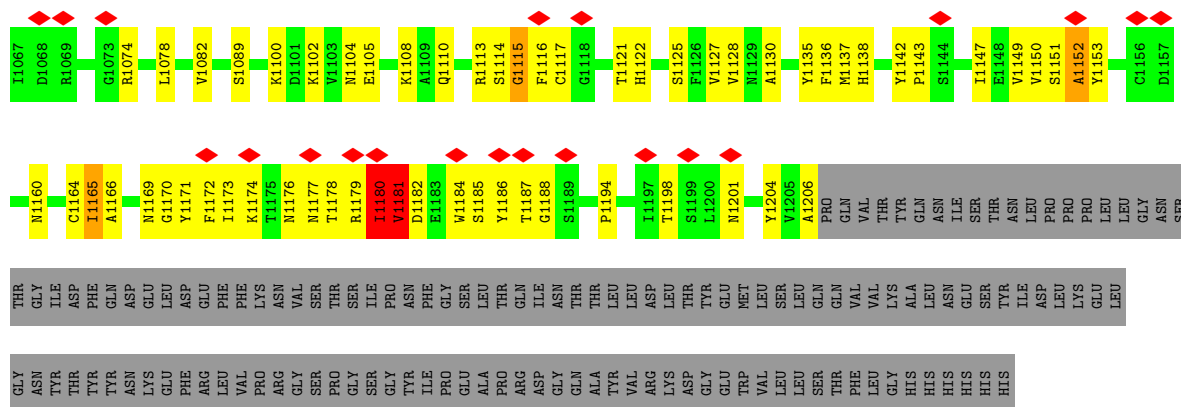
3 Residue-property plots

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.

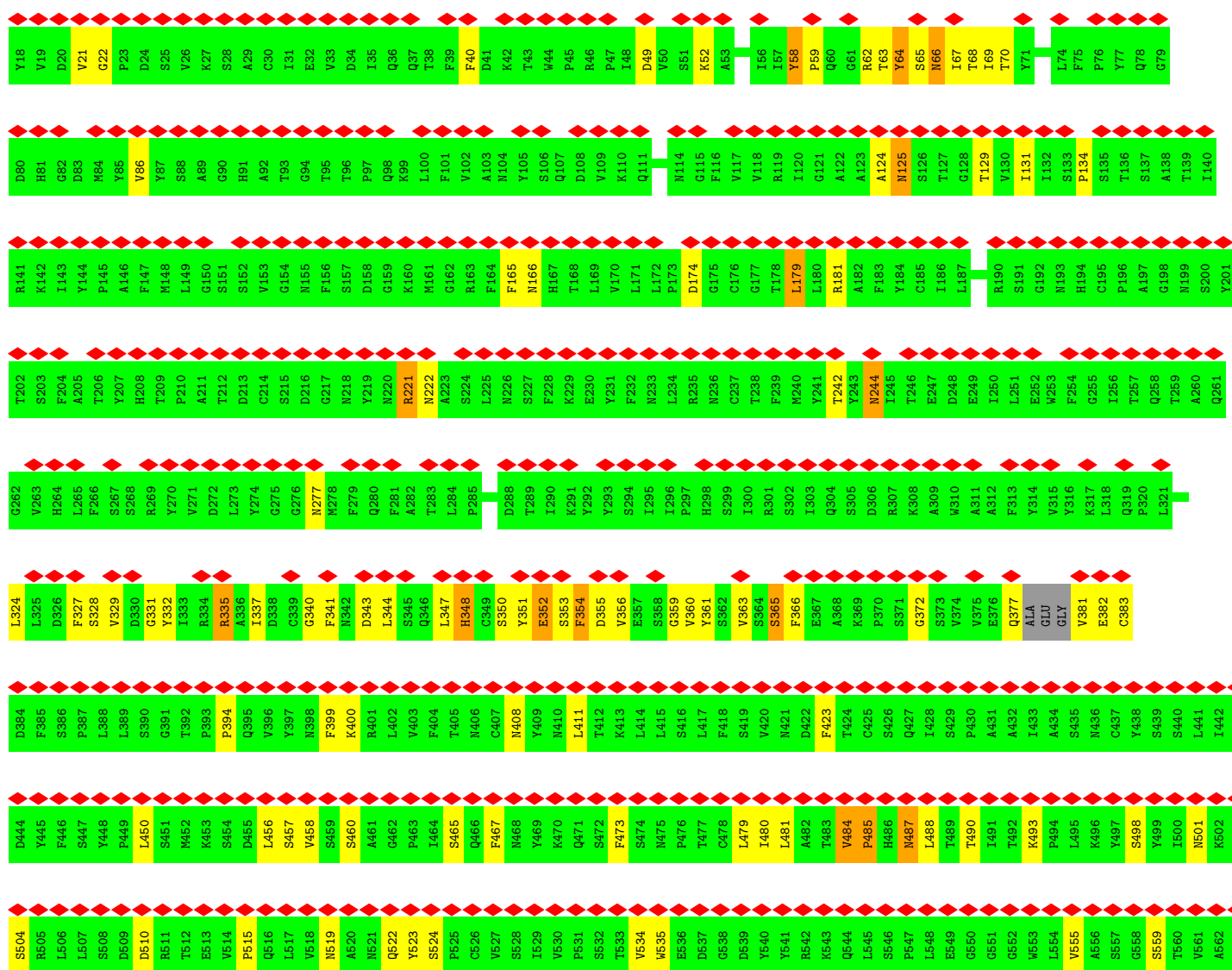
• Molecule 1: S protein







• Molecule 1: S protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.402	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0615	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3, 1.3, 1.3	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	0.51	1/9006 (0.0%)	0.78	21/12245 (0.2%)
1	B	0.51	1/9006 (0.0%)	0.78	21/12245 (0.2%)
1	C	0.51	1/9006 (0.0%)	0.78	21/12245 (0.2%)
All	All	0.51	3/27018 (0.0%)	0.78	63/36735 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	18
1	C	0	18
All	All	0	54

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	PRO	N-CD	5.17	1.55	1.47
1	C	59	PRO	N-CD	5.17	1.55	1.47
1	B	59	PRO	N-CD	5.11	1.55	1.47

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	LEU	CA-CB-CG	11.56	141.88	115.30
1	A	735	LEU	CA-CB-CG	11.55	141.86	115.30
1	C	735	LEU	CA-CB-CG	11.53	141.83	115.30
1	C	1040	LEU	CA-CB-CG	7.83	133.32	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1040	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	1040	LEU	CA-CB-CG	7.83	133.30	115.30
1	B	1151	SER	C-N-CA	7.39	140.18	121.70
1	A	1151	SER	C-N-CA	7.39	140.16	121.70
1	C	1151	SER	C-N-CA	7.38	140.15	121.70
1	B	697	LEU	CA-CB-CG	7.29	132.08	115.30
1	A	697	LEU	CA-CB-CG	7.28	132.04	115.30
1	C	697	LEU	CA-CB-CG	7.27	132.01	115.30
1	C	1018	ALA	N-CA-C	7.14	130.27	111.00
1	A	1018	ALA	N-CA-C	7.12	130.24	111.00
1	B	1018	ALA	N-CA-C	7.12	130.22	111.00
1	A	729	LEU	CA-CB-CG	6.81	130.96	115.30
1	B	729	LEU	CA-CB-CG	6.79	130.92	115.30
1	C	729	LEU	CA-CB-CG	6.79	130.91	115.30
1	B	731	LEU	CA-CB-CG	6.67	130.63	115.30
1	A	731	LEU	CA-CB-CG	6.66	130.62	115.30
1	C	731	LEU	CA-CB-CG	6.66	130.61	115.30
1	B	1152	ALA	C-N-CA	6.46	137.84	121.70
1	A	1152	ALA	C-N-CA	6.45	137.83	121.70
1	B	365	SER	C-N-CA	6.45	137.82	121.70
1	C	1152	ALA	C-N-CA	6.44	137.81	121.70
1	A	365	SER	C-N-CA	6.44	137.80	121.70
1	C	365	SER	C-N-CA	6.42	137.76	121.70
1	C	1180	ILE	CG1-CB-CG2	-6.16	97.84	111.40
1	A	1180	ILE	CG1-CB-CG2	-6.15	97.87	111.40
1	B	1180	ILE	CG1-CB-CG2	-6.13	97.91	111.40
1	C	651	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	651	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	651	LEU	CA-CB-CG	6.08	129.27	115.30
1	C	1116	PHE	N-CA-C	5.74	126.49	111.00
1	A	1116	PHE	N-CA-C	5.73	126.47	111.00
1	B	1116	PHE	N-CA-C	5.72	126.43	111.00
1	C	729	LEU	C-N-CD	-5.59	108.31	120.60
1	A	729	LEU	C-N-CD	-5.59	108.31	120.60
1	B	729	LEU	C-N-CD	-5.58	108.31	120.60
1	B	759	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	C	759	LEU	CB-CG-CD1	-5.49	101.68	111.00
1	A	759	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	C	985	ILE	CG1-CB-CG2	-5.44	99.44	111.40
1	A	985	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	B	985	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	C	902	ASP	C-N-CD	-5.37	108.79	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	902	ASP	C-N-CD	-5.37	108.80	120.60
1	A	902	ASP	C-N-CD	-5.36	108.80	120.60
1	C	724	VAL	C-N-CA	5.26	134.84	121.70
1	A	724	VAL	C-N-CA	5.25	134.82	121.70
1	B	724	VAL	C-N-CA	5.25	134.81	121.70
1	A	997	ILE	N-CA-C	5.22	125.10	111.00
1	C	997	ILE	N-CA-C	5.22	125.10	111.00
1	B	997	ILE	N-CA-C	5.22	125.10	111.00
1	C	638	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	638	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	638	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	799	ILE	CG1-CB-CG2	-5.09	100.19	111.40
1	B	799	ILE	CG1-CB-CG2	-5.09	100.19	111.40
1	C	799	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	B	1017	GLU	C-N-CA	5.06	134.35	121.70
1	C	1017	GLU	C-N-CA	5.05	134.34	121.70
1	A	1017	GLU	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1115	GLY	Peptide
1	A	1152	ALA	Peptide
1	A	1170	GLY	Peptide
1	A	1180	ILE	Peptide
1	A	1188	GLY	Peptide
1	A	1204	TYR	Peptide
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	733	GLN	Peptide
1	A	736	CYS	Peptide
1	A	788	PHE	Peptide
1	A	792	GLN	Peptide
1	A	795	ILE	Peptide
1	A	809	TYR	Peptide
1	A	856	SER	Peptide
1	A	967	PHE	Peptide
1	A	984	GLY	Peptide
1	A	996	LEU	Peptide
1	B	1115	GLY	Peptide
1	B	1152	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	1170	GLY	Peptide
1	B	1180	ILE	Peptide
1	B	1188	GLY	Peptide
1	B	1204	TYR	Peptide
1	B	639	VAL	Peptide
1	B	642	TYR	Peptide
1	B	733	GLN	Peptide
1	B	736	CYS	Peptide
1	B	788	PHE	Peptide
1	B	792	GLN	Peptide
1	B	795	ILE	Peptide
1	B	809	TYR	Peptide
1	B	856	SER	Peptide
1	B	967	PHE	Peptide
1	B	984	GLY	Peptide
1	B	996	LEU	Peptide
1	C	1115	GLY	Peptide
1	C	1152	ALA	Peptide
1	C	1170	GLY	Peptide
1	C	1180	ILE	Peptide
1	C	1188	GLY	Peptide
1	C	1204	TYR	Peptide
1	C	639	VAL	Peptide
1	C	642	TYR	Peptide
1	C	733	GLN	Peptide
1	C	736	CYS	Peptide
1	C	788	PHE	Peptide
1	C	792	GLN	Peptide
1	C	795	ILE	Peptide
1	C	809	TYR	Peptide
1	C	856	SER	Peptide
1	C	967	PHE	Peptide
1	C	984	GLY	Peptide
1	C	996	LEU	Peptide

5.2 Too-close contacts ⓘ

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	8806	0	8505	481	0
1	B	8806	0	8506	478	0
1	C	8806	0	8506	489	0
2	A	140	140	130	39	0
2	B	140	140	130	38	0
2	C	140	140	130	40	0
All	All	26838	420	25907	1213	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 23.

