Full wwPDB EM Validation Report ⓘ

Oct 11, 2023 – 02:37 PM JST

PDB ID	:	7YSQ
EMDB ID	:	EMD-34080
Title	:	GTPgammaS Tube decorated with kinesin
Authors	:	Zhou, J.; Wang, H.-W.
Deposited on	:	2022-08-12
Resolution	:	6.80 Å(reported)

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

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

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

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

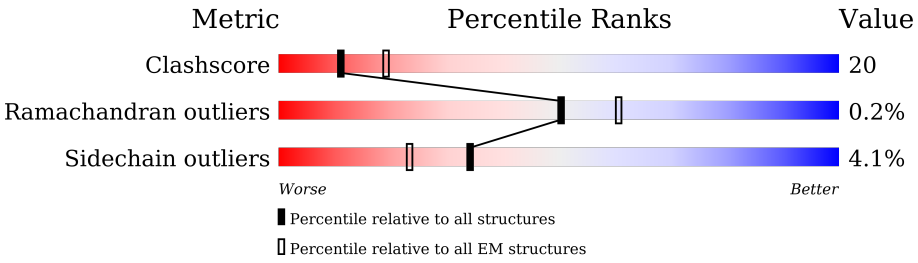
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 6.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	450	56% 34% 6%
1	D	450	55% 34% 6%
1	E	450	56% 34% 6%
1	F	450	56% 33% 6%
2	B	447	55% 36% 5%
2	G	447	57% 35% 5%
2	H	447	57% 35% 5%
2	I	447	54% 37% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26912 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.

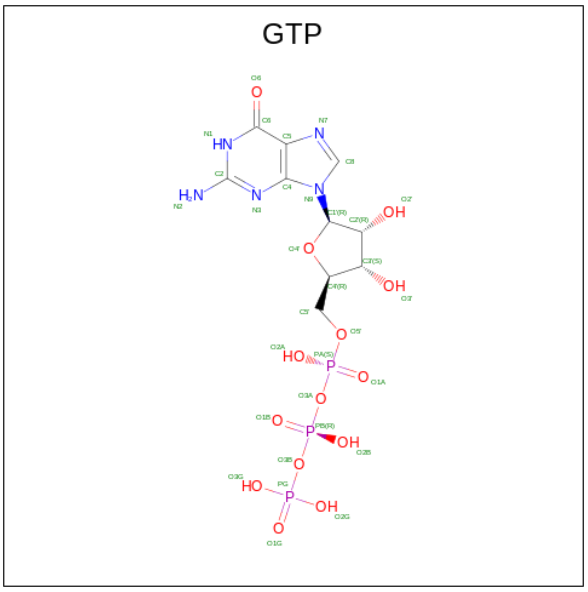
- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	422	Total	C	N	O	S	0	0
			3314	2104	565	623	22		
1	D	422	Total	C	N	O	S	0	0
			3314	2104	565	623	22		
1	E	422	Total	C	N	O	S	0	0
			3314	2104	565	623	22		
1	F	422	Total	C	N	O	S	0	0
			3314	2104	565	623	22		

- Molecule 2 is a protein called Tubulin beta-1 chain.

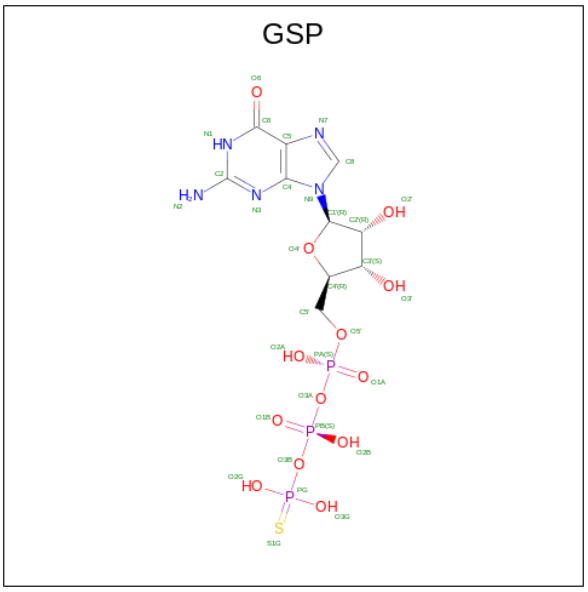
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3350	2107	574	643	26		
2	G	426	Total	C	N	O	S	0	0
			3350	2107	574	643	26		
2	H	426	Total	C	N	O	S	0	0
			3350	2107	574	643	26		
2	I	426	Total	C	N	O	S	0	0
			3350	2107	574	643	26		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).



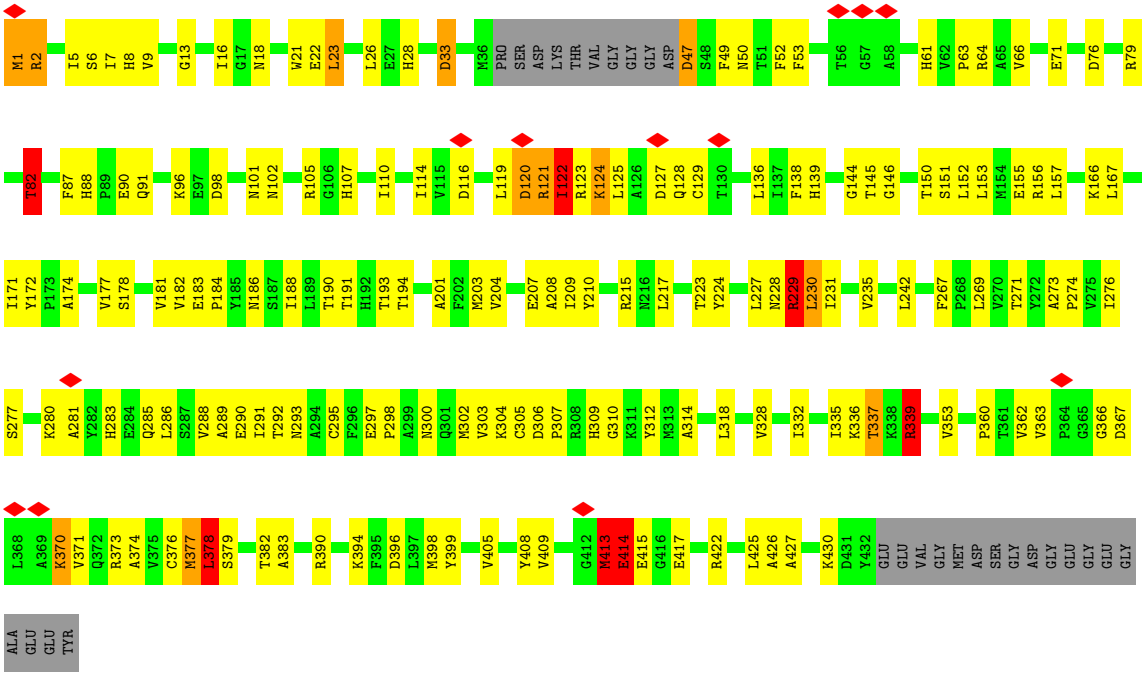
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
4	G	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
4	H	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
4	I	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

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.

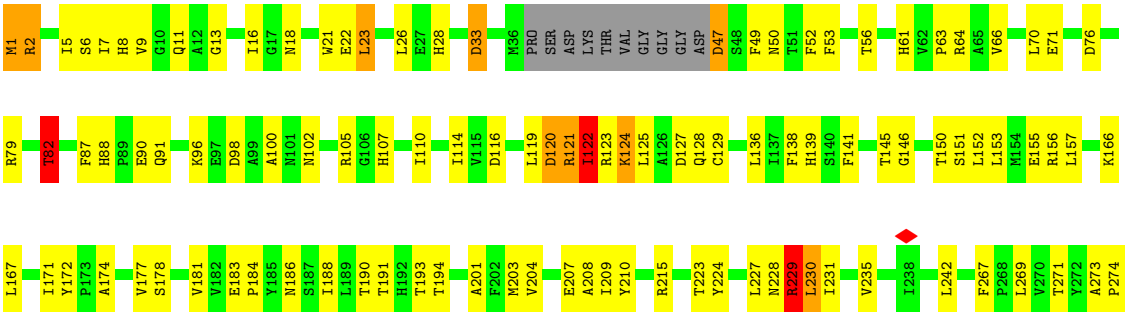
• Molecule 1: Tubulin alpha chain

Chain A:



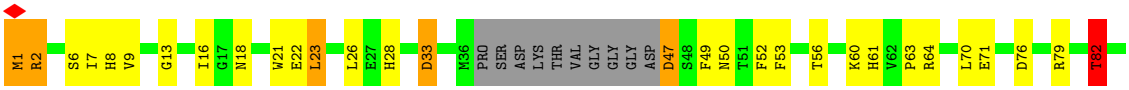
• Molecule 1: Tubulin alpha chain

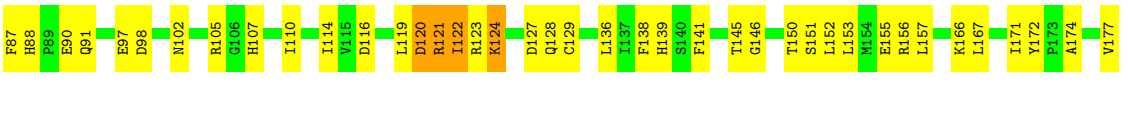
Chain D:

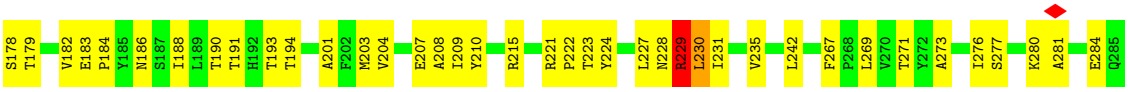


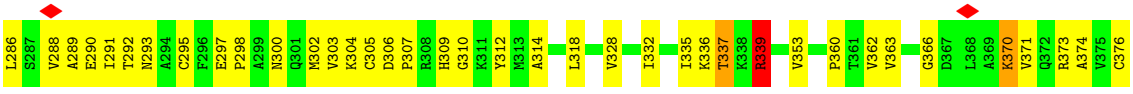
• Molecule 1: Tubulin alpha chain

Chain E:



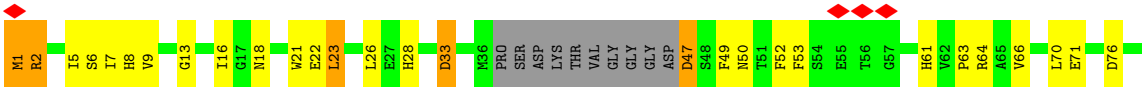


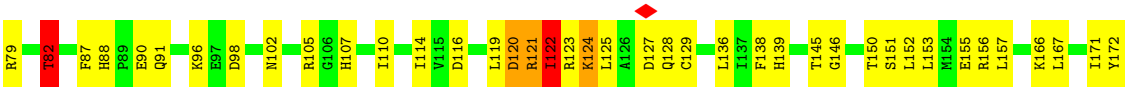


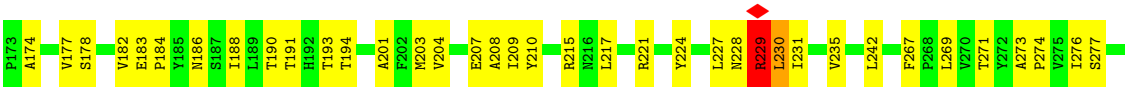


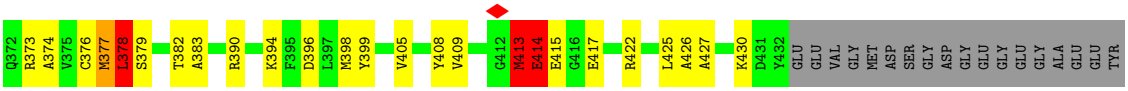
• Molecule 1: Tubulin alpha chain

Chain F:



