Full wwPDB EM Validation Report

Mar 31, 2025 – 12:25 PM JST

PDB ID	:	8GWG
EMDB ID	:	EMD-34312
Title	:	SARS-CoV-2 E-RTC complex with SMP-nsp9 and GMPPNP
Authors	:	Yan, L.M.; Huang, Y.C.; Ge, J.; Liu, Z.Y.; Gao, Y.; Rao, Z.H.; Lou, Z.Y.
Deposited on	:	2022-09-17
Resolution	:	3.37 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:

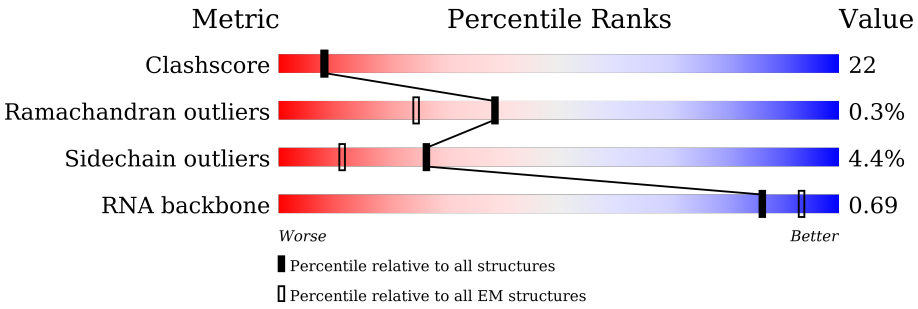
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.37 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
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	932	73% 25% ·
2	B	198	8% 70% 22% · · 6%
2	D	198	7% 67% 24% · 6%
3	C	83	61% 24% · 13%
4	E	601	72% 51% 44% · ·
4	F	601	57% 49% 47% · ·
5	G	113	22% 48% 49% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	I	25	16% 72% 12%
7	J	27	15% 81%

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
11	6GS	G	200	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21905 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	928	7477	4777	1254	1392	54	0	0

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	187	1400	873	241	275	11	0	0
2	D	186	1418	892	243	272	11	0	0

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	72	553	349	91	107	6	0	0

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	585	4508	2875	750	848	35	1	0
4	F	585	4508	2875	750	848	35	1	0

- Molecule 5 is a protein called Viral protein genome-linked nsp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	113	868	549	150	164	5	0	0

- Molecule 6 is a RNA chain called primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

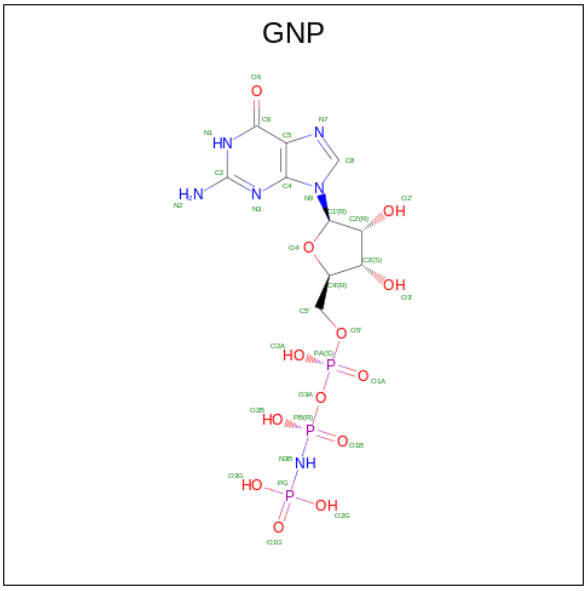
- Molecule 7 is a RNA chain called Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	27	Total	C	N	O	P	0	0
			565	253	95	190	27		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	E	3	Total	Zn	0
			3	3	
8	F	3	Total	Zn	0
			3	3	

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

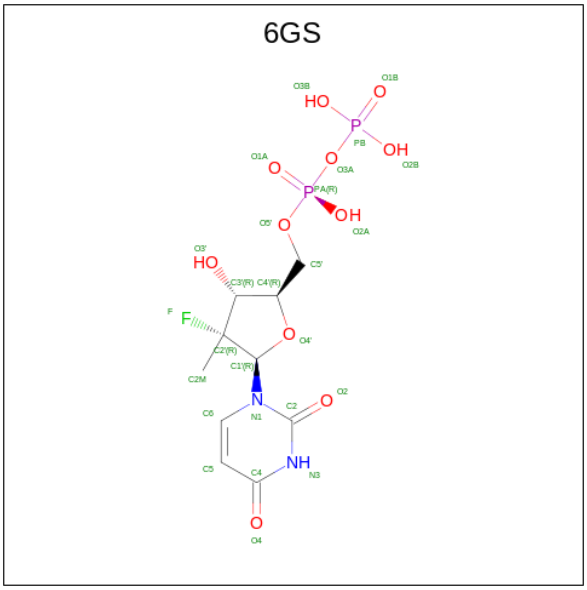


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mg 1 1	0

- Molecule 11 is 2'-deoxy-2'-fluoro-2'-methyluridine 5'-(trihydrogen diphosphate) (three-letter code: 6GS) (formula: $C_{10}H_{15}FN_2O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	G	1	Total C F N O P 21 10 1 2 7 1	0

- Molecule 12 is water.

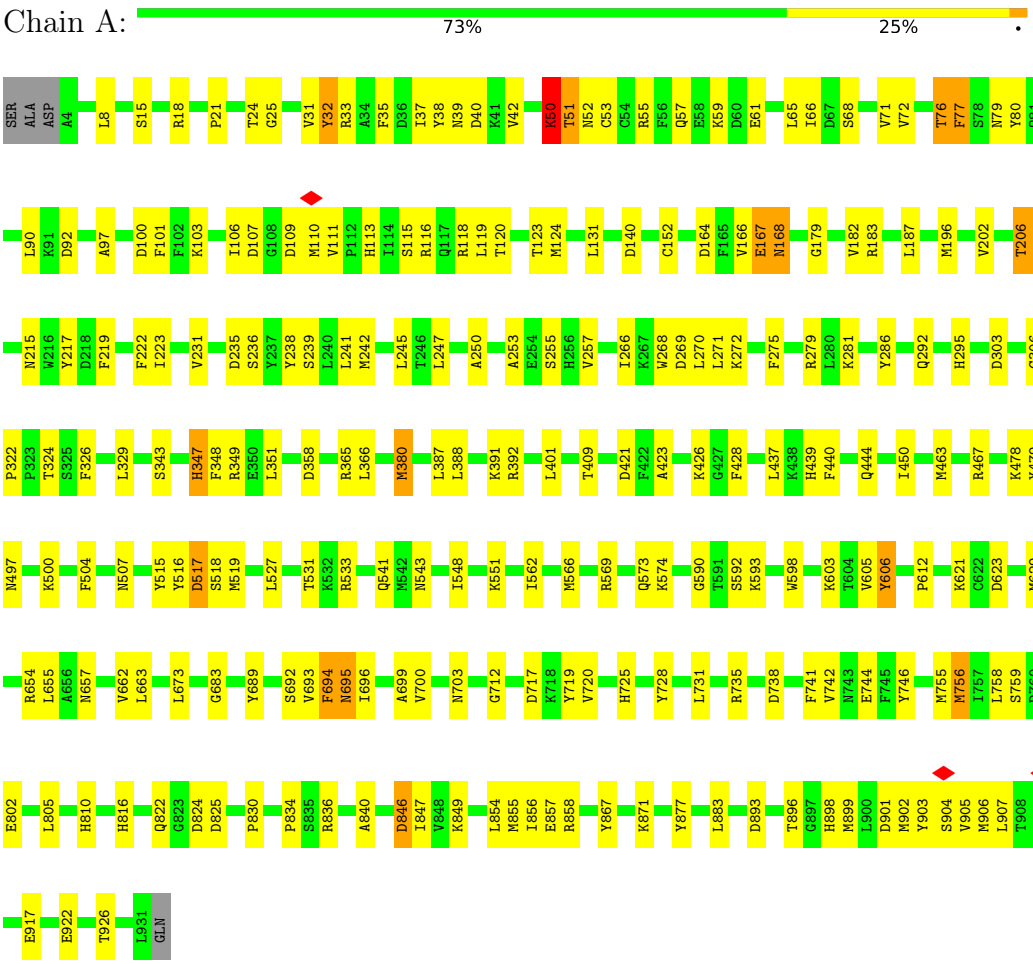
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total O 1 1	0

3 Residue-property plots (i)

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

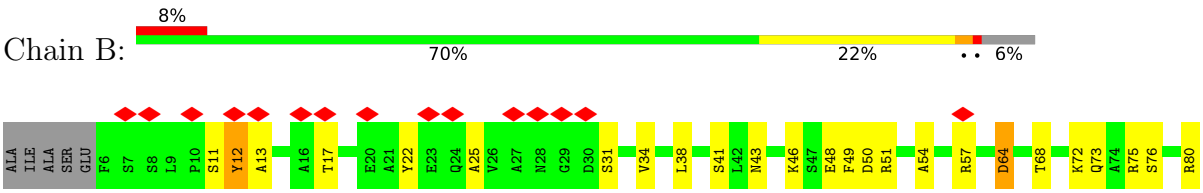
• Molecule 1: RNA-directed RNA polymerase

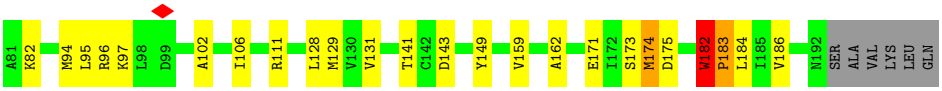
Chain A:



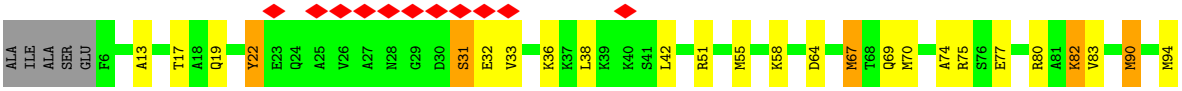
• Molecule 2: Non-structural protein 8

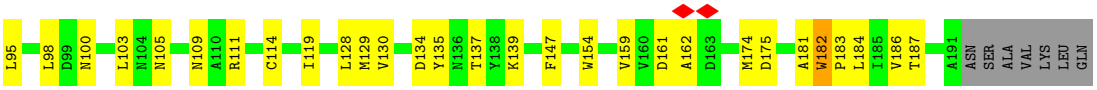
Chain B:





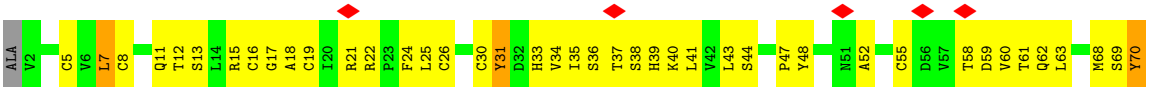
• Molecule 2: Non-structural protein 8

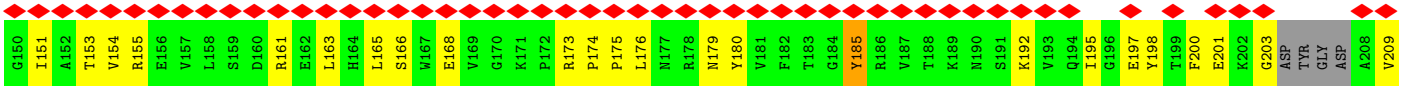


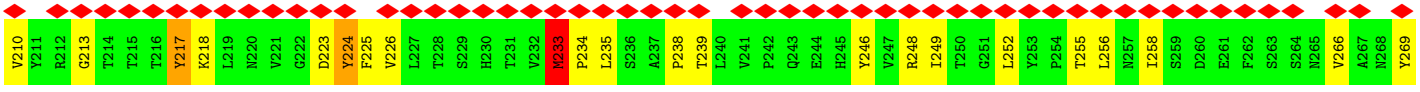


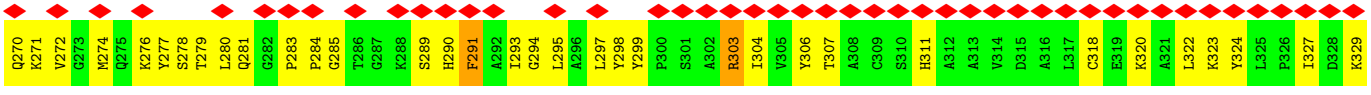
• Molecule 3: Non-structural protein 7

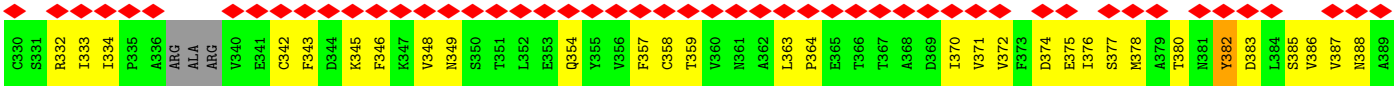
• Molecule 4: Helicase

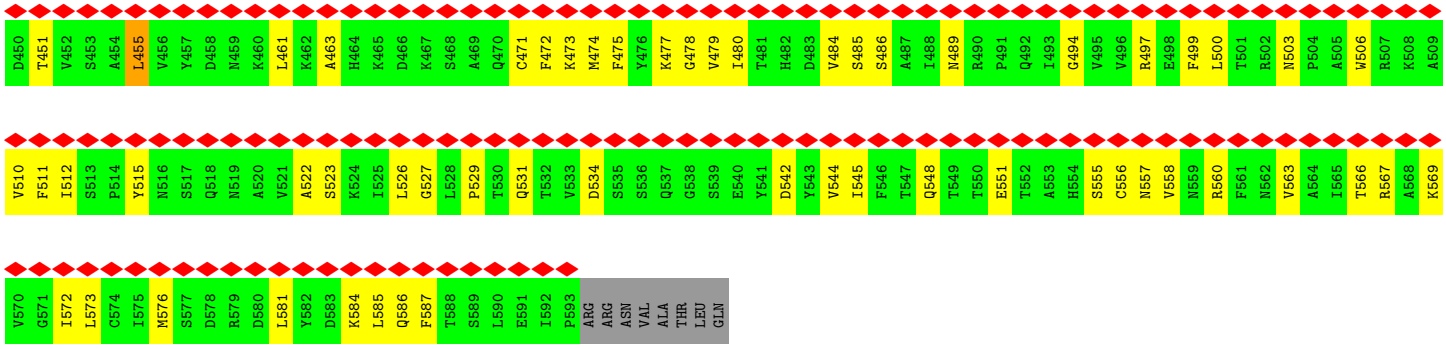






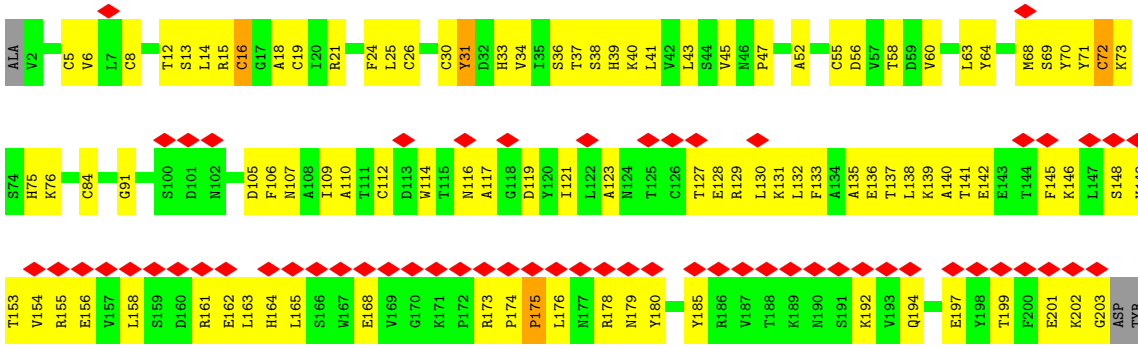






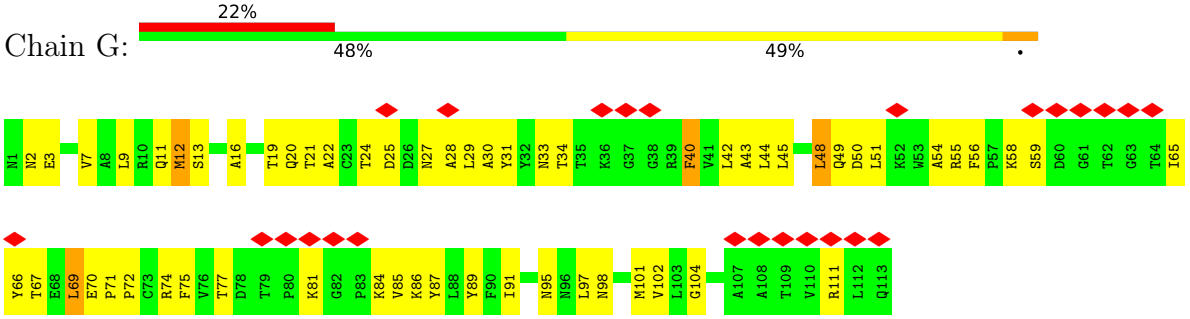
• Molecule 4: Helicase

Chain F:



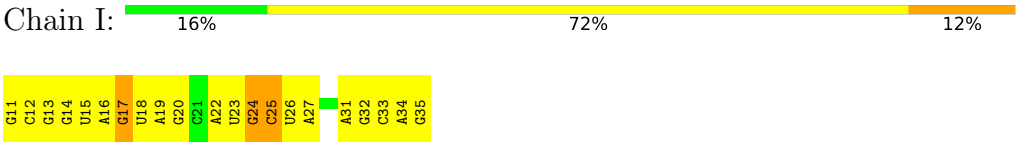
• Molecule 5: Viral protein genome-linked nsp9

Chain G:



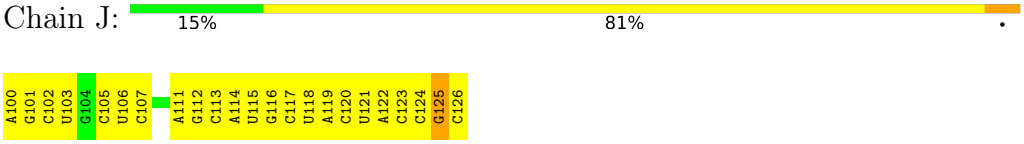
• Molecule 6: primer

Chain I:



• Molecule 7: Template

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3131527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.602	Depositor
Minimum map value	-0.912	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 6GS, GNP, MG

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	0.31	0/7666	0.54	2/10404 (0.0%)
2	B	0.33	0/1418	0.54	0/1927
2	D	0.27	0/1437	0.52	0/1948
3	C	0.27	0/556	0.50	0/749
4	E	0.28	0/4610	0.58	2/6283 (0.0%)
4	F	0.54	4/4610 (0.1%)	0.69	5/6283 (0.1%)
5	G	0.33	0/884	0.83	4/1200 (0.3%)
6	I	0.27	0/611	0.85	0/953
7	J	0.30	0/628	0.83	0/974
All	All	0.36	4/22420 (0.0%)	0.62	13/30721 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	175	PRO	CG-CD	-21.77	0.78	1.50
4	F	175	PRO	CB-CG	19.82	2.49	1.50
4	F	175	PRO	N-CD	8.97	1.60	1.47
4	F	175	PRO	CA-CB	-5.18	1.43	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	175	PRO	CB-CG-CD	-21.90	21.08	106.50
4	F	175	PRO	CA-N-CD	-12.36	94.20	111.50
4	F	175	PRO	N-CA-CB	-10.50	90.70	103.30
4	F	175	PRO	CA-CB-CG	-9.82	85.33	104.00
4	F	175	PRO	N-CD-CG	-9.25	89.33	103.20
5	G	2	ASN	N-CA-C	-8.83	87.15	111.00
5	G	3	GLU	N-CA-CB	7.73	124.52	110.60
5	G	48	LEU	CB-CG-CD2	6.90	122.73	111.00
5	G	3	GLU	N-CA-C	-6.64	93.08	111.00
4	E	7	LEU	CB-CG-CD1	-5.61	101.47	111.00
4	E	233	MET	CA-CB-CG	5.45	122.56	113.30
1	A	207	LEU	CB-CG-CD2	-5.16	102.24	111.00
1	A	910	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	606	TYR	Peptide
2	B	182	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7477	0	7222	211	0
2	B	1400	0	1372	55	0
2	D	1418	0	1427	50	0
3	C	553	0	585	41	0
4	E	4508	0	4423	236	0
4	F	4508	0	4423	251	0
5	G	868	0	877	58	0
6	I	545	0	272	32	0
7	J	565	0	292	37	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	32	0	13	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	1	0	0	0	0
11	G	21	0	12	16	0
12	A	1	0	0	4	0
All	All	21905	0	20918	925	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 22.