All (1213) 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:625:VAL:HG21	1:B:63:THR:CB	1.29	1.59
1:A:63:THR:CB	1:C:625:VAL:HG21	1.02	1.50
1:B:625:VAL:HG21	1:C:63:THR:CB	1.36	1.48
1:A:63:THR:CB	1:C:625:VAL:CG2	1.92	1.47
1:A:63:THR:OG1	1:C:625:VAL:CG2	1.66	1.43
1:B:179:LEU:HD22	1:B:221:ARG:NE	1.31	1.42
1:C:179:LEU:HD22	1:C:221:ARG:NE	1.31	1.41
1:C:348:HIS:CE1	1:C:663:TYR:HE1	1.40	1.40
1:A:179:LEU:HD22	1:A:221:ARG:NE	1.31	1.39
1:B:348:HIS:CE1	1:B:663:TYR:HE1	1.40	1.39
1:A:348:HIS:CE1	1:A:663:TYR:HE1	1.40	1.39
1:A:65:SER:HB2	1:C:623:VAL:CG1	1.52	1.36
1:B:58:TYR:OH	1:B:332:TYR:HA	1.18	1.34
1:B:677:VAL:HG21	1:C:909:TYR:CD2	1.65	1.30
1:A:271:VAL:HG22	1:C:627:GLN:OE1	1.25	1.30
1:C:58:TYR:OH	1:C:332:TYR:HA	1.18	1.30
1:A:58:TYR:OH	1:A:332:TYR:HA	1.18	1.30
1:A:271:VAL:CG2	1:C:627:GLN:OE1	1.81	1.28
1:A:623:VAL:CG1	1:B:65:SER:HB2	1.63	1.28
1:A:63:THR:HB	1:C:625:VAL:CG2	1.54	1.27
1:A:625:VAL:CG2	1:B:63:THR:HB	1.64	1.24
1:A:63:THR:CG2	1:C:628:GLN:HE21	1.49	1.24
1:A:625:VAL:CG2	1:B:63:THR:CB	2.14	1.24
1:B:625:VAL:CG2	1:C:63:THR:HB	1.67	1.22
1:B:348:HIS:CE1	1:B:663:TYR:CE1	2.28	1.21
1:A:348:HIS:CE1	1:A:663:TYR:CE1	2.28	1.21
1:B:677:VAL:HG11	1:C:909:TYR:CE2	1.73	1.21
1:B:58:TYR:HE1	1:B:277:ASN:OD1	1.25	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ALA:HB2	1:C:67:ILE:HD11	1.24	1.20
1:B:125:ASN:ND2	2:B:1402:NAG:C5	2.05	1.20
1:C:125:ASN:ND2	2:C:1402:NAG:C5	2.05	1.19
1:A:343:ASP:HB3	1:A:661:VAL:CG2	1.73	1.19
1:B:343:ASP:CB	1:B:661:VAL:CG2	2.21	1.19
1:A:125:ASN:ND2	2:A:1402:NAG:C5	2.05	1.19
1:B:625:VAL:CG2	1:C:63:THR:CB	2.18	1.19
1:A:909:TYR:CD2	1:C:677:VAL:HG21	1.77	1.18
1:B:165:PHE:CD1	2:B:1408:NAG:O7	1.96	1.18
1:C:348:HIS:CE1	1:C:663:TYR:CE1	2.28	1.18
1:A:58:TYR:HE1	1:A:277:ASN:OD1	1.25	1.18
1:C:343:ASP:CB	1:C:661:VAL:CG2	2.21	1.18
1:B:125:ASN:ND2	2:B:1402:NAG:H5	1.58	1.18
1:B:623:VAL:CG1	1:C:65:SER:HB2	1.73	1.18
1:C:125:ASN:ND2	2:C:1402:NAG:H5	1.58	1.18
1:B:244:ASN:HD21	2:B:1401:NAG:C1	1.56	1.18
1:C:165:PHE:CD1	2:C:1408:NAG:O7	1.96	1.18
1:C:343:ASP:HB3	1:C:661:VAL:CG2	1.73	1.18
1:A:125:ASN:ND2	2:A:1402:NAG:H5	1.58	1.17
1:A:165:PHE:CD1	2:A:1408:NAG:O7	1.96	1.17
1:A:343:ASP:CB	1:A:661:VAL:CG2	2.21	1.17
1:B:343:ASP:HB3	1:B:661:VAL:CG2	1.73	1.17
1:A:244:ASN:HD21	2:A:1401:NAG:C1	1.56	1.17
1:C:244:ASN:HD21	2:C:1401:NAG:C1	1.56	1.16
1:C:58:TYR:HE1	1:C:277:ASN:OD1	1.25	1.16
1:A:677:VAL:HG11	1:B:909:TYR:CE2	1.80	1.15
1:B:350:SER:O	1:B:351:TYR:HD2	1.27	1.15
1:C:343:ASP:HB3	1:C:661:VAL:HG23	1.18	1.15
1:C:350:SER:O	1:C:351:TYR:HD2	1.28	1.15
1:A:822:ARG:HE	1:C:694:ARG:NH1	1.44	1.15
1:B:343:ASP:HB3	1:B:661:VAL:HG23	1.18	1.14
1:A:63:THR:CG2	1:C:628:GLN:NE2	2.11	1.14
1:A:63:THR:OG1	1:C:625:VAL:HG23	1.36	1.14
1:B:179:LEU:CD2	1:B:221:ARG:HE	1.60	1.14
1:A:65:SER:CB	1:C:623:VAL:CG1	2.25	1.14
1:C:58:TYR:CE1	1:C:277:ASN:OD1	2.01	1.14
1:C:179:LEU:CD2	1:C:221:ARG:HE	1.61	1.14
1:A:58:TYR:CE1	1:A:277:ASN:OD1	2.01	1.13
1:A:350:SER:O	1:A:351:TYR:HD2	1.27	1.13
1:A:179:LEU:CD2	1:A:221:ARG:HE	1.61	1.13
1:A:63:THR:HG22	1:C:628:GLN:NE2	1.61	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:VAL:HG21	1:B:909:TYR:CD2	1.84	1.12
1:B:58:TYR:CE1	1:B:277:ASN:OD1	2.01	1.12
1:A:341:PHE:O	1:A:696:MET:O	1.68	1.12
1:A:634:ALA:HB2	1:B:67:ILE:HD11	1.21	1.12
1:B:634:ALA:HB2	1:C:67:ILE:CD1	1.78	1.12
1:A:625:VAL:CG2	1:B:63:THR:OG1	1.98	1.11
1:B:341:PHE:O	1:B:696:MET:O	1.68	1.11
1:B:677:VAL:HG21	1:C:909:TYR:HD2	0.95	1.11
1:A:343:ASP:HB3	1:A:661:VAL:HG23	1.18	1.11
1:B:244:ASN:ND2	2:B:1401:NAG:O5	1.84	1.10
1:C:244:ASN:ND2	2:C:1401:NAG:O5	1.84	1.10
1:A:628:GLN:HE21	1:B:63:THR:CG2	1.62	1.10
1:B:343:ASP:CB	1:B:661:VAL:HG23	1.80	1.10
1:A:343:ASP:CB	1:A:661:VAL:HG23	1.80	1.10
1:C:341:PHE:O	1:C:696:MET:O	1.68	1.10
1:C:347:LEU:HD13	1:C:361:TYR:CD2	1.88	1.09
1:A:347:LEU:HD13	1:A:361:TYR:CD2	1.88	1.09
1:A:634:ALA:HB2	1:B:67:ILE:CD1	1.83	1.09
1:B:343:ASP:OD1	1:B:363:VAL:HG11	1.52	1.09
1:A:623:VAL:HG11	1:B:65:SER:HB2	1.09	1.08
1:B:347:LEU:HD13	1:B:361:TYR:CD2	1.88	1.08
1:A:244:ASN:ND2	2:A:1401:NAG:O5	1.84	1.08
1:B:58:TYR:OH	1:B:332:TYR:CA	2.02	1.08
1:C:58:TYR:OH	1:C:332:TYR:CA	2.02	1.08
1:A:628:GLN:HE21	1:B:63:THR:HG22	0.95	1.07
1:B:628:GLN:HE21	1:C:63:THR:HG22	1.11	1.07
1:A:343:ASP:OD1	1:A:363:VAL:HG11	1.52	1.07
1:B:623:VAL:HG11	1:C:65:SER:HB2	1.11	1.07
1:B:625:VAL:CG2	1:C:63:THR:OG1	2.03	1.07
1:C:343:ASP:CB	1:C:661:VAL:HG23	1.80	1.07
1:C:343:ASP:OD1	1:C:363:VAL:HG11	1.52	1.07
1:A:818:GLU:OE1	1:C:691:ARG:NH2	1.89	1.06
1:A:58:TYR:OH	1:A:332:TYR:CA	2.02	1.06
1:A:348:HIS:HA	1:A:356:VAL:HG21	1.37	1.06
1:A:677:VAL:HG21	1:B:909:TYR:HD2	1.11	1.06
1:A:623:VAL:HG13	1:B:329:VAL:O	1.55	1.06
1:B:677:VAL:CG2	1:C:909:TYR:CD2	2.37	1.05
1:C:348:HIS:HA	1:C:356:VAL:HG21	1.38	1.05
1:A:350:SER:O	1:A:351:TYR:CD2	2.10	1.05
1:B:348:HIS:HA	1:B:356:VAL:HG21	1.38	1.05
1:A:67:ILE:HD11	1:C:634:ALA:HB2	1.35	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:O	1:B:351:TYR:CD2	2.10	1.04
1:C:350:SER:O	1:C:351:TYR:CD2	2.10	1.04
1:A:335:ARG:HB3	1:A:354:PHE:CZ	1.93	1.04
1:C:335:ARG:HB3	1:C:354:PHE:CZ	1.93	1.03
1:B:335:ARG:HB3	1:B:354:PHE:CZ	1.93	1.03
1:A:65:SER:CB	1:C:623:VAL:HG12	1.86	1.02
1:A:65:SER:O	1:A:67:ILE:N	1.92	1.02
1:B:623:VAL:HG13	1:C:329:VAL:O	1.57	1.02
1:B:65:SER:O	1:B:67:ILE:N	1.92	1.01
1:C:65:SER:O	1:C:67:ILE:N	1.92	1.00
1:A:222:ASN:ND2	2:A:1409:NAG:O5	1.94	1.00
1:C:222:ASN:ND2	2:C:1409:NAG:O5	1.94	1.00
1:A:822:ARG:NH2	1:C:694:ARG:HH11	1.59	1.00
1:B:222:ASN:ND2	2:B:1409:NAG:O5	1.95	0.99
1:A:909:TYR:CE2	1:C:677:VAL:HG11	1.96	0.99
1:B:625:VAL:HG23	1:C:63:THR:OG1	1.62	0.99
1:B:628:GLN:HE21	1:C:63:THR:CG2	1.74	0.99
1:A:623:VAL:CG1	1:B:65:SER:CB	2.41	0.99
1:A:822:ARG:NE	1:C:694:ARG:HH12	1.61	0.99
1:A:822:ARG:NE	1:C:694:ARG:NH1	2.10	0.98
1:A:628:GLN:NE2	1:B:63:THR:HG22	1.79	0.98
1:C:21:VAL:C	2:C:1409:NAG:H82	1.84	0.98
1:A:625:VAL:HG23	1:B:63:THR:OG1	1.64	0.98
1:B:343:ASP:C	1:B:661:VAL:HG21	1.85	0.98
1:A:222:ASN:ND2	2:A:1409:NAG:C1	2.27	0.97
1:A:343:ASP:C	1:A:661:VAL:HG21	1.85	0.97
1:A:348:HIS:HA	1:A:356:VAL:CG2	1.95	0.97
1:A:628:GLN:CG	1:B:63:THR:CG2	2.42	0.97
1:A:21:VAL:C	2:A:1409:NAG:H82	1.84	0.97
1:A:124:ALA:O	1:A:125:ASN:HB2	1.65	0.97
1:C:222:ASN:ND2	2:C:1409:NAG:C1	2.27	0.97
1:B:125:ASN:HD21	2:B:1402:NAG:C5	1.72	0.97
1:B:222:ASN:ND2	2:B:1409:NAG:C1	2.28	0.97
1:B:348:HIS:HA	1:B:356:VAL:CG2	1.95	0.97
1:A:628:GLN:NE2	1:B:63:THR:CG2	2.27	0.96
1:A:822:ARG:HH21	1:C:694:ARG:NH1	1.62	0.96
1:A:222:ASN:HD21	2:A:1409:NAG:C1	1.79	0.96
1:B:343:ASP:HB2	1:B:661:VAL:CG2	1.96	0.96
1:C:348:HIS:HA	1:C:356:VAL:CG2	1.95	0.96
1:A:936:PRO:HG2	1:C:715:LEU:HD21	1.45	0.96
1:B:124:ALA:O	1:B:125:ASN:HB2	1.65	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:C	2:B:1409:NAG:H82	1.84	0.96
1:B:222:ASN:HD21	2:B:1409:NAG:C1	1.79	0.96
1:C:222:ASN:HD21	2:C:1409:NAG:C1	1.79	0.96
1:C:343:ASP:C	1:C:661:VAL:HG21	1.85	0.95
1:A:65:SER:CB	1:C:623:VAL:HG11	1.89	0.95
1:A:63:THR:HG22	1:C:628:GLN:HE21	0.78	0.95
1:C:124:ALA:O	1:C:125:ASN:HB2	1.65	0.95
1:A:343:ASP:HB2	1:A:661:VAL:CG2	1.96	0.95
1:A:65:SER:HB2	1:C:623:VAL:HG11	0.98	0.94
1:C:343:ASP:OD1	1:C:363:VAL:CG1	2.15	0.94
1:A:343:ASP:OD1	1:A:363:VAL:CG1	2.15	0.94
1:A:348:HIS:HE1	1:A:663:TYR:CE1	1.77	0.94
1:A:623:VAL:HG12	1:B:65:SER:CB	1.97	0.94
1:B:348:HIS:HE1	1:B:663:TYR:CE1	1.77	0.94
1:B:1114:SER:HB3	1:C:1104:ASN:HB3	1.49	0.94
1:A:335:ARG:NE	1:A:354:PHE:HE2	1.65	0.94
1:A:628:GLN:CG	1:B:63:THR:HG21	1.97	0.93
1:C:335:ARG:NE	1:C:354:PHE:HE2	1.65	0.93
1:A:244:ASN:ND2	2:A:1401:NAG:C1	2.32	0.93
1:A:67:ILE:CD1	1:C:634:ALA:HB2	1.98	0.93
1:C:343:ASP:HB2	1:C:661:VAL:CG2	1.96	0.93
1:A:628:GLN:HG2	1:B:63:THR:HG21	1.50	0.93
1:B:1032:ALA:O	1:B:1036:LEU:HB2	1.69	0.93
1:B:335:ARG:NE	1:B:354:PHE:HE2	1.65	0.93
1:C:1032:ALA:O	1:C:1036:LEU:HB2	1.69	0.93
1:B:244:ASN:ND2	2:B:1401:NAG:C1	2.32	0.92
1:B:343:ASP:OD1	1:B:363:VAL:CG1	2.15	0.92
1:A:909:TYR:HD2	1:C:677:VAL:HG21	1.23	0.92
1:B:623:VAL:CG1	1:C:65:SER:CB	2.47	0.92
1:A:1032:ALA:O	1:A:1036:LEU:HB2	1.69	0.91
1:C:348:HIS:HE1	1:C:663:TYR:CE1	1.77	0.91
1:B:343:ASP:CG	1:B:363:VAL:HB	1.91	0.91
1:C:343:ASP:CG	1:C:363:VAL:HB	1.91	0.91
1:C:350:SER:C	1:C:351:TYR:CD2	2.44	0.91
1:C:244:ASN:ND2	2:C:1401:NAG:C1	2.32	0.91
1:A:65:SER:HB3	1:C:623:VAL:HG12	1.53	0.90
1:B:691:ARG:NH2	1:C:818:GLU:OE1	2.03	0.90
1:A:343:ASP:CG	1:A:363:VAL:HB	1.91	0.90
1:A:350:SER:C	1:A:351:TYR:CD2	2.44	0.90
1:C:125:ASN:HD21	2:C:1402:NAG:C5	1.72	0.90
1:B:1165:ILE:HG12	1:C:960:TRP:HH2	1.37	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:CG2	1:C:628:GLN:CG	2.50	0.89
1:A:125:ASN:HD21	2:A:1402:NAG:C5	1.72	0.89
1:C:179:LEU:CD2	1:C:221:ARG:NE	2.27	0.89
1:B:343:ASP:OD2	1:B:659:VAL:HG13	1.72	0.89
1:A:179:LEU:CD2	1:A:221:ARG:NE	2.27	0.89
1:A:63:THR:HG21	1:C:628:GLN:NE2	1.88	0.89
1:C:347:LEU:HD13	1:C:361:TYR:CG	2.05	0.89
1:B:350:SER:C	1:B:351:TYR:CD2	2.44	0.89
1:A:343:ASP:OD2	1:A:659:VAL:HG13	1.72	0.88
1:B:677:VAL:CG1	1:C:909:TYR:CE2	2.55	0.88
1:C:343:ASP:OD2	1:C:659:VAL:HG13	1.72	0.88
1:A:677:VAL:CG2	1:B:909:TYR:CD2	2.56	0.88
1:A:271:VAL:HG21	1:C:627:GLN:OE1	1.72	0.88
1:B:179:LEU:CD2	1:B:221:ARG:NE	2.27	0.88
1:C:588:LEU:C	1:C:595:LYS:HA	1.95	0.87
1:A:588:LEU:C	1:A:595:LYS:HA	1.95	0.87
1:C:324:LEU:HD22	1:C:354:PHE:CD1	2.10	0.87
1:B:634:ALA:CB	1:C:67:ILE:HD11	2.05	0.86
1:C:343:ASP:CB	1:C:661:VAL:HG21	2.05	0.86
1:B:588:LEU:C	1:B:595:LYS:HA	1.95	0.86
1:B:343:ASP:CB	1:B:661:VAL:HG21	2.05	0.86
1:A:909:TYR:CD2	1:C:677:VAL:CG2	2.59	0.86
1:B:324:LEU:HD22	1:B:354:PHE:CD1	2.10	0.86
1:C:348:HIS:HE1	1:C:663:TYR:HE1	0.87	0.86
1:A:347:LEU:HD13	1:A:361:TYR:CG	2.05	0.85
1:A:324:LEU:HD22	1:A:354:PHE:CD1	2.10	0.85
1:A:343:ASP:CB	1:A:661:VAL:HG21	2.05	0.85
1:C:343:ASP:CB	1:C:363:VAL:HG21	2.07	0.85
1:C:350:SER:C	1:C:351:TYR:HD2	1.80	0.85
1:B:663:TYR:OH	1:B:668:LYS:CE	2.25	0.85
1:A:343:ASP:CB	1:A:363:VAL:HG21	2.07	0.85
1:C:663:TYR:OH	1:C:668:LYS:CE	2.25	0.85
1:B:628:GLN:HG2	1:C:63:THR:HG21	1.58	0.85
1:A:63:THR:CG2	1:C:625:VAL:HG21	2.06	0.85
1:A:348:HIS:HE1	1:A:663:TYR:HE1	0.87	0.84
1:A:822:ARG:NH2	1:C:694:ARG:NH1	2.21	0.84
1:A:663:TYR:OH	1:A:668:LYS:CE	2.25	0.84
1:B:348:HIS:HE1	1:B:663:TYR:HE1	0.87	0.84
1:A:1024:ASP:O	1:A:1028:ASN:HB2	1.78	0.84
1:B:343:ASP:CB	1:B:363:VAL:HG21	2.07	0.84
1:C:1024:ASP:O	1:C:1028:ASN:HB2	1.78	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:HIS:CA	1:C:356:VAL:HG21	2.08	0.84
1:A:348:HIS:CA	1:A:356:VAL:HG21	2.08	0.83
1:A:634:ALA:CB	1:B:67:ILE:HD11	2.06	0.83
1:B:628:GLN:CG	1:C:63:THR:HG21	2.08	0.83
1:B:677:VAL:CB	1:C:909:TYR:CD2	2.61	0.83
1:A:335:ARG:NE	1:A:354:PHE:CE2	2.47	0.83
1:A:335:ARG:CZ	1:A:354:PHE:CD2	2.61	0.83
1:B:335:ARG:CZ	1:B:354:PHE:CD2	2.61	0.83
1:B:625:VAL:HG21	1:C:63:THR:HB	0.84	0.83
1:B:628:GLN:CG	1:C:63:THR:CG2	2.57	0.83
1:C:335:ARG:CZ	1:C:354:PHE:CD2	2.61	0.83
1:B:335:ARG:NE	1:B:354:PHE:CE2	2.47	0.83
1:B:348:HIS:CA	1:B:356:VAL:HG21	2.08	0.82
1:A:1114:SER:HB3	1:B:1104:ASN:HB3	1.59	0.82
1:A:715:LEU:HD21	1:B:936:PRO:HG2	1.62	0.82
1:B:623:VAL:HG12	1:C:65:SER:CB	2.09	0.82
1:C:58:TYR:OH	1:C:331:GLY:O	1.98	0.82
1:A:764:PHE:CD2	1:B:943:MET:SD	2.73	0.82
1:B:1024:ASP:O	1:B:1028:ASN:HB2	1.78	0.82
1:B:350:SER:C	1:B:351:TYR:HD2	1.80	0.82
1:A:377:GLN:O	1:A:381:VAL:HG22	1.80	0.82
1:B:166:ASN:OD1	2:B:1408:NAG:C1	2.28	0.81
1:B:347:LEU:HD13	1:B:361:TYR:CG	2.05	0.81
1:C:335:ARG:NE	1:C:354:PHE:CE2	2.47	0.81
1:A:166:ASN:OD1	2:A:1408:NAG:C1	2.28	0.81
1:A:350:SER:C	1:A:351:TYR:HD2	1.80	0.81
1:B:377:GLN:O	1:B:381:VAL:HG22	1.80	0.81
1:B:628:GLN:NE2	1:C:63:THR:CG2	2.42	0.81
1:A:58:TYR:OH	1:A:331:GLY:O	1.98	0.81
1:C:166:ASN:OD1	2:C:1408:NAG:C1	2.28	0.81
1:B:677:VAL:HG11	1:C:909:TYR:HE2	1.39	0.81
1:C:377:GLN:O	1:C:381:VAL:HG22	1.80	0.80
1:B:58:TYR:OH	1:B:331:GLY:O	1.98	0.80
1:A:1104:ASN:HB3	1:C:1114:SER:HB3	1.64	0.80
1:A:129:THR:HG22	1:A:131:ILE:H	1.47	0.80
1:C:129:THR:HG22	1:C:131:ILE:H	1.47	0.80
1:B:954:SER:O	1:B:958:VAL:HB	1.82	0.80
1:C:954:SER:O	1:C:958:VAL:HB	1.82	0.80
1:C:335:ARG:CZ	1:C:354:PHE:CE2	2.65	0.80
1:A:70:THR:N	1:A:352:GLU:OE2	2.14	0.80
1:B:335:ARG:CZ	1:B:354:PHE:CE2	2.65	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:CZ	1:A:354:PHE:CE2	2.65	0.79
1:A:335:ARG:CD	1:A:354:PHE:HE2	1.95	0.79
1:B:715:LEU:HD21	1:C:936:PRO:HG2	1.63	0.79
1:B:781:SER:OG	1:C:857:GLN:NE2	2.16	0.79
1:B:70:THR:N	1:B:352:GLU:OE2	2.14	0.79
1:B:343:ASP:HB3	1:B:661:VAL:HG21	1.65	0.79
1:A:954:SER:O	1:A:958:VAL:HB	1.82	0.79
1:B:129:THR:HG22	1:B:131:ILE:H	1.47	0.79
1:A:625:VAL:HG21	1:B:63:THR:OG1	1.70	0.79
1:B:335:ARG:CD	1:B:354:PHE:HE2	1.95	0.79
1:A:677:VAL:CG1	1:B:909:TYR:CE2	2.65	0.79
1:C:70:THR:N	1:C:352:GLU:OE2	2.14	0.79
1:A:822:ARG:CZ	1:C:694:ARG:NH1	2.46	0.79
1:C:335:ARG:HB3	1:C:354:PHE:CE2	2.18	0.79
1:A:628:GLN:HG2	1:B:63:THR:CG2	2.08	0.78
1:A:822:ARG:HH21	1:C:694:ARG:HH11	0.83	0.78
1:C:344:LEU:HA	1:C:661:VAL:HG11	1.66	0.78
1:B:365:SER:O	1:C:808:GLN:NE2	2.16	0.78
1:C:335:ARG:CD	1:C:354:PHE:HE2	1.95	0.78
1:C:343:ASP:CG	1:C:363:VAL:CB	2.52	0.78
1:A:335:ARG:HB3	1:A:354:PHE:CE2	2.18	0.78
1:A:343:ASP:HB3	1:A:363:VAL:HG21	1.66	0.78
1:B:344:LEU:HA	1:B:661:VAL:HG11	1.66	0.78
1:C:67:ILE:O	1:C:327:PHE:HD1	1.67	0.78
1:C:343:ASP:HB3	1:C:363:VAL:HG21	1.66	0.78
1:B:335:ARG:HB3	1:B:354:PHE:CE2	2.18	0.77
1:A:63:THR:HG21	1:C:628:GLN:CG	2.14	0.77
1:A:63:THR:CG2	1:C:628:GLN:HG2	2.15	0.77
1:A:343:ASP:CG	1:A:363:VAL:CB	2.52	0.77
1:B:343:ASP:CG	1:B:363:VAL:CB	2.52	0.77
1:B:67:ILE:O	1:B:327:PHE:HD1	1.67	0.77
1:A:628:GLN:NE2	1:B:63:THR:HG21	1.99	0.76
1:A:822:ARG:HE	1:C:694:ARG:HH12	0.79	0.76
1:B:764:PHE:CG	1:C:943:MET:SD	2.78	0.76
1:B:343:ASP:HB3	1:B:363:VAL:HG21	1.66	0.76
1:A:808:GLN:OE1	1:C:365:SER:OG	2.03	0.76
1:A:67:ILE:O	1:A:327:PHE:HD1	1.67	0.76
1:A:179:LEU:HD22	1:A:221:ARG:CD	2.15	0.76
1:A:625:VAL:HG21	1:B:63:THR:HB	0.76	0.76
1:A:344:LEU:HA	1:A:661:VAL:HG11	1.66	0.76
1:A:765:ASN:HD21	1:B:946:ALA:HB1	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:VAL:CB	1:B:909:TYR:CD2	2.69	0.75
1:A:588:LEU:N	1:A:588:LEU:HD23	2.02	0.75
1:A:343:ASP:OD2	1:A:363:VAL:HB	1.86	0.74
1:C:343:ASP:HB3	1:C:661:VAL:HG21	1.65	0.74
1:B:179:LEU:HD22	1:B:221:ARG:CD	2.15	0.74
1:C:343:ASP:OD2	1:C:363:VAL:HB	1.86	0.74
1:B:343:ASP:OD2	1:B:363:VAL:HB	1.86	0.74
1:A:63:THR:HG21	1:C:628:GLN:CD	2.07	0.74
1:A:943:MET:SD	1:C:738:LEU:HD11	2.27	0.74
1:B:588:LEU:N	1:B:588:LEU:HD23	2.02	0.74
1:B:774:ASN:OD1	2:B:1407:NAG:C1	2.36	0.74
1:A:343:ASP:CA	1:A:363:VAL:HG21	2.18	0.74
1:C:179:LEU:HD22	1:C:221:ARG:CD	2.15	0.74
1:A:63:THR:HB	1:C:625:VAL:HG21	0.75	0.74
1:B:778:PHE:HB3	1:C:969:ALA:O	1.88	0.74
1:C:588:LEU:N	1:C:588:LEU:HD23	2.02	0.73
1:C:774:ASN:OD1	2:C:1407:NAG:C1	2.36	0.73
1:C:1179:ARG:HB2	1:C:1184:TRP:HA	1.70	0.73
1:A:1179:ARG:HB2	1:A:1184:TRP:HA	1.70	0.73
1:A:764:PHE:CG	1:B:943:MET:SD	2.82	0.73
1:B:343:ASP:CA	1:B:363:VAL:HG21	2.18	0.73
1:A:774:ASN:OD1	2:A:1407:NAG:C1	2.36	0.73
1:B:764:PHE:CD2	1:C:943:MET:SD	2.82	0.73
1:C:663:TYR:HE2	1:C:668:LYS:HA	1.54	0.73
1:C:343:ASP:CA	1:C:363:VAL:HG21	2.18	0.73
1:A:329:VAL:O	1:C:623:VAL:HG13	1.89	0.72
1:B:1179:ARG:HB2	1:B:1184:TRP:HA	1.70	0.72
1:B:663:TYR:HE2	1:B:668:LYS:HA	1.54	0.72
1:C:22:GLY:N	2:C:1409:NAG:H82	2.05	0.72
1:A:408:ASN:HB3	1:A:587:LYS:HB3	1.71	0.72
1:B:1165:ILE:HG12	1:C:960:TRP:CH2	2.24	0.72
1:B:22:GLY:N	2:B:1409:NAG:H82	2.05	0.72
1:A:628:GLN:CD	1:B:63:THR:HG21	2.10	0.71
1:B:623:VAL:HG11	1:C:65:SER:CB	2.05	0.71
1:A:22:GLY:N	2:A:1409:NAG:H82	2.05	0.71
1:A:63:THR:HG21	1:C:628:GLN:HG2	1.70	0.71
1:A:324:LEU:HD22	1:A:354:PHE:HD1	1.55	0.71
1:A:663:TYR:HE2	1:A:668:LYS:HA	1.54	0.71
1:B:634:ALA:HB2	1:C:67:ILE:HD13	1.68	0.71
1:C:408:ASN:HB3	1:C:587:LYS:HB3	1.71	0.71
1:A:677:VAL:HG11	1:B:909:TYR:CD2	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:ASN:HB3	1:B:587:LYS:HB3	1.71	0.70
1:C:324:LEU:HD11	1:C:353:SER:C	2.12	0.70
1:B:324:LEU:HD11	1:B:353:SER:C	2.12	0.70
1:B:634:ALA:CB	1:C:67:ILE:CD1	2.64	0.70
1:C:181:ARG:NH2	1:C:222:ASN:OD1	2.25	0.70
1:B:40:PHE:HD1	1:B:86:VAL:HG13	1.57	0.70
1:C:324:LEU:HD22	1:C:354:PHE:HD1	1.55	0.70
1:A:324:LEU:HD11	1:A:353:SER:C	2.12	0.70
1:B:819:GLN:O	1:B:822:ARG:HB2	1.92	0.70
1:B:181:ARG:NH2	1:B:222:ASN:OD1	2.25	0.69
1:A:343:ASP:HB3	1:A:661:VAL:HG21	1.65	0.69
1:B:125:ASN:HD22	2:B:1402:NAG:C5	2.05	0.69
1:A:125:ASN:HD22	2:A:1402:NAG:C5	2.05	0.69
1:A:181:ARG:NH2	1:A:222:ASN:OD1	2.25	0.69
1:A:808:GLN:NE2	1:C:365:SER:O	2.25	0.69
1:B:765:ASN:HD21	1:C:946:ALA:HB1	1.56	0.69
1:A:67:ILE:O	1:A:327:PHE:CD1	2.46	0.69
1:A:40:PHE:HD1	1:A:86:VAL:HG13	1.57	0.69
1:A:677:VAL:HG11	1:B:909:TYR:HE2	1.53	0.69
1:C:40:PHE:HD1	1:C:86:VAL:HG13	1.57	0.69
1:C:340:GLY:O	1:C:694:ARG:N	2.26	0.69
1:A:340:GLY:O	1:A:694:ARG:N	2.26	0.68
1:B:67:ILE:O	1:B:327:PHE:CD1	2.45	0.68
1:C:67:ILE:O	1:C:327:PHE:CD1	2.46	0.68
1:B:628:GLN:HG2	1:C:63:THR:CG2	2.20	0.68
1:A:72:GLN:HG3	1:A:322:THR:OG1	1.94	0.68
1:C:335:ARG:CZ	1:C:354:PHE:HD2	2.08	0.67
1:B:221:ARG:HH12	2:B:1401:NAG:H82	1.59	0.67
1:B:628:GLN:NE2	1:C:63:THR:HG21	2.09	0.67
1:A:63:THR:HG23	1:C:628:GLN:CG	2.24	0.67
1:C:337:ILE:HG13	1:C:354:PHE:HE1	1.59	0.67
1:A:63:THR:CG2	1:C:628:GLN:CD	2.61	0.67
1:A:1165:ILE:HG12	1:B:960:TRP:HH2	1.59	0.67
1:B:340:GLY:O	1:B:694:ARG:N	2.26	0.67
1:B:663:TYR:O	1:B:664:ASP:CB	2.43	0.67
1:C:1031:GLN:O	1:C:1035:LYS:HB2	1.95	0.67
1:C:663:TYR:O	1:C:664:ASP:CB	2.43	0.67
1:A:493:LYS:NZ	1:A:565:GLU:O	2.28	0.67
1:A:960:TRP:HH2	1:C:1165:ILE:HG12	1.59	0.67
1:B:337:ILE:HG13	1:B:354:PHE:HE1	1.59	0.67
1:B:493:LYS:NZ	1:B:565:GLU:O	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:TYR:OH	1:C:668:LYS:HE3	1.95	0.67
1:A:738:LEU:HG	1:B:940:ASP:H	1.59	0.66
1:A:66:ASN:HB2	1:A:329:VAL:HA	1.77	0.66
1:B:1031:GLN:O	1:B:1035:LYS:HB2	1.95	0.66
1:C:125:ASN:ND2	2:C:1402:NAG:C6	2.58	0.66
1:C:125:ASN:HD22	2:C:1402:NAG:C5	2.05	0.66
1:C:785:ASN:OD1	2:C:1406:NAG:C1	2.44	0.66
1:A:1031:GLN:O	1:A:1035:LYS:HB2	1.95	0.66
1:A:124:ALA:O	1:A:125:ASN:CB	2.42	0.66
1:C:493:LYS:NZ	1:C:565:GLU:O	2.28	0.66
1:A:125:ASN:ND2	2:A:1402:NAG:C6	2.58	0.66
1:A:221:ARG:HH12	2:A:1401:NAG:H82	1.59	0.66
1:A:663:TYR:O	1:A:664:ASP:CB	2.43	0.66
1:B:324:LEU:HD22	1:B:354:PHE:HD1	1.55	0.66
1:B:663:TYR:OH	1:B:668:LYS:HE3	1.95	0.66
1:B:335:ARG:CZ	1:B:354:PHE:HD2	2.08	0.66
1:A:344:LEU:HD11	1:A:663:TYR:CG	2.31	0.66
1:B:785:ASN:OD1	2:B:1406:NAG:C1	2.44	0.66
1:A:125:ASN:HD22	2:A:1402:NAG:C6	2.09	0.66
1:B:66:ASN:HB2	1:B:329:VAL:HA	1.77	0.66
1:B:324:LEU:CD2	1:B:354:PHE:CD1	2.79	0.66
1:C:125:ASN:HD22	2:C:1402:NAG:C6	2.09	0.66
1:A:337:ILE:HG13	1:A:354:PHE:HE1	1.59	0.65
1:A:785:ASN:OD1	2:A:1406:NAG:H2	1.96	0.65
1:B:72:GLN:OE1	1:C:822:ARG:HG2	1.95	0.65
1:C:221:ARG:HH12	2:C:1401:NAG:H82	1.59	0.65
1:C:344:LEU:HD11	1:C:663:TYR:CG	2.31	0.65
1:A:324:LEU:CD2	1:A:354:PHE:CD1	2.79	0.65
1:A:663:TYR:OH	1:A:668:LYS:HE3	1.95	0.65
1:C:785:ASN:OD1	2:C:1406:NAG:H2	1.97	0.65
1:C:165:PHE:CE1	2:C:1408:NAG:O7	2.50	0.65
1:A:628:GLN:HG3	1:B:63:THR:CG2	2.26	0.65
1:B:344:LEU:HD11	1:B:663:TYR:CG	2.31	0.65
1:C:324:LEU:CD2	1:C:354:PHE:CD1	2.79	0.65
1:B:632:TYR:CE2	1:C:62:ARG:CB	2.80	0.65
1:A:930:ALA:HB3	1:C:656:SER:HB2	1.78	0.65
1:B:125:ASN:HD22	2:B:1402:NAG:C6	2.09	0.65
1:B:347:LEU:HD13	1:B:361:TYR:HD2	1.60	0.65
1:C:66:ASN:HB2	1:C:329:VAL:HA	1.77	0.65
1:C:347:LEU:HD12	1:C:661:VAL:CG1	2.27	0.65
1:A:337:ILE:HG13	1:A:354:PHE:CE1	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:HD11	1:B:943:MET:SD	2.37	0.65
1:B:625:VAL:HG21	1:C:63:THR:CG2	2.22	0.65
1:B:125:ASN:ND2	2:B:1402:NAG:C6	2.58	0.65
1:C:337:ILE:HG13	1:C:354:PHE:CE1	2.32	0.65
1:A:785:ASN:OD1	2:A:1406:NAG:C1	2.44	0.64
1:B:124:ALA:O	1:B:125:ASN:CB	2.42	0.64
1:B:343:ASP:OD2	1:B:659:VAL:CG1	2.45	0.64
1:B:785:ASN:OD1	2:B:1406:NAG:H2	1.97	0.64
1:C:343:ASP:OD2	1:C:659:VAL:CG1	2.45	0.64
1:C:353:SER:OG	1:C:355:ASP:O	2.16	0.64
1:A:678:ALA:HA	1:B:906:MET:SD	2.38	0.64
1:B:337:ILE:HG13	1:B:354:PHE:CE1	2.32	0.64
1:B:764:PHE:CB	1:C:943:MET:SD	2.86	0.64
1:B:779:LYS:O	1:C:969:ALA:HB3	1.98	0.64
1:C:663:TYR:CE2	1:C:668:LYS:HA	2.33	0.64
1:A:930:ALA:HB3	1:C:656:SER:CB	2.26	0.64
1:A:1027:ASN:O	1:A:1031:GLN:HB2	1.98	0.64
1:C:124:ALA:O	1:C:125:ASN:CB	2.42	0.64
1:A:347:LEU:HD12	1:A:661:VAL:CG1	2.27	0.64
1:B:165:PHE:CE1	2:B:1408:NAG:O7	2.50	0.64
1:B:347:LEU:HD12	1:B:661:VAL:CG1	2.27	0.64
1:B:691:ARG:HH12	1:C:818:GLU:CD	2.02	0.64
1:B:774:ASN:HD21	2:B:1407:NAG:C1	2.11	0.64
1:C:774:ASN:HD21	2:C:1407:NAG:C1	2.11	0.64
1:A:353:SER:OG	1:A:355:ASP:O	2.16	0.64
1:A:623:VAL:HG12	1:B:65:SER:HB3	1.78	0.64
1:B:599:GLN:HB3	1:B:600:LEU:HD23	1.80	0.64
1:C:501:ASN:ND2	1:C:559:SER:OG	2.30	0.63
1:A:1110:GLN:O	1:A:1122:HIS:ND1	2.31	0.63
1:B:335:ARG:CB	1:B:354:PHE:CE2	2.81	0.63
1:B:335:ARG:CG	1:B:354:PHE:HE2	2.11	0.63
1:B:1027:ASN:O	1:B:1031:GLN:HB2	1.98	0.63
1:A:335:ARG:CB	1:A:354:PHE:CE2	2.81	0.63
1:A:691:ARG:NH2	1:B:818:GLU:OE1	2.26	0.63
1:B:501:ASN:ND2	1:B:559:SER:OG	2.30	0.63
1:A:335:ARG:CG	1:A:354:PHE:CE2	2.82	0.63
1:A:898:VAL:HA	1:A:1023:GLN:HE21	1.62	0.63
1:C:898:VAL:HA	1:C:1023:GLN:HE21	1.62	0.63
1:B:628:GLN:NE2	1:C:63:THR:HG22	1.95	0.63
1:A:66:ASN:HD21	2:A:1403:NAG:C1	2.12	0.63
1:A:335:ARG:CG	1:A:354:PHE:HE2	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:OD2	1:A:659:VAL:CG1	2.45	0.63
1:A:774:ASN:HD21	2:A:1407:NAG:C1	2.11	0.63
1:B:663:TYR:CE2	1:B:668:LYS:HA	2.33	0.63
1:B:898:VAL:HA	1:B:1023:GLN:HE21	1.62	0.63
1:A:663:TYR:OH	1:A:668:LYS:HD2	1.98	0.63
1:C:335:ARG:CG	1:C:354:PHE:CE2	2.82	0.63
1:B:347:LEU:O	1:B:351:TYR:CE2	2.52	0.63
1:C:335:ARG:CB	1:C:354:PHE:CE2	2.81	0.63
1:C:1027:ASN:O	1:C:1031:GLN:HB2	1.98	0.63
1:B:335:ARG:CG	1:B:354:PHE:CE2	2.82	0.62
1:B:353:SER:OG	1:B:355:ASP:O	2.16	0.62
1:B:663:TYR:OH	1:B:668:LYS:HD2	1.98	0.62
1:A:66:ASN:ND2	2:A:1403:NAG:C1	2.62	0.62
1:A:335:ARG:CZ	1:A:354:PHE:HD2	2.07	0.62
1:A:634:ALA:HB2	1:B:67:ILE:HD13	1.80	0.62
1:C:66:ASN:ND2	2:C:1403:NAG:C1	2.62	0.62
1:C:1110:GLN:O	1:C:1122:HIS:ND1	2.31	0.62
1:C:343:ASP:HB3	1:C:363:VAL:CG2	2.29	0.62
1:C:599:GLN:HB3	1:C:600:LEU:HD23	1.80	0.62
1:A:347:LEU:HD13	1:A:361:TYR:HD2	1.60	0.62
1:C:663:TYR:OH	1:C:668:LYS:HD2	1.98	0.62
1:A:964:LEU:HD22	1:A:965:SER:HB3	1.82	0.62
1:B:66:ASN:ND2	2:B:1403:NAG:C1	2.62	0.62
1:B:964:LEU:HD22	1:B:965:SER:HB3	1.82	0.62
1:C:66:ASN:HD21	2:C:1403:NAG:C1	2.12	0.62
1:A:347:LEU:O	1:A:351:TYR:CE2	2.52	0.62
1:B:781:SER:CB	1:C:857:GLN:OE1	2.47	0.62
1:B:1110:GLN:O	1:B:1122:HIS:ND1	2.31	0.62
1:C:68:THR:O	1:C:69:ILE:CG2	2.48	0.62
1:A:344:LEU:N	1:A:661:VAL:HG21	2.15	0.62
1:A:599:GLN:HB3	1:A:600:LEU:HD23	1.80	0.62
1:B:66:ASN:HD21	2:B:1403:NAG:C1	2.12	0.62
1:B:343:ASP:HB3	1:B:363:VAL:CG2	2.29	0.62
1:C:335:ARG:CG	1:C:354:PHE:HE2	2.11	0.62
1:C:347:LEU:O	1:C:351:TYR:CE2	2.52	0.62
1:B:174:ASP:CG	1:B:221:ARG:O	2.38	0.62
1:A:335:ARG:CB	1:A:354:PHE:CZ	2.79	0.62
1:B:344:LEU:N	1:B:661:VAL:HG21	2.14	0.62
1:A:501:ASN:ND2	1:A:559:SER:OG	2.30	0.62
1:A:663:TYR:CE2	1:A:668:LYS:HA	2.33	0.61
1:C:174:ASP:CG	1:C:221:ARG:O	2.38	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:HB3	1:A:363:VAL:CG2	2.29	0.61
1:A:634:ALA:CB	1:B:67:ILE:CD1	2.70	0.61
1:C:344:LEU:N	1:C:661:VAL:HG21	2.15	0.61
1:A:165:PHE:CE1	2:A:1408:NAG:O7	2.50	0.61
1:B:68:THR:O	1:B:69:ILE:CG2	2.48	0.61
1:A:63:THR:OG1	1:C:625:VAL:HG21	1.44	0.61
1:A:1181:VAL:HB	1:B:967:PHE:CE2	2.35	0.61
1:B:343:ASP:CG	1:B:363:VAL:CG1	2.69	0.61
1:B:765:ASN:HD21	1:C:946:ALA:CB	2.14	0.61
1:A:68:THR:O	1:A:69:ILE:CG2	2.48	0.61
1:C:812:ASN:ND2	1:C:1050:SER:OG	2.34	0.61
1:C:964:LEU:HD22	1:C:965:SER:HB3	1.82	0.61
1:A:174:ASP:CG	1:A:221:ARG:O	2.38	0.61
1:B:588:LEU:HD23	1:B:588:LEU:H	1.66	0.61
1:A:628:GLN:CG	1:B:63:THR:HG23	2.29	0.60
1:A:812:ASN:ND2	1:A:1050:SER:OG	2.34	0.60
1:B:735:LEU:HD22	1:B:736:CYS:H	1.66	0.60
1:B:623:VAL:HG12	1:C:65:SER:HB3	1.84	0.60
1:A:343:ASP:CG	1:A:363:VAL:CG1	2.69	0.60
1:C:735:LEU:HD22	1:C:736:CYS:H	1.67	0.60
1:A:735:LEU:HD22	1:A:736:CYS:H	1.66	0.59
1:B:662:ILE:O	1:B:663:TYR:O	2.21	0.59
1:C:343:ASP:CG	1:C:363:VAL:CG1	2.69	0.59
1:C:588:LEU:HD23	1:C:588:LEU:H	1.66	0.59
1:A:67:ILE:HD11	1:C:634:ALA:CB	2.24	0.59
1:B:335:ARG:CB	1:B:354:PHE:CZ	2.79	0.59
1:C:662:ILE:O	1:C:663:TYR:O	2.21	0.59
1:A:352:GLU:HA	1:A:352:GLU:OE1	2.02	0.59
1:A:662:ILE:O	1:A:663:TYR:O	2.21	0.59
1:B:812:ASN:ND2	1:B:1050:SER:OG	2.34	0.59
1:A:663:TYR:OH	1:A:668:LYS:CD	2.51	0.59
1:C:343:ASP:CG	1:C:363:VAL:HG11	2.23	0.59
1:C:663:TYR:OH	1:C:668:LYS:CD	2.51	0.59
1:C:335:ARG:CB	1:C:354:PHE:CZ	2.79	0.59
1:C:352:GLU:HA	1:C:352:GLU:OE1	2.03	0.59
1:A:271:VAL:CG2	1:C:627:GLN:CD	2.69	0.58
1:B:352:GLU:OE1	1:B:352:GLU:HA	2.02	0.58
1:B:457:SER:HB3	1:B:460:SER:HB3	1.85	0.58
1:B:663:TYR:OH	1:B:668:LYS:CD	2.51	0.58
1:A:588:LEU:HD23	1:A:588:LEU:H	1.65	0.58
1:B:663:TYR:O	1:B:664:ASP:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLN:CD	1:B:63:THR:CG2	2.70	0.58
1:A:812:ASN:ND2	1:A:1050:SER:O	2.37	0.58
1:C:812:ASN:ND2	1:C:1050:SER:O	2.37	0.58
1:A:663:TYR:O	1:A:664:ASP:HB3	2.04	0.58
1:A:457:SER:HB3	1:A:460:SER:HB3	1.86	0.58
1:C:783:PRO:HG3	1:C:1143:PRO:HB3	1.86	0.58
1:A:343:ASP:HA	1:A:363:VAL:HG21	1.86	0.58
1:C:1179:ARG:H	1:C:1186:TYR:H	1.52	0.58
1:A:960:TRP:H	1:A:961:THR:HA	1.68	0.58
1:A:969:ALA:O	1:C:778:PHE:HB3	2.04	0.58
1:B:343:ASP:HA	1:B:363:VAL:HG21	1.86	0.58
1:C:343:ASP:HB2	1:C:661:VAL:HG22	1.85	0.58
1:C:602:ASN:ND2	1:C:617:PHE:O	2.37	0.58
1:C:960:TRP:H	1:C:961:THR:HA	1.68	0.58
1:A:602:ASN:ND2	1:A:617:PHE:O	2.37	0.58
1:B:1181:VAL:HB	1:C:967:PHE:CE2	2.38	0.58
1:A:347:LEU:O	1:A:351:TYR:CD2	2.57	0.58
1:A:1179:ARG:H	1:A:1186:TYR:H	1.52	0.58
1:B:677:VAL:HB	1:C:909:TYR:CD2	2.39	0.58
1:B:343:ASP:CG	1:B:363:VAL:HG11	2.23	0.57
1:C:347:LEU:HD13	1:C:361:TYR:HD2	1.60	0.57
1:B:347:LEU:O	1:B:351:TYR:CD2	2.57	0.57
1:B:812:ASN:ND2	1:B:1050:SER:O	2.37	0.57
1:A:343:ASP:HB2	1:A:661:VAL:HG22	1.85	0.57
1:B:1179:ARG:H	1:B:1186:TYR:H	1.52	0.57
1:C:343:ASP:HA	1:C:363:VAL:HG21	1.86	0.57
1:A:605:GLU:HG3	1:A:614:ARG:HG2	1.86	0.57
1:A:943:MET:SD	1:C:764:PHE:CD2	2.98	0.57
1:C:457:SER:HB3	1:C:460:SER:HB3	1.85	0.57
1:C:1027:ASN:O	1:C:1031:GLN:CB	2.53	0.57
1:A:64:TYR:N	1:A:64:TYR:CD2	2.73	0.57
1:B:67:ILE:O	1:B:327:PHE:HB2	2.05	0.57
1:B:340:GLY:O	1:B:693:THR:O	2.23	0.57
1:B:783:PRO:HG3	1:B:1143:PRO:HB3	1.86	0.57
1:B:1027:ASN:O	1:B:1031:GLN:CB	2.53	0.57
1:B:602:ASN:ND2	1:B:617:PHE:O	2.37	0.57
1:C:663:TYR:O	1:C:664:ASP:HB3	2.04	0.57
1:A:1023:GLN:O	1:A:1027:ASN:HB2	2.04	0.57
1:C:340:GLY:O	1:C:693:THR:O	2.23	0.57
1:C:1105:GLU:OE1	1:C:1113:ARG:NH2	2.38	0.57
1:A:1105:GLU:OE1	1:A:1113:ARG:NH2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:GLU:HG3	1:B:614:ARG:HG2	1.87	0.57
1:B:960:TRP:H	1:B:961:THR:HA	1.68	0.57
1:C:1023:GLN:O	1:C:1027:ASN:HB2	2.04	0.57
1:A:340:GLY:O	1:A:693:THR:O	2.23	0.57
1:A:857:GLN:NE2	1:C:781:SER:OG	2.34	0.57
1:A:1027:ASN:O	1:A:1031:GLN:CB	2.53	0.57
1:C:347:LEU:O	1:C:351:TYR:CD2	2.57	0.57