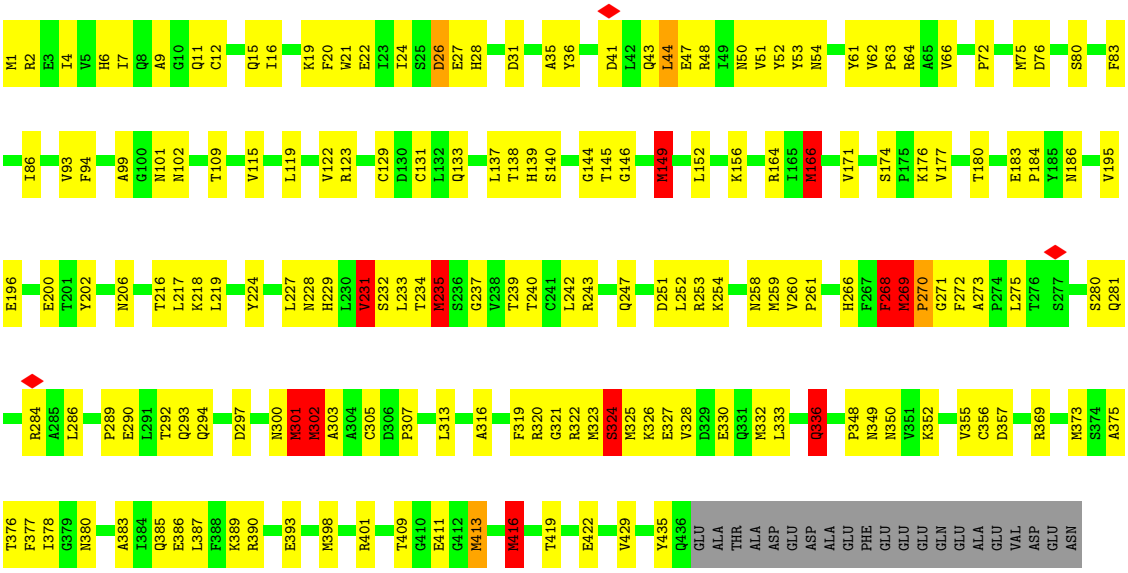






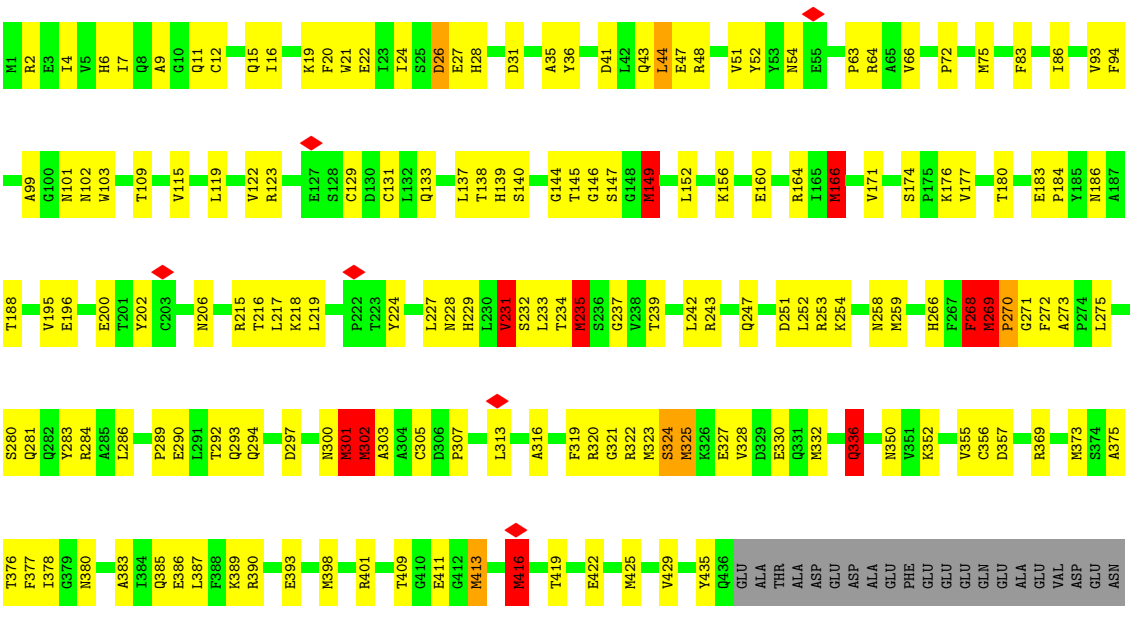
• Molecule 2: Tubulin beta-1 chain

Chain B:



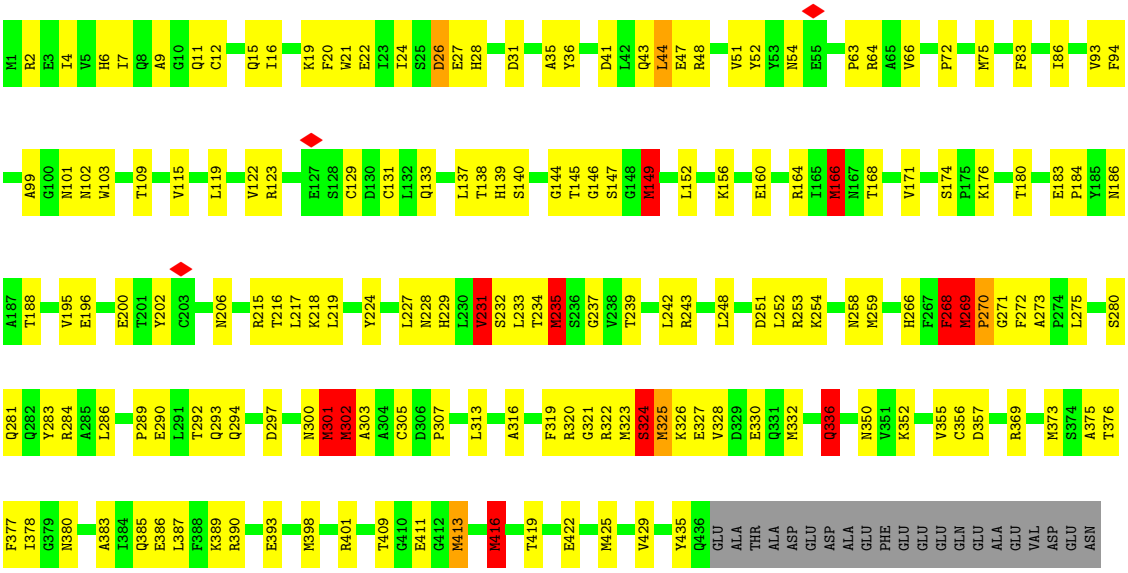
• Molecule 2: Tubulin beta-1 chain

Chain G:



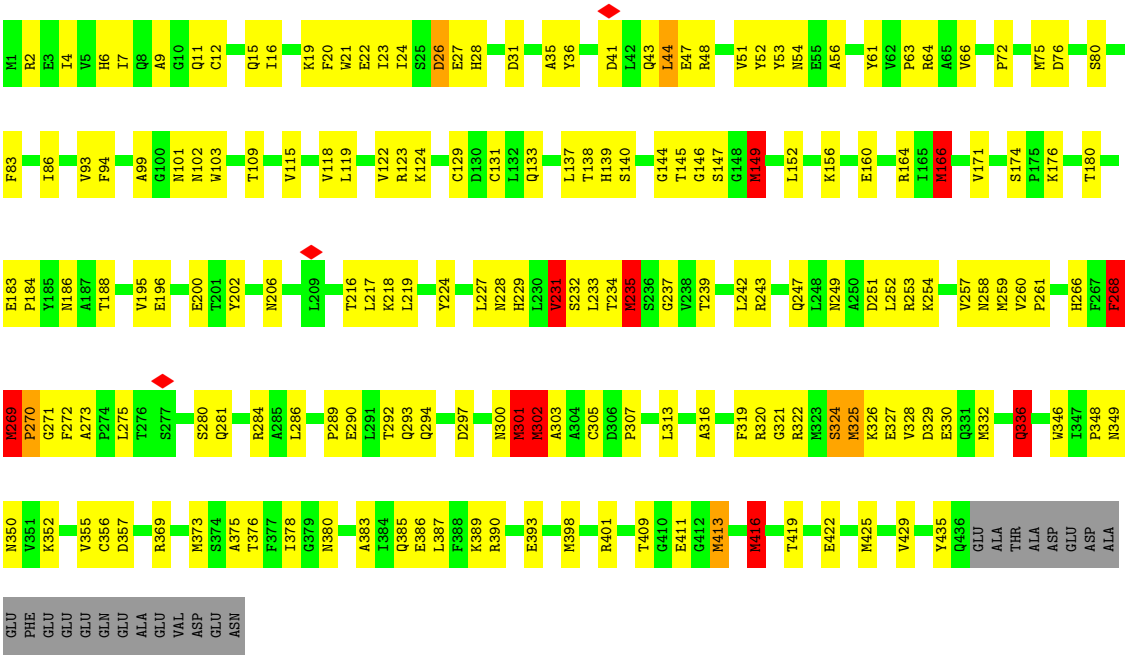
• Molecule 2: Tubulin beta-1 chain

Chain H:



• Molecule 2: Tubulin beta-1 chain

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=22.71°, rise=17.92 Å, axial sym=C1	Depositor
Number of segments used	74919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	1064.0, 1064.0, 1064.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.40	1/3390 (0.0%)	0.89	26/4602 (0.6%)
1	D	0.40	1/3390 (0.0%)	0.89	26/4602 (0.6%)
1	E	0.40	1/3390 (0.0%)	0.89	26/4602 (0.6%)
1	F	0.40	1/3390 (0.0%)	0.89	26/4602 (0.6%)
2	B	0.43	1/3424 (0.0%)	1.00	27/4637 (0.6%)
2	G	0.43	1/3424 (0.0%)	1.00	27/4637 (0.6%)
2	H	0.43	1/3424 (0.0%)	1.00	27/4637 (0.6%)
2	I	0.43	1/3424 (0.0%)	1.00	27/4637 (0.6%)
All	All	0.42	8/27256 (0.0%)	0.95	212/36956 (0.6%)

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	3
1	D	0	3
1	E	0	3
1	F	0	3
2	B	0	5
2	G	0	5
2	H	0	5
2	I	0	5
All	All	0	32