All (925) 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)
4:F:175:PRO:N	4:F:175:PRO:CG	1.77	1.42
3:C:59:LEU:HA	3:C:62:MET:CE	1.51	1.38
1:A:271:LEU:HD21	2:B:106:ILE:CD1	1.54	1.37
5:G:74:ARG:NH2	5:G:85:VAL:HG22	1.46	1.27
1:A:39:ASN:ND2	11:G:200:6GS:O4	1.77	1.17
5:G:74:ARG:HH22	5:G:85:VAL:CG2	1.59	1.16
4:E:16:CYS:SG	4:E:19:CYS:HB2	1.87	1.15
1:A:37:ILE:HD13	11:G:200:6GS:C6	1.77	1.14
3:C:58:VAL:O	3:C:62:MET:SD	2.06	1.13
3:C:58:VAL:HG22	2:D:119:ILE:HD12	1.25	1.11
5:G:74:ARG:CZ	5:G:85:VAL:HG13	1.79	1.11
3:C:59:LEU:HD12	3:C:62:MET:HE2	1.35	1.09
4:F:175:PRO:CD	4:F:175:PRO:HG3	1.56	1.07
4:F:175:PRO:CD	4:F:175:PRO:HG2	1.56	1.07
1:A:271:LEU:CD2	2:B:106:ILE:HD11	1.83	1.07
1:A:271:LEU:HD21	2:B:106:ILE:HD11	1.09	1.04
3:C:59:LEU:HA	3:C:62:MET:HE1	1.12	1.03
3:C:59:LEU:CA	3:C:62:MET:CE	2.35	1.03
5:G:74:ARG:HH22	5:G:85:VAL:HG22	0.86	1.02
5:G:74:ARG:NH2	5:G:85:VAL:HG13	1.76	1.00
3:C:59:LEU:O	3:C:62:MET:HE2	1.60	1.00
3:C:59:LEU:HD12	3:C:62:MET:CE	1.92	0.99
4:F:175:PRO:CG	4:F:175:PRO:HD3	1.48	0.98
1:A:271:LEU:HD21	2:B:106:ILE:HD12	1.45	0.97
4:F:175:PRO:CG	4:F:175:PRO:HD2	1.48	0.96
3:C:59:LEU:CA	3:C:62:MET:HE1	1.96	0.94
1:A:38:TYR:CD2	1:A:728:TYR:HE2	1.85	0.94
3:C:59:LEU:HA	3:C:62:MET:SD	2.08	0.93
5:G:74:ARG:NH2	5:G:85:VAL:CG2	2.25	0.92
1:A:38:TYR:HE1	1:A:725:HIS:HE2	1.18	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:175:PRO:CG	4:F:175:PRO:CB	2.49	0.91
4:F:375:GLU:HG3	4:F:378:MET:HB2	1.53	0.90
1:A:903:TYR:HE1	1:A:905:VAL:HG12	1.36	0.90
6:I:11:G:O6	7:J:126:C:N4	2.06	0.88
3:C:58:VAL:HG22	2:D:119:ILE:CD1	2.04	0.87
1:A:903:TYR:CE1	1:A:905:VAL:HG12	2.09	0.87
4:F:419:PRO:HA	4:F:422:PHE:HE1	1.40	0.86
3:C:59:LEU:CD1	3:C:62:MET:CE	2.54	0.85
1:A:38:TYR:CD2	1:A:728:TYR:CE2	2.66	0.82
1:A:392:ARG:HH11	2:B:131:VAL:HG11	1.42	0.82
1:A:37:ILE:HD11	11:G:200:6GS:O4'	1.79	0.82
6:I:17:G:N1	7:J:120:C:N3	2.25	0.82
4:E:165:LEU:HB2	4:E:209:VAL:HG21	1.62	0.81
4:F:176:LEU:HG	4:F:201:GLU:HA	1.63	0.80
4:E:185:TYR:HB2	4:E:192:LYS:HG2	1.63	0.80
3:C:68:ILE:HD13	2:D:111:ARG:HG2	1.63	0.80
4:F:275:GLN:NE2	4:F:278:SER:OG	2.15	0.80
4:F:250:THR:O	4:F:394:LYS:NZ	2.15	0.79
4:F:370:ILE:HG12	4:F:395:HIS:HB2	1.65	0.79
4:E:375:GLU:HG3	4:E:378:MET:HB2	1.65	0.78
1:A:271:LEU:CD2	2:B:106:ILE:CD1	2.48	0.78
4:F:175:PRO:CG	4:F:175:PRO:CD	0.78	0.78
1:A:759:SER:OG	6:I:35:G:O2'	2.01	0.78
4:E:380:THR:HG23	4:E:382:TYR:H	1.47	0.78
5:G:12:MET:SD	5:G:13:SER:N	2.57	0.77
1:A:717:ASP:OD1	1:A:720:VAL:HG23	1.84	0.77
1:A:689:TYR:O	1:A:693:VAL:HG23	1.85	0.77
4:E:473:LYS:HG2	4:E:587:PHE:HB2	1.66	0.77
4:F:5:CYS:SG	4:F:8:CYS:HB2	2.25	0.77
4:F:174:PRO:HB2	4:F:175:PRO:HG3	1.67	0.77
4:E:374:ASP:HA	4:E:399:ILE:HB	1.64	0.76
1:A:217:TYR:HE2	9:A:1003:GNP:H5'2	1.49	0.76
1:A:904:SER:OG	4:E:95:ASN:ND2	2.18	0.76
1:A:907:LEU:HD12	1:A:910:ASP:OD2	1.86	0.76
5:G:74:ARG:NH2	5:G:85:VAL:CG1	2.49	0.76
4:F:6:VAL:HA	4:F:129:ARG:HH12	1.50	0.76
1:A:38:TYR:HD2	1:A:728:TYR:HE2	1.34	0.76
2:B:82:LYS:HE3	2:B:82:LYS:HA	1.66	0.75
7:J:118:U:H2'	7:J:119:A:H8	1.51	0.75
1:A:207:LEU:HD21	1:A:241:LEU:HD12	1.67	0.75
4:F:185:TYR:HB2	4:F:192:LYS:HD2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:127:THR:HG22	4:F:130:LEU:HD12	1.68	0.74
4:F:203:GLY:HA2	4:F:210:VAL:HG23	1.69	0.74
4:F:175:PRO:N	4:F:175:PRO:HG3	1.78	0.74
4:E:318:CYS:SG	4:E:332:ARG:NH2	2.60	0.74
1:A:37:ILE:CD1	11:G:200:6GS:C6	2.63	0.73
1:A:380:MET:HG2	2:B:94:MET:CE	2.18	0.73
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.71	0.73
4:E:449:VAL:HG11	4:E:463:ALA:HA	1.70	0.73
2:B:102:ALA:O	2:B:106:ILE:HG22	1.87	0.73
4:E:71:TYR:HD2	4:E:76:LYS:HA	1.54	0.73
6:I:17:G:N2	7:J:120:C:O2	2.17	0.72
4:F:280:LEU:HD22	4:F:399:ILE:HA	1.72	0.72
5:G:74:ARG:NH1	5:G:85:VAL:HG13	2.04	0.72
4:E:37:THR:HG23	4:E:107:ASN:HD22	1.54	0.72
4:F:269:TYR:HA	4:F:272:VAL:HG12	1.70	0.72
1:A:699:ALA:O	1:A:703:ASN:ND2	2.23	0.72
1:A:76:THR:HG22	1:A:79:ASN:H	1.54	0.71
1:A:31:VAL:HB	1:A:33:ARG:NH1	2.05	0.71
4:E:129:ARG:HA	4:E:132:LEU:HD12	1.72	0.71
4:E:239:THR:O	4:E:388:ASN:ND2	2.23	0.71
4:E:5:CYS:SG	4:E:8:CYS:HB2	2.30	0.71
4:E:499:PHE:O	4:E:503:ASN:ND2	2.23	0.71
4:E:132:LEU:HD22	4:E:235:LEU:HD11	1.71	0.71
4:E:280:LEU:HD23	4:E:436:MET:HB3	1.73	0.71
4:E:419:PRO:HA	4:E:422:PHE:HE1	1.56	0.71
4:E:136:GLU:HA	4:E:382:TYR:HE1	1.56	0.71
4:F:71:TYR:HD2	4:F:76:LYS:HA	1.56	0.70
5:G:48:LEU:HD22	5:G:51:LEU:HD12	1.74	0.70
4:F:37:THR:HG23	4:F:107:ASN:HD22	1.55	0.70
1:A:822:GLN:NE2	1:A:922:GLU:OE2	2.24	0.70
4:F:174:PRO:CB	4:F:175:PRO:HG3	2.22	0.70
4:F:255:THR:OG1	4:F:298:TYR:O	2.10	0.69
4:E:255:THR:OG1	4:E:298:TYR:O	2.11	0.69
3:C:59:LEU:CA	3:C:62:MET:SD	2.80	0.69
5:G:74:ARG:HH22	5:G:85:VAL:CB	2.05	0.69
5:G:48:LEU:HD23	5:G:50:ASP:H	1.57	0.69
4:E:153:THR:HA	4:E:224:TYR:HB3	1.74	0.69
4:F:305:VAL:HB	4:F:371:VAL:HG12	1.73	0.69
4:F:318:CYS:SG	4:F:332:ARG:NH1	2.66	0.69
2:B:12:TYR:HD2	2:B:49:PHE:CZ	2.10	0.69
4:E:303:ARG:HD2	4:E:354:GLN:HA	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:24:G:H1	7:J:113:C:H42	1.42	0.68
4:F:473:LYS:HG2	4:F:587:PHE:HB2	1.76	0.68
4:F:307:THR:HG23	4:F:373:PHE:HD1	1.59	0.68
2:D:109:ASN:HB3	2:D:114:CYS:HB2	1.75	0.68
1:A:35:PHE:CE2	11:G:200:6GS:H10	2.28	0.68
6:I:31:A:H2'	6:I:32:G:H8	1.59	0.68
4:F:303:ARG:HD2	4:F:354:GLN:HA	1.76	0.68
3:C:58:VAL:CG2	2:D:119:ILE:HD12	2.14	0.67
4:F:280:LEU:HA	4:F:436:MET:SD	2.34	0.67
4:F:293:ILE:HD13	4:F:320:LYS:HB3	1.75	0.67
4:E:7:LEU:HD11	4:E:106:PHE:CD2	2.29	0.67
1:A:235:ASP:O	1:A:239:SER:OG	2.10	0.67
4:F:479:VAL:O	4:F:489:ASN:ND2	2.28	0.67
1:A:855:MET:O	1:A:857:GLU:N	2.24	0.67
4:E:443:ARG:HH12	4:E:567:ARG:HD3	1.59	0.67
4:F:418:GLU:HG2	4:F:420:GLU:H	1.60	0.67
4:E:60:VAL:HA	4:E:63:LEU:HD12	1.76	0.67
7:J:118:U:H2'	7:J:119:A:C8	2.30	0.67
2:B:173:SER:OG	2:B:175:ASP:OD1	2.12	0.66
2:B:73:GLN:OE1	4:F:45:VAL:CG2	2.43	0.66
4:E:192:LYS:HE2	4:E:224:TYR:CD2	2.31	0.66
4:F:174:PRO:C	4:F:175:PRO:HG3	2.16	0.66
2:B:11:SER:OG	2:B:48:GLU:HG2	1.95	0.66
4:E:363:LEU:HD22	4:E:390:ARG:HB3	1.78	0.66
4:F:363:LEU:HD12	4:F:364:PRO:HD2	1.77	0.66
1:A:238:TYR:O	1:A:242:MET:HG2	1.94	0.66
4:E:128:GLU:HA	4:E:131:LYS:HE2	1.77	0.66
4:E:409:ARG:HH22	4:E:417:LEU:HD23	1.60	0.66
4:E:443:ARG:NH1	4:E:567:ARG:HD3	2.11	0.66
4:E:523:SER:HA	4:E:527:GLY:H	1.59	0.66
4:E:557:ASN:HB3	4:E:560:ARG:HB2	1.77	0.66
2:B:22:TYR:HA	2:B:38:LEU:HD13	1.76	0.66
1:A:38:TYR:HE1	1:A:725:HIS:NE2	1.92	0.65
4:E:281:GLN:O	4:E:283:PRO:HD3	1.95	0.65
1:A:531:THR:OG1	1:A:654:ARG:NH1	2.29	0.65
4:E:21:ARG:HH21	4:E:234:PRO:HD3	1.61	0.65
4:E:563:VAL:O	4:E:567:ARG:HG2	1.95	0.65
4:F:523:SER:HA	4:F:527:GLY:H	1.62	0.65
5:G:9:LEU:HD13	5:G:34:THR:H	1.61	0.65
4:E:545:ILE:HA	4:E:573:LEU:HB2	1.77	0.65
4:F:374:ASP:HA	4:F:399:ILE:HB	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:424:SER:HA	4:F:427:ARG:HH21	1.61	0.65
5:G:30:ALA:HA	5:G:43:ALA:O	1.97	0.65
1:A:80:TYR:HE1	1:A:101:PHE:HB3	1.59	0.65
4:F:292:ALA:HB3	4:F:317:LEU:HD21	1.78	0.65
7:J:106:U:H2'	7:J:107:C:H6	1.61	0.65
1:A:111:VAL:HG23	1:A:113:HIS:HE1	1.62	0.65
1:A:217:TYR:CE2	9:A:1003:GNP:H5'2	2.32	0.64
4:F:448:ILE:O	4:F:452:VAL:HG23	1.97	0.64
1:A:37:ILE:HD13	11:G:200:6GS:N1	2.11	0.64
4:F:5:CYS:O	4:F:129:ARG:NH2	2.28	0.64
5:G:98:ASN:HA	5:G:101:MET:HG2	1.80	0.64
1:A:55:ARG:HG2	1:A:71:VAL:HG12	1.78	0.64
1:A:116:ARG:HH12	1:A:119:LEU:HD13	1.63	0.64
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.79	0.64
4:F:419:PRO:HA	4:F:422:PHE:CE1	2.28	0.64
4:E:284:PRO:O	4:E:443:ARG:NH2	2.31	0.64
2:B:64:ASP:O	2:B:68:THR:HG23	1.96	0.64
4:F:280:LEU:HB3	4:F:398:TYR:O	1.98	0.64
6:I:17:G:O6	7:J:120:C:N4	2.21	0.64
1:A:57:GLN:HG2	1:A:65:LEU:HD12	1.80	0.64
4:E:332:ARG:HB2	4:E:346:PHE:HD2	1.62	0.64
4:E:409:ARG:NH2	4:E:417:LEU:HB3	2.13	0.64
3:C:59:LEU:C	3:C:62:MET:HE2	2.17	0.63
5:G:75:PHE:CE2	5:G:77:THR:HG23	2.33	0.63
2:B:54:ALA:HA	2:B:57:ARG:HD3	1.79	0.63
5:G:75:PHE:HE2	5:G:77:THR:HG23	1.61	0.63
3:C:59:LEU:CD1	3:C:62:MET:HE1	2.29	0.63
4:F:406:PRO:HB3	4:F:422:PHE:CD2	2.34	0.63
1:A:592:SER:HB2	7:J:105:C:H4'	1.79	0.63
2:B:128:LEU:HD11	2:B:149:TYR:HD2	1.64	0.63
2:B:75:ARG:HA	2:B:75:ARG:NE	2.14	0.62
4:E:479:VAL:O	4:E:489:ASN:ND2	2.31	0.62
1:A:717:ASP:OD1	1:A:720:VAL:CG2	2.48	0.62
1:A:836:ARG:HH12	1:A:840:ALA:HB2	1.64	0.62
4:F:449:VAL:HG11	4:F:463:ALA:HA	1.81	0.62
4:E:348:VAL:HG12	4:E:349:ASN:OD1	1.99	0.62
4:E:383:ASP:HA	4:E:386:VAL:HG22	1.80	0.62
4:E:151:ILE:H	4:E:168:GLU:HG2	1.64	0.62
1:A:391:LYS:NZ	2:B:141:THR:OG1	2.32	0.62
1:A:392:ARG:HH21	1:A:450:ILE:HG21	1.63	0.62
4:E:26:CYS:O	4:E:30:CYS:N	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:N	1:A:140:ASP:OD1	2.33	0.62
4:F:376:ILE:HG21	4:F:398:TYR:HB3	1.82	0.62
3:C:42:ALA:C	3:C:43:LYS:HD3	2.20	0.62
1:A:329:LEU:HD21	1:A:347:HIS:HB2	1.81	0.61
4:E:375:GLU:OE1	4:E:404:GLN:NE2	2.33	0.61
2:D:105:ASN:OD1	2:D:109:ASN:ND2	2.33	0.61
4:F:557:ASN:HB3	4:F:560:ARG:HB2	1.83	0.61
1:A:518:SER:O	2:B:80:ARG:NH1	2.34	0.61
4:F:378:MET:HE1	4:F:407:ALA:HA	1.83	0.61
4:E:419:PRO:HA	4:E:422:PHE:CE1	2.35	0.61
1:A:631:ARG:HG2	1:A:663:LEU:HD13	1.83	0.61
2:D:162:ALA:HB2	2:D:183:PRO:HG2	1.83	0.61
4:F:174:PRO:CA	4:F:175:PRO:HG3	2.31	0.61
4:F:26:CYS:O	4:F:30:CYS:N	2.26	0.60
1:A:206:THR:CB	12:A:1101:HOH:O	2.50	0.60
5:G:97:LEU:HG	5:G:101:MET:CE	2.31	0.60
1:A:906:MET:SD	1:A:907:LEU:N	2.75	0.60
3:C:59:LEU:O	3:C:62:MET:CE	2.44	0.60
4:F:60:VAL:HA	4:F:63:LEU:HD12	1.83	0.60
4:E:311:HIS:CG	4:E:342:CYS:HG	2.18	0.60
4:F:378:MET:CE	4:F:407:ALA:HA	2.31	0.60
2:D:33:VAL:HA	2:D:36:LYS:HB2	1.84	0.60
4:F:383:ASP:HA	4:F:386:VAL:HG22	1.83	0.60
4:E:363:LEU:HD11	4:E:391:LEU:HD11	1.83	0.60
4:F:531:GLN:HE22	4:F:536:SER:HA	1.67	0.60
1:A:605:VAL:HG21	1:A:756:MET:HE2	1.83	0.60
4:E:322:LEU:HD22	4:E:343:PHE:HZ	1.67	0.60
4:F:306:TYR:HD2	4:F:317:LEU:HD13	1.67	0.60
1:A:907:LEU:CD1	1:A:910:ASP:OD2	2.49	0.59
4:F:176:LEU:HD21	4:F:202:LYS:H	1.66	0.59
4:F:255:THR:HG22	4:F:256:LEU:H	1.66	0.59
1:A:241:LEU:HD23	1:A:245:LEU:HD11	1.84	0.59
1:A:86:ILE:HG22	1:A:90:LEU:HD12	1.84	0.59
4:E:31:TYR:O	4:E:35:ILE:HG12	2.02	0.59
4:F:320:LYS:HZ1	4:F:442:ARG:HH12	1.50	0.59
4:F:522:ALA:O	4:F:526:LEU:N	2.32	0.59
7:J:112:G:H2'	7:J:113:C:C6	2.37	0.59
4:E:106:PHE:HB2	4:E:130:LEU:HD11	1.83	0.59
4:E:258:ILE:HG12	4:E:266:VAL:HG21	1.84	0.59
4:F:226:VAL:HG23	4:F:228:THR:HG22	1.85	0.59
4:E:138:LEU:O	4:E:141:THR:OG1	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:151:ILE:HG22	4:F:168:GLU:HG2	1.84	0.59
4:F:406:PRO:HB3	4:F:422:PHE:CE2	2.37	0.59
6:I:24:G:H2'	6:I:25:C:H6	1.67	0.59
2:B:50:ASP:OD2	2:B:51:ARG:NH1	2.35	0.58
4:E:203:GLY:HA2	4:E:210:VAL:HG23	1.85	0.58
6:I:25:C:H2'	6:I:26:U:H6	1.68	0.58
6:I:25:C:H2'	6:I:26:U:C6	2.38	0.58
4:F:106:PHE:HA	4:F:109:ILE:HG12	1.86	0.58
4:F:192:LYS:HE2	4:F:224:TYR:CE2	2.38	0.58
3:C:2:LYS:NZ	2:D:98:LEU:O	2.34	0.58
6:I:11:G:H1	7:J:126:C:N4	2.02	0.58
6:I:24:G:H2'	6:I:25:C:C6	2.38	0.58
1:A:275:PHE:O	1:A:279:ARG:HG3	2.04	0.58
1:A:836:ARG:NH1	1:A:840:ALA:HB2	2.19	0.58
4:E:19:CYS:O	4:E:22:ARG:NH1	2.37	0.58
4:E:409:ARG:HD3	4:E:409:ARG:N	2.19	0.58
4:F:534:ASP:OD1	4:F:560:ARG:NH1	2.37	0.58
1:A:179:GLY:O	1:A:182:VAL:HG12	2.03	0.58
4:E:151:ILE:HG23	4:E:226:VAL:HG12	1.85	0.58
1:A:50:LYS:HG2	1:A:52:ASN:H	1.69	0.58
1:A:116:ARG:NH1	1:A:119:LEU:HD13	2.18	0.58
4:F:306:TYR:HA	4:F:372:VAL:HG23	1.86	0.58
1:A:312:ASN:HA	1:A:629:MET:CE	2.34	0.57
4:E:142:GLU:O	4:E:146:LYS:HG3	2.03	0.57
1:A:847:ILE:HG12	2:D:83:VAL:HG11	1.84	0.57
4:E:44:SER:HB2	4:E:48:TYR:HE2	1.69	0.57
4:E:371:VAL:HG22	4:E:396:TYR:HA	1.85	0.57
4:E:371:VAL:O	4:E:397:VAL:HB	2.04	0.57
4:F:43:LEU:HD12	4:F:47:PRO:HA	1.87	0.57
6:I:31:A:H2'	6:I:32:G:C8	2.38	0.57
6:I:11:G:C6	7:J:126:C:N4	2.64	0.57
1:A:478:LYS:HD3	1:A:742:VAL:HG12	1.85	0.57
1:A:825:ASP:OD1	1:A:825:ASP:N	2.38	0.57
4:E:133:PHE:HA	4:E:136:GLU:HG2	1.87	0.57
3:C:59:LEU:CA	3:C:62:MET:HE2	2.28	0.57
4:E:175:PRO:HD2	4:E:180:TYR:CE2	2.39	0.57
4:F:409:ARG:HH22	4:F:422:PHE:HD2	1.50	0.57
1:A:37:ILE:HG21	11:G:200:6GS:C5	2.35	0.57
1:A:83:GLU:OE2	1:A:219:PHE:N	2.34	0.57
4:E:105:ASP:OD1	4:E:106:PHE:N	2.36	0.57
4:E:522:ALA:O	4:E:526:LEU:N	2.31	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:278:SER:HB3	4:F:435:ASP:HB2	1.87	0.57
1:A:109:ASP:OD2	1:A:109:ASP:N	2.38	0.57
1:A:292:GLN:OE1	1:A:735:ARG:NH1	2.37	0.57
1:A:123:THR:HG22	9:A:1003:GNP:HN22	1.70	0.56
2:D:105:ASN:O	2:D:109:ASN:ND2	2.38	0.56
4:E:155:ARG:HB3	4:F:253:TYR:HE1	1.71	0.56
4:E:585:LEU:HD12	4:E:586:GLN:H	1.70	0.56
4:F:128:GLU:O	4:F:131:LYS:HG2	2.06	0.56
2:B:143:ASP:N	2:B:143:ASP:OD1	2.37	0.56
4:E:477:LYS:HG3	4:E:478:GLY:H	1.69	0.56
2:D:22:TYR:CD1	2:D:38:LEU:HB2	2.41	0.56
1:A:426:LYS:HE2	1:A:883:LEU:HB2	1.88	0.56
3:C:54:SER:O	3:C:57:SER:OG	2.23	0.56
4:E:255:THR:HG22	4:E:256:LEU:H	1.71	0.56
4:F:105:ASP:OD1	4:F:106:PHE:N	2.38	0.56
4:F:369:ASP:OD1	4:F:370:ILE:HG13	2.05	0.56
7:J:112:G:H2'	7:J:113:C:H6	1.69	0.56
1:A:612:PRO:HB2	1:A:805:LEU:HD21	1.88	0.56
4:E:33:HIS:HA	4:E:107:ASN:HD21	1.70	0.56
5:G:16:ALA:HA	5:G:54:ALA:HA	1.86	0.56
4:F:137:THR:O	4:F:141:THR:HG23	2.04	0.56
1:A:37:ILE:HD11	11:G:200:6GS:C1'	2.35	0.55
1:A:57:GLN:NE2	1:A:66:ILE:O	2.35	0.55
2:B:12:TYR:HD2	2:B:49:PHE:HZ	1.53	0.55
4:E:43:LEU:CD1	4:E:47:PRO:HA	2.36	0.55
4:F:320:LYS:HA	4:F:323:LYS:HE3	1.88	0.55
5:G:58:LYS:HD3	5:G:59:SER:H	1.70	0.55
1:A:38:TYR:CE1	1:A:725:HIS:NE2	2.72	0.55
1:A:392:ARG:NH1	2:B:131:VAL:HG11	2.19	0.55
4:E:306:TYR:HA	4:E:372:VAL:HG23	1.88	0.55
4:E:62:GLN:HE21	4:E:73:LYS:HG2	1.71	0.55
4:E:409:ARG:HH22	4:E:417:LEU:HB3	1.71	0.55
4:E:542:ASP:HB3	4:E:569:LYS:HE3	1.89	0.55
1:A:692:SER:O	1:A:696:ILE:HG13	2.07	0.55
4:E:132:LEU:O	4:E:136:GLU:HG2	2.06	0.55
1:A:55:ARG:HD2	9:A:1003:GNP:N7	2.22	0.55
4:F:151:ILE:CG2	4:F:168:GLU:HG2	2.37	0.55
4:F:178:ARG:HA	4:F:199:THR:HG21	1.89	0.55
5:G:48:LEU:HD23	5:G:50:ASP:N	2.20	0.55
1:A:485:GLY:HA2	1:A:574:LYS:HG2	1.89	0.55
1:A:636:LEU:HD11	1:A:655:LEU:HD22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:GLU:OE1	1:A:810:HIS:N	2.40	0.54
1:A:910:ASP:HB3	1:A:912:THR:HG23	1.88	0.54
1:A:103:LYS:HG2	1:A:110:MET:HB3	1.90	0.54
2:D:74:ALA:O	2:D:77:GLU:HG3	2.07	0.54
2:B:106:ILE:HD12	2:B:106:ILE:O	2.07	0.54
2:D:162:ALA:HB3	2:D:181:ALA:HB1	1.89	0.54
4:F:306:TYR:HB2	4:F:357:PHE:HD1	1.72	0.54
1:A:206:THR:HG21	12:A:1101:HOH:O	2.07	0.54
2:B:159:VAL:HG13	2:B:186:VAL:HG22	1.88	0.54
4:E:68:MET:SD	4:E:68:MET:N	2.81	0.54
4:E:358:CYS:SG	4:E:359:THR:N	2.81	0.54
4:F:151:ILE:HD11	4:F:224:TYR:CD2	2.43	0.54
4:F:513:SER:HB3	4:F:519:ASN:HB2	1.90	0.54
4:E:39:HIS:CE1	4:E:110:ALA:HB1	2.43	0.54
4:F:43:LEU:CD1	4:F:47:PRO:HA	2.38	0.54
5:G:111:ARG:HA	5:G:111:ARG:NE	2.23	0.54
1:A:401:LEU:HD11	1:A:673:LEU:HD12	1.88	0.54
2:D:90:MET:HG2	2:D:94:MET:CE	2.37	0.54
4:F:542:ASP:HB3	4:F:569:LYS:HE3	1.90	0.54
4:F:6:VAL:HA	4:F:129:ARG:NH1	2.20	0.54
1:A:111:VAL:HG23	1:A:113:HIS:CE1	2.42	0.53
4:E:25:LEU:HD21	4:E:106:PHE:HZ	1.73	0.53
4:F:116:ASN:N	4:F:119:ASP:OD2	2.38	0.53
4:F:142:GLU:O	4:F:146:LYS:HG2	2.08	0.53
4:F:281:GLN:HB3	4:F:437:PHE:HB3	1.89	0.53
1:A:82:HIS:NE2	1:A:86:ILE:HD11	2.23	0.53
4:E:69:SER:OG	4:E:70:TYR:N	2.42	0.53
4:E:176:LEU:HD12	4:E:201:GLU:HA	1.91	0.53
4:F:285:GLY:HA3	4:F:443:ARG:NE	2.23	0.53
5:G:77:THR:OG1	5:G:84:LYS:HB2	2.08	0.53
5:G:98:ASN:HA	5:G:101:MET:CG	2.38	0.53
4:E:370:ILE:HG12	4:E:395:HIS:HB2	1.90	0.53
5:G:16:ALA:O	5:G:27:ASN:ND2	2.21	0.53
5:G:20:GLN:HE21	5:G:21:THR:HG22	1.73	0.53
1:A:131:LEU:HD21	1:A:247:LEU:HD23	1.89	0.53
4:E:280:LEU:HD11	4:E:397:VAL:HG13	1.90	0.53
4:E:329:LYS:HE3	4:E:354:GLN:NE2	2.23	0.53
2:B:31:SER:HB3	2:B:34:VAL:HG23	1.90	0.53
4:E:269:TYR:HA	4:E:272:VAL:HG12	1.91	0.53
4:F:174:PRO:C	4:F:175:PRO:CG	2.70	0.53
6:I:14:G:H2'	6:I:15:U:C6	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ASN:OD1	7:J:100:A:O2'	2.22	0.53
1:A:758:LEU:CD2	1:A:759:SER:H	2.20	0.53
2:D:31:SER:OG	2:D:32:GLU:N	2.41	0.53
1:A:303:ASP:N	1:A:303:ASP:OD1	2.39	0.53
1:A:206:THR:HB	12:A:1101:HOH:O	2.08	0.53
4:E:320:LYS:HZ3	4:E:442:ARG:HH12	1.57	0.53
1:A:268:TRP:CD1	1:A:322:PRO:HD3	2.43	0.53
4:F:383:ASP:OD1	4:F:383:ASP:N	2.42	0.53
7:J:121:U:H2'	7:J:122:A:H8	1.72	0.53
3:C:47:GLU:HA	3:C:50:GLU:HG2	1.90	0.52
4:E:382:TYR:O	4:E:386:VAL:HG13	2.09	0.52
4:F:424:SER:HA	4:F:427:ARG:NH2	2.23	0.52
4:E:145:PHE:O	4:E:148:SER:OG	2.20	0.52
4:E:185:TYR:O	4:E:192:LYS:NZ	2.30	0.52
4:E:375:GLU:CG	4:E:378:MET:HB2	2.37	0.52
4:F:131:LYS:NZ	4:F:427:ARG:HH22	2.07	0.52
3:C:59:LEU:C	3:C:62:MET:CE	2.76	0.52
2:B:54:ALA:HB1	2:B:57:ARG:NH1	2.25	0.52
4:E:534:ASP:OD1	4:E:560:ARG:NH1	2.43	0.52
6:I:11:G:N1	7:J:126:C:N4	2.58	0.52
7:J:106:U:H2'	7:J:107:C:C6	2.42	0.52
2:D:64:ASP:O	2:D:67:MET:HE3	2.10	0.52
4:F:13:SER:O	4:F:13:SER:OG	2.23	0.52
4:F:428:LEU:HD13	4:F:432:ILE:HD11	1.91	0.52
1:A:569:ARG:O	1:A:573:GLN:HB2	2.10	0.52
2:D:19:GLN:OE1	2:D:42:LEU:HD11	2.09	0.52
1:A:119:LEU:HD12	1:A:211:ASP:HB3	1.92	0.52
4:F:306:TYR:CD2	4:F:317:LEU:HD13	2.45	0.52
4:F:69:SER:OG	4:F:70:TYR:N	2.42	0.52
1:A:401:LEU:HD12	1:A:401:LEU:H	1.74	0.52
4:E:451:THR:HG21	4:E:585:LEU:HD13	1.92	0.52
4:E:506:TRP:CZ3	4:E:573:LEU:HD21	2.45	0.52
4:E:132:LEU:HD11	4:E:238:PRO:HA	1.92	0.52
6:I:11:G:H2'	6:I:12:C:C6	2.44	0.52
1:A:97:ALA:HB2	1:A:215:ASN:HB3	1.91	0.51
1:A:816:HIS:O	1:A:830:PRO:HA	2.10	0.51
4:E:41:LEU:HD21	4:E:58:THR:HB	1.91	0.51
4:E:105:ASP:O	4:E:109:ILE:HG13	2.09	0.51
4:E:19:CYS:HA	4:E:39:HIS:CE1	2.44	0.51
4:E:494:GLY:HA2	4:E:497:ARG:HB2	1.92	0.51
2:B:12:TYR:CD2	2:B:49:PHE:CZ	2.97	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:195:ILE:HG21	4:E:225:PHE:CZ	2.45	0.51
7:J:113:C:H2'	7:J:114:A:C8	2.46	0.51
4:F:320:LYS:NZ	4:F:442:ARG:HH12	2.08	0.51
2:B:182:TRP:CZ3	2:B:184:LEU:HD12	2.45	0.51
4:E:284:PRO:HB3	4:E:567:ARG:CZ	2.40	0.51
4:E:293:ILE:HD13	4:E:320:LYS:HB3	1.92	0.51
4:E:332:ARG:O	4:E:348:VAL:HA	2.11	0.51
4:E:500:LEU:HA	4:E:503:ASN:HD21	1.75	0.51
1:A:24:THR:OG1	1:A:25:GLY:N	2.43	0.51
1:A:77:PHE:O	1:A:80:TYR:HB3	2.11	0.51
2:B:43:ASN:HB3	7:J:123:C:H5'	1.93	0.51
4:E:428:LEU:HD13	4:E:432:ILE:HD11	1.92	0.51
4:F:176:LEU:HD21	4:F:202:LYS:HG2	1.93	0.51
1:A:358:ASP:OD1	1:A:533:ARG:NH2	2.42	0.51
4:F:332:ARG:HB2	4:F:346:PHE:HB2	1.92	0.51
5:G:55:ARG:HD3	5:G:66:TYR:CZ	2.45	0.51
1:A:37:ILE:CD1	11:G:200:6GS:O4'	2.55	0.51
4:E:255:THR:HG22	4:E:256:LEU:N	2.26	0.51
5:G:54:ALA:HB3	5:G:67:THR:OG1	2.11	0.51
2:B:174:MET:HE3	2:B:174:MET:O	2.10	0.50
3:C:47:GLU:OE1	3:C:47:GLU:N	2.29	0.50
2:D:182:TRP:O	2:D:184:LEU:N	2.43	0.50
4:E:402:PRO:HB3	4:E:426:CYS:SG	2.52	0.50
1:A:8:LEU:HD21	1:A:21:PRO:HG3	1.92	0.50
1:A:257:VAL:HA	1:A:266:ILE:HG12	1.94	0.50
1:A:696:ILE:O	1:A:700:VAL:HG23	2.11	0.50
1:A:899:MET:CE	1:A:906:MET:HA	2.41	0.50
2:B:25:ALA:HB3	2:B:38:LEU:HD11	1.93	0.50
4:E:13:SER:O	4:E:13:SER:OG	2.24	0.50
4:E:139:LYS:HA	4:E:142:GLU:OE1	2.11	0.50
4:F:152:ALA:HB1	4:F:165:LEU:HD23	1.93	0.50
5:G:74:ARG:HH12	5:G:85:VAL:CA	2.23	0.50
1:A:902:MET:CE	1:A:903:TYR:HB2	2.41	0.50
4:E:62:GLN:NE2	4:E:73:LYS:HG2	2.26	0.50
4:E:370:ILE:HG23	4:E:395:HIS:HB2	1.94	0.50
4:F:146:LYS:NZ	4:F:180:TYR:OH	2.41	0.50
4:F:156:GLU:HB3	4:F:164:HIS:ND1	2.27	0.50
4:F:420:GLU:OE2	4:F:430:LYS:HG3	2.11	0.50
4:F:585:LEU:HD23	4:F:586:GLN:N	2.27	0.50
4:E:52:ALA:HB3	4:E:75:HIS:ND1	2.27	0.50
4:F:332:ARG:HB2	4:F:346:PHE:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:115:U:C2	7:J:116:G:C8	3.00	0.50
1:A:738:ASP:O	1:A:741:PHE:N	2.44	0.50
2:B:43:ASN:ND2	7:J:123:C:OP1	2.45	0.50
7:J:123:C:H2'	7:J:124:C:C6	2.46	0.50
2:B:12:TYR:CD2	2:B:49:PHE:HZ	2.29	0.50
2:D:22:TYR:HD1	2:D:38:LEU:HB2	1.75	0.50
4:E:322:LEU:HD22	4:E:343:PHE:CZ	2.46	0.50
4:E:327:ILE:HG13	4:E:345:LYS:HZ2	1.75	0.50
4:F:112:CYS:SG	4:F:119:ASP:HB3	2.52	0.50
1:A:187:LEU:HD21	1:A:286:TYR:HE1	1.76	0.50
4:E:124:ASN:O	4:E:427:ARG:NH1	2.45	0.50
4:F:284:PRO:O	4:F:443:ARG:NH2	2.44	0.50
4:F:404:GLN:O	4:F:405:LEU:HG	2.12	0.50
5:G:44:LEU:HD22	5:G:89:TYR:HB2	1.93	0.50
2:D:51:ARG:HE	6:I:19:A:H5'	1.77	0.49
4:E:291:PHE:CD2	4:E:438:LEU:HG	2.47	0.49
4:F:305:VAL:HG13	4:F:356:VAL:HG23	1.94	0.49
4:F:494:GLY:HA2	4:F:497:ARG:HB2	1.93	0.49
1:A:167:GLU:OE2	1:A:168:ASN:HB2	2.12	0.49
1:A:507:ASN:ND2	1:A:541:GLN:OE1	2.44	0.49
4:E:114:TRP:CZ3	4:E:123:ALA:HB2	2.46	0.49
4:E:585:LEU:HD12	4:E:586:GLN:N	2.26	0.49
5:G:91:ILE:HD12	5:G:91:ILE:H	1.77	0.49
1:A:235:ASP:OD1	1:A:236:SER:N	2.46	0.49
1:A:272:LYS:HE3	1:A:275:PHE:CE1	2.47	0.49
1:A:380:MET:HG2	2:B:94:MET:HE2	1.93	0.49
4:E:289:SER:HB3	4:E:320:LYS:HZ1	1.77	0.49
4:E:311:HIS:CE1	4:E:342:CYS:HG	2.29	0.49
4:E:446:ALA:HA	4:E:449:VAL:HG12	1.93	0.49
4:F:41:LEU:HD11	4:F:58:THR:HB	1.93	0.49
4:F:512:ILE:HD12	4:F:531:GLN:HG3	1.95	0.49
5:G:97:LEU:O	5:G:101:MET:HE2	2.12	0.49
1:A:82:HIS:CD2	1:A:86:ILE:HD11	2.47	0.49
1:A:905:VAL:HG22	1:A:906:MET:H	1.78	0.49
2:B:11:SER:CB	2:B:48:GLU:HG2	2.41	0.49
4:E:503:ASN:OD1	4:E:506:TRP:HB2	2.12	0.49
4:F:185:TYR:HB2	4:F:192:LYS:CD	2.39	0.49
4:F:373:PHE:HD2	4:F:376:ILE:HG22	1.77	0.49
5:G:24:THR:OG1	5:G:25:ASP:N	2.45	0.49
5:G:74:ARG:HH12	5:G:85:VAL:HA	1.77	0.49
1:A:42:VAL:HG23	1:A:712:GLY:HA3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG13	1:A:107:ASP:H	1.78	0.49
1:A:484:ASP:OD1	1:A:484:ASP:N	2.43	0.49
4:F:447:GLU:CD	4:F:467:LYS:HZ2	2.15	0.49
7:J:113:C:C2	7:J:114:A:C8	3.00	0.49
1:A:207:LEU:HD11	1:A:241:LEU:HB2	1.93	0.49
3:C:9:THR:HG21	2:D:98:LEU:HD11	1.94	0.49
2:D:175:ASP:N	2:D:175:ASP:OD1	2.46	0.49
4:F:248:ARG:HG2	4:F:249:ILE:N	2.27	0.49
1:A:695:ASN:C	1:A:695:ASN:HD22	2.16	0.49
1:A:867:TYR:OH	1:A:871:LYS:NZ	2.41	0.49
9:A:1003:GNP:PG	11:G:200:6GS:O1A	2.70	0.49
4:E:285:GLY:HA3	4:E:443:ARG:NE	2.28	0.49
4:F:139:LYS:NZ	4:F:382:TYR:HB3	2.28	0.49
1:A:326:PHE:CE2	1:A:349:ARG:HG2	2.48	0.49
2:D:38:LEU:O	2:D:42:LEU:HB3	2.13	0.49
4:F:145:PHE:O	4:F:148:SER:OG	2.24	0.49
4:F:158:LEU:HD22	4:F:162:GLU:HB2	1.94	0.49
4:F:449:VAL:HG22	4:F:461:LEU:HB3	1.95	0.49
1:A:183:ARG:HG3	1:A:250:ALA:O	2.13	0.49
6:I:33:C:H2'	6:I:34:A:C8	2.47	0.49
9:A:1003:GNP:N3B	11:G:200:6GS:O1A	2.46	0.49
4:F:302:ALA:HB1	4:F:369:ASP:OD1	2.12	0.49
1:A:32:TYR:H	1:A:33:ARG:NH1	2.11	0.48
1:A:86:ILE:HD13	1:A:222:PHE:HB2	1.94	0.48
1:A:683:GLY:O	7:J:101:G:O2'	2.31	0.48
4:E:303:ARG:HH11	4:E:354:GLN:HG3	1.78	0.48
1:A:517:ASP:OD1	2:B:76:SER:OG	2.24	0.48
1:A:834:PRO:HG2	1:A:877:TYR:CE1	2.47	0.48
4:E:15:ARG:HD3	4:E:24:PHE:CE1	2.49	0.48
4:F:185:TYR:HD1	4:F:194:GLN:H	1.61	0.48
5:G:31:TYR:O	5:G:42:LEU:N	2.36	0.48
1:A:18:ARG:HB3	1:A:59:LYS:HB2	1.95	0.48
3:C:59:LEU:HD13	3:C:62:MET:CE	2.41	0.48
2:D:174:MET:SD	2:D:174:MET:N	2.86	0.48
4:E:116:ASN:HB3	4:E:414:LYS:HE2	1.96	0.48
4:F:14:LEU:HD21	4:F:91:GLY:HA3	1.95	0.48
4:F:114:TRP:CH2	4:F:123:ALA:HB2	2.49	0.48
4:F:217:TYR:HD1	4:F:218:LYS:H	1.62	0.48
4:E:117:ALA:O	4:E:121:ILE:HG12	2.14	0.48
4:F:39:HIS:CE1	4:F:110:ALA:HB1	2.49	0.48
1:A:119:LEU:HG	1:A:120:THR:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:MET:CE	1:A:182:VAL:HG23	2.44	0.48
4:E:43:LEU:HD12	4:E:47:PRO:HA	1.96	0.48
4:E:306:TYR:HB2	4:E:357:PHE:HD1	1.77	0.48
4:E:404:GLN:O	4:E:405:LEU:HG	2.14	0.48
4:F:158:LEU:HB2	4:F:164:HIS:CE1	2.48	0.48
4:E:295:LEU:HD21	4:E:370:ILE:HG21	1.95	0.48
4:F:252:LEU:HB3	4:F:299:TYR:CE1	2.47	0.48
4:F:256:LEU:H	4:F:256:LEU:HD23	1.78	0.48
1:A:39:ASN:ND2	11:G:200:6GS:C4	2.74	0.48
1:A:758:LEU:HD23	1:A:759:SER:H	1.77	0.48
4:E:155:ARG:HD3	4:E:166:SER:HB2	1.96	0.48
4:E:217:TYR:HD1	4:E:218:LYS:H	1.61	0.48
4:E:375:GLU:OE2	4:E:377:SER:OG	2.31	0.48
7:J:113:C:H2'	7:J:114:A:H8	1.78	0.48
2:D:162:ALA:H	2:D:181:ALA:HB3	1.79	0.48
4:E:473:LYS:NZ	4:E:586:GLN:HA	2.29	0.48
4:F:33:HIS:HA	4:F:107:ASN:HD21	1.78	0.48
4:F:443:ARG:NH2	4:F:566:THR:OG1	2.47	0.48
5:G:28:ALA:HB1	5:G:44:LEU:HG	1.96	0.48
1:A:605:VAL:HG21	1:A:756:MET:CE	2.43	0.47
2:B:162:ALA:HB2	2:B:183:PRO:HD2	1.95	0.47
2:D:58:LYS:HZ2	4:E:79:ILE:HG12	1.79	0.47
5:G:20:GLN:O	5:G:66:TYR:OH	2.28	0.47
1:A:623:ASP:OD1	1:A:623:ASP:N	2.46	0.47
4:E:239:THR:HA	4:E:385:SER:OG	2.14	0.47
4:E:290:HIS:ND1	4:E:320:LYS:HD3	2.29	0.47
4:E:409:ARG:HD3	4:E:409:ARG:H	1.79	0.47
4:E:477:LYS:HG3	4:E:478:GLY:N	2.29	0.47
4:F:153:THR:HA	4:F:224:TYR:HB3	1.95	0.47
6:I:33:C:H2'	6:I:34:A:H8	1.80	0.47
1:A:913:SER:OG	1:A:917:GLU:OE1	2.25	0.47
4:E:484:VAL:HG13	4:E:485:SER:H	1.79	0.47
4:F:56:ASP:OD1	4:F:56:ASP:O	2.31	0.47
2:D:159:VAL:HG22	2:D:186:VAL:HG13	1.96	0.47
4:E:376:ILE:HD12	4:E:425:VAL:HG11	1.96	0.47
4:E:551:GLU:N	4:E:551:GLU:OE2	2.47	0.47
1:A:467:ARG:HG3	1:A:731:LEU:O	2.14	0.47
4:E:279:THR:HG22	4:E:398:TYR:HD2	1.80	0.47
4:E:376:ILE:HD13	4:E:398:TYR:HB3	1.96	0.47
4:F:151:ILE:HD11	4:F:224:TYR:HD2	1.78	0.47
5:G:11:GLN:HE21	5:G:29:LEU:HB3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:269:TYR:HB2	4:F:298:TYR:CD2	2.49	0.47
4:F:445:PRO:HB3	4:F:465:LYS:NZ	2.29	0.47
1:A:31:VAL:HB	1:A:33:ARG:HH12	1.76	0.47
1:A:202:VAL:HG22	1:A:231:VAL:CG1	2.44	0.47
1:A:504:PHE:HB2	1:A:541:GLN:HG3	1.97	0.47
1:A:899:MET:HE3	1:A:906:MET:HA	1.96	0.47
2:B:95:LEU:C	2:B:95:LEU:HD23	2.34	0.47
3:C:41:LEU:O	3:C:43:LYS:NZ	2.47	0.47
3:C:59:LEU:HD13	3:C:62:MET:HE1	1.96	0.47
2:D:13:ALA:O	2:D:17:THR:HG23	2.15	0.47
4:E:18:ALA:N	4:E:41:LEU:HB2	2.30	0.47
4:E:333:ILE:HB	4:E:358:CYS:HB2	1.97	0.47
4:F:262:PHE:HE2	4:F:290:HIS:O	1.98	0.47
4:F:353:GLU:HG3	4:F:354:GLN:H	1.80	0.47
4:F:402:PRO:HB3	4:F:426:CYS:SG	2.54	0.47
5:G:19:THR:H	5:G:22:ALA:HB3	1.80	0.47
6:I:26:U:H2'	6:I:27:A:C8	2.50	0.47
3:C:21:ARG:O	3:C:21:ARG:HG3	2.15	0.47
4:F:322:LEU:HD23	4:F:343:PHE:CZ	2.50	0.47
2:B:73:GLN:OE1	4:F:45:VAL:HG21	2.15	0.47
4:F:5:CYS:HB2	4:F:25:LEU:HA	1.96	0.47
5:G:75:PHE:C	5:G:75:PHE:CD2	2.87	0.47
1:A:612:PRO:HG2	1:A:805:LEU:HD11	1.96	0.47
4:E:116:ASN:N	4:E:119:ASP:OD2	2.42	0.47
1:A:423:ALA:O	1:A:428:PHE:HB2	2.15	0.46
1:A:898:HIS:O	1:A:901:ASP:OD1	2.33	0.46
4:E:62:GLN:HE22	4:E:72:CYS:HB2	1.80	0.46
4:F:274:MET:SD	4:F:275:GLN:HB3	2.55	0.46
4:F:396:TYR:HD2	4:F:398:TYR:HE1	1.63	0.46
5:G:43:ALA:HB2	5:G:102:VAL:HG21	1.97	0.46
6:I:11:G:H2'	6:I:12:C:H6	1.80	0.46
7:J:123:C:H2'	7:J:124:C:H6	1.81	0.46
1:A:40:ASP:C	1:A:725:HIS:HE1	2.18	0.46
4:F:31:TYR:OH	4:F:84:CYS:HB3	2.15	0.46
4:F:255:THR:HG22	4:F:256:LEU:N	2.30	0.46
5:G:74:ARG:HH12	5:G:85:VAL:C	2.17	0.46
1:A:387:LEU:HD12	1:A:388:LEU:H	1.80	0.46
4:E:276:LYS:HD3	4:E:277:TYR:N	2.30	0.46
4:F:163:LEU:O	4:F:209:VAL:N	2.46	0.46
4:F:322:LEU:HD12	4:F:323:LYS:HG2	1.97	0.46
4:F:375:GLU:CG	4:F:378:MET:HB2	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:484:VAL:HG13	4:F:485:SER:H	1.79	0.46
1:A:183:ARG:HH11	1:A:253:ALA:HB3	1.80	0.46
3:C:43:LYS:HD3	3:C:43:LYS:N	2.31	0.46
4:E:21:ARG:HH11	4:E:140:ALA:HB2	1.80	0.46
4:E:154:VAL:HG12	4:E:223:ASP:O	2.15	0.46
5:G:48:LEU:HD23	5:G:49:GLN:N	2.31	0.46
4:E:113:ASP:HB3	4:E:115:THR:HG23	1.97	0.46
4:E:449:VAL:HG22	4:E:461:LEU:HB3	1.97	0.46
4:E:455:LEU:HD21	4:E:558:VAL:HG22	1.98	0.46
4:E:198:TYR:CD2	4:E:225:PHE:HE1	2.34	0.46
4:E:510:VAL:HG13	4:E:529:PRO:HB2	1.98	0.46
4:F:19:CYS:HA	4:F:39:HIS:CE1	2.50	0.46
4:F:139:LYS:HZ3	4:F:382:TYR:HB3	1.80	0.46
4:F:295:LEU:HD21	4:F:370:ILE:HG21	1.98	0.46
4:F:490:ARG:NH2	4:F:491:PRO:HG3	2.30	0.46
1:A:621:LYS:HA	1:A:621:LYS:HD3	1.63	0.46
1:A:717:ASP:OD1	1:A:720:VAL:CB	2.64	0.46
6:I:22:A:H2'	6:I:23:U:C6	2.50	0.46
1:A:72:VAL:CG2	1:A:113:HIS:HB3	2.46	0.46
1:A:124:MET:HE1	1:A:182:VAL:HG23	1.97	0.46
2:D:95:LEU:HD23	2:D:95:LEU:HA	1.83	0.46
4:E:11:GLN:HB3	4:E:93:TYR:CD2	2.50	0.46
4:E:320:LYS:NZ	4:E:442:ARG:HH12	2.14	0.46
4:F:114:TRP:CZ3	4:F:123:ALA:HB2	2.51	0.46
4:F:244:GLU:O	4:F:275:GLN:HB2	2.16	0.46
4:F:288:LYS:NZ	4:F:404:GLN:HE22	2.14	0.46
1:A:805:LEU:H	1:A:805:LEU:HD12	1.82	0.46
2:B:11:SER:C	2:B:49:PHE:HE1	2.19	0.46
4:F:332:ARG:HG2	4:F:343:PHE:O	2.15	0.46
5:G:98:ASN:O	5:G:101:MET:HG2	2.15	0.46
1:A:605:VAL:CG2	1:A:756:MET:HE2	2.44	0.45
2:B:73:GLN:OE1	4:F:45:VAL:HG22	2.14	0.45
4:F:246:TYR:HB2	4:F:274:MET:O	2.16	0.45
4:F:394:LYS:O	4:F:395:HIS:ND1	2.49	0.45
1:A:467:ARG:HA	1:A:467:ARG:HD3	1.78	0.45
4:E:7:LEU:HD21	4:E:106:PHE:HB3	1.97	0.45
4:E:486:SER:HA	4:E:515:TYR:CD2	2.51	0.45
4:F:156:GLU:HA	4:F:221:VAL:HG12	1.98	0.45
6:I:18:U:H2'	6:I:19:A:C8	2.51	0.45
2:D:82:LYS:O	2:D:82:LYS:HG3	2.15	0.45
4:F:486:SER:HA	4:F:515:TYR:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:CE1	1:A:101:PHE:HB3	2.46	0.45
2:D:100:ASN:HB3	2:D:103:LEU:HD12	1.97	0.45
1:A:223:ILE:HD13	5:G:104:GLY:HA2	1.97	0.45
1:A:593:LYS:HB3	1:A:598:TRP:HE3	1.82	0.45
2:B:162:ALA:HB2	2:B:183:PRO:CD	2.46	0.45
4:F:15:ARG:HD2	4:F:24:PHE:CE1	2.51	0.45
4:F:565:ILE:HD12	4:F:572:ILE:HD13	1.99	0.45
1:A:35:PHE:HE2	11:G:200:6GS:H9	1.63	0.45
1:A:893:ASP:HA	1:A:896:THR:HG22	1.99	0.45
2:D:134:ASP:OD2	2:D:137:THR:OG1	2.25	0.45
4:E:233:MET:HA	4:E:234:PRO:HD2	1.85	0.45
4:F:64:TYR:HE1	4:F:73:LYS:HZ2	1.65	0.45
4:F:382:TYR:O	4:F:386:VAL:HG13	2.16	0.45
7:J:115:U:H2'	7:J:116:G:O4'	2.16	0.45
1:A:37:ILE:CD1	11:G:200:6GS:N1	2.77	0.45
1:A:72:VAL:HG23	1:A:113:HIS:HB3	1.98	0.45
1:A:847:ILE:HD13	2:D:80:ARG:HB2	1.99	0.45
2:B:96:ARG:NH2	2:B:97:LYS:HG2	2.32	0.45
4:E:16:CYS:SG	4:E:39:HIS:HB3	2.57	0.45
4:E:252:LEU:HB3	4:E:299:TYR:CE1	2.52	0.45
4:E:409:ARG:HH12	4:E:417:LEU:HD23	1.81	0.45
4:F:52:ALA:HB3	4:F:75:HIS:ND1	2.31	0.45
3:C:47:GLU:HA	3:C:50:GLU:CG	2.47	0.45
2:D:95:LEU:HD23	2:D:98:LEU:HD12	1.98	0.45
4:E:548:GLN:OE1	4:E:555:SER:OG	2.21	0.45
4:F:245:HIS:HA	4:F:275:GLN:HB2	1.99	0.45
1:A:37:ILE:CD1	11:G:200:6GS:C1'	2.95	0.45
1:A:322:PRO:HB2	1:A:324:THR:HG22	1.99	0.45
4:E:378:MET:O	4:E:407:ALA:HB2	2.17	0.45
4:E:48:TYR:HA	4:E:70:TYR:CD2	2.51	0.45
4:E:327:ILE:HG13	4:E:345:LYS:NZ	2.32	0.45
4:F:117:ALA:O	4:F:121:ILE:HG12	2.17	0.45
4:F:252:LEU:HD11	4:F:370:ILE:HD11	1.99	0.44
4:F:358:CYS:SG	4:F:359:THR:N	2.90	0.44
4:F:383:ASP:O	4:F:387:VAL:HG13	2.17	0.44
1:A:903:TYR:CD1	1:A:905:VAL:HG12	2.51	0.44
2:D:51:ARG:HG2	6:I:19:A:H4'	1.99	0.44
4:E:59:ASP:OD1	4:E:61:THR:OG1	2.22	0.44
4:E:127:THR:OG1	4:E:128:GLU:N	2.49	0.44
4:F:235:LEU:HD21	4:F:382:TYR:CZ	2.52	0.44
5:G:74:ARG:HD2	5:G:87:TYR:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:116:G:H2'	7:J:117:C:H6	1.82	0.44
3:C:14:LEU:HD12	3:C:14:LEU:HA	1.68	0.44
3:C:68:ILE:CD1	2:D:111:ARG:HG2	2.42	0.44
4:E:140:ALA:HA	4:E:143:GLU:OE2	2.17	0.44
4:E:323:LYS:HG3	4:E:324:TYR:CD2	2.52	0.44
1:A:15:SER:HB3	1:A:118:ARG:HH22	1.81	0.44
1:A:380:MET:HG2	2:B:94:MET:HE1	1.95	0.44
3:C:47:GLU:HB2	3:C:51:LYS:HZ1	1.83	0.44
4:E:165:LEU:HD12	4:E:209:VAL:HG11	1.98	0.44
4:F:285:GLY:H	4:F:288:LYS:HD2	1.82	0.44
5:G:72:PRO:HB3	5:G:89:TYR:CZ	2.52	0.44
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.43	0.44
2:D:161:ASP:HB2	2:D:181:ALA:HB3	1.98	0.44
4:F:154:VAL:HG12	4:F:223:ASP:O	2.17	0.44
7:J:116:G:H2'	7:J:117:C:C6	2.53	0.44
2:B:50:ASP:O	2:B:54:ALA:HB3	2.17	0.44
3:C:59:LEU:CB	3:C:62:MET:HE1	2.46	0.44
4:F:114:TRP:CD1	4:F:138:LEU:HA	2.52	0.44
6:I:23:U:H2'	6:I:24:G:C8	2.52	0.44
7:J:121:U:H2'	7:J:122:A:C8	2.52	0.44
1:A:164:ASP:OD1	1:A:166:VAL:N	2.51	0.44
4:E:278:SER:HB2	4:E:435:ASP:HB2	2.00	0.44
4:E:484:VAL:HG13	4:E:485:SER:N	2.33	0.44
4:F:426:CYS:O	4:F:430:LYS:NZ	2.43	0.44
5:G:74:ARG:NH1	5:G:85:VAL:CG1	2.79	0.44
1:A:527:LEU:O	1:A:531:THR:HG23	2.18	0.44
4:E:165:LEU:HD23	4:E:165:LEU:HA	1.80	0.44
4:F:149:TYR:HB3	4:F:174:PRO:HD3	2.00	0.44
5:G:95:ASN:OD1	5:G:95:ASN:N	2.51	0.44
1:A:196:MET:SD	1:A:222:PHE:HE2	2.41	0.43
1:A:574:LYS:HB2	1:A:574:LYS:HE3	1.86	0.43
4:E:266:VAL:HA	4:E:269:TYR:CD2	2.53	0.43
4:E:581:LEU:HA	4:E:584:LYS:HB3	2.00	0.43
4:F:237:ALA:O	4:F:385:SER:OG	2.36	0.43
4:F:258:ILE:HG12	4:F:266:VAL:HG21	1.99	0.43
1:A:18:ARG:HH21	1:A:61:GLU:HA	1.82	0.43
1:A:497:ASN:ND2	1:A:500:LYS:HE3	2.33	0.43
4:F:31:TYR:HA	4:F:34:VAL:HG12	1.99	0.43
4:F:484:VAL:HG13	4:F:485:SER:N	2.33	0.43
7:J:122:A:H2'	7:J:123:C:H6	1.83	0.43
1:A:68:SER:HA	1:A:119:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:ALA:O	2:B:17:THR:HG23	2.18	0.43
4:E:154:VAL:HG21	4:E:163:LEU:HD13	2.00	0.43
4:E:290:HIS:CE1	4:E:320:LYS:HD3	2.53	0.43
4:E:294:GLY:HA2	4:E:297:LEU:HB2	2.00	0.43
4:F:282:GLY:O	4:F:404:GLN:NE2	2.51	0.43
4:F:510:VAL:HG13	4:F:529:PRO:HB2	2.00	0.43
2:B:171:GLU:N	2:B:171:GLU:OE1	2.51	0.43
3:C:58:VAL:C	3:C:62:MET:SD	2.89	0.43
4:E:307:THR:HA	4:E:358:CYS:O	2.18	0.43
4:F:471:CYS:SG	4:F:572:ILE:HG22	2.59	0.43
1:A:365:ARG:NH1	1:A:366:LEU:H	2.17	0.43
4:E:252:LEU:HD11	4:E:370:ILE:HD11	2.00	0.43
4:E:269:TYR:HB2	4:E:298:TYR:CD2	2.54	0.43
1:A:242:MET:HE3	1:A:463:MET:HE2	2.01	0.43
1:A:348:PHE:CD2	1:A:351:LEU:HB2	2.53	0.43
2:B:128:LEU:HD23	2:B:129:MET:N	2.34	0.43
4:E:441:CYS:SG	4:E:461:LEU:HD12	2.59	0.43
4:F:18:ALA:N	4:F:41:LEU:HB2	2.34	0.43
4:F:220:ASN:OD1	4:F:221:VAL:N	2.51	0.43
4:F:332:ARG:O	4:F:348:VAL:HA	2.19	0.43
4:F:403:ALA:O	4:F:559:ASN:HB2	2.19	0.43
1:A:321:PHE:HB3	1:A:322:PRO:HD2	2.01	0.43
5:G:9:LEU:HD23	5:G:9:LEU:HA	1.82	0.43
1:A:242:MET:CE	1:A:463:MET:HE3	2.48	0.43
2:B:175:ASP:OD1	2:B:175:ASP:N	2.50	0.43
2:D:90:MET:HG2	2:D:94:MET:HE2	2.01	0.43
4:E:12:THR:OG1	4:E:26:CYS:HA	2.19	0.43
4:F:135:ALA:HB2	4:F:381:ASN:HB2	2.00	0.43
4:F:512:ILE:HB	4:F:546:PHE:CD1	2.54	0.43
6:I:19:A:H2'	6:I:20:G:H8	1.84	0.43
1:A:100:ASP:HB3	1:A:115:SER:O	2.19	0.43
1:A:409:THR:OG1	1:A:444:GLN:O	2.35	0.43
4:E:417:LEU:HD21	4:E:422:PHE:HA	2.01	0.43
4:E:449:VAL:CG2	4:E:461:LEU:HB3	2.49	0.43
4:F:73:LYS:HA	4:F:73:LYS:HD3	1.87	0.43
4:F:311:HIS:HA	4:F:314:VAL:HG12	2.00	0.43
4:F:21:ARG:HH11	4:F:140:ALA:HB2	1.84	0.42
4:F:248:ARG:HG2	4:F:249:ILE:H	1.84	0.42
1:A:437:LEU:HB3	1:A:440:PHE:CZ	2.55	0.42
4:E:280:LEU:HB2	4:E:398:TYR:O	2.19	0.42
4:E:293:ILE:HD12	4:E:324:TYR:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:161:ARG:O	4:F:210:VAL:HA	2.18	0.42
5:G:33:ASN:N	5:G:40:PHE:O	2.26	0.42
5:G:45:LEU:HD11	5:G:86:LYS:HD2	2.01	0.42
5:G:84:LYS:O	5:G:86:LYS:NZ	2.52	0.42
2:B:75:ARG:HA	2:B:75:ARG:HE	1.80	0.42
4:E:174:PRO:HB2	4:E:180:TYR:HD2	1.84	0.42
4:E:405:LEU:HD22	4:E:534:ASP:O	2.20	0.42
4:E:512:ILE:HA	4:E:531:GLN:HB3	2.00	0.42
4:F:261:GLU:HG2	4:F:262:PHE:CE1	2.55	0.42
2:D:135:TYR:HB2	2:D:182:TRP:CZ2	2.55	0.42
4:E:161:ARG:O	4:E:210:VAL:HA	2.19	0.42
4:E:544:VAL:HG23	4:E:572:ILE:HG13	2.01	0.42
4:F:127:THR:CG2	4:F:130:LEU:HD12	2.45	0.42
4:F:377:SER:OG	4:F:402:PRO:HA	2.19	0.42
4:F:396:TYR:HB3	4:F:398:TYR:CE1	2.54	0.42
2:B:182:TRP:CH2	2:B:184:LEU:HD12	2.53	0.42
2:D:19:GLN:OE1	2:D:19:GLN:HA	2.20	0.42
4:F:109:ILE:HG13	4:F:110:ALA:N	2.34	0.42
4:F:282:GLY:N	4:F:401:ASP:OD1	2.52	0.42
4:F:417:LEU:HD11	4:F:421:TYR:O	2.18	0.42
4:F:450:ASP:O	4:F:453:SER:OG	2.37	0.42
4:F:452:VAL:HG13	4:F:562:ASN:HD21	1.83	0.42
7:J:101:G:H2'	7:J:102:C:C6	2.54	0.42
1:A:82:HIS:O	1:A:86:ILE:HG13	2.20	0.42
1:A:206:THR:CG2	12:A:1101:HOH:O	2.65	0.42
4:E:31:TYR:O	4:E:34:VAL:HG12	2.20	0.42
4:F:151:ILE:HG13	4:F:225:PHE:O	2.20	0.42
7:J:125:G:H2'	7:J:126:C:O4'	2.20	0.42
4:E:155:ARG:HE	4:F:248:ARG:HH22	1.66	0.42
4:E:376:ILE:HG21	4:E:398:TYR:HB3	2.02	0.42
4:F:273:GLY:HA2	4:F:395:HIS:CD2	2.54	0.42
4:F:327:ILE:HG12	4:F:345:LYS:NZ	2.35	0.42
5:G:74:ARG:HH12	5:G:86:LYS:N	2.17	0.42
6:I:13:G:H2'	6:I:14:G:C8	2.54	0.42
1:A:51:THR:HG23	1:A:53:CYS:SG	2.60	0.42
1:A:119:LEU:HG	1:A:120:THR:H	1.85	0.42
1:A:719:TYR:OH	1:A:744:GLU:OE2	2.33	0.42
4:F:68:MET:SD	4:F:68:MET:N	2.79	0.42
4:F:446:ALA:HA	4:F:449:VAL:HG12	2.01	0.42
7:J:122:A:H2'	7:J:123:C:C6	2.54	0.42
1:A:515:TYR:O	1:A:519:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LYS:HE2	1:A:551:LYS:HB3	1.73	0.42
4:E:153:THR:CA	4:E:224:TYR:HB3	2.48	0.42
4:E:266:VAL:HA	4:E:269:TYR:HD2	1.85	0.42
6:I:24:G:HO2'	6:I:25:C:P	2.41	0.42
6:I:26:U:H2'	6:I:27:A:H8	1.85	0.42
1:A:630:LEU:HD23	1:A:694:PHE:CD1	2.55	0.42
3:C:44:ASP:HB3	3:C:47:GLU:OE2	2.19	0.42
4:E:114:TRP:CD1	4:E:138:LEU:HA	2.55	0.42
4:E:163:LEU:O	4:E:209:VAL:N	2.49	0.42
4:E:248:ARG:CZ	4:E:249:ILE:HG12	2.50	0.42
4:E:475:PHE:HA	4:E:576:MET:O	2.20	0.42
4:F:12:THR:OG1	4:F:25:LEU:O	2.33	0.42
4:F:452:VAL:CG1	4:F:562:ASN:HD21	2.33	0.42
4:F:519:ASN:ND2	4:F:530:THR:HA	2.35	0.42
7:J:113:C:H2'	7:J:114:A:O4'	2.20	0.42
4:E:38:SER:HA	4:E:40:LYS:NZ	2.35	0.41
4:E:175:PRO:HD2	4:E:180:TYR:HE2	1.83	0.41
4:E:198:TYR:CD1	4:E:213:GLY:HA2	2.55	0.41
4:E:200:PHE:HZ	4:E:225:PHE:CD1	2.37	0.41
4:E:376:ILE:HG12	4:E:400:GLY:HA3	2.02	0.41
4:E:378:MET:SD	4:E:407:ALA:HA	2.60	0.41
4:F:31:TYR:O	4:F:34:VAL:HG12	2.20	0.41
4:F:266:VAL:HA	4:F:269:TYR:CD2	2.53	0.41
1:A:562:ILE:O	1:A:566:MET:HB2	2.20	0.41
1:A:902:MET:HE3	1:A:903:TYR:N	2.35	0.41
4:E:21:ARG:NH2	4:E:234:PRO:HD3	2.33	0.41
4:E:271:LYS:HA	4:E:274:MET:HG2	2.03	0.41
4:F:72:CYS:SG	4:F:73:LYS:N	2.93	0.41
4:F:155:ARG:NH1	4:F:156:GLU:OE2	2.53	0.41
4:F:220:ASN:CG	4:F:221:VAL:H	2.23	0.41
4:F:244:GLU:O	4:F:244:GLU:HG2	2.19	0.41
4:F:251:GLY:HA3	4:F:394:LYS:HZ1	1.85	0.41
4:F:471:CYS:HA	4:F:572:ILE:H	1.85	0.41
4:F:562:ASN:HA	4:F:565:ILE:HG22	2.02	0.41
1:A:295:HIS:HE1	1:A:306:CYS:SG	2.43	0.41
1:A:590:GLY:O	7:J:105:C:H5'	2.20	0.41
2:D:51:ARG:HB3	2:D:51:ARG:NH1	2.35	0.41
2:D:130:VAL:HG21	2:D:147:PHE:HE2	1.85	0.41
4:E:284:PRO:HB3	4:E:567:ARG:NH1	2.35	0.41
4:F:473:LYS:HB2	4:F:576:MET:SD	2.61	0.41
4:F:586:GLN:N	4:F:586:GLN:OE1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:81:LYS:HD2	5:G:84:LYS:HG2	2.02	0.41
1:A:242:MET:CE	1:A:463:MET:CE	2.98	0.41
2:B:11:SER:HG	2:B:49:PHE:HD1	1.61	0.41
4:E:471:CYS:HA	4:E:572:ILE:H	1.86	0.41
4:F:21:ARG:HB2	4:F:133:PHE:CZ	2.55	0.41
5:G:98:ASN:HA	5:G:101:MET:SD	2.60	0.41
9:A:1003:GNP:O3G	11:G:200:6GS:O1A	2.38	0.41
2:D:135:TYR:CZ	2:D:139:LYS:HD3	2.55	0.41
4:E:304:ILE:HA	4:E:370:ILE:O	2.20	0.41
4:F:315:ASP:O	4:F:319:GLU:HG2	2.20	0.41
1:A:365:ARG:NH1	1:A:366:LEU:HD12	2.35	0.41
1:A:562:ILE:HD12	1:A:562:ILE:HA	1.87	0.41
1:A:631:ARG:HH12	1:A:662:VAL:HG23	1.85	0.41
4:E:270:GLN:NE2	4:E:271:LYS:HB3	2.35	0.41
4:E:383:ASP:O	4:E:387:VAL:HG13	2.20	0.41
6:I:18:U:H2'	6:I:19:A:H8	1.85	0.41
1:A:202:VAL:HG22	1:A:231:VAL:HG12	2.03	0.41
1:A:606:TYR:CE2	1:A:805:LEU:HB3	2.55	0.41
3:C:41:LEU:O	3:C:43:LYS:CE	2.68	0.41
3:C:68:ILE:HD12	3:C:68:ILE:HA	1.88	0.41
4:E:332:ARG:HD2	4:E:334:ILE:CD1	2.50	0.41
4:E:417:LEU:HD11	4:E:421:TYR:HB2	2.03	0.41
4:E:443:ARG:NH1	4:E:566:THR:O	2.54	0.41
4:F:56:ASP:OD1	4:F:56:ASP:C	2.59	0.41
4:F:477:LYS:HD2	4:F:477:LYS:HA	1.74	0.41
1:A:439:HIS:HB3	1:A:548:ILE:HG12	2.01	0.41
4:E:480:ILE:HD13	4:E:480:ILE:HA	1.81	0.41
4:F:38:SER:HA	4:F:40:LYS:NZ	2.36	0.41
4:F:375:GLU:N	4:F:399:ILE:O	2.54	0.41
1:A:717:ASP:OD1	1:A:720:VAL:HB	2.21	0.41
1:A:822:GLN:HE21	1:A:926:THR:HG23	1.86	0.41
4:E:36:SER:HB2	4:E:107:ASN:ND2	2.35	0.41
4:E:92:LEU:HD12	4:E:92:LEU:HA	1.93	0.41
4:E:276:LYS:HE2	4:E:396:TYR:HB2	2.03	0.41
4:F:16:CYS:SG	4:F:39:HIS:HB3	2.61	0.41
4:F:128:GLU:O	4:F:132:LEU:HD23	2.21	0.41
4:F:551:GLU:OE2	4:F:578:ASP:HB3	2.20	0.41
4:F:586:GLN:HG2	4:F:586:GLN:O	2.21	0.41
7:J:111:A:H2'	7:J:112:G:C8	2.56	0.41
2:D:55:MET:HE3	2:D:58:LYS:HB3	2.03	0.41
4:E:113:ASP:HB3	4:E:115:THR:CG2	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:551:GLU:HA	4:E:556:CYS:SG	2.61	0.41
4:F:21:ARG:HD3	4:F:136:GLU:HB3	2.03	0.41
4:F:447:GLU:HG3	4:F:587:PHE:CE1	2.55	0.41
1:A:269:ASP:OD1	1:A:270:LEU:N	2.54	0.40
1:A:281:LYS:HB3	1:A:281:LYS:HE2	1.84	0.40
2:B:51:ARG:NH2	6:I:16:A:H4'	2.36	0.40
2:D:98:LEU:HD23	2:D:98:LEU:HA	1.95	0.40
4:E:246:TYR:HB2	4:E:274:MET:O	2.21	0.40
4:F:319:GLU:O	4:F:322:LEU:HG	2.21	0.40
4:F:480:ILE:HD11	4:F:549:THR:O	2.21	0.40
4:F:559:ASN:OD1	4:F:560:ARG:N	2.54	0.40
1:A:854:LEU:HD11	2:D:75:ARG:HG2	2.03	0.40
2:D:182:TRP:N	2:D:183:PRO:HD2	2.36	0.40
4:E:17:GLY:N	4:E:41:LEU:O	2.53	0.40
4:E:185:TYR:HB2	4:E:192:LYS:CG	2.43	0.40
4:E:376:ILE:HG12	4:E:376:ILE:H	1.77	0.40
4:E:443:ARG:HE	4:E:443:ARG:HB2	1.66	0.40
4:F:43:LEU:HD12	4:F:43:LEU:HA	1.50	0.40
4:F:274:MET:HE1	4:F:275:GLN:HB3	2.03	0.40
4:F:322:LEU:HD23	4:F:343:PHE:HZ	1.84	0.40
4:E:185:TYR:C	4:E:195:ILE:HG12	2.42	0.40
4:E:363:LEU:HD23	4:E:364:PRO:O	2.21	0.40
5:G:44:LEU:HD13	5:G:69:LEU:HD11	2.03	0.40
5:G:56:PHE:O	5:G:65:ILE:HG13	2.21	0.40
1:A:450:ILE:HD12	1:A:450:ILE:HA	1.90	0.40
1:A:479:TYR:HA	1:A:746:TYR:HE2	1.86	0.40
4:F:151:ILE:HD13	4:F:151:ILE:HG21	1.84	0.40
4:F:217:TYR:HD1	4:F:218:LYS:N	2.20	0.40
4:F:329:LYS:HG3	4:F:355:TYR:CE2	2.56	0.40
4:F:581:LEU:HA	4:F:584:LYS:HE3	2.04	0.40
3:C:14:LEU:HD22	3:C:36:HIS:HB2	2.03	0.40
2:D:128:LEU:O	2:D:187:THR:HA	2.21	0.40
4:E:405:LEU:HD21	4:E:563:VAL:HG21	2.02	0.40
4:F:36:SER:HB2	4:F:107:ASN:ND2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	926/932 (99%)	832 (90%)	90 (10%)	4 (0%)	30 60
2	B	185/198 (93%)	173 (94%)	11 (6%)	1 (0%)	25 54
2	D	184/198 (93%)	166 (90%)	18 (10%)	0	100 100
3	C	70/83 (84%)	66 (94%)	4 (6%)	0	100 100
4	E	580/601 (96%)	526 (91%)	54 (9%)	0	100 100
4	F	580/601 (96%)	524 (90%)	56 (10%)	0	100 100
5	G	111/113 (98%)	102 (92%)	7 (6%)	2 (2%)	7 26
All	All	2636/2726 (97%)	2389 (91%)	240 (9%)	7 (0%)	38 66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	7	VAL
5	G	71	PRO
1	A	50	LYS
1	A	76	THR
1	A	846	ASP
2	B	183	PRO
1	A	856	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	820/823 (100%)	793 (97%)	27 (3%)	33	59
2	B	146/167 (87%)	138 (94%)	8 (6%)	18	44
2	D	150/167 (90%)	141 (94%)	9 (6%)	16	42
3	C	67/77 (87%)	63 (94%)	4 (6%)	16	42
4	E	498/523 (95%)	475 (95%)	23 (5%)	23	50
4	F	498/523 (95%)	472 (95%)	26 (5%)	19	46
5	G	94/94 (100%)	90 (96%)	4 (4%)	25	51
All	All	2273/2374 (96%)	2172 (96%)	101 (4%)	26	51