1:A:783:PRO:HG3	1:A:1143:PRO:HB3	1.86	0.56
1:B:1023:GLN:O	1:B:1027:ASN:HB2	2.04	0.56
1:C:67:ILE:O	1:C:327:PHE:HB2	2.05	0.56
1:A:67:ILE:O	1:A:327:PHE:HB2	2.05	0.56
1:B:64:TYR:N	1:B:64:TYR:CD2	2.73	0.56
1:C:605:GLU:HG3	1:C:614:ARG:HG2	1.87	0.56
1:A:343:ASP:CG	1:A:363:VAL:HG11	2.23	0.56
1:C:343:ASP:CB	1:C:363:VAL:CG2	2.82	0.56
1:A:677:VAL:CG1	1:B:909:TYR:CD2	2.88	0.56
1:B:985:ILE:HD11	1:C:962:ALA:O	2.06	0.56
1:A:765:ASN:HD21	1:B:946:ALA:CB	2.17	0.56
1:A:967:PHE:CE2	1:C:1181:VAL:HB	2.41	0.56
1:C:673:LEU:HD13	1:C:735:LEU:HD21	1.88	0.56
1:C:1102:LYS:HB3	1:C:1136:PHE:HE2	1.71	0.56
1:A:63:THR:OG1	1:C:625:VAL:CB	2.49	0.56
1:B:787:SER:H	1:B:1000:LYS:HD3	1.71	0.56
1:B:793:GLU:HA	1:B:1018:ALA:HB2	1.88	0.56
1:B:1105:GLU:OE1	1:B:1113:ARG:NH2	2.38	0.56
1:A:787:SER:H	1:A:1000:LYS:HD3	1.71	0.56
1:B:377:GLN:O	1:B:381:VAL:CG2	2.53	0.56
1:C:343:ASP:CA	1:C:661:VAL:HG21	2.36	0.56
1:A:787:SER:OG	1:A:1142:TYR:O	2.24	0.55
1:B:343:ASP:CB	1:B:363:VAL:CG2	2.82	0.55
1:C:66:ASN:HA	1:C:328:SER:O	2.06	0.55
1:C:787:SER:OG	1:C:1142:TYR:O	2.24	0.55
1:C:793:GLU:HA	1:C:1018:ALA:HB2	1.88	0.55
1:C:888:SER:OG	1:C:889:ALA:N	2.39	0.55
1:B:66:ASN:HA	1:B:328:SER:O	2.06	0.55
1:C:64:TYR:N	1:C:64:TYR:CD2	2.73	0.55
1:B:343:ASP:HB2	1:B:661:VAL:HG22	1.84	0.55
1:C:125:ASN:ND2	2:C:1402:NAG:O5	2.14	0.55
1:A:377:GLN:O	1:A:381:VAL:CG2	2.53	0.55
1:A:673:LEU:HD13	1:A:735:LEU:HD21	1.88	0.55
1:B:628:GLN:CD	1:C:63:THR:HG21	2.26	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:VAL:HG21	1:B:63:THR:CG2	2.26	0.55
1:C:677:VAL:HG22	1:C:678:ALA:HB2	1.89	0.55
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.89	0.55
1:B:68:THR:C	1:B:69:ILE:HG23	2.26	0.55
1:B:831:ILE:HG23	1:B:1082:VAL:HG21	1.89	0.55
1:B:996:LEU:HD23	1:B:998:ALA:HB3	1.89	0.55
1:A:68:THR:C	1:A:69:ILE:HG23	2.27	0.55
1:B:787:SER:OG	1:B:1142:TYR:O	2.24	0.55
1:B:1102:LYS:HB3	1:B:1136:PHE:HE2	1.71	0.55
1:A:677:VAL:HG22	1:A:678:ALA:HB2	1.89	0.55
1:C:68:THR:C	1:C:69:ILE:HG23	2.26	0.55
1:A:66:ASN:HA	1:A:328:SER:O	2.06	0.55
1:A:343:ASP:CA	1:A:661:VAL:HG21	2.36	0.55
1:B:343:ASP:CA	1:B:661:VAL:HG21	2.36	0.55
1:B:1174:LYS:O	1:B:1177:ASN:ND2	2.40	0.55
1:C:348:HIS:HA	1:C:356:VAL:HG23	1.87	0.55
1:A:335:ARG:NH1	1:A:354:PHE:HD2	2.06	0.54
1:B:888:SER:OG	1:B:889:ALA:N	2.40	0.54
1:A:1174:LYS:O	1:A:1177:ASN:ND2	2.40	0.54
1:C:787:SER:H	1:C:1000:LYS:HD3	1.71	0.54
1:C:996:LEU:HD23	1:C:998:ALA:HB3	1.89	0.54
1:A:1102:LYS:HB3	1:A:1136:PHE:HE2	1.71	0.54
1:B:673:LEU:HD13	1:B:735:LEU:HD21	1.88	0.54
1:B:738:LEU:HG	1:C:940:ASP:H	1.73	0.54
1:C:831:ILE:HG23	1:C:1082:VAL:HG21	1.89	0.54
1:C:1174:LYS:O	1:C:1177:ASN:ND2	2.40	0.54
1:C:335:ARG:NH1	1:C:354:PHE:HD2	2.06	0.54
1:A:781:SER:OG	1:B:857:GLN:NE2	2.36	0.54
1:A:888:SER:OG	1:A:889:ALA:N	2.39	0.54
1:B:1169:ASN:OD1	1:C:967:PHE:CE1	2.61	0.54
1:A:996:LEU:HD23	1:A:998:ALA:HB3	1.89	0.54
1:C:21:VAL:C	2:C:1409:NAG:C8	2.70	0.54
1:C:989:VAL:HB	1:C:1186:TYR:HE1	1.72	0.54
1:A:793:GLU:HA	1:A:1018:ALA:HB2	1.88	0.54
1:A:989:VAL:HB	1:A:1186:TYR:HE1	1.72	0.54
1:B:399:PHE:O	1:B:523:TYR:OH	2.15	0.54
1:C:796:GLN:O	1:C:798:THR:N	2.40	0.54
1:C:377:GLN:O	1:C:381:VAL:CG2	2.53	0.54
1:B:335:ARG:NH1	1:B:354:PHE:HD2	2.06	0.54
1:B:1166:ALA:HB2	1:B:1194:PRO:HD3	1.90	0.54
1:A:63:THR:HG23	1:C:628:GLN:HG2	1.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:C	2:A:1409:NAG:C8	2.70	0.53
1:A:1166:ALA:HB2	1:A:1194:PRO:HD3	1.90	0.53
1:A:909:TYR:CE2	1:C:677:VAL:CG1	2.84	0.53
1:A:936:PRO:HG2	1:C:715:LEU:CD2	2.29	0.53
1:B:989:VAL:HB	1:B:1186:TYR:HE1	1.73	0.53
1:A:737:ALA:HB1	1:B:940:ASP:OD1	2.09	0.53
1:C:1166:ALA:HB2	1:C:1194:PRO:HD3	1.90	0.53
1:C:619:ASN:ND2	2:C:1404:NAG:O6	2.42	0.53
1:A:946:ALA:HB1	1:C:765:ASN:HD21	1.74	0.53
1:B:179:LEU:CD2	1:B:221:ARG:CD	2.83	0.53
1:B:480:ILE:HB	1:B:571:PHE:HB2	1.91	0.53
1:B:677:VAL:HG22	1:B:678:ALA:HB2	1.89	0.53
1:B:677:VAL:HG11	1:C:909:TYR:CD2	2.37	0.52
1:B:631:VAL:HA	1:C:63:THR:O	2.08	0.52
1:A:697:LEU:HD13	1:A:698:LYS:H	1.74	0.52
1:B:467:PHE:O	1:B:524:SER:HB2	2.10	0.52
1:B:619:ASN:ND2	2:B:1404:NAG:O6	2.42	0.52
1:C:125:ASN:HD22	2:C:1402:NAG:H5	1.66	0.52
1:C:977:PHE:O	1:C:981:ASN:HB2	2.10	0.52
1:A:179:LEU:CD2	1:A:221:ARG:CD	2.83	0.52
1:A:181:ARG:HG3	1:A:242:THR:HG22	1.92	0.52
1:A:1117:CYS:HB3	1:A:1122:HIS:CD2	2.45	0.52
1:B:21:VAL:C	2:B:1409:NAG:C8	2.70	0.52
1:B:181:ARG:HG3	1:B:242:THR:HG22	1.92	0.52
1:C:129:THR:HG23	1:C:134:PRO:HA	1.91	0.52
1:A:774:ASN:ND2	2:A:1407:NAG:C1	2.73	0.52
1:A:789:GLY:HA3	1:A:1004:ALA:HB1	1.92	0.52
1:B:677:VAL:CG1	1:C:909:TYR:CD2	2.92	0.52
1:C:181:ARG:HG3	1:C:242:THR:HG22	1.92	0.52
1:A:619:ASN:ND2	2:A:1404:NAG:O6	2.42	0.52
1:A:628:GLN:HG3	1:B:63:THR:HG23	1.89	0.52
1:A:1147:ILE:HD12	1:A:1184:TRP:HE1	1.75	0.52
1:B:347:LEU:CD1	1:B:361:TYR:CD2	2.76	0.52
1:B:697:LEU:HD13	1:B:698:LYS:H	1.74	0.52
1:B:977:PHE:O	1:B:981:ASN:HB2	2.10	0.52
1:C:480:ILE:HB	1:C:571:PHE:HB2	1.91	0.52
1:A:347:LEU:CD1	1:A:361:TYR:CD2	2.76	0.52
1:A:660:SER:N	1:A:673:LEU:O	2.42	0.52
1:A:677:VAL:HB	1:B:909:TYR:CD2	2.45	0.52
1:B:21:VAL:HA	2:B:1409:NAG:H81	1.92	0.52
1:B:129:THR:HG23	1:B:134:PRO:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:LEU:HD22	1:B:354:PHE:CE1	2.45	0.52
1:B:628:GLN:HG3	1:C:63:THR:CG2	2.37	0.52
1:B:1117:CYS:HB3	1:B:1122:HIS:CD2	2.45	0.52
1:C:21:VAL:HA	2:C:1409:NAG:H81	1.92	0.52
1:A:343:ASP:CB	1:A:363:VAL:CG2	2.82	0.52
1:C:697:LEU:HD13	1:C:698:LYS:H	1.74	0.52
1:A:977:PHE:O	1:A:981:ASN:HB2	2.10	0.52
1:C:619:ASN:ND2	2:C:1404:NAG:O5	2.43	0.52
1:A:399:PHE:O	1:A:523:TYR:OH	2.15	0.51
1:A:958:VAL:HG11	1:A:1108:LYS:HD2	1.92	0.51
1:B:677:VAL:CB	1:C:909:TYR:CE2	2.93	0.51
1:B:1147:ILE:HD12	1:B:1184:TRP:HE1	1.75	0.51
1:C:774:ASN:ND2	2:C:1407:NAG:C1	2.73	0.51
1:C:1117:CYS:HB3	1:C:1122:HIS:CD2	2.45	0.51
1:C:68:THR:HG22	1:C:69:ILE:N	2.26	0.51
1:A:21:VAL:HA	2:A:1409:NAG:H81	1.92	0.51
1:A:870:ASN:N	1:A:1002:ASN:OD1	2.43	0.51
1:B:348:HIS:HA	1:B:356:VAL:HG23	1.87	0.51
1:B:588:LEU:N	1:B:588:LEU:CD2	2.73	0.51
1:B:619:ASN:ND2	2:B:1404:NAG:O5	2.44	0.51
1:B:870:ASN:N	1:B:1002:ASN:OD1	2.43	0.51
1:B:958:VAL:HG11	1:B:1108:LYS:HD2	1.92	0.51
1:C:1169:ASN:OD1	1:C:1169:ASN:N	2.43	0.51
1:A:68:THR:HG22	1:A:69:ILE:N	2.26	0.51
1:A:129:THR:HG23	1:A:134:PRO:HA	1.91	0.51
1:A:467:PHE:O	1:A:524:SER:HB2	2.10	0.51
1:A:619:ASN:ND2	2:A:1404:NAG:O5	2.44	0.51
1:B:799:ILE:HD11	1:B:1089:SER:HA	1.93	0.51
1:A:480:ILE:HB	1:A:571:PHE:HB2	1.91	0.51
1:A:799:ILE:HD11	1:A:1089:SER:HA	1.93	0.51
1:A:1031:GLN:HG2	1:A:1035:LYS:HD3	1.92	0.51
1:C:467:PHE:O	1:C:524:SER:HB2	2.10	0.51
1:C:383:CYS:N	1:C:408:ASN:O	2.44	0.51
1:A:335:ARG:CD	1:A:354:PHE:CE2	2.86	0.51
1:B:789:GLY:HA3	1:B:1004:ALA:HB1	1.92	0.51
1:B:1153:TYR:OH	1:C:970:ILE:HG23	2.11	0.51
1:A:125:ASN:ND2	2:A:1402:NAG:O5	2.14	0.51
1:A:221:ARG:NH1	2:A:1401:NAG:H2	2.26	0.51
1:C:221:ARG:NH1	2:C:1401:NAG:H2	2.26	0.51
1:C:799:ILE:HD11	1:C:1089:SER:HA	1.93	0.51
1:A:796:GLN:O	1:A:798:THR:N	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASN:HA	1:B:327:PHE:O	2.12	0.50
1:B:221:ARG:NH1	2:B:1401:NAG:H2	2.26	0.50
1:C:399:PHE:O	1:C:523:TYR:OH	2.15	0.50
1:C:789:GLY:HA3	1:C:1004:ALA:HB1	1.92	0.50
1:C:872:THR:OG1	1:C:1009:GLN:NE2	2.39	0.50
1:A:66:ASN:HA	1:A:327:PHE:O	2.11	0.50
1:A:588:LEU:N	1:A:588:LEU:CD2	2.73	0.50
1:A:621:THR:HG23	2:A:1404:NAG:O7	2.12	0.50
1:A:960:TRP:CH2	1:C:1165:ILE:HG12	2.45	0.50
1:B:785:ASN:OD1	2:B:1406:NAG:C2	2.59	0.50
1:A:324:LEU:HD22	1:A:354:PHE:CE1	2.45	0.50
1:A:943:MET:SD	1:C:764:PHE:CG	3.04	0.50
1:B:383:CYS:N	1:B:408:ASN:O	2.44	0.50
1:B:596:ILE:C	1:B:598:SER:H	2.15	0.50
1:B:796:GLN:O	1:B:798:THR:N	2.40	0.50
1:C:621:THR:HG23	2:C:1404:NAG:O7	2.11	0.50
1:A:335:ARG:NH1	1:A:354:PHE:CD2	2.79	0.50
1:A:983:VAL:HG12	1:A:1121:THR:HB	1.93	0.50
1:B:335:ARG:NH1	1:B:354:PHE:CD2	2.79	0.50
1:B:774:ASN:ND2	2:B:1407:NAG:C1	2.73	0.50
1:C:350:SER:O	1:C:351:TYR:CB	2.60	0.50
1:C:1147:ILE:HD12	1:C:1184:TRP:HE1	1.75	0.50
1:B:621:THR:HG23	2:B:1404:NAG:O7	2.12	0.50
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	1.93	0.50
1:C:335:ARG:NH1	1:C:354:PHE:CD2	2.79	0.50
1:C:958:VAL:HG11	1:C:1108:LYS:HD2	1.92	0.50
1:B:68:THR:HG22	1:B:69:ILE:N	2.26	0.50
1:B:660:SER:N	1:B:673:LEU:O	2.42	0.50
1:B:967:PHE:HB3	1:B:968:ALA:HB2	1.94	0.50
1:C:660:SER:N	1:C:673:LEU:O	2.42	0.50
1:C:1031:GLN:HG2	1:C:1035:LYS:HD3	1.92	0.50
1:A:1008:MET:HB3	1:A:1137:MET:HE3	1.93	0.50
1:B:626:ARG:HA	1:B:642:TYR:HE2	1.76	0.50
1:B:663:TYR:C	1:B:663:TYR:CD2	2.85	0.50
1:C:626:ARG:HA	1:C:642:TYR:HE2	1.76	0.50
1:C:870:ASN:N	1:C:1002:ASN:OD1	2.43	0.50
1:A:626:ARG:HA	1:A:642:TYR:HE2	1.76	0.50
1:A:778:PHE:HB3	1:B:969:ALA:O	2.12	0.50
1:A:383:CYS:N	1:A:408:ASN:O	2.44	0.50
1:C:324:LEU:HD22	1:C:354:PHE:CE1	2.45	0.50
1:C:738:LEU:HD13	1:C:762:ILE:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG23	1:C:628:GLN:HG3	1.93	0.49
1:A:1130:ALA:HB2	1:A:1135:TYR:HB2	1.93	0.49
1:B:1031:GLN:HG2	1:B:1035:LYS:HD3	1.92	0.49
1:A:348:HIS:HA	1:A:356:VAL:HG23	1.86	0.49
1:A:804:VAL:HA	1:A:932:TYR:HA	1.94	0.49
1:C:596:ILE:C	1:C:598:SER:H	2.15	0.49
1:C:1130:ALA:HB2	1:C:1135:TYR:HB2	1.93	0.49
1:A:372:GLY:HA2	1:A:596:ILE:HG22	1.94	0.49
1:A:632:TYR:CE2	1:B:62:ARG:CB	2.96	0.49
1:A:738:LEU:HD13	1:A:762:ILE:HG23	1.94	0.49
1:C:49:ASP:HB3	1:C:52:LYS:HD2	1.95	0.49
1:C:735:LEU:HD12	1:C:739:PRO:HB2	1.95	0.49
1:A:179:LEU:HD22	1:A:221:ARG:HE	0.70	0.49
1:B:350:SER:O	1:B:351:TYR:CB	2.60	0.49
1:B:663:TYR:OH	1:B:668:LYS:HE2	2.12	0.49
1:A:68:THR:O	1:A:69:ILE:HG23	2.13	0.49
1:A:663:TYR:OH	1:A:668:LYS:HE2	2.12	0.49
1:A:663:TYR:CD2	1:A:663:TYR:C	2.85	0.49
1:A:764:PHE:CB	1:B:943:MET:SD	3.00	0.49
1:A:909:TYR:CD2	1:C:677:VAL:CB	2.95	0.49
1:A:350:SER:O	1:A:351:TYR:CB	2.60	0.49
1:B:49:ASP:HB3	1:B:52:LYS:HD2	1.95	0.49
1:B:68:THR:O	1:B:69:ILE:HG23	2.12	0.49
1:B:1179:ARG:HB2	1:B:1185:SER:HA	1.95	0.49
1:C:785:ASN:OD1	2:C:1406:NAG:C2	2.59	0.49
1:A:677:VAL:HG21	1:B:910:ASP:OD1	2.13	0.49
1:B:738:LEU:HD13	1:B:762:ILE:HG23	1.94	0.49
1:C:372:GLY:HA2	1:C:596:ILE:HG22	1.94	0.49
1:A:384:ASP:OD1	1:A:386:SER:OG	2.23	0.49
1:A:596:ILE:C	1:A:598:SER:H	2.15	0.49
1:A:967:PHE:HB3	1:A:968:ALA:HB2	1.94	0.49
1:C:663:TYR:OH	1:C:668:LYS:HE2	2.12	0.49
1:A:663:TYR:C	1:A:663:TYR:HD2	2.16	0.49
1:C:1172:PHE:O	1:C:1176:ASN:OD1	2.31	0.49
1:A:728:LYS:H	1:A:761:SER:HG	1.61	0.49
1:A:735:LEU:HD12	1:A:739:PRO:HB2	1.94	0.49
1:B:519:ASN:HB2	1:B:522:GLN:OE1	2.13	0.49
1:B:983:VAL:HG12	1:B:1121:THR:HB	1.94	0.49
1:C:720:SER:HG	1:C:757:MET:N	2.11	0.49
1:B:125:ASN:ND2	2:B:1402:NAG:O5	2.14	0.48
1:C:663:TYR:C	1:C:663:TYR:CD2	2.85	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:VAL:HA	1:C:932:TYR:HA	1.94	0.48
1:C:983:VAL:HG12	1:C:1121:THR:HB	1.94	0.48
1:A:631:VAL:HA	1:B:63:THR:O	2.12	0.48
1:B:335:ARG:CD	1:B:354:PHE:CE2	2.86	0.48
1:C:663:TYR:C	1:C:663:TYR:HD2	2.16	0.48
1:C:686:MET:SD	1:C:686:MET:N	2.75	0.48
1:C:967:PHE:HB3	1:C:968:ALA:HB2	1.94	0.48
1:A:785:ASN:OD1	2:A:1406:NAG:C2	2.59	0.48
1:B:1008:MET:HB3	1:B:1137:MET:HE3	1.94	0.48
1:C:66:ASN:HA	1:C:327:PHE:O	2.11	0.48
1:C:519:ASN:HB2	1:C:522:GLN:OE1	2.13	0.48
1:B:372:GLY:HA2	1:B:596:ILE:HG22	1.94	0.48
1:B:691:ARG:NH1	1:C:818:GLU:CD	2.65	0.48
1:B:720:SER:HG	1:B:757:MET:N	2.11	0.48
1:B:735:LEU:HD12	1:B:739:PRO:HB2	1.94	0.48
1:B:804:VAL:HA	1:B:932:TYR:HA	1.94	0.48
1:A:720:SER:HG	1:A:757:MET:N	2.11	0.48
1:B:68:THR:O	1:B:69:ILE:HG22	2.14	0.48
1:C:68:THR:O	1:C:69:ILE:HG22	2.14	0.48
1:C:1008:MET:HB3	1:C:1137:MET:HE3	1.94	0.48
1:A:629:ARG:HB2	1:A:642:TYR:HB3	1.96	0.48
1:A:872:THR:OG1	1:A:1009:GLN:NE2	2.39	0.48
1:A:1165:ILE:HG12	1:B:960:TRP:CH2	2.45	0.48
1:A:1172:PHE:O	1:A:1176:ASN:OD1	2.31	0.48
1:B:663:TYR:C	1:B:663:TYR:HD2	2.16	0.48
1:C:68:THR:O	1:C:69:ILE:HG23	2.12	0.48
1:C:179:LEU:CD2	1:C:221:ARG:CD	2.83	0.48
1:C:990:LEU:HD11	1:C:1179:ARG:HD3	1.96	0.48
1:C:179:LEU:HD22	1:C:221:ARG:HE	0.71	0.48
1:A:990:LEU:HD11	1:A:1179:ARG:HD3	1.96	0.48
1:C:335:ARG:CD	1:C:354:PHE:CE2	2.86	0.48
1:C:1179:ARG:HB2	1:C:1185:SER:HA	1.95	0.48
1:A:49:ASP:HB3	1:A:52:LYS:HD2	1.95	0.48
1:A:581:THR:O	1:A:583:SER:N	2.47	0.48
1:B:129:THR:CG2	1:B:131:ILE:H	2.24	0.48
1:A:836:HIS:CE1	1:C:360:VAL:O	2.67	0.47
1:B:764:PHE:HB2	1:C:943:MET:SD	2.54	0.47
1:C:800:GLN:HE21	1:C:934:VAL:HG11	1.78	0.47
1:A:365:SER:O	1:B:808:GLN:NE2	2.47	0.47
1:C:804:VAL:HG11	1:C:1078:LEU:HD11	1.96	0.47
1:A:68:THR:O	1:A:69:ILE:HG22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:ARG:HB2	1:A:1185:SER:HA	1.95	0.47
1:B:581:THR:O	1:B:583:SER:N	2.47	0.47
1:B:1172:PHE:O	1:B:1176:ASN:OD1	2.31	0.47
1:A:798:THR:HB	1:A:842:GLN:HE21	1.80	0.47
1:C:629:ARG:HB2	1:C:642:TYR:HB3	1.96	0.47
1:A:519:ASN:HB2	1:A:522:GLN:OE1	2.13	0.47
1:A:804:VAL:HG11	1:A:1078:LEU:HD11	1.96	0.47
1:B:485:PRO:O	1:B:566:GLN:HG2	2.15	0.47
1:B:800:GLN:HE21	1:B:934:VAL:HG11	1.78	0.47
1:B:1181:VAL:HA	1:B:1182:ASP:HA	1.61	0.47
1:C:798:THR:HB	1:C:842:GLN:HE21	1.80	0.47
1:A:68:THR:C	1:A:69:ILE:CG2	2.83	0.47
1:A:485:PRO:O	1:A:566:GLN:HG2	2.15	0.47
1:A:984:GLY:O	1:A:986:THR:N	2.48	0.47
1:B:804:VAL:HG11	1:B:1078:LEU:HD11	1.96	0.47
1:B:984:GLY:O	1:B:986:THR:N	2.48	0.47
1:B:990:LEU:HD11	1:B:1179:ARG:HD3	1.96	0.47
1:B:1160:ASN:HB3	1:B:1198:THR:HG21	1.97	0.47
1:C:845:SER:O	1:C:849:LEU:HB2	2.15	0.47
1:C:867:GLY:HA2	1:C:868:ASP:HA	1.63	0.47
1:A:800:GLN:HE21	1:A:934:VAL:HG11	1.78	0.47
1:B:384:ASP:OD1	1:B:386:SER:OG	2.23	0.47
1:B:845:SER:O	1:B:849:LEU:HB2	2.15	0.47
1:C:984:GLY:O	1:C:986:THR:N	2.48	0.47
1:A:907:GLN:O	1:A:911:ASP:CB	2.63	0.47
1:C:68:THR:C	1:C:69:ILE:CG2	2.83	0.47
1:A:347:LEU:HD11	1:A:361:TYR:HB2	0.93	0.47
1:A:686:MET:SD	1:A:686:MET:N	2.75	0.47
1:A:940:ASP:H	1:C:738:LEU:HG	1.79	0.47
1:B:691:ARG:CZ	1:C:818:GLU:OE1	2.60	0.47
1:B:872:THR:OG1	1:B:1009:GLN:NE2	2.39	0.47
1:B:907:GLN:O	1:B:911:ASP:CB	2.63	0.47
1:C:581:THR:O	1:C:583:SER:N	2.47	0.47
1:C:728:LYS:HA	1:C:729:LEU:HA	1.72	0.47
1:B:408:ASN:HA	1:B:585:CYS:O	2.15	0.46
1:B:807:LYS:HA	1:B:821:LEU:HD13	1.97	0.46
1:C:408:ASN:HA	1:C:585:CYS:O	2.15	0.46
1:C:642:TYR:HA	1:C:643:SER:HA	1.63	0.46
1:B:629:ARG:HB2	1:B:642:TYR:HB3	1.96	0.46
1:C:933:LYS:NZ	1:C:934:VAL:O	2.47	0.46
1:A:716:GLY:HA2	1:B:906:MET:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:SER:O	1:A:849:LEU:HB2	2.15	0.46
1:C:588:LEU:N	1:C:588:LEU:CD2	2.73	0.46
1:C:1171:TYR:H	1:C:1178:THR:HG22	1.81	0.46
1:A:807:LYS:HA	1:A:821:LEU:HD13	1.97	0.46
1:A:1128:VAL:HG23	1:A:1135:TYR:HB3	1.98	0.46
1:C:350:SER:HB2	1:C:351:TYR:CE2	2.51	0.46
1:C:1160:ASN:HB3	1:C:1198:THR:HG21	1.97	0.46
1:B:738:LEU:HD11	1:C:943:MET:SD	2.56	0.46
1:C:485:PRO:O	1:C:566:GLN:HG2	2.15	0.46
1:C:658:PRO:HG2	1:C:675:GLY:HA3	1.98	0.46
1:C:907:GLN:O	1:C:911:ASP:CB	2.63	0.46
1:A:63:THR:CG2	1:C:628:GLN:HG3	2.42	0.46
1:A:1160:ASN:HB3	1:A:1198:THR:HG21	1.97	0.46
1:B:658:PRO:HG2	1:B:675:GLY:HA3	1.98	0.46
1:A:408:ASN:HA	1:A:585:CYS:O	2.15	0.46
1:A:1169:ASN:OD1	1:A:1169:ASN:N	2.43	0.46
1:A:1171:TYR:H	1:A:1178:THR:HG22	1.81	0.46
1:B:1128:VAL:HG23	1:B:1135:TYR:HB3	1.98	0.46
1:C:807:LYS:HA	1:C:821:LEU:HD13	1.97	0.46
1:B:691:ARG:NH1	1:C:818:GLU:OE1	2.48	0.46
1:B:798:THR:HB	1:B:842:GLN:HE21	1.80	0.46
1:A:63:THR:HG21	1:C:625:VAL:HG11	1.97	0.46
1:B:1149:VAL:HG12	1:B:1150:VAL:H	1.81	0.46
1:A:779:LYS:O	1:B:969:ALA:HB3	2.15	0.46
1:B:691:ARG:HB2	1:C:808:GLN:HE22	1.81	0.46
1:C:1128:VAL:HG23	1:C:1135:TYR:HB3	1.98	0.46
1:A:993:ASN:HA	1:A:994:GLN:HA	1.75	0.45
1:B:642:TYR:HA	1:B:643:SER:HA	1.63	0.45
1:B:1171:TYR:H	1:B:1178:THR:HG22	1.81	0.45
1:A:658:PRO:HG2	1:A:675:GLY:HA3	1.98	0.45
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.99	0.45
1:B:501:ASN:HD22	1:B:559:SER:HG	1.60	0.45
1:C:1149:VAL:HG12	1:C:1150:VAL:H	1.81	0.45
1:B:359:GLY:HA2	1:B:733:GLN:HB2	1.98	0.45
1:B:867:GLY:HA2	1:B:868:ASP:HA	1.63	0.45
1:B:1165:ILE:CG1	1:C:960:TRP:HH2	2.16	0.45
1:C:359:GLY:HA2	1:C:733:GLN:HB2	1.98	0.45
1:B:348:HIS:O	1:B:353:SER:O	2.35	0.45
1:B:350:SER:HB2	1:B:351:TYR:CE2	2.51	0.45
1:C:803:THR:HG22	1:C:839:ASN:HD21	1.81	0.45
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:TYR:HH	1:A:668:LYS:CE	2.29	0.45
1:C:68:THR:CG2	1:C:69:ILE:N	2.80	0.45
1:C:722:LEU:HG	1:C:758:ARG:HA	1.98	0.45
1:A:350:SER:HB2	1:A:351:TYR:CE2	2.51	0.45
1:B:803:THR:HG22	1:B:839:ASN:HD21	1.81	0.45
1:C:964:LEU:HA	1:C:965:SER:HA	1.78	0.45
1:A:68:THR:CG2	1:A:69:ILE:N	2.80	0.45
1:A:340:GLY:O	1:A:693:THR:C	2.55	0.45
1:A:969:ALA:HB3	1:C:779:LYS:O	2.17	0.45
1:A:1181:VAL:HB	1:B:967:PHE:CZ	2.51	0.45
1:B:335:ARG:HB3	1:B:354:PHE:HZ	1.71	0.45
1:B:347:LEU:HD11	1:B:361:TYR:HB2	0.92	0.45
1:B:621:THR:CG2	2:B:1404:NAG:O7	2.65	0.45
1:B:722:LEU:HG	1:B:758:ARG:HA	1.98	0.45
1:C:498:SER:HB3	1:C:534:VAL:HG23	1.99	0.45
1:A:722:LEU:HG	1:A:758:ARG:HA	1.98	0.45
1:B:340:GLY:O	1:B:693:THR:C	2.55	0.45
1:B:68:THR:C	1:B:69:ILE:CG2	2.83	0.45
1:B:179:LEU:HD22	1:B:221:ARG:HE	0.70	0.45
1:B:1164:CYS:HA	1:B:1165:ILE:HA	1.69	0.45
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.99	0.45
1:A:803:THR:HG22	1:A:839:ASN:HD21	1.81	0.45
1:C:340:GLY:O	1:C:693:THR:C	2.55	0.45
1:C:348:HIS:O	1:C:353:SER:O	2.35	0.45
1:A:354:PHE:HD1	1:A:354:PHE:HA	1.73	0.44
1:A:359:GLY:HA2	1:A:733:GLN:HB2	1.98	0.44
1:A:728:LYS:HA	1:A:729:LEU:HA	1.71	0.44
1:B:792:GLN:HG3	1:B:1138:HIS:HB2	1.99	0.44
1:B:1165:ILE:CD1	1:C:960:TRP:CH2	3.00	0.44
1:A:498:SER:HB3	1:A:534:VAL:HG23	1.99	0.44
1:A:778:PHE:CD1	1:B:971:PRO:HD3	2.52	0.44
1:A:778:PHE:CZ	1:B:971:PRO:HG3	2.53	0.44
1:C:21:VAL:HA	2:C:1409:NAG:C8	2.48	0.44
1:A:324:LEU:CD1	1:A:353:SER:O	2.66	0.44
1:B:728:LYS:H	1:B:761:SER:HG	1.62	0.44
1:C:347:LEU:CD1	1:C:361:TYR:CD2	2.76	0.44
1:A:63:THR:C	1:A:64:TYR:CD2	2.91	0.44
1:A:628:GLN:HG2	1:B:63:THR:HG23	1.95	0.44
1:A:792:GLN:HG3	1:A:1138:HIS:HB2	1.99	0.44
1:B:63:THR:C	1:B:64:TYR:CD2	2.91	0.44
1:B:498:SER:HB3	1:B:534:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:O	1:A:353:SER:O	2.35	0.44
1:B:933:LYS:NZ	1:B:934:VAL:O	2.47	0.44
1:C:63:THR:C	1:C:64:TYR:CD2	2.91	0.44
1:C:129:THR:CG2	1:C:131:ILE:H	2.24	0.44
1:C:621:THR:CG2	2:C:1404:NAG:O7	2.65	0.44
1:C:792:GLN:HG3	1:C:1138:HIS:HB2	1.99	0.44
1:A:718:VAL:HG11	1:A:759:LEU:HD11	2.00	0.44
1:A:964:LEU:HA	1:A:965:SER:HA	1.78	0.44
1:B:344:LEU:HD13	1:B:661:VAL:CG1	2.48	0.44
1:B:347:LEU:HD12	1:B:661:VAL:HG11	1.99	0.44
1:B:350:SER:O	1:B:351:TYR:CG	2.68	0.44
1:B:1169:ASN:OD1	1:B:1169:ASN:N	2.43	0.44
1:C:324:LEU:CD1	1:C:353:SER:O	2.66	0.44
1:C:718:VAL:HG11	1:C:759:LEU:HD11	2.00	0.44
1:A:1149:VAL:HG12	1:A:1150:VAL:H	1.81	0.44
1:A:1181:VAL:HA	1:A:1182:ASP:HA	1.61	0.44
1:C:596:ILE:C	1:C:598:SER:N	2.71	0.44
1:A:21:VAL:HA	2:A:1409:NAG:C8	2.47	0.44
1:B:68:THR:CG2	1:B:69:ILE:N	2.80	0.44
1:B:324:LEU:CD1	1:B:353:SER:O	2.66	0.44
1:B:485:PRO:HB2	1:B:486:HIS:H	1.61	0.44
1:B:712:GLY:HA3	1:B:713:CYS:HA	1.67	0.44
1:C:979:ARG:O	1:C:1110:GLN:NE2	2.51	0.44
1:B:993:ASN:HA	1:B:994:GLN:HA	1.75	0.44
1:A:72:GLN:HE21	1:A:72:GLN:HB3	1.60	0.43
1:A:1037:ALA:HA	1:A:1040:LEU:HD12	2.00	0.43
1:B:21:VAL:HA	2:B:1409:NAG:C8	2.48	0.43
1:B:1186:TYR:HB3	1:B:1187:THR:H	1.53	0.43
1:C:765:ASN:HB2	1:C:766:HIS:HA	2.00	0.43
1:A:372:GLY:HA2	1:A:596:ILE:CG2	2.48	0.43
1:C:372:GLY:HA2	1:C:596:ILE:CG2	2.48	0.43
1:C:1114:SER:OG	1:C:1115:GLY:N	2.51	0.43
1:A:221:ARG:HH12	2:A:1401:NAG:H2	1.83	0.43
1:A:638:LEU:HG	1:A:651:LEU:HD21	2.00	0.43
1:A:933:LYS:NZ	1:A:934:VAL:O	2.47	0.43
1:A:979:ARG:O	1:A:1110:GLN:NE2	2.51	0.43
1:B:628:GLN:CG	1:C:63:THR:HG23	2.46	0.43
1:C:484:VAL:HA	1:C:485:PRO:HD3	1.72	0.43
1:C:638:LEU:HG	1:C:651:LEU:HD21	2.00	0.43
1:A:350:SER:O	1:A:351:TYR:CG	2.68	0.43
1:A:656:SER:CB	1:B:930:ALA:HB3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:GLY:HA2	1:A:868:ASP:HA	1.63	0.43
1:A:1173:ILE:HG22	1:A:1174:LYS:H	1.83	0.43
1:B:372:GLY:HA2	1:B:596:ILE:CG2	2.48	0.43
1:B:1180:ILE:HG22	1:C:967:PHE:CZ	2.53	0.43
1:C:1173:ILE:HG22	1:C:1174:LYS:H	1.83	0.43
1:A:344:LEU:HD13	1:A:661:VAL:CG1	2.48	0.43
1:A:596:ILE:C	1:A:598:SER:N	2.71	0.43
1:A:621:THR:CG2	2:A:1404:NAG:O7	2.65	0.43
1:A:726:ASP:HB2	1:A:727:CYS:HB3	2.01	0.43
1:B:221:ARG:HH12	2:B:1401:NAG:H2	1.84	0.43
1:B:335:ARG:HG2	1:B:354:PHE:CE2	2.54	0.43
1:B:596:ILE:C	1:B:598:SER:N	2.71	0.43
1:B:718:VAL:HG11	1:B:759:LEU:HD11	2.00	0.43
1:A:1122:HIS:NE2	1:A:1125:SER:HB3	2.34	0.43
1:C:1037:ALA:HA	1:C:1040:LEU:HD12	2.00	0.43
1:A:129:THR:CG2	1:A:134:PRO:HA	2.49	0.43
1:B:129:THR:CG2	1:B:134:PRO:HA	2.49	0.43
1:B:726:ASP:HB2	1:B:727:CYS:HB3	2.01	0.43
1:A:335:ARG:HG2	1:A:354:PHE:CE2	2.54	0.43
1:B:621:THR:HG21	2:B:1404:NAG:H81	2.01	0.43
1:C:58:TYR:OH	1:C:332:TYR:C	2.56	0.43
1:C:693:THR:HA	1:C:694:ARG:HA	1.80	0.43
1:A:765:ASN:HB2	1:A:766:HIS:HA	2.00	0.43
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.88	0.43
1:B:1114:SER:OG	1:B:1115:GLY:N	2.51	0.43
1:A:738:LEU:HG	1:B:940:ASP:N	2.32	0.43
1:B:765:ASN:HB2	1:B:766:HIS:HA	2.00	0.43
1:B:1122:HIS:NE2	1:B:1125:SER:HB3	2.34	0.43
1:A:485:PRO:HB2	1:A:486:HIS:H	1.61	0.42
1:B:979:ARG:O	1:B:1110:GLN:NE2	2.51	0.42
1:C:129:THR:CG2	1:C:134:PRO:HA	2.49	0.42
1:C:344:LEU:HD13	1:C:661:VAL:CG1	2.48	0.42
1:C:377:GLN:C	1:C:381:VAL:HG22	2.39	0.42
1:C:1013:THR:HA	1:C:1014:THR:HA	1.76	0.42
1:A:484:VAL:HA	1:A:485:PRO:HD3	1.72	0.42
1:B:677:VAL:HG21	1:C:910:ASP:OD1	2.19	0.42
1:B:693:THR:HA	1:B:694:ARG:HA	1.80	0.42
1:C:347:LEU:HD12	1:C:661:VAL:HG11	1.99	0.42
1:C:1181:VAL:HA	1:C:1182:ASP:HA	1.61	0.42
1:A:179:LEU:CD1	1:A:221:ARG:HD3	2.50	0.42
1:A:347:LEU:HD12	1:A:661:VAL:HG11	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1173:ILE:HG22	1:B:1174:LYS:H	1.83	0.42
1:C:1122:HIS:NE2	1:C:1125:SER:HB3	2.34	0.42
1:B:727:CYS:HB2	1:B:763:ALA:HA	2.02	0.42
1:C:347:LEU:O	1:C:351:TYR:HE2	2.02	0.42
1:B:638:LEU:HG	1:B:651:LEU:HD21	2.00	0.42
1:B:976:ILE:O	1:B:980:LEU:CB	2.68	0.42
1:C:456:LEU:HD12	1:C:456:LEU:HA	1.88	0.42
1:A:778:PHE:CE1	1:B:971:PRO:HD3	2.55	0.42
1:A:985:ILE:HD11	1:B:962:ALA:O	2.19	0.42
1:B:656:SER:CB	1:C:930:ALA:HB3	2.49	0.42
1:C:165:PHE:CG	2:C:1408:NAG:O7	2.65	0.42
1:C:366:PHE:N	1:C:691:ARG:O	2.51	0.42
1:C:621:THR:HG21	2:C:1404:NAG:H81	2.01	0.42
1:C:990:LEU:HD23	1:C:990:LEU:HA	1.87	0.42
1:B:728:LYS:HA	1:B:729:LEU:HA	1.72	0.42
1:B:1037:ALA:HA	1:B:1040:LEU:HD12	2.00	0.42
1:C:179:LEU:CD1	1:C:221:ARG:HD3	2.50	0.42
1:A:871:LEU:HA	1:A:871:LEU:HD23	1.84	0.42
1:A:976:ILE:O	1:A:980:LEU:CB	2.68	0.42
1:A:1114:SER:OG	1:A:1115:GLY:N	2.51	0.42
1:B:350:SER:O	1:B:351:TYR:HB2	2.20	0.42
1:B:1201:ASN:HB2	1:B:1206:ALA:HB3	2.02	0.42
1:C:1201:ASN:HB2	1:C:1206:ALA:HB3	2.02	0.42
1:A:731:LEU:HD22	1:A:732:GLY:H	1.85	0.42
1:A:350:SER:O	1:A:351:TYR:HB2	2.20	0.42
1:A:530:VAL:HA	1:A:531:PRO:HD2	1.90	0.42
1:A:764:PHE:HA	1:A:765:ASN:HA	1.81	0.42
1:A:1036:LEU:HD23	1:A:1036:LEU:HA	1.87	0.42
1:C:774:ASN:CG	2:C:1407:NAG:C1	2.89	0.42
1:A:271:VAL:HG22	1:C:627:GLN:CD	2.21	0.41
1:A:727:CYS:HB2	1:A:763:ALA:HA	2.02	0.41
1:B:179:LEU:CD1	1:B:221:ARG:HD3	2.50	0.41
1:B:617:PHE:HB3	1:B:649:TYR:HB3	2.02	0.41
1:B:810:VAL:HG22	1:B:1074:ARG:HD2	2.02	0.41
1:C:726:ASP:HB2	1:C:727:CYS:HB3	2.01	0.41
1:A:818:GLU:O	1:A:822:ARG:HG3	2.20	0.41
1:C:129:THR:HG22	1:C:131:ILE:N	2.26	0.41
1:C:782:ILE:H	1:C:782:ILE:HG13	1.59	0.41
1:A:906:MET:SD	1:C:678:ALA:HA	2.59	0.41
1:C:617:PHE:HB3	1:C:649:TYR:HB3	2.03	0.41
1:C:726:ASP:OD1	1:C:726:ASP:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:GLY:HA2	1:C:734:SER:HB2	2.02	0.41
1:A:1201:ASN:HB2	1:A:1206:ALA:HB3	2.02	0.41
1:B:686:MET:SD	1:B:686:MET:N	2.75	0.41
1:B:1127:VAL:HG13	1:B:1136:PHE:HE1	1.86	0.41
1:B:1165:ILE:CG1	1:C:960:TRP:CH2	2.99	0.41
1:C:221:ARG:HH12	2:C:1401:NAG:H2	1.84	0.41
1:C:727:CYS:HB2	1:C:763:ALA:HA	2.02	0.41
1:A:728:LYS:N	1:A:761:SER:OG	2.45	0.41
1:A:810:VAL:HG22	1:A:1074:ARG:HD2	2.02	0.41
1:A:1164:CYS:HA	1:A:1165:ILE:HA	1.69	0.41
1:C:663:TYR:HH	1:C:668:LYS:CE	2.29	0.41
1:C:731:LEU:HD22	1:C:732:GLY:H	1.85	0.41
1:A:725:GLU:OE2	1:A:728:LYS:NZ	2.43	0.41
1:B:484:VAL:O	1:B:566:GLN:HB3	2.21	0.41
1:B:774:ASN:CG	2:B:1407:NAG:C1	2.89	0.41
1:C:335:ARG:HB3	1:C:354:PHE:HZ	1.71	0.41
1:C:335:ARG:HG2	1:C:354:PHE:CE2	2.54	0.41
1:C:350:SER:O	1:C:351:TYR:HB2	2.20	0.41
1:C:810:VAL:HG22	1:C:1074:ARG:HD2	2.02	0.41
1:A:63:THR:HB	1:C:625:VAL:HG22	1.78	0.41
1:A:65:SER:HB3	1:C:623:VAL:CG1	2.23	0.41
1:A:967:PHE:CZ	1:C:1181:VAL:HB	2.56	0.41
1:B:731:LEU:HD22	1:B:732:GLY:H	1.85	0.41
1:C:484:VAL:O	1:C:566:GLN:HB3	2.21	0.41
1:C:1164:CYS:HA	1:C:1165:ILE:HA	1.69	0.41
1:A:484:VAL:O	1:A:566:GLN:HB3	2.21	0.41
1:B:343:ASP:HA	1:B:363:VAL:HG11	2.03	0.41
1:B:691:ARG:HB3	1:B:693:THR:HG22	2.03	0.41
1:C:504:SER:HB3	1:C:515:PRO:HA	2.03	0.41
1:C:712:GLY:HA3	1:C:713:CYS:HA	1.67	0.41
1:C:1186:TYR:HB3	1:C:1187:THR:H	1.52	0.41
1:A:347:LEU:HD12	1:A:661:VAL:HG12	2.01	0.41
1:A:347:LEU:O	1:A:351:TYR:HE2	2.02	0.41
1:A:366:PHE:N	1:A:691:ARG:O	2.51	0.41
1:A:621:THR:HG21	2:A:1404:NAG:H81	2.01	0.41
1:A:642:TYR:HD1	1:A:642:TYR:HA	1.76	0.41
1:A:774:ASN:CG	2:A:1407:NAG:C1	2.89	0.41
1:B:58:TYR:OH	1:B:332:TYR:C	2.56	0.41
1:B:347:LEU:HD12	1:B:661:VAL:HG12	2.01	0.41
1:B:347:LEU:O	1:B:351:TYR:HE2	2.02	0.41
1:B:732:GLY:HA2	1:B:734:SER:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:LEU:HA	1:B:965:SER:HA	1.78	0.41
1:C:343:ASP:HA	1:C:363:VAL:HG11	2.03	0.41
1:C:350:SER:O	1:C:351:TYR:CG	2.68	0.41
1:C:598:SER:OG	1:C:599:GLN:N	2.54	0.41
1:C:822:ARG:O	1:C:823:GLU:C	2.58	0.41
1:B:598:SER:OG	1:B:599:GLN:N	2.54	0.41
1:C:487:ASN:OD1	1:C:487:ASN:N	2.54	0.41
1:C:728:LYS:H	1:C:761:SER:HG	1.64	0.41
1:C:976:ILE:O	1:C:980:LEU:CB	2.68	0.41
1:A:165:PHE:CG	2:A:1408:NAG:O7	2.65	0.40
1:A:487:ASN:OD1	1:A:487:ASN:N	2.54	0.40
1:A:641:TYR:CD2	1:A:648:TYR:HA	2.56	0.40
1:A:1127:VAL:HG13	1:A:1136:PHE:HE1	1.86	0.40
1:B:179:LEU:CD2	1:B:221:ARG:HD3	2.51	0.40
1:B:835:LEU:HD23	1:B:835:LEU:HA	1.89	0.40
1:B:909:TYR:O	1:B:928:TYR:OH	2.39	0.40
1:C:691:ARG:HB3	1:C:693:THR:HG22	2.03	0.40
1:C:1100:LYS:O	1:C:1104:ASN:ND2	2.54	0.40
1:B:853:VAL:HG13	1:B:951:LEU:HD22	2.03	0.40
1:B:990:LEU:HD23	1:B:990:LEU:HA	1.87	0.40
1:B:1100:LYS:O	1:B:1104:ASN:ND2	2.54	0.40
1:C:1180:ILE:HG22	1:C:1181:VAL:H	1.86	0.40
1:A:392:THR:HG1	1:A:492:THR:HG1	1.68	0.40
1:A:448:TYR:OH	1:A:452:MET:O	2.36	0.40
1:A:943:MET:SD	1:C:764:PHE:CB	3.10	0.40
1:C:1127:VAL:HG13	1:C:1136:PHE:HE1	1.86	0.40
1:A:58:TYR:OH	1:A:332:TYR:C	2.56	0.40
1:A:129:THR:CG2	1:A:131:ILE:H	2.24	0.40
1:A:712:GLY:HA3	1:A:713:CYS:HA	1.67	0.40
1:A:1100:LYS:O	1:A:1104:ASN:ND2	2.54	0.40
1:B:72:GLN:OE1	1:C:822:ARG:HB3	2.22	0.40
1:A:808:GLN:HE22	1:C:691:ARG:HB2	1.86	0.40
1:A:990:LEU:HA	1:A:990:LEU:HD23	1.86	0.40
1:B:634:ALA:CB	1:C:67:ILE:HD13	2.42	0.40
1:B:641:TYR:CD2	1:B:648:TYR:HA	2.56	0.40
1:C:645:ASP:HA	1:C:646:GLY:HA2	1.81	0.40
1:C:871:LEU:HD23	1:C:871:LEU:HA	1.84	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	1128/1323 (85%)	964 (86%)	149 (13%)	15 (1%)	10	40
1	B	1128/1323 (85%)	964 (86%)	149 (13%)	15 (1%)	10	40
1	C	1128/1323 (85%)	964 (86%)	149 (13%)	15 (1%)	10	40
All	All	3384/3969 (85%)	2892 (86%)	447 (13%)	45 (1%)	13	40