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	GLU	CD-OE2	5.45	1.31	1.25
1	F	414	GLU	CD-OE2	5.44	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	414	GLU	CD-OE2	5.38	1.31	1.25
1	E	414	GLU	CD-OE2	5.35	1.31	1.25
2	B	336	GLN	CB-CG	5.23	1.66	1.52
2	G	336	GLN	CB-CG	5.21	1.66	1.52
2	I	336	GLN	CB-CG	5.21	1.66	1.52
2	H	336	GLN	CB-CG	5.18	1.66	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	325	MET	CB-CG-SD	22.53	179.98	112.40
2	G	325	MET	CB-CG-SD	22.52	179.97	112.40
2	H	325	MET	CB-CG-SD	22.52	179.97	112.40
2	B	325	MET	CB-CG-SD	22.52	179.97	112.40
2	H	269	MET	CA-CB-CG	17.39	142.86	113.30
2	G	269	MET	CA-CB-CG	17.36	142.81	113.30
2	I	269	MET	CA-CB-CG	17.36	142.81	113.30
2	B	269	MET	CA-CB-CG	17.35	142.80	113.30
1	A	122	ILE	CG1-CB-CG2	-13.72	81.21	111.40
1	D	122	ILE	CG1-CB-CG2	-13.72	81.22	111.40
1	E	122	ILE	CG1-CB-CG2	-13.71	81.23	111.40
1	F	122	ILE	CG1-CB-CG2	-13.71	81.23	111.40
1	D	33	ASP	CB-CG-OD1	13.05	130.05	118.30
1	E	33	ASP	CB-CG-OD1	13.02	130.02	118.30
1	A	33	ASP	CB-CG-OD1	12.98	129.98	118.30
1	F	33	ASP	CB-CG-OD1	12.97	129.98	118.30
2	H	269	MET	N-CA-C	-12.84	76.33	111.00
2	G	269	MET	N-CA-C	-12.83	76.35	111.00
2	B	269	MET	N-CA-C	-12.83	76.37	111.00
2	I	269	MET	N-CA-C	-12.82	76.39	111.00
1	D	1	MET	CA-CB-CG	12.76	134.99	113.30
1	A	1	MET	CA-CB-CG	12.75	134.98	113.30
1	F	1	MET	CA-CB-CG	12.74	134.97	113.30
1	E	1	MET	CA-CB-CG	12.72	134.93	113.30
2	B	302	MET	CB-CG-SD	12.31	149.32	112.40
2	G	302	MET	CB-CG-SD	12.30	149.29	112.40
2	H	302	MET	CB-CG-SD	12.29	149.27	112.40
2	I	302	MET	CB-CG-SD	12.29	149.25	112.40
2	I	235	MET	CG-SD-CE	11.44	118.50	100.20
2	B	235	MET	CG-SD-CE	11.43	118.48	100.20
2	H	235	MET	CG-SD-CE	11.43	118.48	100.20
2	G	235	MET	CG-SD-CE	11.42	118.47	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	416	MET	CG-SD-CE	10.43	116.89	100.20
2	B	416	MET	CG-SD-CE	10.43	116.88	100.20
2	H	416	MET	CG-SD-CE	10.42	116.87	100.20
2	G	416	MET	CG-SD-CE	10.41	116.86	100.20
2	B	166	MET	CB-CG-SD	-10.41	81.17	112.40
2	H	166	MET	CB-CG-SD	-10.40	81.19	112.40
2	G	166	MET	CB-CG-SD	-10.40	81.19	112.40
2	I	166	MET	CB-CG-SD	-10.40	81.20	112.40
1	D	230	LEU	CB-CG-CD1	10.12	128.21	111.00
1	E	230	LEU	CB-CG-CD1	10.12	128.20	111.00
1	A	230	LEU	CB-CG-CD1	10.10	128.17	111.00
1	F	230	LEU	CB-CG-CD1	10.09	128.15	111.00
1	E	33	ASP	CB-CG-OD2	-9.58	109.67	118.30
2	I	301	MET	CG-SD-CE	9.55	115.48	100.20
2	G	301	MET	CG-SD-CE	9.55	115.48	100.20
2	H	301	MET	CG-SD-CE	9.54	115.47	100.20
1	A	33	ASP	CB-CG-OD2	-9.54	109.72	118.30
1	D	33	ASP	CB-CG-OD2	-9.54	109.72	118.30
2	B	301	MET	CG-SD-CE	9.52	115.42	100.20
1	F	33	ASP	CB-CG-OD2	-9.50	109.75	118.30
2	H	231	VAL	CG1-CB-CG2	-9.34	95.96	110.90
2	G	231	VAL	CG1-CB-CG2	-9.33	95.97	110.90
2	I	231	VAL	CG1-CB-CG2	-9.32	96.00	110.90
2	B	231	VAL	CG1-CB-CG2	-9.31	96.01	110.90
2	B	301	MET	CB-CG-SD	-9.11	85.07	112.40
2	H	301	MET	CB-CG-SD	-9.10	85.09	112.40
2	G	301	MET	CB-CG-SD	-9.10	85.10	112.40
2	I	301	MET	CB-CG-SD	-9.10	85.09	112.40
2	B	398	MET	CA-CB-CG	8.94	128.49	113.30
2	I	398	MET	CA-CB-CG	8.94	128.49	113.30
2	G	398	MET	CA-CB-CG	8.93	128.47	113.30
2	H	398	MET	CA-CB-CG	8.92	128.47	113.30
2	B	325	MET	CG-SD-CE	-8.88	85.99	100.20
2	G	325	MET	CG-SD-CE	-8.87	86.01	100.20
2	I	325	MET	CG-SD-CE	-8.87	86.01	100.20
2	H	325	MET	CG-SD-CE	-8.86	86.02	100.20
2	H	324	SER	C-N-CA	-8.73	99.87	121.70
2	I	324	SER	C-N-CA	-8.73	99.87	121.70
2	B	324	SER	C-N-CA	-8.73	99.88	121.70
2	G	324	SER	C-N-CA	-8.72	99.89	121.70
1	E	82	THR	CA-CB-CG2	-8.57	100.40	112.40
1	A	413	MET	CG-SD-CE	-8.56	86.50	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	THR	CA-CB-CG2	-8.56	100.42	112.40
1	D	82	THR	CA-CB-CG2	-8.56	100.42	112.40
1	F	82	THR	CA-CB-CG2	-8.56	100.42	112.40
1	F	413	MET	CG-SD-CE	-8.55	86.52	100.20
1	E	413	MET	CG-SD-CE	-8.55	86.53	100.20
1	D	413	MET	CG-SD-CE	-8.54	86.54	100.20
2	B	268	PHE	C-N-CA	-8.36	100.80	121.70
2	G	268	PHE	C-N-CA	-8.35	100.83	121.70
2	H	268	PHE	C-N-CA	-8.34	100.85	121.70
2	I	268	PHE	C-N-CA	-8.33	100.87	121.70
1	D	120	ASP	N-CA-CB	-7.99	96.23	110.60
1	A	120	ASP	N-CA-CB	-7.98	96.24	110.60
1	E	120	ASP	N-CA-CB	-7.96	96.27	110.60
1	F	120	ASP	N-CA-CB	-7.95	96.29	110.60
1	E	337	THR	CA-CB-CG2	-7.81	101.46	112.40
1	F	337	THR	CA-CB-CG2	-7.80	101.47	112.40
1	A	337	THR	CA-CB-CG2	-7.80	101.49	112.40
1	D	337	THR	CA-CB-CG2	-7.79	101.50	112.40
2	B	398	MET	CG-SD-CE	7.78	112.64	100.20
2	H	398	MET	CG-SD-CE	7.77	112.63	100.20
2	I	398	MET	CG-SD-CE	7.75	112.59	100.20
2	G	398	MET	CG-SD-CE	7.73	112.57	100.20
2	B	269	MET	CB-CG-SD	7.61	135.22	112.40
2	G	269	MET	CB-CG-SD	7.60	135.20	112.40
2	H	269	MET	CB-CG-SD	7.59	135.18	112.40
2	I	269	MET	CB-CG-SD	7.59	135.17	112.40
1	A	121	ARG	CB-CG-CD	-7.44	92.25	111.60
1	F	121	ARG	CB-CG-CD	-7.44	92.25	111.60
1	D	121	ARG	CB-CG-CD	-7.44	92.27	111.60
1	E	121	ARG	CB-CG-CD	-7.44	92.27	111.60
1	F	1	MET	CG-SD-CE	-7.37	88.41	100.20
1	D	1	MET	CG-SD-CE	-7.37	88.42	100.20
1	E	337	THR	OG1-CB-CG2	-7.36	93.08	110.00
1	A	1	MET	CG-SD-CE	-7.35	88.44	100.20
1	E	1	MET	CG-SD-CE	-7.35	88.45	100.20
1	D	337	THR	OG1-CB-CG2	-7.34	93.11	110.00
1	A	337	THR	OG1-CB-CG2	-7.34	93.12	110.00
1	F	337	THR	OG1-CB-CG2	-7.33	93.14	110.00
2	G	416	MET	CB-CG-SD	-7.32	90.43	112.40
2	I	416	MET	CB-CG-SD	-7.31	90.47	112.40
2	B	416	MET	CB-CG-SD	-7.31	90.48	112.40
2	H	416	MET	CB-CG-SD	-7.30	90.49	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	82	THR	OG1-CB-CG2	-7.21	93.42	110.00
1	E	82	THR	OG1-CB-CG2	-7.21	93.42	110.00
1	D	82	THR	OG1-CB-CG2	-7.20	93.43	110.00
1	A	82	THR	OG1-CB-CG2	-7.20	93.44	110.00
2	G	301	MET	CA-CB-CG	-7.11	101.21	113.30
2	H	301	MET	CA-CB-CG	-7.10	101.23	113.30
2	I	301	MET	CA-CB-CG	-7.10	101.23	113.30
2	B	301	MET	CA-CB-CG	-7.08	101.27	113.30
2	H	166	MET	CG-SD-CE	6.76	111.02	100.20
2	B	166	MET	CG-SD-CE	6.76	111.01	100.20
2	G	166	MET	CG-SD-CE	6.75	111.01	100.20
2	I	166	MET	CG-SD-CE	6.74	110.98	100.20
2	B	149	MET	CG-SD-CE	6.73	110.97	100.20
2	G	149	MET	CG-SD-CE	6.73	110.97	100.20
2	I	149	MET	CG-SD-CE	6.72	110.96	100.20
2	H	149	MET	CG-SD-CE	6.72	110.95	100.20
2	G	149	MET	CB-CG-SD	-6.67	92.38	112.40
2	H	149	MET	CB-CG-SD	-6.67	92.39	112.40
2	I	149	MET	CB-CG-SD	-6.67	92.40	112.40
2	B	149	MET	CB-CG-SD	-6.66	92.41	112.40
2	B	336	GLN	N-CA-CB	6.63	122.53	110.60
2	I	336	GLN	N-CA-CB	6.62	122.52	110.60
2	G	336	GLN	N-CA-CB	6.61	122.50	110.60
2	H	336	GLN	N-CA-CB	6.61	122.50	110.60
1	E	229	ARG	CB-CG-CD	-6.51	94.68	111.60
1	A	229	ARG	CB-CG-CD	-6.50	94.69	111.60
1	F	229	ARG	CB-CG-CD	-6.50	94.69	111.60
1	D	229	ARG	CB-CG-CD	-6.50	94.71	111.60
1	E	378	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	F	378	LEU	CB-CG-CD1	-6.47	99.99	111.00
1	D	378	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	A	378	LEU	CB-CG-CD1	-6.47	100.01	111.00
1	F	23	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	A	23	LEU	CB-CG-CD2	-6.39	100.13	111.00
1	D	23	LEU	CB-CG-CD2	-6.38	100.14	111.00
1	E	23	LEU	CB-CG-CD2	-6.38	100.14	111.00
1	D	413	MET	C-N-CA	6.22	137.26	121.70
1	A	413	MET	C-N-CA	6.22	137.25	121.70
1	E	413	MET	C-N-CA	6.22	137.25	121.70
1	F	413	MET	C-N-CA	6.22	137.24	121.70
2	G	195	VAL	C-N-CA	6.14	137.05	121.70
1	D	229	ARG	CG-CD-NE	6.13	124.68	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	195	VAL	C-N-CA	6.13	137.03	121.70
2	B	195	VAL	C-N-CA	6.13	137.03	121.70
2	H	195	VAL	C-N-CA	6.12	137.01	121.70
1	E	229	ARG	CG-CD-NE	6.11	124.64	111.80
1	A	229	ARG	CG-CD-NE	6.10	124.61	111.80
1	F	229	ARG	CG-CD-NE	6.10	124.60	111.80
1	E	1	MET	N-CA-C	5.96	127.10	111.00
1	A	1	MET	N-CA-C	5.96	127.09	111.00
1	D	1	MET	N-CA-C	5.96	127.09	111.00
1	F	1	MET	N-CA-C	5.96	127.09	111.00
1	F	398	MET	CB-CG-SD	5.89	130.06	112.40
1	D	398	MET	CB-CG-SD	5.88	130.03	112.40
1	A	398	MET	CB-CG-SD	5.87	130.02	112.40
1	E	398	MET	CB-CG-SD	5.87	130.02	112.40
1	E	120	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	F	120	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	A	120	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	D	120	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	D	121	ARG	CG-CD-NE	5.51	123.36	111.80
1	F	121	ARG	CG-CD-NE	5.50	123.34	111.80
1	E	121	ARG	CG-CD-NE	5.48	123.32	111.80
1	A	121	ARG	CG-CD-NE	5.48	123.31	111.80
2	H	270	PRO	CA-C-N	5.48	127.15	116.20
2	I	270	PRO	CA-C-N	5.47	127.14	116.20
2	B	270	PRO	CA-C-N	5.47	127.13	116.20
1	F	398	MET	CA-CB-CG	5.46	122.58	113.30
1	A	398	MET	CA-CB-CG	5.46	122.58	113.30
1	E	398	MET	CA-CB-CG	5.46	122.57	113.30
2	G	270	PRO	CA-C-N	5.45	127.11	116.20
1	D	398	MET	CA-CB-CG	5.45	122.56	113.30
2	H	336	GLN	CA-CB-CG	5.43	125.35	113.40
2	G	336	GLN	CA-CB-CG	5.42	125.33	113.40
2	I	336	GLN	CA-CB-CG	5.42	125.32	113.40
2	B	336	GLN	CA-CB-CG	5.41	125.29	113.40
2	G	196	GLU	CB-CA-C	5.40	121.20	110.40
2	H	196	GLU	CB-CA-C	5.40	121.20	110.40
2	B	196	GLU	CB-CA-C	5.40	121.20	110.40
2	I	196	GLU	CB-CA-C	5.40	121.19	110.40
1	D	1	MET	CA-C-N	-5.25	105.65	117.20
1	A	1	MET	CA-C-N	-5.25	105.65	117.20
1	F	1	MET	CA-C-N	-5.25	105.65	117.20
1	E	1	MET	CA-C-N	-5.23	105.70	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	336	GLN	CG-CD-NE2	-5.22	104.18	116.70
2	I	336	GLN	CG-CD-NE2	-5.21	104.21	116.70
2	B	336	GLN	CG-CD-NE2	-5.20	104.21	116.70
2	G	336	GLN	CG-CD-NE2	-5.20	104.22	116.70
1	E	370	LYS	CA-CB-CG	5.17	124.78	113.40
1	F	370	LYS	CA-CB-CG	5.16	124.76	113.40
1	D	370	LYS	CA-CB-CG	5.16	124.75	113.40
1	E	1	MET	N-CA-CB	-5.15	101.32	110.60
1	A	370	LYS	CA-CB-CG	5.15	124.72	113.40
1	A	1	MET	N-CA-CB	-5.14	101.35	110.60
1	D	1	MET	N-CA-CB	-5.13	101.36	110.60
1	F	1	MET	N-CA-CB	-5.12	101.39	110.60

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	413	MET	Peptide
2	B	234	THR	Peptide
2	B	268	PHE	Peptide
2	B	303	ALA	Peptide
2	B	324	SER	Peptide
2	B	336	GLN	Sidechain
1	D	229	ARG	Sidechain
1	D	339	ARG	Sidechain
1	D	413	MET	Peptide
1	E	229	ARG	Sidechain
1	E	339	ARG	Sidechain
1	E	413	MET	Peptide
1	F	229	ARG	Sidechain
1	F	339	ARG	Sidechain
1	F	413	MET	Peptide
2	G	234	THR	Peptide
2	G	268	PHE	Peptide
2	G	303	ALA	Peptide
2	G	324	SER	Peptide
2	G	336	GLN	Sidechain
2	H	234	THR	Peptide
2	H	268	PHE	Peptide
2	H	303	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	H	324	SER	Peptide
2	H	336	GLN	Sidechain
2	I	234	THR	Peptide
2	I	268	PHE	Peptide
2	I	303	ALA	Peptide
2	I	324	SER	Peptide
2	I	336	GLN	Sidechain

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	3314	0	3239	135	0
1	D	3314	0	3239	144	0
1	E	3314	0	3239	138	0
1	F	3314	0	3239	137	0
2	B	3350	0	3242	140	0
2	G	3350	0	3242	134	0
2	H	3350	0	3242	139	0
2	I	3350	0	3242	150	0
3	A	32	0	12	1	0
3	D	32	0	12	1	0
3	E	32	0	12	1	0
3	F	32	0	12	1	0
4	B	32	0	12	3	0
4	G	32	0	12	3	0
4	H	32	0	12	3	0
4	I	32	0	12	3	0
All	All	26912	0	26020	1081	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 20.