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	50	LYS
1	A	51	THR
1	A	77	PHE
1	A	92	ASP
1	A	152	CYS
1	A	167	GLU
1	A	168	ASN
1	A	206	THR
1	A	209	ASN
1	A	255	SER
1	A	343	SER
1	A	347	HIS
1	A	380	MET
1	A	421	ASP
1	A	516	TYR
1	A	517	ASP
1	A	603	LYS
1	A	657	ASN
1	A	694	PHE
1	A	695	ASN
1	A	756	MET
1	A	761	ASP
1	A	824	ASP
1	A	846	ASP
1	A	849	LYS
1	A	858	ARG
2	B	12	TYR
2	B	41	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	46	LYS
2	B	64	ASP
2	B	72	LYS
2	B	111	ARG
2	B	174	MET
2	B	182	TRP
3	C	27	LYS
3	C	34	GLN
3	C	52	MET
3	C	62	MET
2	D	22	TYR
2	D	31	SER
2	D	67	MET
2	D	69	GLN
2	D	70	MET
2	D	82	LYS
2	D	90	MET
2	D	129	MET
2	D	182	TRP
4	E	31	TYR
4	E	55	CYS
4	E	70	TYR
4	E	106	PHE
4	E	129	ARG
4	E	147	LEU
4	E	173	ARG
4	E	179	ASN
4	E	185	TYR
4	E	197	GLU
4	E	217	TYR
4	E	224	TYR
4	E	233	MET
4	E	291	PHE
4	E	303	ARG
4	E	382	TYR
4	E	409	ARG
4	E	437	PHE
4	E	455	LEU
4	E	472	PHE
4	E	474[A]	MET
4	E	474[B]	MET
4	E	511	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	16	CYS
4	F	31	TYR
4	F	55	CYS
4	F	72	CYS
4	F	173	ARG
4	F	179	ASN
4	F	197	GLU
4	F	217	TYR
4	F	233	MET
4	F	248	ARG
4	F	269	TYR
4	F	291	PHE
4	F	303	ARG
4	F	343	PHE
4	F	347	LYS
4	F	414	LYS
4	F	427	ARG
4	F	436	MET
4	F	472	PHE
4	F	474[A]	MET
4	F	474[B]	MET
4	F	476	TYR
4	F	492	GLN
4	F	511	PHE
4	F	517	SER
4	F	584	LYS
5	G	12	MET
5	G	40	PHE
5	G	69	LEU
5	G	70	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	703	ASN
4	E	95	ASN
4	F	275	GLN
4	F	404	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	24/25 (96%)	2 (8%)	1 (4%)
7	J	26/27 (96%)	2 (7%)	0
All	All	50/52 (96%)	4 (8%)	1 (2%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	17	G
6	I	25	C
7	J	103	U
7	J	125	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	I	24	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
11	6GS	G	200	5	15,22,27	4.49	9 (60%)	18,33,43	2.26	9 (50%)
9	GNP	A	1003	10	29,34,34	1.61	7 (24%)	33,54,54	2.15	6 (18%)