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	663	TYR
1	A	664	ASP
1	A	797	THR
1	B	66	ASN
1	B	663	TYR
1	B	664	ASP
1	B	797	THR
1	C	66	ASN
1	C	663	TYR
1	C	664	ASP
1	C	797	THR
1	A	125	ASN
1	A	485	PRO
1	A	582	ASN
1	A	997	ILE
1	B	125	ASN
1	B	485	PRO
1	B	582	ASN
1	B	997	ILE
1	C	125	ASN
1	C	485	PRO
1	C	582	ASN
1	C	997	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	855	SER
1	B	855	SER
1	C	855	SER
1	A	382	GLU
1	B	382	GLU
1	C	382	GLU
1	A	642	TYR
1	B	642	TYR
1	C	642	TYR
1	A	736	CYS
1	B	736	CYS
1	C	736	CYS
1	A	1181	VAL
1	B	1181	VAL
1	C	1181	VAL
1	A	1054	ILE
1	B	1054	ILE
1	C	1054	ILE
1	A	985	ILE
1	B	985	ILE
1	C	985	ILE

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	973/1143 (85%)	930 (96%)	43 (4%)	24	50
1	B	973/1143 (85%)	931 (96%)	42 (4%)	25	50
1	C	973/1143 (85%)	930 (96%)	43 (4%)	24	50
All	All	2919/3429 (85%)	2791 (96%)	128 (4%)	26	50