All (1081) 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:D:121:ARG:HE	1:D:124:LYS:HG2	1.07	1.18
1:E:121:ARG:HE	1:E:124:LYS:HG2	1.07	1.16
1:F:121:ARG:HE	1:F:124:LYS:HG2	1.07	1.13
1:A:121:ARG:HE	1:A:124:LYS:HG2	1.07	1.09
1:E:116:ASP:O	1:E:120:ASP:HB2	1.52	1.09
1:D:116:ASP:O	1:D:120:ASP:HB2	1.52	1.09
1:A:116:ASP:O	1:A:120:ASP:HB2	1.52	1.08
1:F:116:ASP:O	1:F:120:ASP:HB2	1.52	1.07
1:A:47:ASP:OD1	1:A:50:ASN:ND2	1.90	1.05
1:D:47:ASP:OD1	1:D:50:ASN:ND2	1.90	1.05
1:F:26:LEU:HD21	1:F:229:ARG:HH12	1.21	1.05
1:A:26:LEU:HD21	1:A:229:ARG:HH12	1.21	1.03
1:E:26:LEU:HD21	1:E:229:ARG:HH12	1.21	1.03
1:D:26:LEU:HD21	1:D:229:ARG:HH12	1.21	1.03
2:B:232:SER:HA	2:B:235:MET:HG3	1.40	1.03
1:E:47:ASP:OD1	1:E:50:ASN:ND2	1.90	1.03
1:F:47:ASP:OD1	1:F:50:ASN:ND2	1.90	1.02
2:H:232:SER:HA	2:H:235:MET:HG3	1.40	1.02
2:I:232:SER:HA	2:I:235:MET:HG3	1.40	1.02
2:G:232:SER:HA	2:G:235:MET:HG3	1.40	1.02
2:I:72:PRO:HA	2:I:75:MET:HG3	1.41	0.99
2:G:72:PRO:HA	2:G:75:MET:HG3	1.41	0.99
2:H:72:PRO:HA	2:H:75:MET:HG3	1.41	0.99
2:B:72:PRO:HA	2:B:75:MET:HG3	1.41	0.98
1:F:121:ARG:NE	1:F:124:LYS:HG2	1.80	0.96
1:A:121:ARG:NE	1:A:124:LYS:HG2	1.80	0.95
2:G:336:GLN:HE21	2:G:336:GLN:HA	1.31	0.95
1:D:121:ARG:NE	1:D:124:LYS:HG2	1.81	0.95
1:E:121:ARG:NE	1:E:124:LYS:HG2	1.80	0.94
2:H:336:GLN:HE21	2:H:336:GLN:HA	1.31	0.94
2:I:336:GLN:HE21	2:I:336:GLN:HA	1.31	0.94
2:B:336:GLN:HE21	2:B:336:GLN:HA	1.31	0.94
2:H:416:MET:SD	2:H:419:THR:HB	2.23	0.79
2:G:416:MET:SD	2:G:419:THR:HB	2.23	0.78
2:B:416:MET:SD	2:B:419:THR:HB	2.23	0.78
2:I:416:MET:SD	2:I:419:THR:HB	2.23	0.78
2:G:239:THR:HG23	2:G:243:ARG:HE	1.49	0.78
2:H:239:THR:HG23	2:H:243:ARG:HE	1.49	0.78
1:F:228:ASN:O	1:F:231:ILE:HG22	1.84	0.78
1:A:228:ASN:O	1:A:231:ILE:HG22	1.84	0.77
1:A:229:ARG:NH1	1:A:363:VAL:HB	1.99	0.77
1:A:285:GLN:H	1:E:56:THR:HB	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:HB3	1:D:61:HIS:HB3	1.66	0.77
2:I:239:THR:HG23	2:I:243:ARG:HE	1.49	0.77
1:E:53:PHE:HB3	1:E:61:HIS:HB3	1.67	0.77
1:E:228:ASN:O	1:E:231:ILE:HG22	1.84	0.77
1:F:229:ARG:NH1	1:F:363:VAL:HB	1.99	0.77
1:D:229:ARG:NH1	1:D:363:VAL:HB	1.99	0.77
1:F:53:PHE:HB3	1:F:61:HIS:HB3	1.67	0.77
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.67	0.77
1:D:228:ASN:O	1:D:231:ILE:HG22	1.85	0.76
2:B:75:MET:SD	2:B:94:PHE:HB3	2.25	0.76
2:H:75:MET:SD	2:H:94:PHE:HB3	2.25	0.76
1:E:229:ARG:NH1	1:E:363:VAL:HB	1.99	0.76
2:G:75:MET:SD	2:G:94:PHE:HB3	2.25	0.76
2:I:75:MET:SD	2:I:94:PHE:HB3	2.25	0.76
2:B:239:THR:HG23	2:B:243:ARG:HE	1.49	0.76
1:D:56:THR:HB	1:F:285:GLN:H	1.52	0.75
2:H:232:SER:O	2:H:235:MET:HB2	1.88	0.74
2:I:232:SER:O	2:I:235:MET:HB2	1.88	0.74
2:B:232:SER:O	2:B:235:MET:HB2	1.88	0.74
2:G:232:SER:O	2:G:235:MET:HB2	1.88	0.74
1:D:398:MET:HB3	2:I:348:PRO:HD2	1.71	0.73
2:H:387:LEU:HD12	2:H:390:ARG:HH12	1.53	0.73
2:B:387:LEU:HD12	2:B:390:ARG:HH12	1.53	0.73
2:I:387:LEU:HD12	2:I:390:ARG:HH12	1.53	0.73
2:I:259:MET:HE1	2:I:380:ASN:HB2	1.70	0.72
2:G:387:LEU:HD12	2:G:390:ARG:HH12	1.53	0.72
1:F:88:HIS:CE1	1:F:90:GLU:HB2	2.25	0.72
1:E:88:HIS:CE1	1:E:90:GLU:HB2	2.25	0.71
1:F:362:VAL:HG12	1:F:370:LYS:HD3	1.71	0.71
1:D:88:HIS:CE1	1:D:90:GLU:HB2	2.25	0.71
1:D:362:VAL:HG12	1:D:370:LYS:HD3	1.71	0.71
1:E:119:LEU:HD21	1:E:156:ARG:HB3	1.73	0.71
1:D:119:LEU:HD21	1:D:156:ARG:HB3	1.73	0.71
1:E:362:VAL:HG12	1:E:370:LYS:HD3	1.71	0.71
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.25	0.71
1:F:362:VAL:CG1	1:F:370:LYS:HD3	2.21	0.71
1:D:26:LEU:HD21	1:D:229:ARG:NH1	2.03	0.70
1:E:26:LEU:HD21	1:E:229:ARG:NH1	2.03	0.70
1:D:362:VAL:CG1	1:D:370:LYS:HD3	2.20	0.70
1:A:26:LEU:HD21	1:A:229:ARG:NH1	2.03	0.70
1:F:26:LEU:HD21	1:F:229:ARG:NH1	2.03	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:CG1	1:A:370:LYS:HD3	2.20	0.70
2:G:259:MET:HE1	2:G:380:ASN:HB2	1.74	0.70
1:A:362:VAL:HG12	1:A:370:LYS:HD3	1.71	0.70
1:A:119:LEU:HD21	1:A:156:ARG:HB3	1.73	0.69
1:E:362:VAL:CG1	1:E:370:LYS:HD3	2.20	0.69
1:F:119:LEU:HD21	1:F:156:ARG:HB3	1.73	0.69
2:H:259:MET:HE1	2:H:380:ASN:HB2	1.76	0.68
1:A:413:MET:SD	1:A:414:GLU:O	2.52	0.68
2:B:20:PHE:HB2	2:B:235:MET:SD	2.34	0.67
2:G:336:GLN:HE21	2:G:336:GLN:CA	1.99	0.67
1:F:413:MET:SD	1:F:414:GLU:O	2.52	0.67
2:H:20:PHE:HB2	2:H:235:MET:SD	2.35	0.67
1:D:413:MET:SD	1:D:414:GLU:O	2.52	0.67
1:E:413:MET:SD	1:E:414:GLU:O	2.52	0.67
2:G:20:PHE:HB2	2:G:235:MET:SD	2.35	0.67
2:I:20:PHE:HB2	2:I:235:MET:SD	2.34	0.67
2:B:64:ARG:NE	2:B:129:CYS:SG	2.69	0.66
1:F:209:ILE:HG21	1:F:227:LEU:HG	1.78	0.66
1:F:174:ALA:HB3	1:F:177:VAL:HB	1.78	0.66
1:A:209:ILE:HG21	1:A:227:LEU:HG	1.78	0.66
2:G:180:THR:HB	2:G:183:GLU:HB3	1.77	0.66
2:I:64:ARG:NE	2:I:129:CYS:SG	2.69	0.66
2:H:180:THR:HB	2:H:183:GLU:HB3	1.77	0.66
2:G:64:ARG:NE	2:G:129:CYS:SG	2.69	0.66
1:A:174:ALA:HB3	1:A:177:VAL:HB	1.78	0.66
2:B:269:MET:HE2	2:B:269:MET:O	1.96	0.65
2:B:180:THR:HB	2:B:183:GLU:HB3	1.77	0.65
2:H:28:HIS:ND1	2:H:43:GLN:O	2.30	0.65
1:E:174:ALA:HB3	1:E:177:VAL:HB	1.78	0.65
1:E:271:THR:HB	1:E:377:MET:HB3	1.79	0.65
2:G:28:HIS:ND1	2:G:43:GLN:O	2.30	0.65
2:I:28:HIS:ND1	2:I:43:GLN:O	2.30	0.65
2:I:180:THR:HB	2:I:183:GLU:HB3	1.77	0.65
2:B:28:HIS:ND1	2:B:43:GLN:O	2.30	0.65
2:H:115:VAL:HB	2:H:152:LEU:HD21	1.78	0.65
2:H:64:ARG:NE	2:H:129:CYS:SG	2.68	0.65
1:F:2:ARG:NH2	1:F:242:LEU:O	2.29	0.65
2:B:15:GLN:NE2	4:B:501:GSP:O6	2.30	0.64
1:D:174:ALA:HB3	1:D:177:VAL:HB	1.78	0.64
1:D:271:THR:HB	1:D:377:MET:HB3	1.79	0.64
2:G:115:VAL:HB	2:G:152:LEU:HD21	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HG2	2:B:133:GLN:HE21	1.62	0.64
2:H:15:GLN:NE2	4:H:501:GSP:O6	2.30	0.64
1:A:2:ARG:NH2	1:A:242:LEU:O	2.29	0.64
2:B:115:VAL:HB	2:B:152:LEU:HD21	1.77	0.64
2:I:115:VAL:HB	2:I:152:LEU:HD21	1.78	0.64
1:E:208:ALA:HB2	1:E:304:LYS:HG2	1.80	0.64
2:H:2:ARG:HG2	2:H:133:GLN:HE21	1.62	0.64
1:D:2:ARG:NH2	1:D:242:LEU:O	2.29	0.64
1:D:208:ALA:HB2	1:D:304:LYS:HG2	1.80	0.64
1:E:2:ARG:NH2	1:E:242:LEU:O	2.29	0.64
2:G:15:GLN:NE2	4:G:501:GSP:O6	2.30	0.64
1:E:88:HIS:ND1	1:E:90:GLU:HB2	2.13	0.64
2:G:301:MET:HG2	2:G:302:MET:N	2.13	0.64
2:H:301:MET:HG2	2:H:302:MET:N	2.12	0.64
2:I:2:ARG:HG2	2:I:133:GLN:HE21	1.62	0.64
1:A:285:GLN:N	1:E:56:THR:HB	2.12	0.64
1:D:88:HIS:ND1	1:D:90:GLU:HB2	2.13	0.64
2:B:301:MET:HG2	2:B:302:MET:N	2.13	0.63
1:F:121:ARG:O	1:F:124:LYS:HG3	1.99	0.63
1:D:121:ARG:O	1:D:124:LYS:HG3	1.99	0.63
1:D:209:ILE:HG21	1:D:227:LEU:HG	1.78	0.63
2:B:259:MET:HE1	2:B:380:ASN:HB2	1.79	0.63
1:F:88:HIS:ND1	1:F:90:GLU:HB2	2.13	0.63
1:F:271:THR:HB	1:F:377:MET:HB3	1.79	0.63
2:G:2:ARG:HG2	2:G:133:GLN:HE21	1.62	0.63
1:E:121:ARG:O	1:E:124:LYS:HG3	1.99	0.63
2:I:301:MET:HG2	2:I:302:MET:N	2.13	0.63
2:I:15:GLN:NE2	4:I:501:GSP:O6	2.30	0.63
1:A:121:ARG:O	1:A:124:LYS:HG3	1.99	0.63
1:F:183:GLU:HG3	1:F:184:PRO:HD3	1.81	0.63
1:E:209:ILE:HG21	1:E:227:LEU:HG	1.78	0.63
1:A:88:HIS:ND1	1:A:90:GLU:HB2	2.13	0.63
1:A:183:GLU:HG3	1:A:184:PRO:HD3	1.81	0.63
1:A:271:THR:HB	1:A:377:MET:HB3	1.79	0.63
1:D:404:PHE:H	2:I:261:PRO:HA	1.64	0.62
2:H:336:GLN:HE21	2:H:336:GLN:CA	1.99	0.62
2:B:51:VAL:HG11	2:B:243:ARG:HG2	1.81	0.62
2:H:416:MET:SD	2:H:416:MET:O	2.57	0.62
1:A:208:ALA:HB2	1:A:304:LYS:HG2	1.80	0.62