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
11	6GS	G	200	5	-	0/7/29/36	0/2/2/2
9	GNP	A	1003	10	-	8/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	200	6GS	C4'-C3'	-8.76	1.34	1.53
11	G	200	6GS	O4-C4	8.32	1.40	1.24
11	G	200	6GS	O4'-C4'	7.97	1.62	1.45
11	G	200	6GS	O4'-C1'	-6.28	1.32	1.42
9	A	1003	GNP	PB-O3A	4.54	1.64	1.59
11	G	200	6GS	O2-C2	-4.25	1.15	1.23
9	A	1003	GNP	PG-N3B	2.99	1.71	1.63
11	G	200	6GS	C2-N3	-2.91	1.32	1.38
11	G	200	6GS	C6-N1	-2.88	1.31	1.38
9	A	1003	GNP	C6-N1	2.88	1.38	1.33
11	G	200	6GS	C4-N3	-2.87	1.33	1.38
9	A	1003	GNP	PB-O1B	2.85	1.50	1.46
9	A	1003	GNP	PG-O1G	2.53	1.50	1.46
11	G	200	6GS	O5'-C5'	-2.48	1.38	1.44
9	A	1003	GNP	PB-O2B	-2.29	1.50	1.56
9	A	1003	GNP	C5-C6	2.05	1.44	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1003	GNP	C5-C6-N1	-8.32	112.06	123.43
9	A	1003	GNP	C2-N1-C6	5.82	125.17	115.93
11	G	200	6GS	N3-C2-N1	4.45	120.79	114.89
11	G	200	6GS	O3'-C3'-C4'	3.40	120.44	112.40
11	G	200	6GS	C1'-N1-C6	-3.28	118.18	121.51
11	G	200	6GS	O4-C4-N3	3.27	124.10	119.31
11	G	200	6GS	O4-C4-C5	-3.10	119.71	125.16
11	G	200	6GS	O4'-C4'-C3'	2.91	107.60	104.42
9	A	1003	GNP	PB-O3A-PA	-2.83	122.64	132.62
9	A	1003	GNP	N3-C2-N1	-2.79	123.50	127.22
9	A	1003	GNP	C4-C5-C6	-2.51	118.40	120.80
11	G	200	6GS	O2-C2-N1	-2.50	119.47	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	200	6GS	C4-N3-C2	-2.16	123.73	126.58
11	G	200	6GS	C6-N1-C2	-2.12	118.28	120.99
9	A	1003	GNP	C2-N3-C4	-2.02	113.05	115.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	GNP	PG-N3B-PB-O1B
9	A	1003	GNP	PA-O3A-PB-O1B
9	A	1003	GNP	PA-O3A-PB-O2B
9	A	1003	GNP	C5'-O5'-PA-O3A
9	A	1003	GNP	O4'-C4'-C5'-O5'
9	A	1003	GNP	C3'-C4'-C5'-O5'
9	A	1003	GNP	C5'-O5'-PA-O1A
9	A	1003	GNP	C4'-C5'-O5'-PA