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	TYR
1	A	72	GLN
1	A	179	LEU
1	A	221	ARG
1	A	244	ASN
1	A	335	ARG
1	A	348	HIS
1	A	352	GLU
1	A	354	PHE
1	A	411	LEU
1	A	423	PHE
1	A	450	LEU
1	A	458	VAL
1	A	465	SER
1	A	473	PHE
1	A	479	LEU
1	A	481	LEU
1	A	484	VAL
1	A	487	ASN
1	A	488	LEU
1	A	490	THR
1	A	510	ASP
1	A	535	TRP
1	A	555	VAL
1	A	565	GLU
1	A	573	ILE
1	A	588	LEU
1	A	595	LYS
1	A	602	ASN
1	A	663	TYR
1	A	665	LYS
1	A	677	VAL
1	A	722	LEU
1	A	785	ASN
1	A	799	ILE
1	A	832	ASN
1	A	848	ASN
1	A	854	LYS
1	A	870	ASN
1	A	1028	ASN
1	A	1165	ILE
1	A	1181	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	58	TYR
1	B	64	TYR
1	B	179	LEU
1	B	221	ARG
1	B	244	ASN
1	B	335	ARG
1	B	348	HIS
1	B	352	GLU
1	B	354	PHE
1	B	411	LEU
1	B	423	PHE
1	B	450	LEU
1	B	458	VAL
1	B	465	SER
1	B	473	PHE
1	B	479	LEU
1	B	481	LEU
1	B	484	VAL
1	B	487	ASN
1	B	488	LEU
1	B	490	THR
1	B	510	ASP
1	B	535	TRP
1	B	555	VAL
1	B	565	GLU
1	B	573	ILE
1	B	588	LEU
1	B	595	LYS
1	B	602	ASN
1	B	663	TYR
1	B	665	LYS
1	B	677	VAL
1	B	722	LEU
1	B	785	ASN
1	B	799	ILE
1	B	832	ASN
1	B	848	ASN
1	B	854	LYS
1	B	870	ASN
1	B	1028	ASN
1	B	1165	ILE
1	B	1181	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	58	TYR
1	C	64	TYR
1	C	179	LEU
1	C	221	ARG
1	C	244	ASN
1	C	335	ARG
1	C	348	HIS
1	C	352	GLU
1	C	354	PHE
1	C	411	LEU
1	C	423	PHE
1	C	450	LEU
1	C	458	VAL
1	C	465	SER
1	C	473	PHE
1	C	479	LEU
1	C	481	LEU
1	C	484	VAL
1	C	487	ASN
1	C	488	LEU
1	C	490	THR
1	C	510	ASP
1	C	535	TRP
1	C	555	VAL
1	C	565	GLU
1	C	573	ILE
1	C	588	LEU
1	C	595	LYS
1	C	602	ASN
1	C	663	TYR
1	C	665	LYS
1	C	677	VAL
1	C	722	LEU
1	C	785	ASN
1	C	799	ILE
1	C	822	ARG
1	C	832	ASN
1	C	848	ASN
1	C	854	LYS
1	C	870	ASN
1	C	1028	ASN
1	C	1165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	72	GLN
1	A	125	ASN
1	A	244	ASN
1	A	348	HIS
1	A	599	GLN
1	A	602	ASN
1	A	619	ASN
1	A	628	GLN
1	A	765	ASN
1	A	792	GLN
1	A	800	GLN
1	A	812	ASN
1	A	832	ASN
1	A	836	HIS
1	A	839	ASN
1	A	842	GLN
1	A	1009	GLN
1	A	1023	GLN
1	A	1028	ASN
1	A	1072	ASN
1	A	1104	ASN
1	A	1176	ASN
1	B	66	ASN
1	B	125	ASN
1	B	244	ASN
1	B	346	GLN
1	B	348	HIS
1	B	501	ASN
1	B	599	GLN
1	B	602	ASN
1	B	619	ASN
1	B	628	GLN
1	B	765	ASN
1	B	792	GLN
1	B	800	GLN
1	B	812	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	832	ASN
1	B	839	ASN
1	B	842	GLN
1	B	848	ASN
1	B	1009	GLN
1	B	1023	GLN
1	B	1028	ASN
1	B	1072	ASN
1	B	1104	ASN
1	B	1176	ASN
1	C	66	ASN
1	C	125	ASN
1	C	244	ASN
1	C	346	GLN
1	C	348	HIS
1	C	599	GLN
1	C	602	ASN
1	C	619	ASN
1	C	628	GLN
1	C	792	GLN
1	C	800	GLN
1	C	812	ASN
1	C	832	ASN
1	C	839	ASN
1	C	842	GLN
1	C	848	ASN
1	C	1009	GLN
1	C	1023	GLN
1	C	1028	ASN
1	C	1072	ASN
1	C	1104	ASN
1	C	1176	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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
2	NAG	B	1407	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	B	1409	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	C	1408	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	A	1405	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	A	1404	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	B	1408	-	14,14,15	1.37	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	A	1408	-	14,14,15	1.36	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	B	1402	-	14,14,15	0.36	0	17,19,21	0.85	0
2	NAG	B	1406	-	14,14,15	1.36	3 (21%)	17,19,21	0.97	1 (5%)
2	NAG	C	1401	-	14,14,15	0.27	0	17,19,21	0.67	0
2	NAG	A	1403	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	B	1403	-	14,14,15	1.35	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	A	1407	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	B	1405	-	14,14,15	1.37	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	A	1401	-	14,14,15	0.27	0	17,19,21	0.66	0
2	NAG	B	1404	-	14,14,15	1.36	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	C	1406	-	14,14,15	1.34	3 (21%)	17,19,21	0.97	1 (5%)
2	NAG	C	1410	-	14,14,15	1.35	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	B	1401	-	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	C	1405	-	14,14,15	1.35	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	A	1410	-	14,14,15	1.35	3 (21%)	17,19,21	0.99	1 (5%)
2	NAG	C	1402	-	14,14,15	0.37	0	17,19,21	0.85	0
2	NAG	C	1409	-	14,14,15	1.36	3 (21%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1402	-	14,14,15	0.37	0	17,19,21	0.85	0
2	NAG	C	1403	-	14,14,15	1.35	3 (21%)	17,19,21	1.00	1 (5%)
2	NAG	C	1407	-	14,14,15	1.35	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	A	1406	-	14,14,15	1.35	3 (21%)	17,19,21	0.97	1 (5%)
2	NAG	C	1404	-	14,14,15	1.35	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	A	1409	-	14,14,15	1.37	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	B	1410	-	14,14,15	1.35	3 (21%)	17,19,21	0.99	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
2	NAG	B	1407	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1409	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1408	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1405	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1404	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1408	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1408	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1402	-	-	4/6/23/26	0/1/1/1
2	NAG	B	1406	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1401	-	-	4/6/23/26	0/1/1/1
2	NAG	A	1403	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1403	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1407	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1405	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1401	-	-	4/6/23/26	0/1/1/1
2	NAG	B	1404	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1406	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1410	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1401	-	-	4/6/23/26	0/1/1/1
2	NAG	C	1405	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1410	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1402	-	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1409	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1402	-	-	4/6/23/26	0/1/1/1
2	NAG	C	1403	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1407	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1406	-	-	2/6/23/26	0/1/1/1
2	NAG	C	1404	-	-	2/6/23/26	0/1/1/1
2	NAG	A	1409	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1410	-	-	2/6/23/26	0/1/1/1