2:B:72:PRO:O	2:B:75:MET:HB2	2.00	0.62
1:D:88:HIS:HB3	1:D:91:GLN:OE1	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:PRO:O	2:H:75:MET:HB2	2.00	0.62
2:I:72:PRO:O	2:I:75:MET:HB2	2.00	0.62
1:F:208:ALA:HB2	1:F:304:LYS:HG2	1.80	0.62
2:G:416:MET:SD	2:G:416:MET:O	2.57	0.62
2:B:328:VAL:O	2:B:332:MET:HG2	2.00	0.62
1:E:88:HIS:HB3	1:E:91:GLN:OE1	2.00	0.62
2:G:72:PRO:O	2:G:75:MET:HB2	2.00	0.62
2:I:416:MET:SD	2:I:416:MET:O	2.58	0.62
2:H:269:MET:CE	2:H:270:PRO:O	2.48	0.62
2:I:269:MET:HE2	2:I:269:MET:O	2.00	0.62
2:B:269:MET:CE	2:B:270:PRO:O	2.48	0.61
2:H:20:PHE:CD1	2:H:235:MET:SD	2.93	0.61
2:B:416:MET:SD	2:B:416:MET:O	2.57	0.61
2:G:20:PHE:CD1	2:G:235:MET:SD	2.93	0.61
2:I:269:MET:CE	2:I:270:PRO:O	2.48	0.61
1:E:139:HIS:ND1	1:E:146:GLY:O	2.32	0.61
1:E:183:GLU:HG3	1:E:184:PRO:HD3	1.80	0.61
2:H:51:VAL:HG11	2:H:243:ARG:HG2	1.81	0.61
2:I:20:PHE:CD1	2:I:235:MET:SD	2.93	0.61
1:A:396:ASP:OD2	1:A:422:ARG:NH2	2.33	0.61
2:B:20:PHE:CD1	2:B:235:MET:SD	2.93	0.61
2:B:301:MET:HG2	2:B:302:MET:H	1.66	0.61
2:B:323:MET:HA	1:E:221:ARG:HD2	1.83	0.61
2:G:301:MET:HG2	2:G:302:MET:H	1.66	0.61
2:G:328:VAL:O	2:G:332:MET:HG2	2.00	0.61
2:I:328:VAL:O	2:I:332:MET:HG2	2.00	0.61
1:E:396:ASP:OD2	1:E:422:ARG:NH2	2.33	0.61
2:G:269:MET:CE	2:G:270:PRO:O	2.48	0.61
2:B:328:VAL:O	2:B:332:MET:HE3	1.99	0.61
1:D:183:GLU:HG3	1:D:184:PRO:HD3	1.81	0.61
1:F:396:ASP:OD2	1:F:422:ARG:NH2	2.33	0.61
2:G:51:VAL:HG11	2:G:243:ARG:HG2	1.81	0.61
2:I:51:VAL:HG11	2:I:243:ARG:HG2	1.81	0.61
1:D:396:ASP:OD2	1:D:422:ARG:NH2	2.33	0.61
1:D:139:HIS:ND1	1:D:146:GLY:O	2.32	0.61
2:G:7:ILE:HB	2:G:137:LEU:HD22	1.83	0.61
2:G:281:GLN:HE22	2:G:286:LEU:HD13	1.66	0.61
2:H:301:MET:HG2	2:H:302:MET:H	1.66	0.61
2:H:328:VAL:O	2:H:332:MET:HG2	2.00	0.61
2:I:281:GLN:HE22	2:I:286:LEU:HD13	1.66	0.61
2:H:281:GLN:HE22	2:H:286:LEU:HD13	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:HB3	1:A:91:GLN:OE1	2.00	0.60
2:B:348:PRO:HD2	1:E:398:MET:HB3	1.81	0.60
2:H:7:ILE:HB	2:H:137:LEU:HD22	1.83	0.60
2:B:281:GLN:HE22	2:B:286:LEU:HD13	1.66	0.60
1:F:88:HIS:HB3	1:F:91:GLN:OE1	2.00	0.60
1:F:298:PRO:HB3	1:F:307:PRO:HD2	1.83	0.60
1:F:409:VAL:HA	1:F:413:MET:O	2.02	0.60
2:H:269:MET:O	2:H:269:MET:HE2	2.01	0.60
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.83	0.60
1:A:409:VAL:HA	1:A:413:MET:O	2.02	0.60
1:E:409:VAL:HA	1:E:413:MET:O	2.02	0.60
1:F:139:HIS:ND1	1:F:146:GLY:O	2.32	0.60
2:G:289:PRO:HA	2:G:292:THR:HG22	1.83	0.60
2:I:301:MET:HG2	2:I:302:MET:H	1.66	0.60
1:D:409:VAL:HA	1:D:413:MET:O	2.02	0.60
2:I:242:LEU:HD12	2:I:251:ASP:HB2	1.84	0.60
2:B:7:ILE:HG13	2:B:66:VAL:HB	1.83	0.59
1:D:298:PRO:HB3	1:D:307:PRO:HD2	1.83	0.59
2:H:19:LYS:HE2	2:H:229:HIS:CD2	2.37	0.59
2:H:289:PRO:HA	2:H:292:THR:HG22	1.83	0.59
2:I:7:ILE:HB	2:I:137:LEU:HD22	1.83	0.59
2:B:289:PRO:HA	2:B:292:THR:HG22	1.83	0.59
1:D:318:LEU:HB2	1:D:376:CYS:HB3	1.84	0.59
2:G:19:LYS:HE2	2:G:229:HIS:CD2	2.37	0.59
2:I:72:PRO:HA	2:I:75:MET:CG	2.25	0.59
1:A:318:LEU:HB2	1:A:376:CYS:HB3	1.84	0.59
2:B:19:LYS:HE2	2:B:229:HIS:CD2	2.37	0.59
2:B:242:LEU:HD12	2:B:251:ASP:HB2	1.84	0.59
1:E:298:PRO:HB3	1:E:307:PRO:HD2	1.83	0.59
1:F:318:LEU:HB2	1:F:376:CYS:HB3	1.84	0.59
2:I:7:ILE:HG13	2:I:66:VAL:HB	1.83	0.59
2:I:289:PRO:HA	2:I:292:THR:HG22	1.83	0.59
1:D:128:GLN:NE2	1:D:129:CYS:SG	2.76	0.59
2:G:7:ILE:HG13	2:G:66:VAL:HB	1.83	0.59
2:H:7:ILE:HG13	2:H:66:VAL:HB	1.83	0.59
1:E:318:LEU:HB2	1:E:376:CYS:HB3	1.84	0.59
1:D:401:LYS:HG3	2:I:346:TRP:CD1	2.37	0.59
1:E:128:GLN:NE2	1:E:129:CYS:SG	2.76	0.59
1:F:269:LEU:HB2	1:F:303:VAL:HG21	1.85	0.59
1:A:128:GLN:NE2	1:A:129:CYS:SG	2.76	0.59
1:A:269:LEU:HB2	1:A:303:VAL:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HB	2:B:137:LEU:HD22	1.83	0.58
2:G:269:MET:HE2	2:G:269:MET:O	2.03	0.58
2:I:119:LEU:HD21	2:I:156:LYS:HG3	1.85	0.58
2:I:133:GLN:OE1	2:I:253:ARG:NH2	2.36	0.58
1:A:139:HIS:ND1	1:A:146:GLY:O	2.32	0.58
2:B:119:LEU:HD21	2:B:156:LYS:HG3	1.86	0.58
1:D:56:THR:HB	1:F:285:GLN:N	2.19	0.58
1:D:339:ARG:O	1:D:339:ARG:HD3	2.04	0.58
2:G:133:GLN:OE1	2:G:253:ARG:NH2	2.36	0.58
2:I:19:LYS:HE2	2:I:229:HIS:CD2	2.37	0.58
1:E:339:ARG:O	1:E:339:ARG:HD3	2.04	0.58
1:A:7:ILE:N	1:A:136:LEU:O	2.36	0.58
2:B:133:GLN:OE1	2:B:253:ARG:NH2	2.36	0.58
1:D:120:ASP:O	1:D:123:ARG:HB2	2.04	0.58
1:E:269:LEU:HB2	1:E:303:VAL:HG21	1.85	0.58
1:F:128:GLN:NE2	1:F:129:CYS:SG	2.76	0.58
2:H:133:GLN:OE1	2:H:253:ARG:NH2	2.36	0.58
1:D:269:LEU:HB2	1:D:303:VAL:HG21	1.85	0.58
2:H:242:LEU:HD12	2:H:251:ASP:HB2	1.84	0.58
1:D:286:LEU:HB3	1:D:291:ILE:HG21	1.86	0.57
1:E:286:LEU:HB3	1:E:291:ILE:HG21	1.86	0.57
1:E:16:ILE:HG12	1:E:231:ILE:HG21	1.86	0.57
2:G:103:TRP:HD1	2:G:147:SER:HG	1.51	0.57
2:G:242:LEU:HD12	2:G:251:ASP:HB2	1.84	0.57
1:D:7:ILE:N	1:D:136:LEU:O	2.36	0.57
1:E:120:ASP:O	1:E:123:ARG:HB2	2.04	0.57
2:H:328:VAL:O	2:H:332:MET:HE3	2.04	0.57
1:A:120:ASP:O	1:A:123:ARG:HB2	2.04	0.57
2:G:328:VAL:O	2:G:332:MET:HE3	2.03	0.57
2:H:72:PRO:HA	2:H:75:MET:CG	2.25	0.57
1:A:53:PHE:O	1:A:64:ARG:NH2	2.38	0.57
1:A:339:ARG:O	1:A:339:ARG:HD3	2.04	0.57
1:F:339:ARG:O	1:F:339:ARG:HD3	2.04	0.57
1:D:16:ILE:HG12	1:D:231:ILE:HG21	1.86	0.57
1:D:171:ILE:HD12	1:D:204:VAL:HG11	1.87	0.57
1:E:171:ILE:HD12	1:E:204:VAL:HG11	1.87	0.57
1:F:53:PHE:O	1:F:64:ARG:NH2	2.38	0.57
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.87	0.57
1:F:120:ASP:O	1:F:123:ARG:HB2	2.04	0.57
2:H:316:ALA:HB3	2:H:378:ILE:HB	1.87	0.57
1:F:16:ILE:HG12	1:F:231:ILE:HG21	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD11	1:A:171:ILE:HD11	1.88	0.56
1:F:16:ILE:HD11	1:F:171:ILE:HD11	1.88	0.56
2:I:316:ALA:HB3	2:I:378:ILE:HB	1.87	0.56
1:A:16:ILE:HG12	1:A:231:ILE:HG21	1.86	0.56
2:B:20:PHE:CG	2:B:235:MET:SD	2.98	0.56
2:G:20:PHE:CG	2:G:235:MET:SD	2.98	0.56
2:G:316:ALA:HB3	2:G:378:ILE:HB	1.87	0.56
2:H:119:LEU:HD21	2:H:156:LYS:HG3	1.86	0.56
2:G:119:LEU:HD21	2:G:156:LYS:HG3	1.86	0.56
1:A:88:HIS:HD1	1:A:90:GLU:HB2	1.71	0.56
1:A:286:LEU:HB3	1:A:291:ILE:HG21	1.86	0.56
1:F:286:LEU:HB3	1:F:291:ILE:HG21	1.86	0.56
2:H:20:PHE:CG	2:H:235:MET:SD	2.98	0.56
1:D:229:ARG:CZ	1:D:363:VAL:HB	2.36	0.56
1:F:229:ARG:CZ	1:F:363:VAL:HB	2.36	0.56
1:A:288:VAL:O	1:A:292:THR:HG23	2.06	0.56
1:E:7:ILE:N	1:E:136:LEU:O	2.36	0.56
2:G:72:PRO:HA	2:G:75:MET:CG	2.25	0.56
2:G:133:GLN:HG3	2:G:252:LEU:HD21	1.88	0.56
2:B:9:ALA:HB3	2:B:139:HIS:HB3	1.88	0.56
2:B:224:TYR:HA	2:B:227:LEU:HD12	1.88	0.56
1:E:229:ARG:CZ	1:E:363:VAL:HB	2.35	0.56
2:H:275:LEU:H	2:H:294:GLN:HE22	1.54	0.56
2:I:20:PHE:CG	2:I:235:MET:SD	2.98	0.56
1:D:53:PHE:O	1:D:64:ARG:NH2	2.38	0.55
2:I:224:TYR:HA	2:I:227:LEU:HD12	1.88	0.55
2:H:133:GLN:HG3	2:H:252:LEU:HD21	1.88	0.55
1:F:171:ILE:HD12	1:F:204:VAL:HG11	1.87	0.55
2:G:275:LEU:H	2:G:294:GLN:HE22	1.54	0.55
2:I:133:GLN:HG3	2:I:252:LEU:HD21	1.88	0.55
1:A:229:ARG:CZ	1:A:363:VAL:HB	2.35	0.55
1:F:88:HIS:HD1	1:F:90:GLU:HB2	1.71	0.55
2:I:275:LEU:H	2:I:294:GLN:HE22	1.54	0.55
1:A:171:ILE:HD12	1:A:204:VAL:HG11	1.87	0.55
2:B:275:LEU:H	2:B:294:GLN:HE22	1.54	0.55
1:D:210:TYR:CD2	2:I:326:LYS:HB3	2.42	0.55
1:E:16:ILE:HD11	1:E:171:ILE:HD11	1.88	0.55
2:B:133:GLN:HG3	2:B:252:LEU:HD21	1.88	0.55