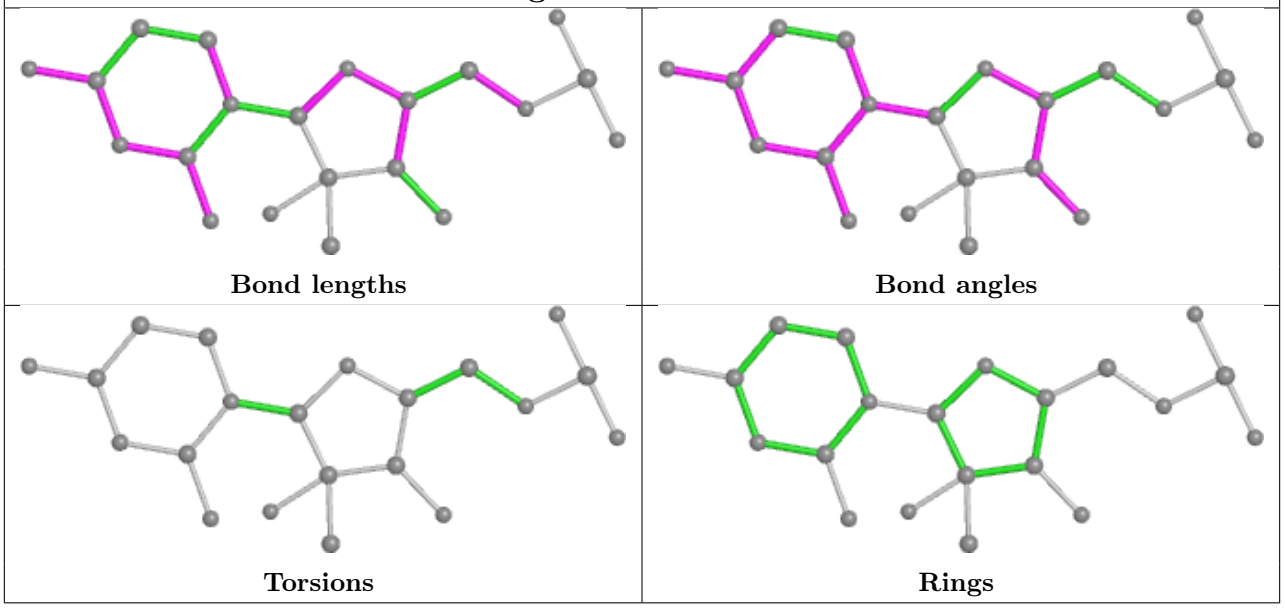
There are no ring outliers.