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1408	NAG	O5-C5	-2.61	1.38	1.43
2	A	1404	NAG	O5-C5	-2.60	1.38	1.43
2	B	1405	NAG	O5-C5	-2.60	1.38	1.43
2	A	1408	NAG	O5-C5	-2.60	1.38	1.43
2	C	1404	NAG	O5-C5	-2.59	1.38	1.43
2	B	1404	NAG	O5-C5	-2.59	1.38	1.43
2	C	1403	NAG	C7-N2	2.58	1.43	1.34
2	B	1407	NAG	C7-N2	2.58	1.43	1.34
2	B	1403	NAG	C7-N2	2.58	1.43	1.34
2	A	1409	NAG	O5-C5	-2.57	1.38	1.43
2	A	1407	NAG	C7-N2	2.57	1.43	1.34
2	B	1406	NAG	O5-C5	-2.57	1.38	1.43
2	A	1403	NAG	C7-N2	2.57	1.43	1.34
2	B	1409	NAG	C7-N2	2.56	1.43	1.34
2	B	1405	NAG	C7-N2	2.56	1.43	1.34
2	B	1408	NAG	C7-N2	2.56	1.43	1.34
2	C	1409	NAG	O5-C5	-2.56	1.38	1.43
2	A	1405	NAG	O5-C5	-2.56	1.38	1.43
2	C	1408	NAG	O5-C5	-2.56	1.38	1.43
2	A	1409	NAG	C7-N2	2.56	1.43	1.34
2	A	1405	NAG	C7-N2	2.56	1.43	1.34
2	A	1408	NAG	C7-N2	2.56	1.43	1.34
2	C	1408	NAG	C7-N2	2.56	1.43	1.34
2	B	1409	NAG	O5-C5	-2.55	1.38	1.43
2	C	1407	NAG	C7-N2	2.55	1.43	1.34
2	A	1403	NAG	O5-C5	-2.55	1.38	1.43
2	C	1410	NAG	C7-N2	2.55	1.43	1.34
2	B	1410	NAG	O5-C5	-2.55	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1406	NAG	O5-C5	-2.55	1.38	1.43
2	A	1410	NAG	O5-C5	-2.55	1.38	1.43
2	B	1404	NAG	C7-N2	2.55	1.43	1.34
2	A	1406	NAG	O5-C5	-2.55	1.38	1.43
2	C	1403	NAG	O5-C5	-2.55	1.38	1.43
2	A	1410	NAG	C7-N2	2.55	1.43	1.34
2	A	1407	NAG	O5-C5	-2.54	1.38	1.43
2	C	1405	NAG	O5-C5	-2.54	1.38	1.43
2	B	1403	NAG	O5-C5	-2.54	1.38	1.43
2	C	1409	NAG	C7-N2	2.54	1.43	1.34
2	C	1405	NAG	C7-N2	2.54	1.43	1.34
2	B	1406	NAG	C7-N2	2.54	1.43	1.34
2	C	1410	NAG	O5-C5	-2.54	1.38	1.43
2	C	1404	NAG	C7-N2	2.53	1.43	1.34
2	C	1407	NAG	O5-C5	-2.53	1.38	1.43
2	A	1404	NAG	C7-N2	2.53	1.43	1.34
2	C	1406	NAG	C7-N2	2.53	1.43	1.34
2	B	1410	NAG	C7-N2	2.53	1.43	1.34
2	A	1406	NAG	C7-N2	2.52	1.43	1.34
2	B	1407	NAG	O5-C5	-2.51	1.38	1.43
2	B	1407	NAG	C2-N2	-2.32	1.42	1.46
2	B	1405	NAG	C2-N2	-2.32	1.42	1.46
2	A	1405	NAG	C2-N2	-2.31	1.42	1.46
2	B	1406	NAG	C2-N2	-2.30	1.42	1.46
2	A	1407	NAG	C2-N2	-2.30	1.42	1.46
2	C	1408	NAG	C2-N2	-2.29	1.42	1.46
2	A	1406	NAG	C2-N2	-2.29	1.42	1.46
2	C	1406	NAG	C2-N2	-2.28	1.42	1.46
2	C	1407	NAG	C2-N2	-2.27	1.42	1.46
2	A	1408	NAG	C2-N2	-2.27	1.42	1.46
2	A	1404	NAG	C2-N2	-2.27	1.42	1.46
2	C	1405	NAG	C2-N2	-2.27	1.42	1.46
2	B	1408	NAG	C2-N2	-2.27	1.42	1.46
2	A	1403	NAG	C2-N2	-2.27	1.42	1.46
2	A	1409	NAG	C2-N2	-2.26	1.42	1.46
2	B	1403	NAG	C2-N2	-2.25	1.42	1.46
2	C	1404	NAG	C2-N2	-2.25	1.42	1.46
2	B	1410	NAG	C2-N2	-2.25	1.42	1.46
2	B	1404	NAG	C2-N2	-2.25	1.42	1.46
2	B	1409	NAG	C2-N2	-2.25	1.42	1.46
2	A	1410	NAG	C2-N2	-2.24	1.42	1.46
2	C	1403	NAG	C2-N2	-2.24	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1409	NAG	C2-N2	-2.23	1.42	1.46
2	C	1410	NAG	C2-N2	-2.23	1.42	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1410	NAG	O5-C1-C2	-2.20	107.81	111.29
2	A	1410	NAG	O5-C1-C2	-2.18	107.84	111.29
2	B	1405	NAG	O5-C1-C2	-2.18	107.85	111.29
2	B	1403	NAG	O5-C1-C2	-2.17	107.86	111.29
2	A	1404	NAG	O5-C1-C2	-2.17	107.87	111.29
2	B	1410	NAG	O5-C1-C2	-2.16	107.87	111.29
2	C	1406	NAG	O5-C1-C2	-2.16	107.87	111.29
2	A	1405	NAG	O5-C1-C2	-2.16	107.88	111.29
2	C	1403	NAG	O5-C1-C2	-2.16	107.88	111.29
2	C	1404	NAG	O5-C1-C2	-2.16	107.88	111.29
2	C	1405	NAG	O5-C1-C2	-2.16	107.88	111.29
2	B	1408	NAG	O5-C1-C2	-2.15	107.89	111.29
2	A	1403	NAG	O5-C1-C2	-2.15	107.90	111.29
2	B	1404	NAG	O5-C1-C2	-2.14	107.91	111.29
2	B	1406	NAG	O5-C1-C2	-2.14	107.91	111.29
2	A	1408	NAG	O5-C1-C2	-2.14	107.91	111.29
2	A	1406	NAG	O5-C1-C2	-2.14	107.92	111.29
2	B	1407	NAG	O5-C1-C2	-2.13	107.92	111.29
2	C	1407	NAG	O5-C1-C2	-2.13	107.93	111.29
2	A	1407	NAG	O5-C1-C2	-2.13	107.93	111.29
2	C	1409	NAG	O5-C1-C2	-2.12	107.94	111.29
2	C	1408	NAG	O5-C1-C2	-2.11	107.96	111.29
2	B	1409	NAG	O5-C1-C2	-2.10	107.97	111.29
2	A	1409	NAG	O5-C1-C2	-2.10	107.97	111.29