1:D:224:TYR:HA	1:D:227:LEU:HD13	1.89	0.55
1:D:288:VAL:O	1:D:292:THR:HG23	2.06	0.55
2:G:224:TYR:HA	2:G:227:LEU:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HD11	1:D:171:ILE:HD11	1.87	0.55
1:E:53:PHE:O	1:E:64:ARG:NH2	2.38	0.55
1:F:288:VAL:O	1:F:292:THR:HG23	2.06	0.55
2:G:254:LYS:O	2:G:258:ASN:ND2	2.40	0.55
2:H:224:TYR:HA	2:H:227:LEU:HD12	1.88	0.55
2:I:103:TRP:HD1	2:I:147:SER:HG	1.54	0.55
2:B:254:LYS:O	2:B:258:ASN:ND2	2.40	0.55
2:I:9:ALA:HB3	2:I:139:HIS:HB3	1.88	0.55
1:D:88:HIS:HD1	1:D:90:GLU:HB2	1.71	0.55
1:E:288:VAL:O	1:E:292:THR:HG23	2.06	0.55
1:E:224:TYR:HA	1:E:227:LEU:HD13	1.89	0.54
2:G:99:ALA:HB3	2:G:145:THR:HB	1.89	0.54
2:G:307:PRO:HA	2:G:383:ALA:HB2	1.90	0.54
2:H:41:ASP:HA	2:H:44:LEU:CD2	2.37	0.54
2:H:99:ALA:HB3	2:H:145:THR:HB	1.89	0.54
2:H:307:PRO:HA	2:H:383:ALA:HB2	1.90	0.54
1:F:177:VAL:HG21	1:F:207:GLU:HB3	1.89	0.54
2:G:9:ALA:HB3	2:G:139:HIS:HB3	1.88	0.54
2:G:41:ASP:HA	2:G:44:LEU:CD2	2.38	0.54
2:H:322:ARG:NH2	2:H:357:ASP:O	2.41	0.54
2:I:254:LYS:O	2:I:258:ASN:ND2	2.40	0.54
1:E:119:LEU:O	1:E:123:ARG:HG2	2.08	0.54
1:E:177:VAL:HG21	1:E:207:GLU:HB3	1.90	0.54
2:H:254:LYS:O	2:H:258:ASN:ND2	2.40	0.54
1:D:177:VAL:HG21	1:D:207:GLU:HB3	1.90	0.54
2:H:9:ALA:HB3	2:H:139:HIS:HB3	1.88	0.54
2:I:307:PRO:HA	2:I:383:ALA:HB2	1.89	0.54
2:B:41:ASP:HA	2:B:44:LEU:CD2	2.38	0.54
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.90	0.54
2:I:319:PHE:HB2	2:I:355:VAL:HG22	1.90	0.54
2:H:313:LEU:HD22	2:H:380:ASN:ND2	2.23	0.53
2:G:313:LEU:HD22	2:G:380:ASN:ND2	2.23	0.53
2:I:328:VAL:O	2:I:332:MET:HE3	2.08	0.53
1:F:7:ILE:N	1:F:136:LEU:O	2.36	0.53
2:I:322:ARG:NH2	2:I:357:ASP:O	2.41	0.53
1:A:177:VAL:HG21	1:A:207:GLU:HB3	1.90	0.53
2:H:36:TYR:OH	2:H:44:LEU:HD22	2.08	0.53
2:I:313:LEU:HD22	2:I:380:ASN:ND2	2.23	0.53
2:B:313:LEU:HD22	2:B:380:ASN:ND2	2.23	0.53
1:F:119:LEU:O	1:F:123:ARG:HG2	2.08	0.53
2:G:36:TYR:OH	2:G:44:LEU:HD22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:41:ASP:HA	2:I:44:LEU:CD2	2.37	0.53
1:A:119:LEU:O	1:A:123:ARG:HG2	2.08	0.53
1:A:224:TYR:HA	1:A:227:LEU:HD13	1.89	0.53
1:D:119:LEU:O	1:D:123:ARG:HG2	2.08	0.53
2:G:322:ARG:NH2	2:G:357:ASP:O	2.41	0.53
1:E:88:HIS:HD1	1:E:90:GLU:HB2	1.71	0.53
1:F:224:TYR:HA	1:F:227:LEU:HD13	1.89	0.53
2:B:72:PRO:HA	2:B:75:MET:CG	2.25	0.53
2:B:99:ALA:HB3	2:B:145:THR:HB	1.89	0.53
2:I:290:GLU:O	2:I:293:GLN:NE2	2.33	0.53
2:B:307:PRO:HA	2:B:383:ALA:HB2	1.89	0.53
2:H:103:TRP:HD1	2:H:147:SER:HG	1.55	0.53
2:B:322:ARG:NH2	2:B:357:ASP:O	2.41	0.52
1:D:6:SER:HB2	1:D:138:PHE:HE2	1.73	0.52
2:B:235:MET:O	2:B:239:THR:HG22	2.09	0.52
1:E:190:THR:O	1:E:194:THR:HG22	2.10	0.52
2:G:235:MET:O	2:G:239:THR:HG22	2.09	0.52
2:G:319:PHE:HB2	2:G:355:VAL:HG22	1.90	0.52
2:H:235:MET:O	2:H:239:THR:HG22	2.09	0.52
2:I:99:ALA:HB3	2:I:145:THR:HB	1.89	0.52
2:B:290:GLU:O	2:B:293:GLN:NE2	2.33	0.52
1:D:190:THR:O	1:D:194:THR:HG22	2.10	0.52
1:A:6:SER:HB2	1:A:138:PHE:HE2	1.73	0.52
2:I:235:MET:O	2:I:239:THR:HG22	2.10	0.52
2:B:11:GLN:NE2	4:B:501:GSP:O2G	2.40	0.52
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.43	0.52
2:H:319:PHE:HB2	2:H:355:VAL:HG22	1.90	0.52
2:I:27:GLU:O	2:I:369:ARG:NH2	2.43	0.52
2:B:27:GLU:O	2:B:369:ARG:NH2	2.43	0.52
1:F:6:SER:HB2	1:F:138:PHE:HE2	1.73	0.52
2:H:183:GLU:HG2	2:H:184:PRO:HD3	1.91	0.52
2:B:183:GLU:HG2	2:B:184:PRO:HD3	1.91	0.52
1:D:276:ILE:HG23	1:D:280:LYS:HB3	1.92	0.52
2:I:11:GLN:NE2	4:I:501:GSP:O2G	2.40	0.52
1:E:6:SER:HB2	1:E:138:PHE:HE2	1.73	0.52
2:H:290:GLU:O	2:H:293:GLN:NE2	2.33	0.52
2:B:36:TYR:OH	2:B:44:LEU:HD22	2.08	0.52
2:H:27:GLU:O	2:H:369:ARG:NH2	2.43	0.52
1:A:190:THR:O	1:A:194:THR:HG22	2.10	0.51
1:D:289:ALA:O	1:D:293:ASN:ND2	2.43	0.51
1:E:276:ILE:HG23	1:E:280:LYS:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:THR:O	1:F:194:THR:HG22	2.10	0.51
1:F:289:ALA:O	1:F:293:ASN:ND2	2.43	0.51
2:I:183:GLU:HG2	2:I:184:PRO:HD3	1.91	0.51
1:E:289:ALA:O	1:E:293:ASN:ND2	2.43	0.51
1:F:221:ARG:HD3	2:H:324:SER:OG	2.09	0.51
1:A:64:ARG:NH1	1:A:129:CYS:SG	2.84	0.51
1:A:289:ALA:O	1:A:293:ASN:ND2	2.43	0.51
2:G:54:ASN:OD1	2:G:64:ARG:NH2	2.43	0.51
2:I:54:ASN:OD1	2:I:64:ARG:NH2	2.43	0.51
1:F:121:ARG:CD	1:F:124:LYS:HG2	2.41	0.51
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.93	0.51
1:F:276:ILE:HG23	1:F:280:LYS:HB3	1.92	0.51
2:G:27:GLU:O	2:G:369:ARG:NH2	2.43	0.51
2:I:36:TYR:OH	2:I:44:LEU:HD22	2.08	0.51
1:D:64:ARG:NH1	1:D:129:CYS:SG	2.84	0.51
1:D:98:ASP:N	1:D:98:ASP:OD1	2.44	0.51
2:B:217:LEU:HD22	2:B:219:LEU:HB2	1.93	0.51
1:E:121:ARG:CD	1:E:124:LYS:HG2	2.41	0.51
1:F:64:ARG:NH1	1:F:129:CYS:SG	2.84	0.51
2:I:217:LEU:HD22	2:I:219:LEU:HB2	1.93	0.51
1:A:229:ARG:HH11	1:A:363:VAL:HB	1.76	0.51
1:A:276:ILE:HG23	1:A:280:LYS:HB3	1.92	0.51
1:D:121:ARG:CD	1:D:124:LYS:HG2	2.41	0.51
1:E:64:ARG:NH1	1:E:129:CYS:SG	2.84	0.51
1:E:229:ARG:HH11	1:E:363:VAL:HB	1.76	0.51
2:G:183:GLU:HG2	2:G:184:PRO:HD3	1.91	0.51
2:B:109:THR:OG1	2:B:411:GLU:OE1	2.25	0.51
1:E:21:TRP:CD2	1:E:63:PRO:HB3	2.46	0.51
1:F:328:VAL:HG11	1:F:353:VAL:HG11	1.93	0.51
2:H:11:GLN:NE2	4:H:501:GSP:O2G	2.40	0.51
1:D:21:TRP:CD2	1:D:63:PRO:HB3	2.46	0.50
1:D:21:TRP:HZ3	1:D:52:PHE:HB3	1.77	0.50
1:E:98:ASP:OD1	1:E:98:ASP:N	2.44	0.50
2:G:137:LEU:HG	2:G:166:MET:HE1	1.93	0.50
2:G:217:LEU:HD22	2:G:219:LEU:HB2	1.93	0.50
2:H:54:ASN:OD1	2:H:64:ARG:NH2	2.43	0.50
1:D:21:TRP:CE2	1:D:63:PRO:HB3	2.47	0.50
1:F:21:TRP:CE2	1:F:63:PRO:HB3	2.47	0.50
1:E:21:TRP:CE2	1:E:63:PRO:HB3	2.47	0.50
2:G:11:GLN:NE2	4:G:501:GSP:O2G	2.40	0.50
2:I:101:ASN:HA	2:I:144:GLY:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CD2	1:A:63:PRO:HB3	2.46	0.50
1:A:188:ILE:HD12	1:A:425:LEU:HD12	1.94	0.50
1:D:292:THR:OG1	1:D:335:ILE:HD11	2.12	0.50
1:E:292:THR:OG1	1:E:335:ILE:HD11	2.12	0.50
2:G:31:ASP:OD1	2:G:35:ALA:N	2.45	0.50
2:H:239:THR:CG2	2:H:243:ARG:HE	2.23	0.50
1:A:21:TRP:HZ3	1:A:52:PHE:HB3	1.77	0.50
1:A:107:HIS:HA	1:A:152:LEU:HD23	1.94	0.50
2:B:259:MET:CE	2:B:380:ASN:HB2	2.41	0.50
1:D:139:HIS:CG	1:D:150:THR:HG21	2.47	0.50
1:D:188:ILE:HD12	1:D:425:LEU:HD12	1.94	0.50
1:E:188:ILE:HD12	1:E:425:LEU:HD12	1.94	0.50
1:F:107:HIS:HA	1:F:152:LEU:HD23	1.94	0.50
2:B:31:ASP:OD1	2:B:35:ALA:N	2.45	0.50
1:D:406:HIS:NE2	2:I:260:VAL:HG12	2.26	0.50
1:E:139:HIS:CG	1:E:150:THR:HG21	2.47	0.50
1:F:188:ILE:HD12	1:F:425:LEU:HD12	1.94	0.50
2:G:290:GLU:O	2:G:293:GLN:NE2	2.33	0.50
2:H:217:LEU:HD22	2:H:219:LEU:HB2	1.93	0.50
2:B:352:LYS:HG2	1:E:179:THR:O	2.12	0.50
1:D:21:TRP:CZ3	1:D:52:PHE:HB3	2.47	0.50
1:A:121:ARG:CD	1:A:124:LYS:HG2	2.41	0.50
1:A:139:HIS:CG	1:A:150:THR:HG21	2.47	0.50
1:D:290:GLU:HA	1:D:293:ASN:HD21	1.77	0.50
1:D:328:VAL:HG11	1:D:353:VAL:HG11	1.93	0.50
1:E:21:TRP:CZ3	1:E:52:PHE:HB3	2.47	0.50
1:F:21:TRP:CD2	1:F:63:PRO:HB3	2.46	0.50
2:G:28:HIS:HA	2:G:43:GLN:HB3	1.94	0.50
2:G:259:MET:CE	2:G:380:ASN:HB2	2.41	0.50
1:A:290:GLU:HA	1:A:293:ASN:HD21	1.77	0.49
1:F:21:TRP:CZ3	1:F:52:PHE:HB3	2.47	0.49
1:F:21:TRP:HZ3	1:F:52:PHE:HB3	1.77	0.49
2:G:63:PRO:HD3	2:G:86:ILE:HG12	1.94	0.49
2:G:101:ASN:HA	2:G:144:GLY:H	1.77	0.49
2:G:119:LEU:HD11	2:G:156:LYS:HB3	1.94	0.49
2:H:31:ASP:OD1	2:H:35:ALA:N	2.45	0.49
2:H:63:PRO:HD3	2:H:86:ILE:HG12	1.94	0.49