2 monomers are involved in 20 short contacts:

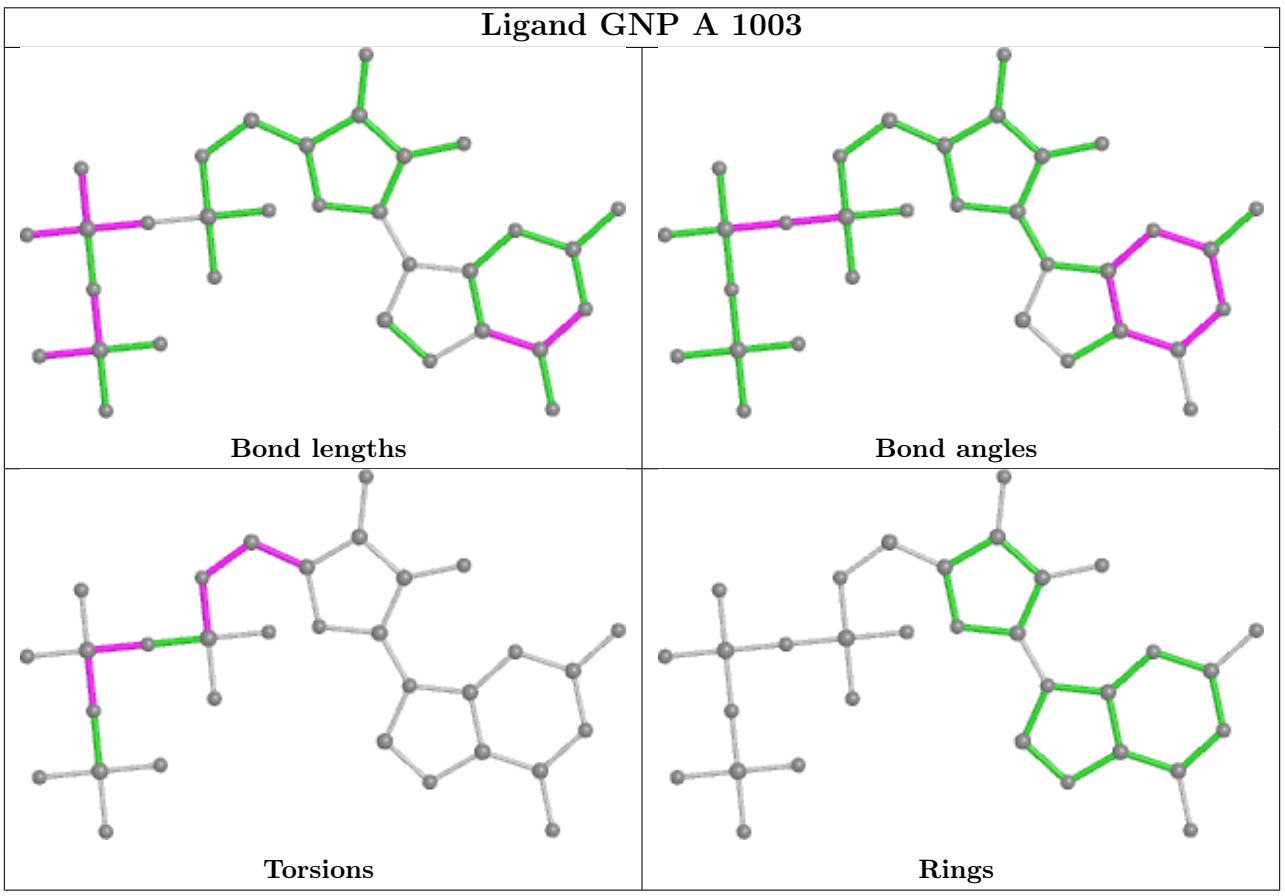
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	200	6GS	16	0
9	A	1003	GNP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 6GS G 200



Ligand GNP A 1003



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.

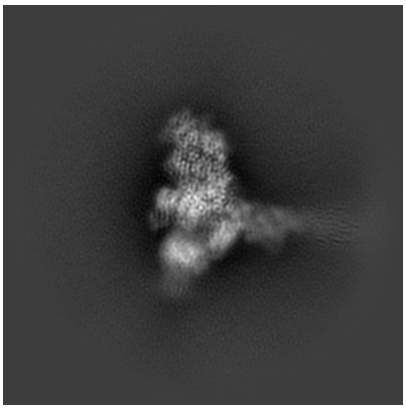
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34312. These allow visual inspection of the internal detail of the map and identification of artifacts.