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1403	NAG	O5-C5-C6-O6
2	A	1404	NAG	O5-C5-C6-O6
2	A	1405	NAG	O5-C5-C6-O6
2	A	1406	NAG	O5-C5-C6-O6
2	A	1407	NAG	O5-C5-C6-O6
2	A	1408	NAG	O5-C5-C6-O6
2	A	1409	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1410	NAG	O5-C5-C6-O6
2	B	1403	NAG	O5-C5-C6-O6
2	B	1404	NAG	O5-C5-C6-O6
2	B	1405	NAG	O5-C5-C6-O6
2	B	1406	NAG	O5-C5-C6-O6
2	B	1407	NAG	O5-C5-C6-O6
2	B	1408	NAG	O5-C5-C6-O6
2	B	1409	NAG	O5-C5-C6-O6
2	B	1410	NAG	O5-C5-C6-O6
2	C	1403	NAG	O5-C5-C6-O6
2	C	1404	NAG	O5-C5-C6-O6
2	C	1405	NAG	O5-C5-C6-O6
2	C	1406	NAG	O5-C5-C6-O6
2	C	1407	NAG	O5-C5-C6-O6
2	C	1408	NAG	O5-C5-C6-O6
2	C	1409	NAG	O5-C5-C6-O6
2	C	1410	NAG	O5-C5-C6-O6
2	A	1402	NAG	O5-C5-C6-O6
2	B	1402	NAG	O5-C5-C6-O6
2	C	1402	NAG	O5-C5-C6-O6
2	A	1402	NAG	C4-C5-C6-O6
2	B	1402	NAG	C4-C5-C6-O6
2	C	1402	NAG	C4-C5-C6-O6
2	A	1403	NAG	C4-C5-C6-O6
2	A	1404	NAG	C4-C5-C6-O6
2	A	1405	NAG	C4-C5-C6-O6
2	A	1406	NAG	C4-C5-C6-O6
2	A	1407	NAG	C4-C5-C6-O6
2	A	1408	NAG	C4-C5-C6-O6
2	A	1409	NAG	C4-C5-C6-O6
2	A	1410	NAG	C4-C5-C6-O6
2	B	1403	NAG	C4-C5-C6-O6
2	B	1404	NAG	C4-C5-C6-O6
2	B	1405	NAG	C4-C5-C6-O6
2	B	1406	NAG	C4-C5-C6-O6
2	B	1407	NAG	C4-C5-C6-O6
2	B	1408	NAG	C4-C5-C6-O6
2	B	1409	NAG	C4-C5-C6-O6
2	B	1410	NAG	C4-C5-C6-O6
2	C	1403	NAG	C4-C5-C6-O6
2	C	1404	NAG	C4-C5-C6-O6
2	C	1405	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1406	NAG	C4-C5-C6-O6
2	C	1407	NAG	C4-C5-C6-O6
2	C	1408	NAG	C4-C5-C6-O6
2	C	1409	NAG	C4-C5-C6-O6
2	C	1410	NAG	C4-C5-C6-O6
2	A	1401	NAG	C8-C7-N2-C2
2	A	1401	NAG	O7-C7-N2-C2
2	A	1402	NAG	C8-C7-N2-C2
2	A	1402	NAG	O7-C7-N2-C2
2	B	1401	NAG	C8-C7-N2-C2
2	B	1401	NAG	O7-C7-N2-C2
2	B	1402	NAG	C8-C7-N2-C2
2	B	1402	NAG	O7-C7-N2-C2
2	C	1401	NAG	C8-C7-N2-C2
2	C	1401	NAG	O7-C7-N2-C2
2	C	1402	NAG	C8-C7-N2-C2
2	C	1402	NAG	O7-C7-N2-C2
2	A	1401	NAG	O5-C5-C6-O6
2	B	1401	NAG	O5-C5-C6-O6
2	C	1401	NAG	O5-C5-C6-O6
2	A	1401	NAG	C4-C5-C6-O6
2	C	1401	NAG	C4-C5-C6-O6
2	B	1401	NAG	C4-C5-C6-O6

There are no ring outliers.

24 monomers are involved in 117 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1407	NAG	4	0
2	B	1409	NAG	8	0
2	C	1408	NAG	4	0
2	A	1404	NAG	5	0
2	B	1408	NAG	3	0
2	A	1408	NAG	4	0
2	B	1402	NAG	7	0
2	B	1406	NAG	3	0
2	C	1401	NAG	6	0
2	A	1403	NAG	2	0
2	B	1403	NAG	2	0
2	A	1407	NAG	4	0
2	A	1401	NAG	6	0
2	B	1404	NAG	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1406	NAG	3	0
2	B	1401	NAG	6	0
2	C	1402	NAG	8	0
2	C	1409	NAG	8	0
2	A	1402	NAG	7	0
2	C	1403	NAG	2	0
2	C	1407	NAG	4	0
2	A	1406	NAG	3	0
2	C	1404	NAG	5	0
2	A	1409	NAG	8	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.

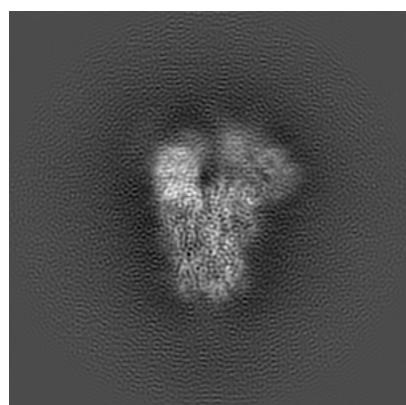
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6704. These allow visual inspection of the internal detail of the map and identification of artifacts.

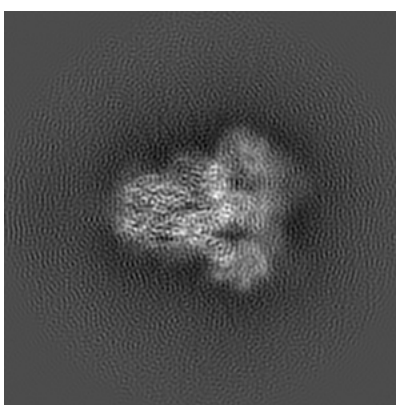
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

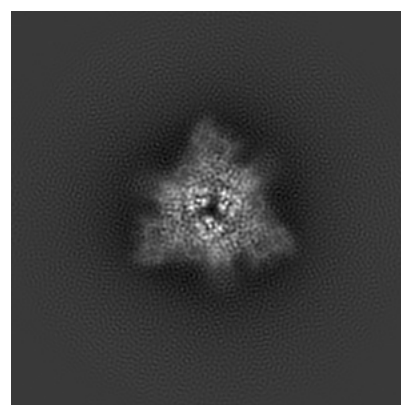
6.1.1 Primary map



X



Y

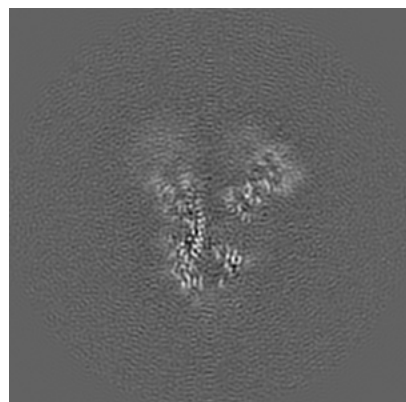


Z

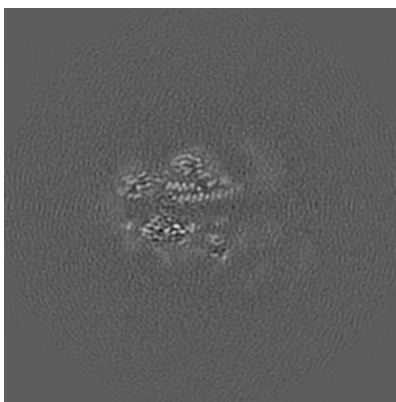
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

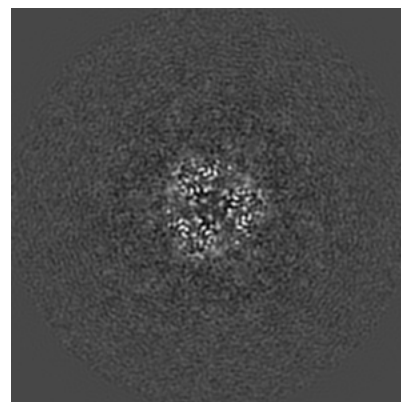
6.2.1 Primary map



X Index: 128



Y Index: 128

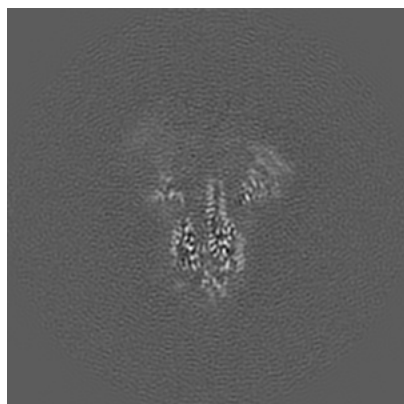


Z Index: 128

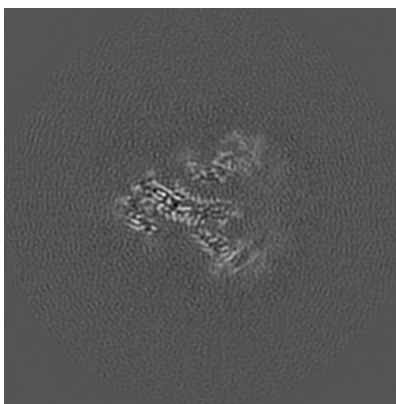
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

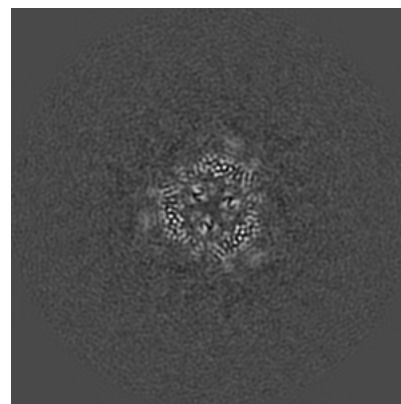
6.3.1 Primary map



X Index: 136



Y Index: 117

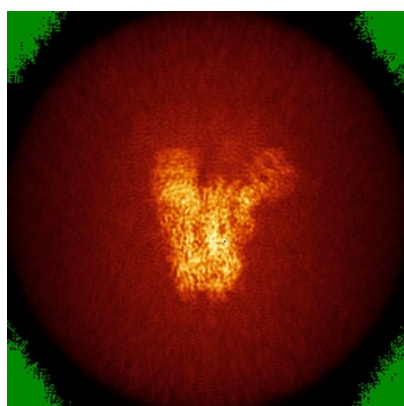


Z Index: 134

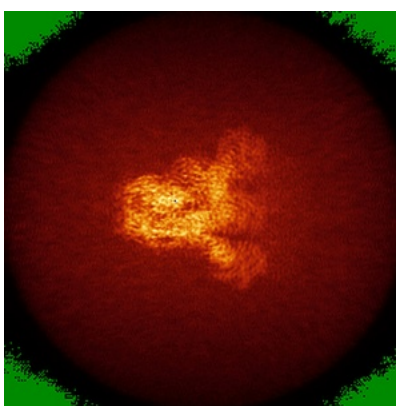
The images above show the largest variance slices of the map in three orthogonal directions.