2:I:31:ASP:OD1	2:I:35:ALA:N	2.45	0.49
1:A:21:TRP:CE2	1:A:63:PRO:HB3	2.47	0.49
2:B:28:HIS:HA	2:B:43:GLN:HB3	1.94	0.49
1:D:145:THR:N	3:D:501:GTP:O2G	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:HIS:HA	2:H:43:GLN:HB3	1.94	0.49
2:H:119:LEU:HD11	2:H:156:LYS:HB3	1.94	0.49
1:E:328:VAL:HG11	1:E:353:VAL:HG11	1.93	0.49
1:F:290:GLU:HA	1:F:293:ASN:HD21	1.77	0.49
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.13	0.49
1:E:21:TRP:HZ3	1:E:52:PHE:HB3	1.77	0.49
2:H:259:MET:CE	2:H:380:ASN:HB2	2.41	0.49
1:A:310:GLY:HA3	1:A:382:THR:HB	1.94	0.49
1:E:145:THR:N	3:E:501:GTP:O2G	2.40	0.49
1:F:139:HIS:CG	1:F:150:THR:HG21	2.47	0.49
1:F:310:GLY:HA3	1:F:382:THR:HB	1.94	0.49
2:G:239:THR:CG2	2:G:243:ARG:HE	2.23	0.49
2:H:101:ASN:HA	2:H:144:GLY:H	1.76	0.49
2:I:28:HIS:HA	2:I:43:GLN:HB3	1.94	0.49
2:I:63:PRO:HD3	2:I:86:ILE:HG12	1.94	0.49
2:I:237:GLY:HA3	2:I:376:THR:OG1	2.13	0.49
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.94	0.49
1:E:76:ASP:HA	1:E:79:ARG:HG2	1.93	0.49
1:F:191:THR:HB	1:F:425:LEU:HD11	1.95	0.49
2:I:119:LEU:HD11	2:I:156:LYS:HB3	1.94	0.49
1:A:21:TRP:CZ3	1:A:52:PHE:HB3	2.47	0.49
1:D:76:ASP:HA	1:D:79:ARG:HG2	1.93	0.49
1:D:224:TYR:CE2	2:I:247:GLN:HB2	2.47	0.49
1:A:191:THR:HB	1:A:425:LEU:HD11	1.95	0.49
1:E:310:GLY:HA3	1:E:382:THR:HB	1.94	0.49
2:H:233:LEU:HD13	2:H:272:PHE:CE2	2.48	0.49
1:E:290:GLU:HA	1:E:293:ASN:HD21	1.77	0.49
1:F:98:ASP:N	1:F:98:ASP:OD1	2.44	0.49
2:H:237:GLY:HA3	2:H:376:THR:OG1	2.13	0.49
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.94	0.49
2:G:233:LEU:HD13	2:G:272:PHE:CE2	2.48	0.49
2:B:101:ASN:HA	2:B:144:GLY:H	1.76	0.48
1:F:292:THR:OG1	1:F:335:ILE:HD11	2.12	0.48
1:A:76:ASP:HA	1:A:79:ARG:HG2	1.93	0.48
1:D:229:ARG:HE	1:D:363:VAL:CG1	2.27	0.48
2:H:273:ALA:O	2:H:375:ALA:N	2.38	0.48
1:A:121:ARG:HD2	1:A:121:ARG:HA	1.37	0.48
1:D:310:GLY:HA3	1:D:382:THR:HB	1.94	0.48
1:E:107:HIS:HA	1:E:152:LEU:HD23	1.94	0.48
2:H:6:HIS:O	2:H:66:VAL:N	2.46	0.48
1:A:98:ASP:OD1	1:A:98:ASP:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:OG1	1:A:335:ILE:HD11	2.12	0.48
2:B:239:THR:CG2	2:B:243:ARG:HE	2.23	0.48
2:G:6:HIS:O	2:G:66:VAL:N	2.45	0.48
2:I:200:GLU:HA	2:I:266:HIS:HB2	1.95	0.48
2:I:239:THR:CG2	2:I:243:ARG:HE	2.23	0.48
1:F:145:THR:N	3:F:501:GTP:O2G	2.40	0.48
2:G:280:SER:O	2:G:284:ARG:N	2.45	0.48
2:I:233:LEU:HD13	2:I:272:PHE:CE2	2.48	0.48
1:A:229:ARG:HE	1:A:363:VAL:CG1	2.27	0.48
1:D:406:HIS:NE2	2:I:260:VAL:O	2.40	0.48
1:E:151:SER:OG	1:E:190:THR:OG1	2.28	0.48
1:F:76:ASP:HA	1:F:79:ARG:HG2	1.93	0.48
2:G:237:GLY:HA3	2:G:376:THR:OG1	2.13	0.48
1:A:119:LEU:HD11	1:A:156:ARG:HD3	1.96	0.48
2:B:26:ASP:O	2:B:369:ARG:NH1	2.47	0.48
1:D:107:HIS:HA	1:D:152:LEU:HD23	1.94	0.48
1:D:191:THR:HB	1:D:425:LEU:HD11	1.95	0.48
1:D:229:ARG:HH11	1:D:363:VAL:HB	1.76	0.48
1:D:422:ARG:NH1	1:D:426:ALA:HB2	2.28	0.48
1:E:422:ARG:NH1	1:E:426:ALA:HB2	2.28	0.48
1:F:119:LEU:HD11	1:F:156:ARG:HD3	1.96	0.48
1:F:269:LEU:HD23	1:F:379:SER:O	2.14	0.48
2:I:26:ASP:O	2:I:369:ARG:NH1	2.47	0.48
1:A:269:LEU:HD23	1:A:379:SER:O	2.14	0.48
2:B:6:HIS:O	2:B:66:VAL:N	2.46	0.48
2:B:36:TYR:CZ	2:B:44:LEU:HB3	2.49	0.48
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.95	0.48
2:H:26:ASP:O	2:H:369:ARG:NH1	2.47	0.48
2:B:280:SER:O	2:B:284:ARG:N	2.45	0.48
2:I:36:TYR:CZ	2:I:44:LEU:HB3	2.49	0.48
1:A:422:ARG:NH1	1:A:426:ALA:HB2	2.28	0.47
1:E:191:THR:HB	1:E:425:LEU:HD11	1.95	0.47
1:D:277:SER:O	1:D:281:ALA:N	2.42	0.47
1:E:136:LEU:HD23	1:E:167:LEU:HB3	1.97	0.47
1:E:229:ARG:HE	1:E:363:VAL:CG1	2.27	0.47
2:H:200:GLU:HA	2:H:266:HIS:HB2	1.95	0.47
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.50	0.47
1:A:145:THR:N	3:A:501:GTP:O2G	2.40	0.47
1:F:422:ARG:NH1	1:F:426:ALA:HB2	2.28	0.47
2:G:409:THR:HA	2:G:413:MET:HB2	1.96	0.47
2:I:6:HIS:O	2:I:66:VAL:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD23	1:D:167:LEU:HB3	1.97	0.47
1:E:139:HIS:CD2	1:E:150:THR:HG21	2.50	0.47
1:E:305:CYS:HB3	1:E:383:ALA:HB1	1.96	0.47
2:G:273:ALA:O	2:G:375:ALA:N	2.38	0.47
2:G:336:GLN:OE1	2:G:350:ASN:OD1	2.32	0.47
2:H:109:THR:OG1	2:H:411:GLU:OE1	2.25	0.47
1:A:157:LEU:HB3	1:A:166:LYS:HD3	1.96	0.47
1:D:139:HIS:CD2	1:D:150:THR:HG21	2.50	0.47
1:D:305:CYS:HB3	1:D:383:ALA:HB1	1.97	0.47
1:F:139:HIS:CD2	1:F:150:THR:HG21	2.50	0.47
1:F:229:ARG:HE	1:F:363:VAL:CG1	2.27	0.47
2:G:26:ASP:O	2:G:369:ARG:NH1	2.47	0.47
1:A:277:SER:O	1:A:281:ALA:N	2.43	0.47
2:G:200:GLU:HA	2:G:266:HIS:HB2	1.95	0.47
2:H:409:THR:HA	2:H:413:MET:HB2	1.96	0.47
2:I:259:MET:CE	2:I:380:ASN:HB2	2.41	0.47
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.97	0.47
2:B:233:LEU:HD13	2:B:272:PHE:CE2	2.48	0.47
1:D:9:VAL:HG21	1:D:153:LEU:HD21	1.96	0.47
1:F:71:GLU:HB3	1:F:98:ASP:HB3	1.97	0.47
1:F:157:LEU:HB3	1:F:166:LYS:HD3	1.96	0.47
1:F:229:ARG:HH11	1:F:363:VAL:HB	1.76	0.47
1:F:277:SER:O	1:F:281:ALA:N	2.42	0.47
2:G:36:TYR:CZ	2:G:44:LEU:HB3	2.49	0.47
2:G:385:GLN:HG2	2:G:429:VAL:HG23	1.97	0.47
2:H:36:TYR:CZ	2:H:44:LEU:HB3	2.49	0.47
2:I:409:THR:HA	2:I:413:MET:HB2	1.96	0.47
1:A:405:VAL:HG11	1:A:415:GLU:HG3	1.97	0.47
1:E:269:LEU:HD23	1:E:379:SER:O	2.14	0.47
1:E:277:SER:O	1:E:281:ALA:N	2.42	0.47
1:F:215:ARG:NH2	1:F:300:ASN:OD1	2.32	0.47
1:F:405:VAL:HG11	1:F:415:GLU:HG3	1.97	0.47
2:B:409:THR:HA	2:B:413:MET:HB2	1.96	0.47
1:D:157:LEU:HB3	1:D:166:LYS:HD3	1.96	0.47
2:G:401:ARG:HA	2:G:401:ARG:HD2	1.81	0.47
2:I:320:ARG:HA	2:I:356:CYS:O	2.15	0.47
2:G:323:MET:HE3	2:G:328:VAL:HG23	1.96	0.47
2:I:386:GLU:HA	2:I:389:LYS:HE2	1.97	0.47
1:A:136:LEU:HD23	1:A:167:LEU:HB3	1.97	0.46
1:A:305:CYS:HB3	1:A:383:ALA:HB1	1.96	0.46
2:B:273:ALA:O	2:B:375:ALA:N	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:SER:OG	1:E:222:PRO:HD2	2.15	0.46
1:D:102:ASN:HB3	1:D:105:ARG:HB2	1.97	0.46
1:E:9:VAL:HG21	1:E:153:LEU:HD21	1.96	0.46
1:F:136:LEU:HD23	1:F:167:LEU:HB3	1.97	0.46
1:F:305:CYS:HB3	1:F:383:ALA:HB1	1.96	0.46
2:H:336:GLN:OE1	2:H:350:ASN:OD1	2.32	0.46
1:A:9:VAL:HG21	1:A:153:LEU:HD21	1.96	0.46
1:A:102:ASN:HB3	1:A:105:ARG:HB2	1.97	0.46
1:A:231:ILE:O	1:A:235:VAL:HG23	2.16	0.46
1:D:269:LEU:HD23	1:D:379:SER:O	2.14	0.46
1:E:157:LEU:HB3	1:E:166:LYS:HD3	1.96	0.46
1:F:102:ASN:HB3	1:F:105:ARG:HB2	1.97	0.46
1:F:231:ILE:O	1:F:235:VAL:HG23	2.16	0.46
2:H:280:SER:O	2:H:284:ARG:N	2.45	0.46
2:I:336:GLN:OE1	2:I:350:ASN:OD1	2.32	0.46
2:I:419:THR:O	2:I:422:GLU:HG3	2.15	0.46
2:B:320:ARG:HA	2:B:356:CYS:O	2.15	0.46
2:B:336:GLN:OE1	2:B:350:ASN:OD1	2.32	0.46
2:B:386:GLU:HA	2:B:389:LYS:HE2	1.97	0.46
1:D:151:SER:OG	1:D:190:THR:OG1	2.28	0.46
1:E:284:GLU:OE1	1:F:120:ASP:OD1	2.32	0.46
1:F:295:CYS:SG	1:F:377:MET:HB2	2.55	0.46
2:H:389:LYS:HE2	2:H:389:LYS:HB3	1.78	0.46
1:A:82:THR:O	1:A:82:THR:OG1	2.34	0.46
1:E:295:CYS:SG	1:E:377:MET:HB2	2.55	0.46
1:E:332:ILE:O	1:E:336:LYS:HG3	2.15	0.46
2:G:320:ARG:HA	2:G:356:CYS:O	2.15	0.46
2:I:280:SER:O	2:I:284:ARG:N	2.45	0.46
1:A:295:CYS:SG	1:A:377:MET:HB2	2.55	0.46
2:B:419:THR:O	2:B:422:GLU:HG3	2.15	0.46
1:D:295:CYS:SG	1:D:377:MET:HB2	2.55	0.46
1:D:306:ASP:HB3	1:D:309:HIS:CE1	2.51	0.46
1:E:102:ASN:HB3	1:E:105:ARG:HB2	1.97	0.46
1:F:9:VAL:HG21	1:F:153:LEU:HD21	1.97	0.46