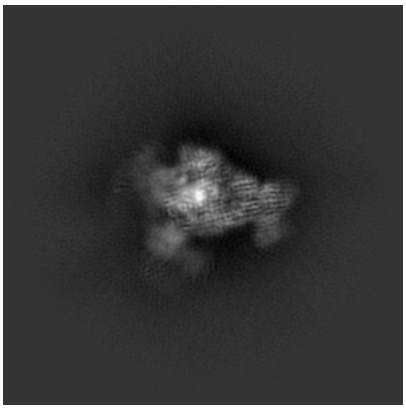
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

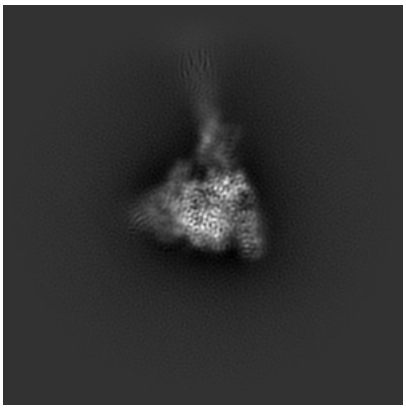
6.1.1 Primary map



X

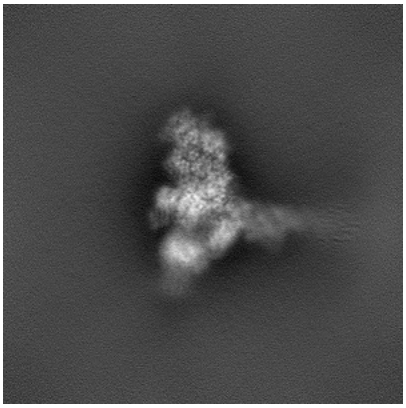


Y

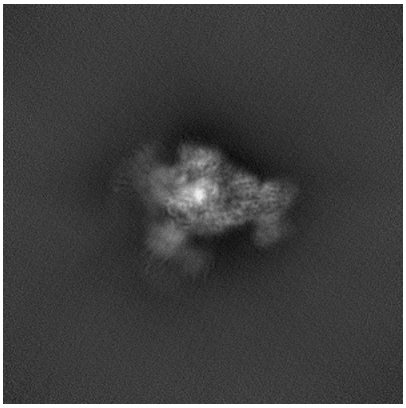


Z

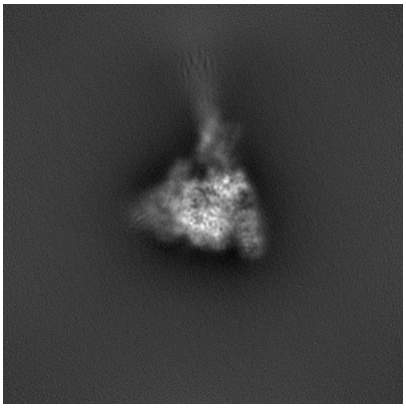
6.1.2 Raw map



X



Y

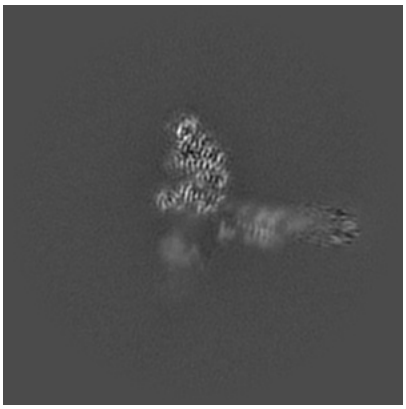


Z

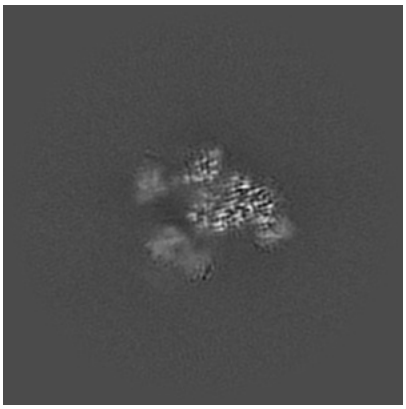
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

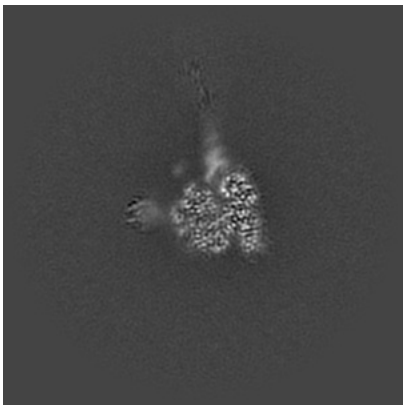
6.2.1 Primary map



X Index: 224

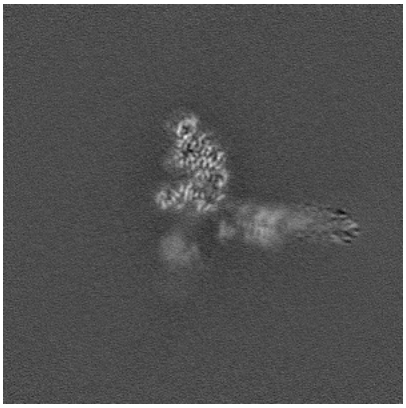


Y Index: 224

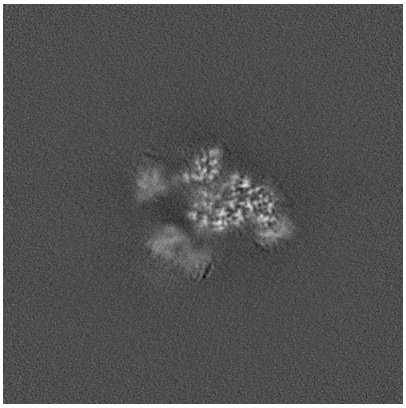


Z Index: 224

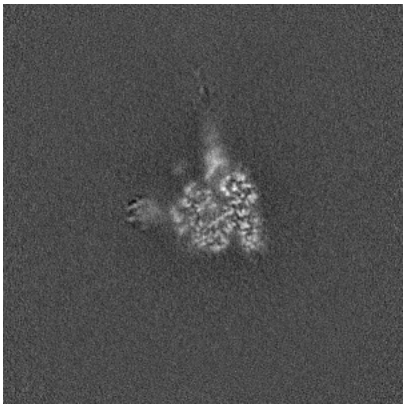
6.2.2 Raw map



X Index: 224



Y Index: 224

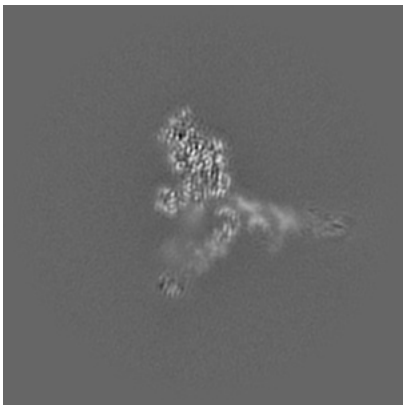


Z Index: 224

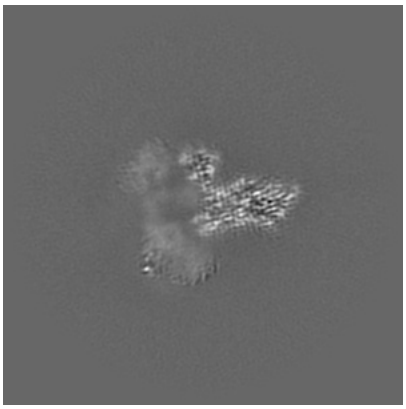
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

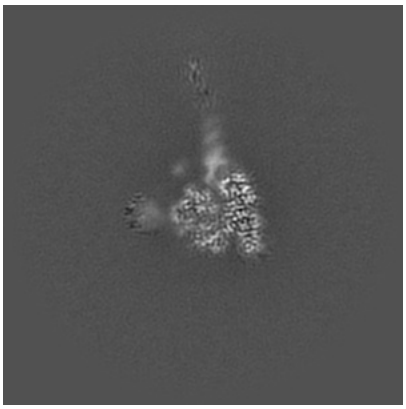
6.3.1 Primary map



X Index: 238

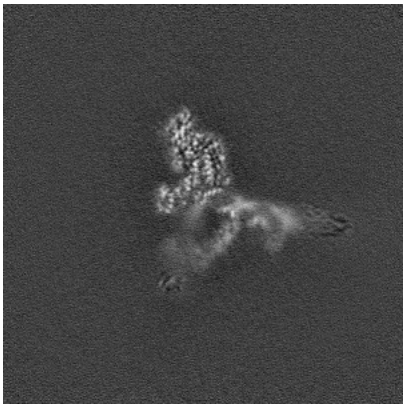


Y Index: 207

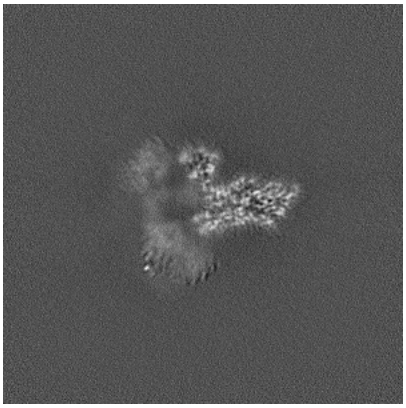


Z Index: 222

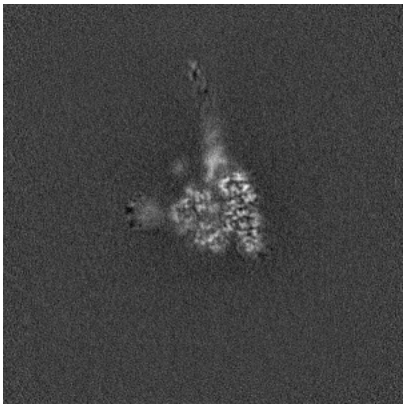
6.3.2 Raw map



X Index: 235



Y Index: 207

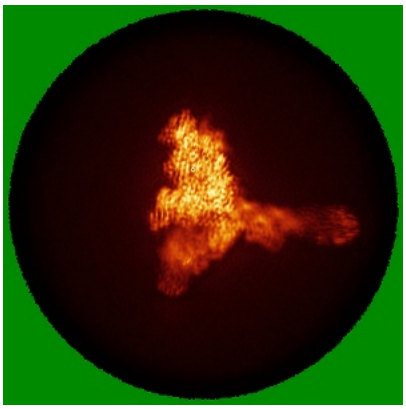


Z Index: 222

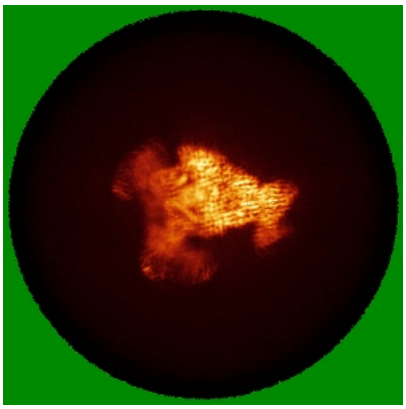
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

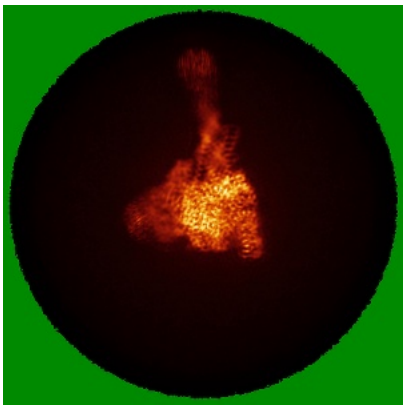
6.4.1 Primary map



X

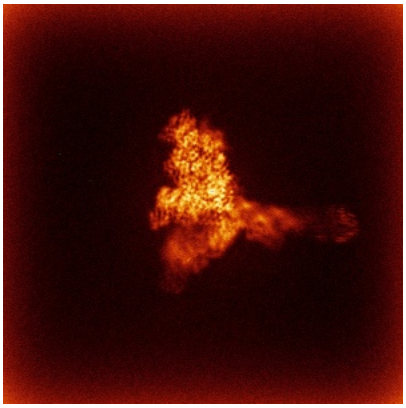


Y

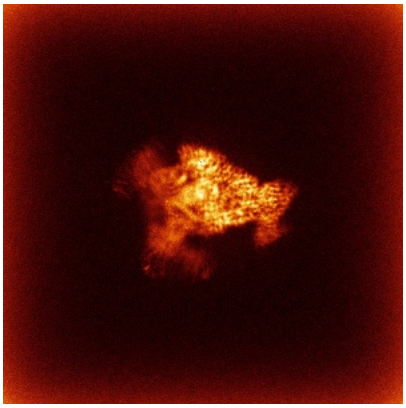


Z

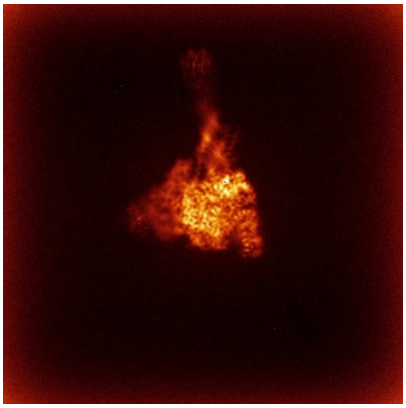
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

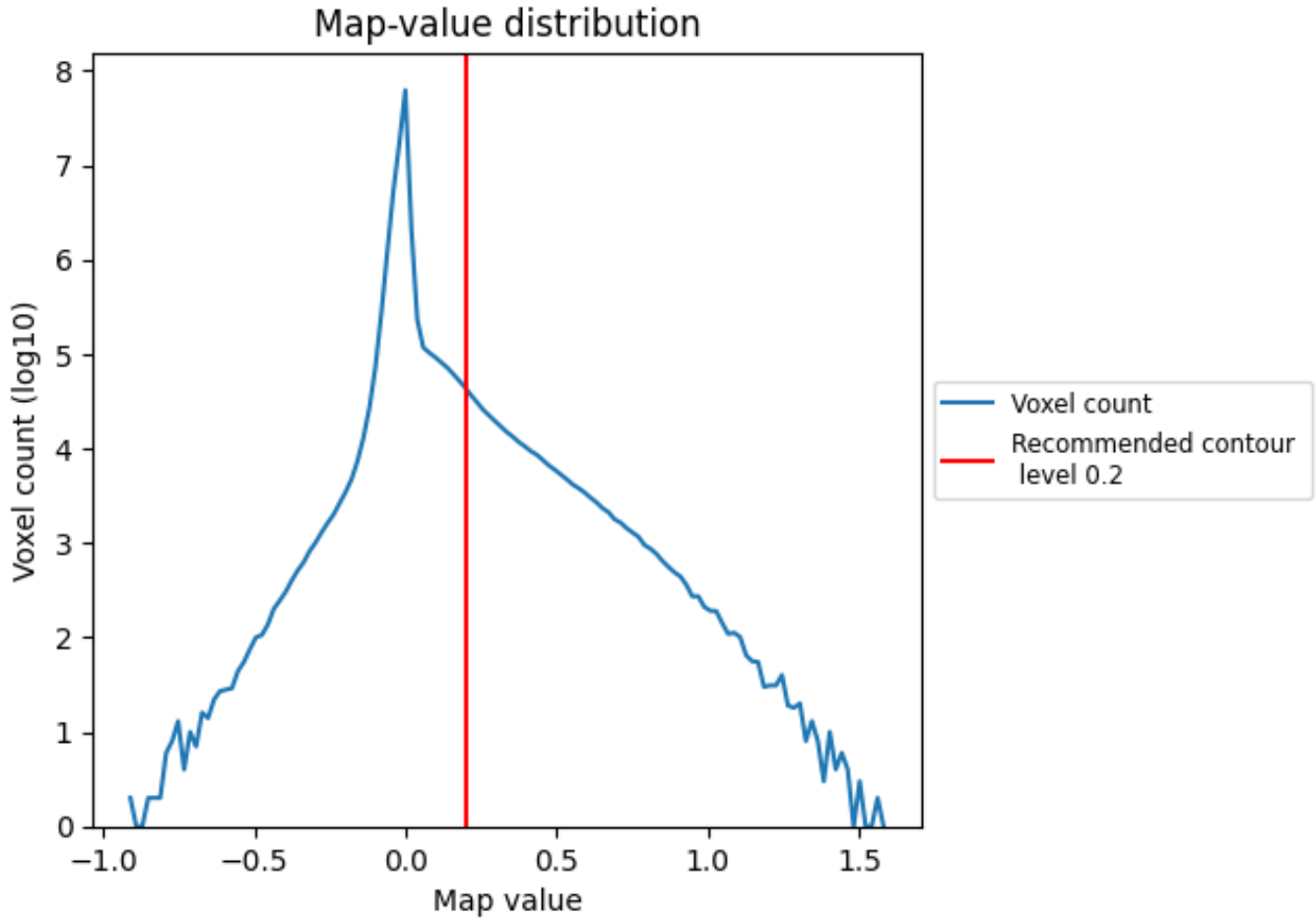
6.6 Mask visualisation (i)