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

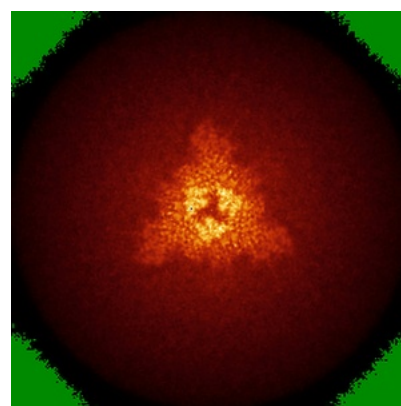
6.4.1 Primary map



X



Y

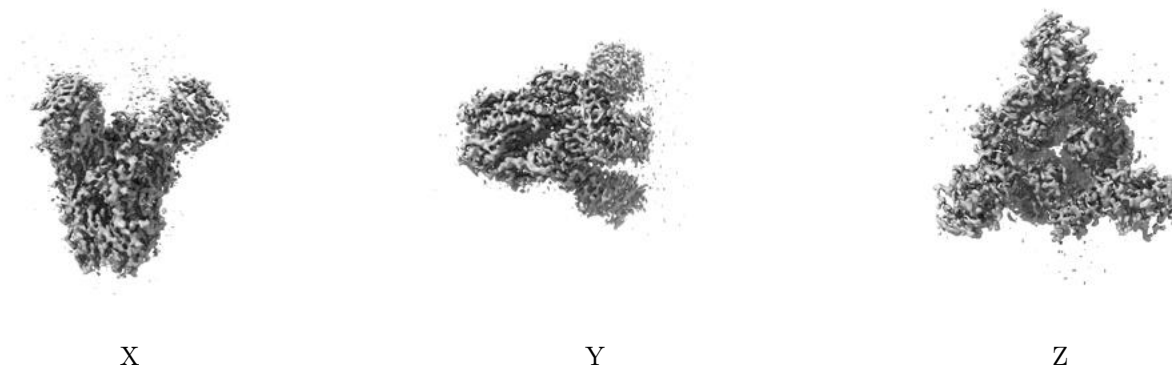


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0615. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

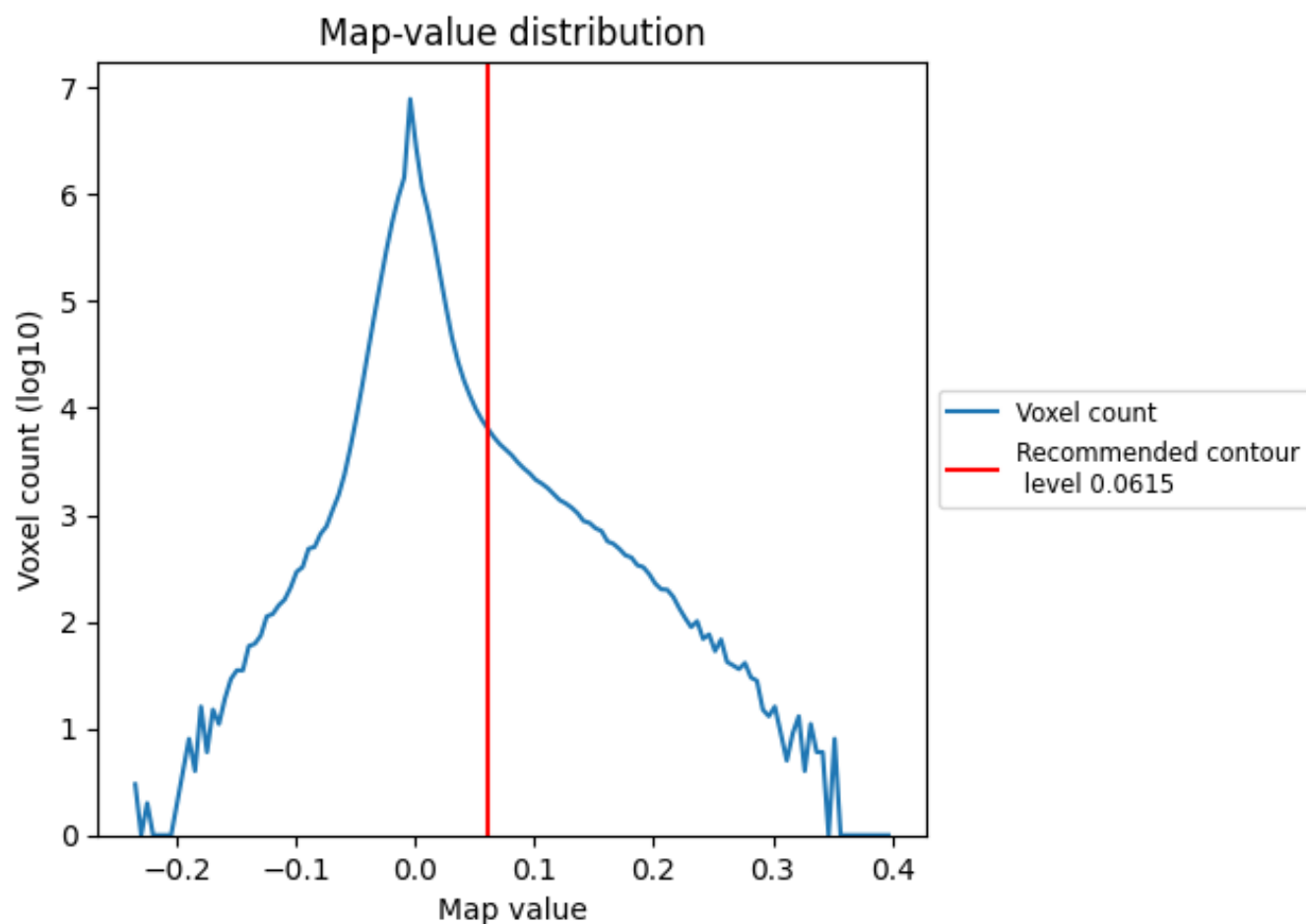
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

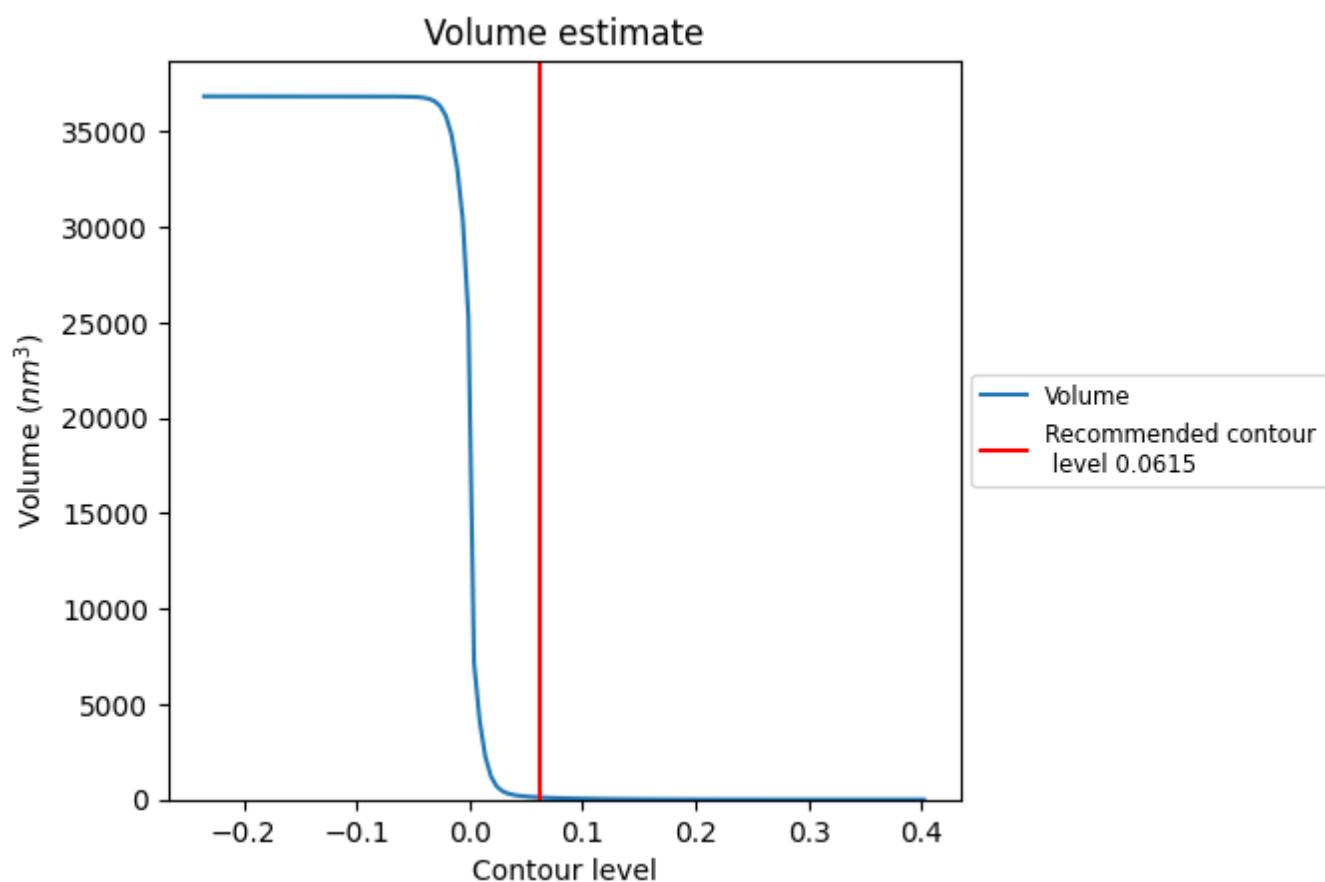
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

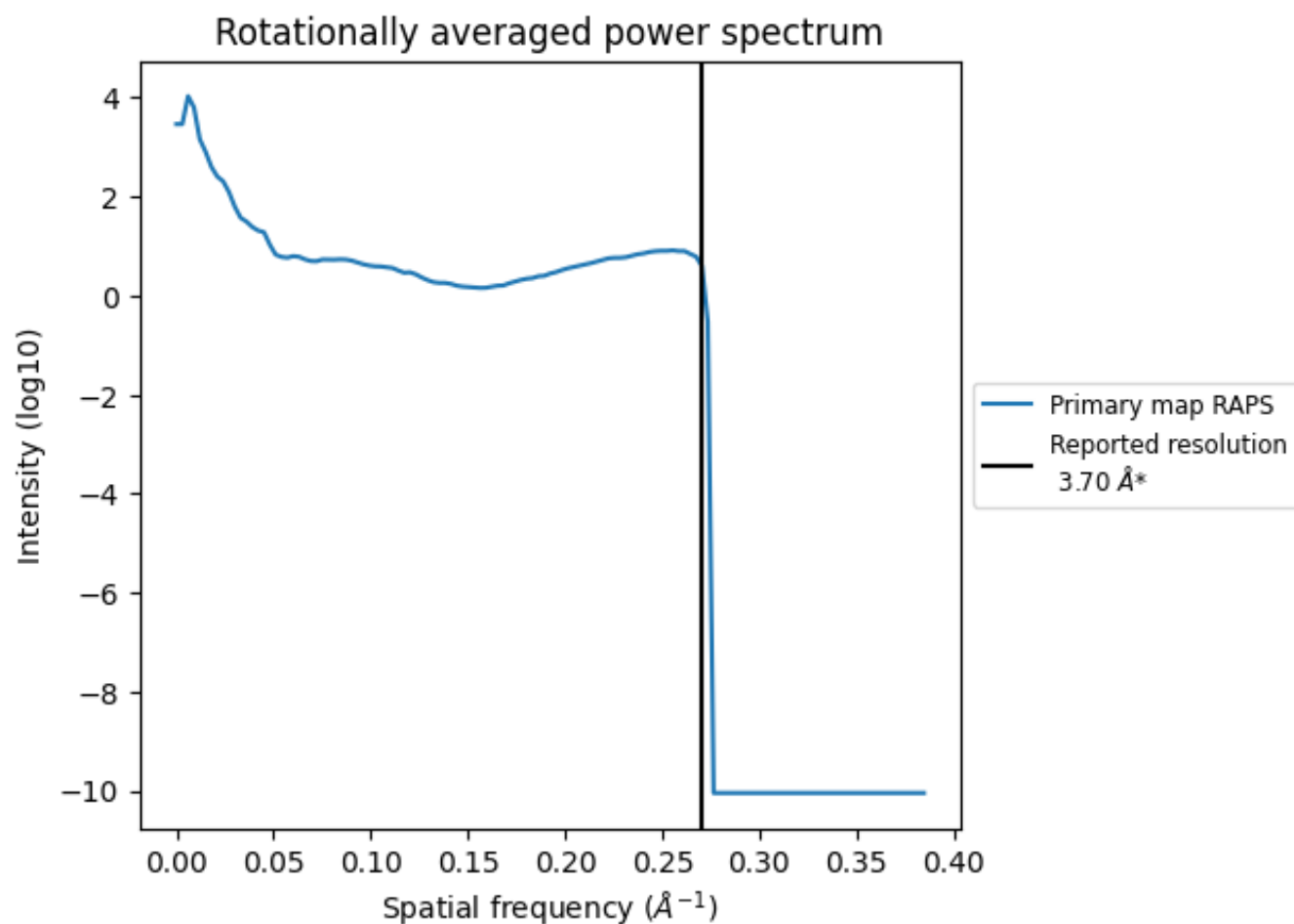
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 0.270 Å⁻¹

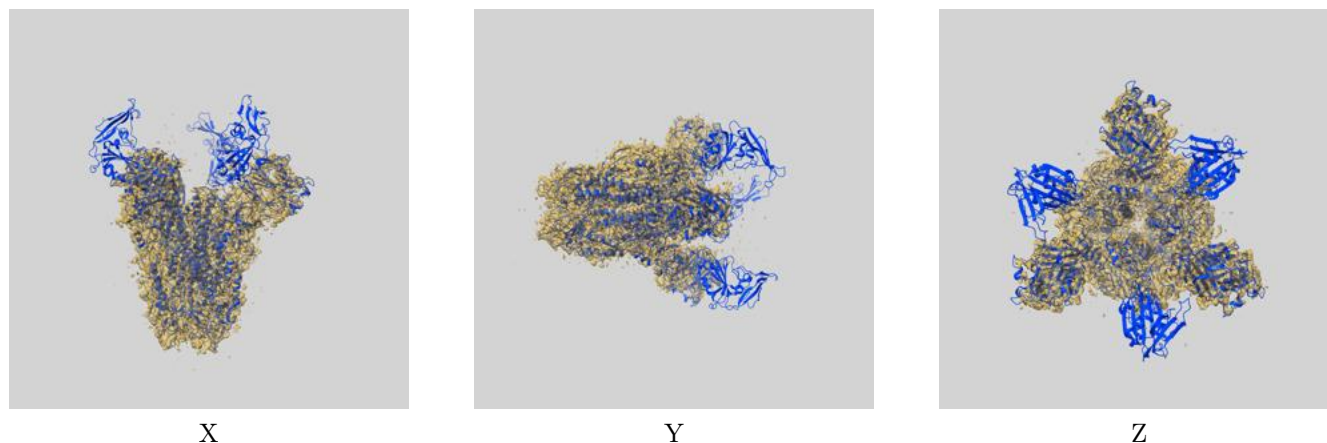
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

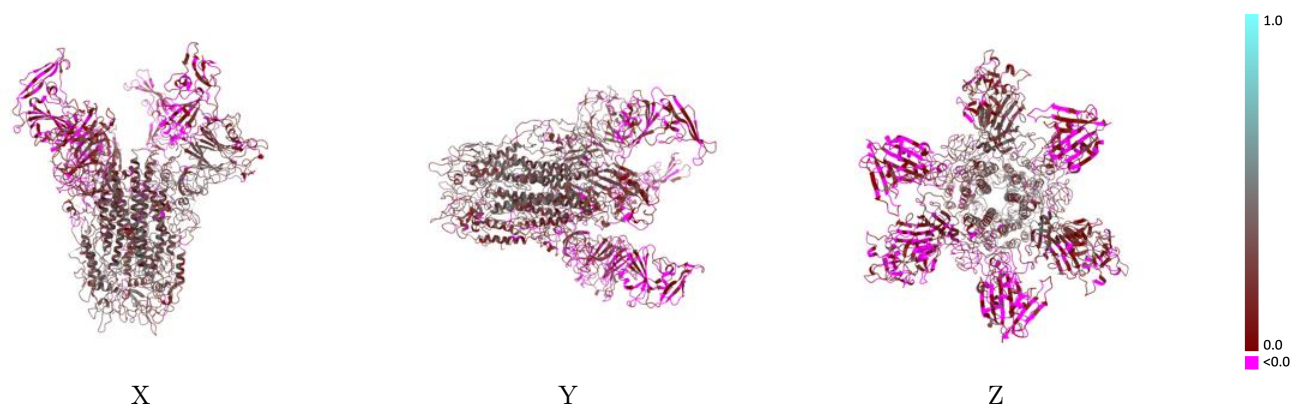
This section contains information regarding the fit between EMDB map EMD-6704 and PDB model 5X59. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



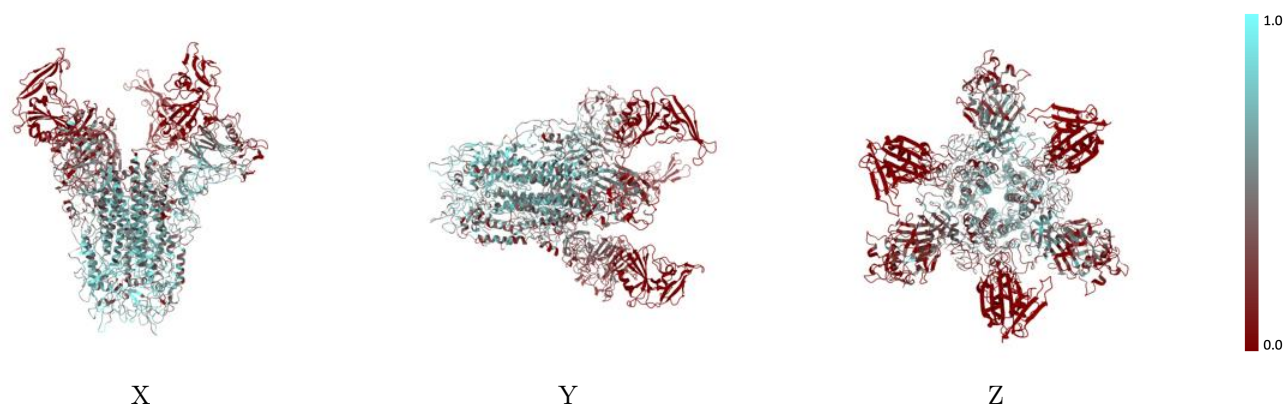
The images above show the 3D surface view of the map at the recommended contour level 0.0615 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



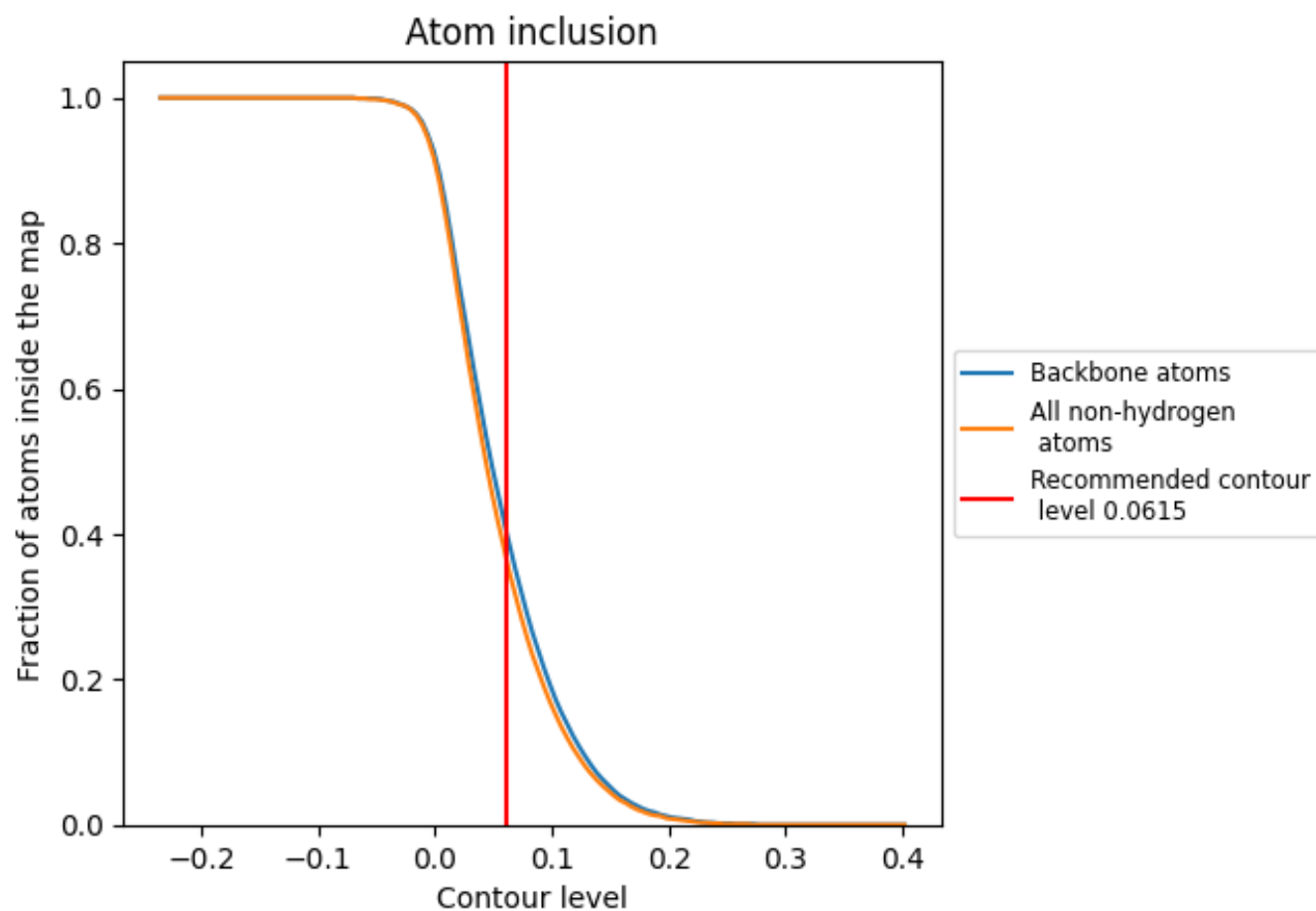
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0615).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 36% 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 (0.0615) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3630	<div></div> 0.1750
A	<div></div> 0.3900	<div></div> 0.2010
B	<div></div> 0.3950	<div></div> 0.2080
C	<div></div> 0.3060	<div></div> 0.1150