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

7 Map analysis

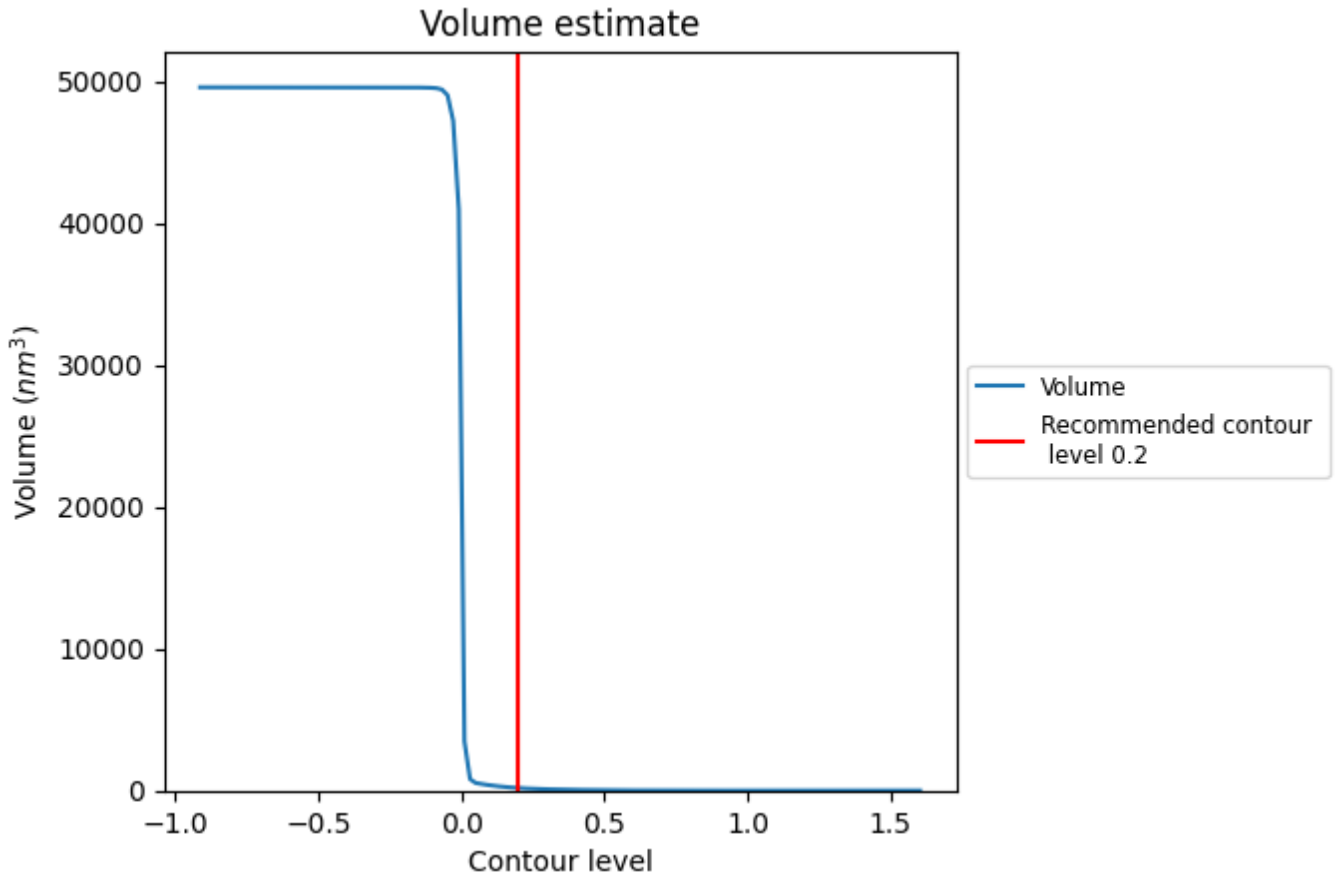
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

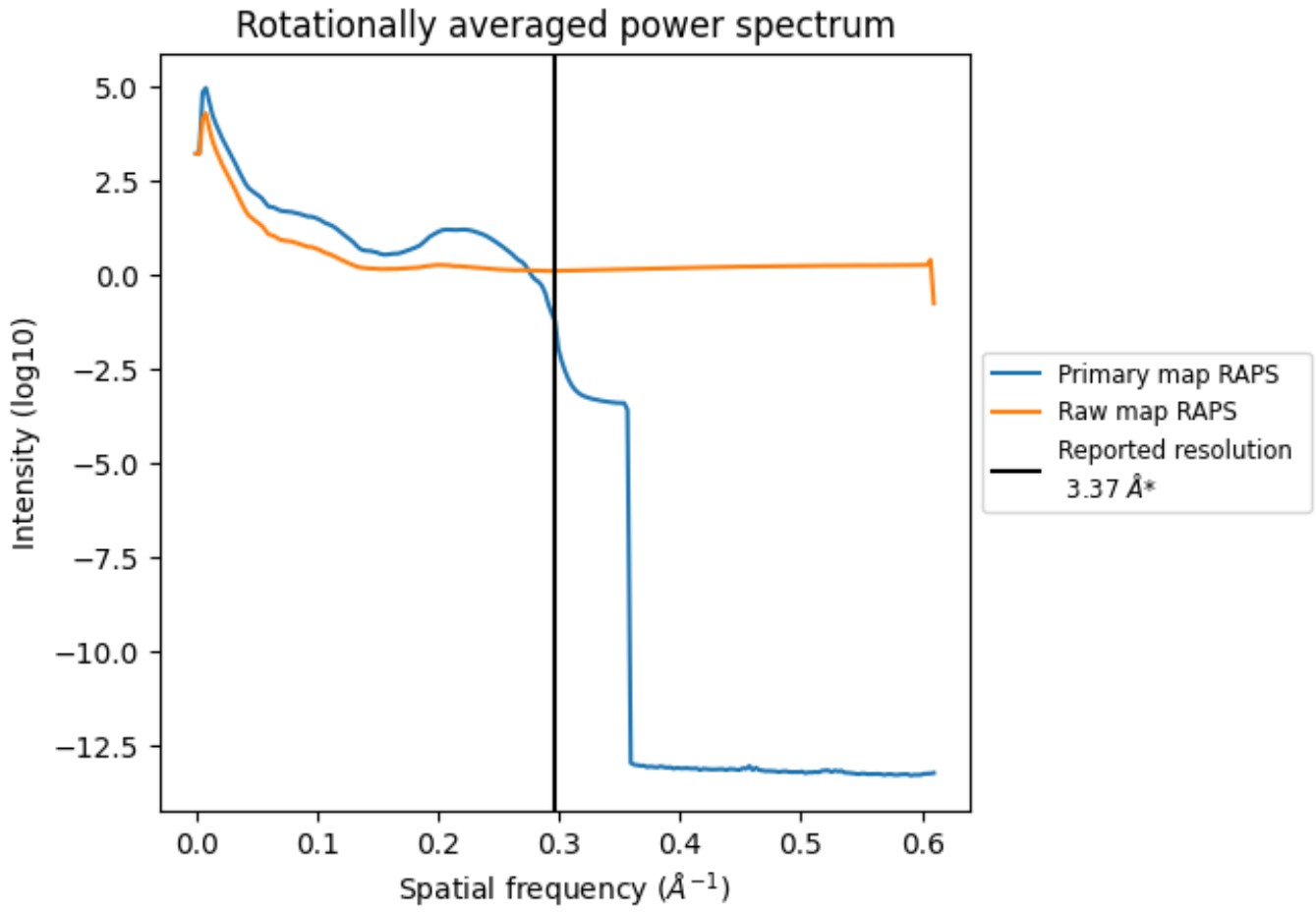
7.2 Volume estimate



The volume at the recommended contour level is 179 nm^3; this corresponds to an approximate mass of 161 kDa.

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

7.3 Rotationally averaged power spectrum (i)

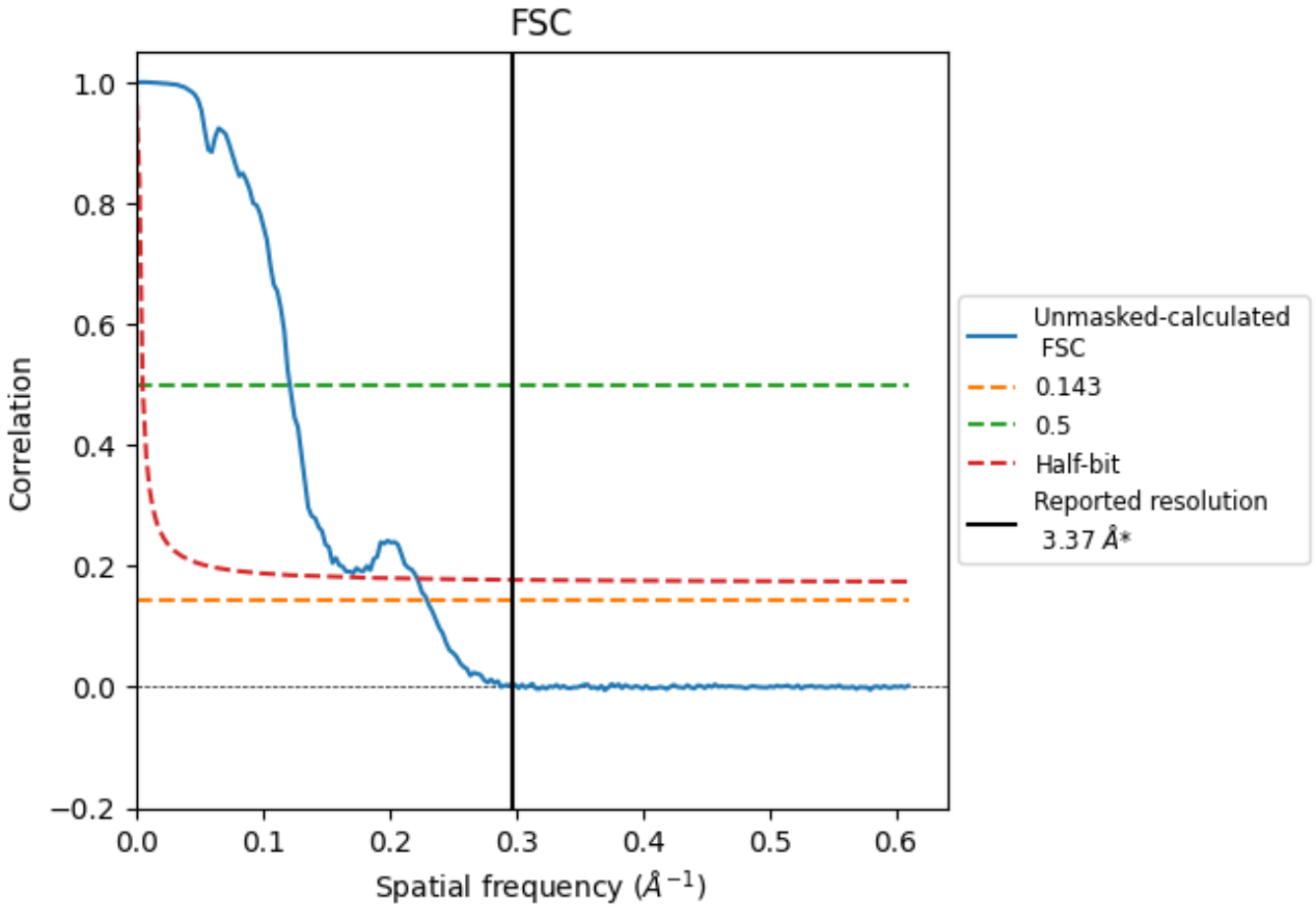


*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

8.2 Resolution estimates (i)

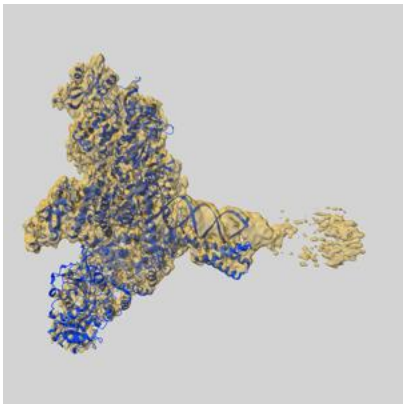
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	8.24	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.37 by more than 10 %

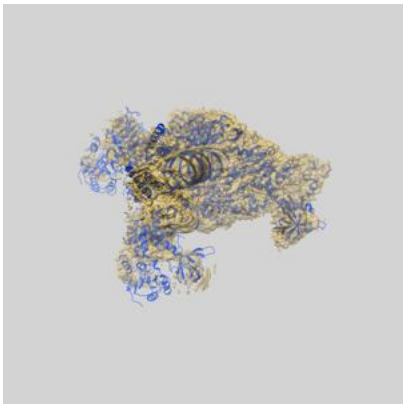
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34312 and PDB model 8GWG. Per-residue inclusion information can be found in section 3 on page 7.

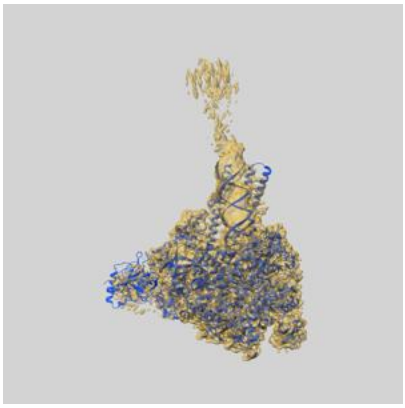
9.1 Map-model overlay



X



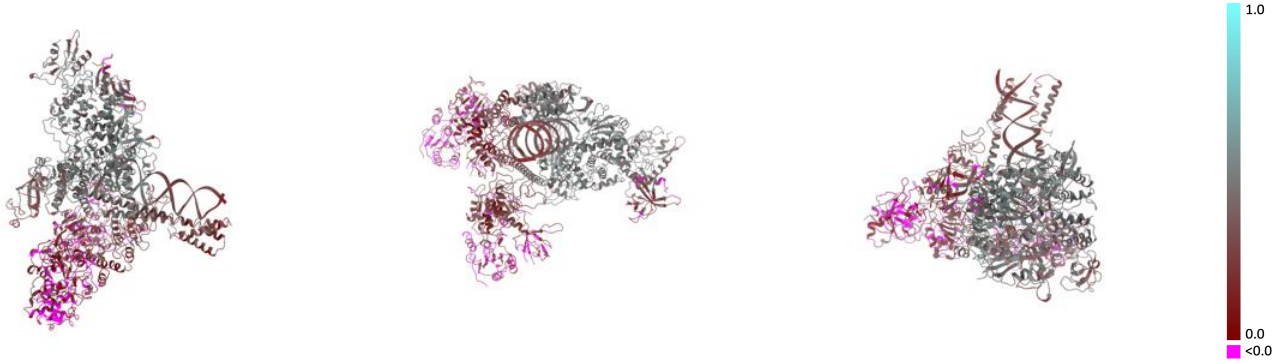
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

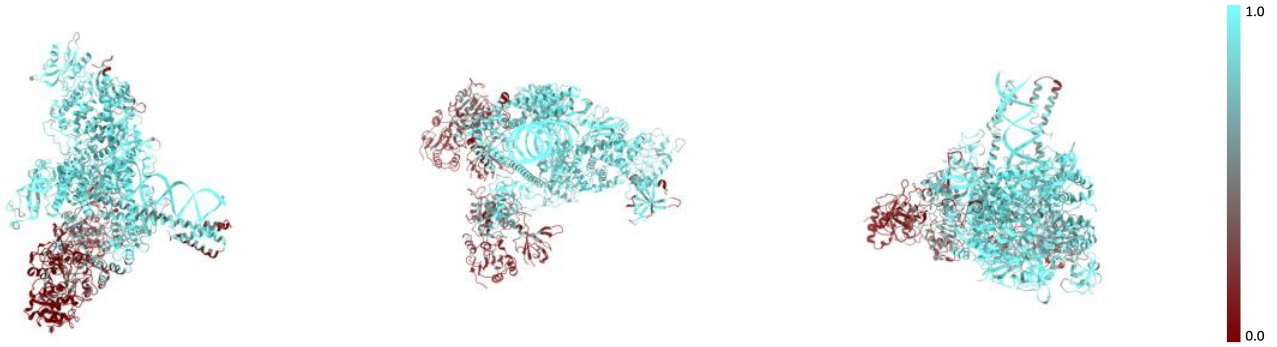
9.2 Q-score mapped to coordinate model



X Y Z

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

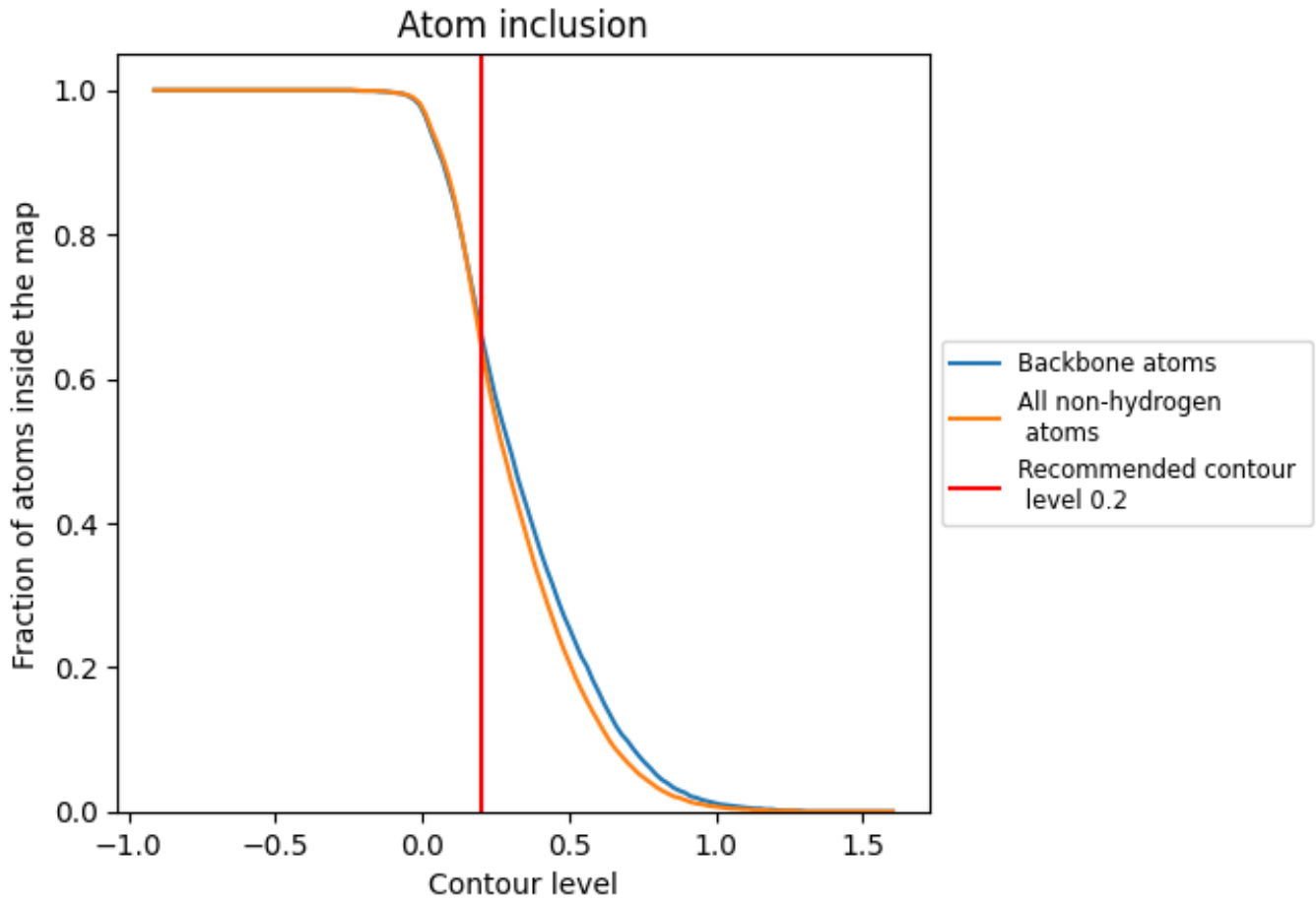
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 65% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6490	0.3040
A	0.9280	0.4710
B	0.8410	0.3940
C	0.9020	0.4380
D	0.8160	0.3680
E	0.2490	0.1170
F	0.3600	0.1400
G	0.6830	0.2660
I	0.9850	0.3580
J	0.9790	0.3590