1:F:151:SER:OG	1:F:190:THR:OG1	2.28	0.46
1:F:332:ILE:O	1:F:336:LYS:HG3	2.15	0.46
2:H:385:GLN:HG2	2:H:429:VAL:HG23	1.97	0.46
2:I:273:ALA:O	2:I:375:ALA:N	2.38	0.46
1:A:306:ASP:HB3	1:A:309:HIS:CE1	2.51	0.46
1:D:231:ILE:O	1:D:235:VAL:HG23	2.15	0.46
1:E:23:LEU:HG	1:E:229:ARG:HH22	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HA	1:A:274:PRO:HA	1.67	0.46
2:B:316:ALA:HA	2:B:352:LYS:HB3	1.97	0.46
1:D:23:LEU:HG	1:D:229:ARG:HH22	1.81	0.46
1:D:119:LEU:HD11	1:D:156:ARG:HD3	1.96	0.46
1:D:332:ILE:O	1:D:336:LYS:HG3	2.15	0.46
1:E:231:ILE:O	1:E:235:VAL:HG23	2.16	0.46
1:F:82:THR:O	1:F:82:THR:OG1	2.34	0.46
2:G:4:ILE:HB	2:G:52:TYR:HE1	1.81	0.46
2:G:419:THR:O	2:G:422:GLU:HG3	2.15	0.46
2:H:401:ARG:HA	2:H:401:ARG:HD2	1.81	0.46
2:H:419:THR:O	2:H:422:GLU:HG3	2.15	0.46
2:I:47:GLU:HG3	2:I:48:ARG:HG3	1.98	0.46
2:I:109:THR:OG1	2:I:411:GLU:OE1	2.25	0.46
2:I:385:GLN:HG2	2:I:429:VAL:HG23	1.97	0.46
1:A:151:SER:OG	1:A:190:THR:OG1	2.28	0.46
1:D:6:SER:HA	1:D:136:LEU:HB2	1.97	0.46
1:D:273:ALA:HB2	1:D:295:CYS:SG	2.56	0.46
1:E:6:SER:HA	1:E:136:LEU:HB2	1.97	0.46
1:E:119:LEU:HD11	1:E:156:ARG:HD3	1.96	0.46
1:E:273:ALA:HB2	1:E:295:CYS:SG	2.56	0.46
1:E:306:ASP:HB3	1:E:309:HIS:CE1	2.51	0.46
2:G:109:THR:OG1	2:G:411:GLU:OE1	2.25	0.46
2:H:301:MET:HE2	2:H:305:CYS:H	1.81	0.46
2:I:316:ALA:HA	2:I:352:LYS:HB3	1.97	0.46
1:A:332:ILE:O	1:A:336:LYS:HG3	2.15	0.46
1:A:413:MET:SD	1:A:417:GLU:HB2	2.56	0.46
2:B:47:GLU:HG3	2:B:48:ARG:HG3	1.98	0.46
1:D:405:VAL:HG11	1:D:415:GLU:HG3	1.97	0.46
1:E:413:MET:SD	1:E:417:GLU:HB2	2.56	0.46
1:F:224:TYR:HD1	1:F:227:LEU:HD13	1.81	0.46
1:F:306:ASP:HB3	1:F:309:HIS:CE1	2.51	0.46
1:A:6:SER:HA	1:A:136:LEU:HB2	1.97	0.46
1:A:273:ALA:HB2	1:A:295:CYS:SG	2.56	0.46
1:D:224:TYR:HD1	1:D:227:LEU:HD13	1.81	0.46
2:G:271:GLY:HA2	2:G:302:MET:SD	2.56	0.46
2:H:271:GLY:HA2	2:H:302:MET:SD	2.56	0.46
2:H:320:ARG:HA	2:H:356:CYS:O	2.15	0.46
2:I:4:ILE:HB	2:I:52:TYR:HE1	1.81	0.46
1:A:28:HIS:CE1	1:A:49:PHE:HB3	2.52	0.45
2:B:261:PRO:HA	1:E:404:PHE:H	1.81	0.45
1:F:6:SER:HA	1:F:136:LEU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:316:ALA:HA	2:G:352:LYS:HB3	1.97	0.45
1:A:201:ALA:HB3	1:A:267:PHE:HD1	1.81	0.45
1:D:201:ALA:HB3	1:D:267:PHE:HD1	1.82	0.45
2:B:321:GLY:HA3	2:B:373:MET:SD	2.57	0.45
1:D:71:GLU:HB3	1:D:98:ASP:HB3	1.97	0.45
1:D:371:VAL:HG22	1:D:373:ARG:H	1.81	0.45
1:F:371:VAL:HG22	1:F:373:ARG:H	1.81	0.45
2:G:321:GLY:HA3	2:G:373:MET:SD	2.57	0.45
1:D:204:VAL:HA	1:D:302:MET:CE	2.47	0.45
1:D:390:ARG:HH11	1:D:394:LYS:HE2	1.82	0.45
1:D:413:MET:SD	1:D:417:GLU:HB2	2.56	0.45
1:E:71:GLU:HB3	1:E:98:ASP:HB3	1.97	0.45
1:F:390:ARG:HH11	1:F:394:LYS:HE2	1.82	0.45
1:F:413:MET:SD	1:F:417:GLU:HB2	2.56	0.45
2:G:386:GLU:HA	2:G:389:LYS:HE2	1.97	0.45
2:B:271:GLY:HA2	2:B:302:MET:SD	2.56	0.45
1:E:82:THR:O	1:E:82:THR:OG1	2.34	0.45
1:E:215:ARG:NH2	1:E:300:ASN:OD1	2.33	0.45
1:E:269:LEU:HD23	1:E:269:LEU:H	1.82	0.45
1:E:371:VAL:HG22	1:E:373:ARG:H	1.81	0.45
1:E:390:ARG:HH11	1:E:394:LYS:HE2	1.82	0.45
1:E:405:VAL:HG11	1:E:415:GLU:HG3	1.97	0.45
1:F:28:HIS:CE1	1:F:49:PHE:HB3	2.52	0.45
1:F:201:ALA:HB3	1:F:267:PHE:HD1	1.82	0.45
1:F:273:ALA:HA	1:F:274:PRO:HA	1.67	0.45
2:H:283:TYR:HA	2:I:56:ALA:HB1	1.99	0.45
2:H:316:ALA:HA	2:H:352:LYS:HB3	1.97	0.45
2:H:321:GLY:HA3	2:H:373:MET:SD	2.57	0.45
2:H:386:GLU:HA	2:H:389:LYS:HE2	1.97	0.45
2:I:271:GLY:HA2	2:I:302:MET:SD	2.56	0.45
1:A:204:VAL:HA	1:A:302:MET:CE	2.47	0.45
1:A:371:VAL:HG22	1:A:373:ARG:H	1.81	0.45
1:A:390:ARG:HH11	1:A:394:LYS:HE2	1.82	0.45
2:B:4:ILE:HB	2:B:52:TYR:HE1	1.81	0.45
2:B:385:GLN:HG2	2:B:429:VAL:HG23	1.97	0.45
1:D:376:CYS:SG	1:D:378:LEU:HD11	2.56	0.45
2:H:4:ILE:HB	2:H:52:TYR:HE1	1.81	0.45
1:D:11:GLN:OE1	2:I:249:ASN:ND2	2.48	0.45
1:E:204:VAL:HA	1:E:302:MET:CE	2.47	0.45
1:F:273:ALA:HB2	1:F:295:CYS:SG	2.56	0.45
2:H:19:LYS:HE2	2:H:229:HIS:NE2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:401:ARG:HA	2:I:401:ARG:HD2	1.81	0.45
1:F:376:CYS:SG	1:F:378:LEU:HD11	2.57	0.45
2:G:216:THR:HG21	2:G:300:ASN:ND2	2.32	0.45
2:H:140:SER:HA	2:H:171:VAL:HB	1.99	0.45
2:I:216:THR:HG21	2:I:300:ASN:ND2	2.32	0.45
1:A:23:LEU:HG	1:A:229:ARG:HH22	1.81	0.45
2:B:216:THR:HG21	2:B:300:ASN:ND2	2.32	0.45
1:E:224:TYR:HD1	1:E:227:LEU:HD13	1.81	0.45
1:F:204:VAL:HA	1:F:302:MET:CE	2.47	0.45
1:F:297:GLU:HG2	1:F:298:PRO:HD2	1.99	0.45
2:I:321:GLY:HA3	2:I:373:MET:SD	2.57	0.45
1:A:184:PRO:O	1:A:188:ILE:HG12	2.17	0.45
1:A:376:CYS:SG	1:A:378:LEU:HD11	2.57	0.45
1:F:184:PRO:O	1:F:188:ILE:HG12	2.17	0.45
1:F:210:TYR:HE1	1:F:227:LEU:HD11	1.82	0.45
2:G:140:SER:HA	2:G:171:VAL:HB	1.99	0.45
1:A:269:LEU:HD23	1:A:269:LEU:H	1.82	0.44
1:A:399:TYR:OH	1:A:415:GLU:HB3	2.17	0.44
2:B:1:MET:N	2:B:50:ASN:OD1	2.45	0.44
2:B:146:GLY:HA2	2:B:149:MET:SD	2.57	0.44
2:B:389:LYS:HE2	2:B:389:LYS:HB3	1.78	0.44
1:E:28:HIS:CE1	1:E:49:PHE:HB3	2.51	0.44
1:E:184:PRO:O	1:E:188:ILE:HG12	2.17	0.44
1:E:201:ALA:HB3	1:E:267:PHE:HD1	1.82	0.44
2:I:336:GLN:HE21	2:I:336:GLN:CA	1.99	0.44
1:A:210:TYR:HE1	1:A:227:LEU:HD11	1.82	0.44
1:A:297:GLU:HG2	1:A:298:PRO:HD2	1.99	0.44
1:D:82:THR:O	1:D:82:THR:OG1	2.34	0.44
1:D:399:TYR:OH	1:D:415:GLU:HB3	2.17	0.44
1:F:23:LEU:HG	1:F:229:ARG:HH22	1.81	0.44
2:I:218:LYS:HD3	2:I:218:LYS:HA	1.83	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.44
1:F:121:ARG:HD2	1:F:121:ARG:HA	1.37	0.44
1:F:269:LEU:HD23	1:F:269:LEU:H	1.82	0.44
2:H:21:TRP:CE3	2:H:63:PRO:HB3	2.52	0.44
2:H:216:THR:HG21	2:H:300:ASN:ND2	2.32	0.44
1:A:18:ASN:O	1:A:22:GLU:HG2	2.17	0.44
1:A:224:TYR:HD1	1:A:227:LEU:HD13	1.81	0.44
1:D:269:LEU:HD23	1:D:269:LEU:H	1.82	0.44
1:D:297:GLU:HG2	1:D:298:PRO:HD2	1.99	0.44
1:F:18:ASN:O	1:F:22:GLU:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:TRP:CE3	2:G:63:PRO:HB3	2.53	0.44
2:I:146:GLY:HA2	2:I:149:MET:SD	2.57	0.44
2:B:119:LEU:HA	2:B:122:VAL:HG12	1.99	0.44
2:G:146:GLY:HA2	2:G:149:MET:SD	2.57	0.44
2:G:228:ASN:O	2:G:231:VAL:HG12	2.18	0.44
2:H:228:ASN:O	2:H:231:VAL:HG12	2.18	0.44
1:D:172:TYR:OH	1:D:390:ARG:NH2	2.50	0.44
1:E:376:CYS:SG	1:E:378:LEU:HD11	2.56	0.44
1:F:427:ALA:HA	1:F:430:LYS:HG2	2.00	0.44
2:G:19:LYS:HE2	2:G:229:HIS:NE2	2.32	0.44
2:G:119:LEU:HA	2:G:122:VAL:HG12	1.99	0.44
2:H:47:GLU:HG3	2:H:48:ARG:HG3	1.98	0.44
2:H:232:SER:C	2:H:235:MET:HB2	2.37	0.44
2:H:293:GLN:HG2	2:I:124:LYS:HZ2	1.83	0.44
1:A:172:TYR:OH	1:A:390:ARG:NH2	2.50	0.44
2:B:174:SER:HB2	2:B:206:ASN:HB2	2.00	0.44
1:E:172:TYR:OH	1:E:390:ARG:NH2	2.50	0.44
1:E:297:GLU:HG2	1:E:298:PRO:HD2	1.99	0.44
1:F:172:TYR:OH	1:F:390:ARG:NH2	2.50	0.44
2:G:47:GLU:HG3	2:G:48:ARG:HG3	1.98	0.44
2:I:174:SER:HB2	2:I:206:ASN:HB2	2.00	0.44
1:A:427:ALA:HA	1:A:430:LYS:HG2	2.00	0.44
2:B:19:LYS:HE2	2:B:229:HIS:NE2	2.32	0.44
2:B:232:SER:C	2:B:235:MET:HB2	2.37	0.44
1:D:210:TYR:HE1	1:D:227:LEU:HD11	1.82	0.44
1:D:215:ARG:NH2	1:D:300:ASN:OD1	2.33	0.44
1:E:210:TYR:HE1	1:E:227:LEU:HD11	1.82	0.44
2:G:232:SER:C	2:G:235:MET:HB2	2.37	0.44
2:G:301:MET:CG	2:G:302:MET:N	2.80	0.44
2:H:146:GLY:HA2	2:H:149:MET:SD	2.57	0.44
2:H:269:MET:CE	2:H:269:MET:O	2.66	0.44
1:A:188:ILE:HG23	1:A:425:LEU:HD12	2.00	0.44
1:F:221:ARG:HD2	2:H:323:MET:HA	1.99	0.44
2:G:269:MET:CE	2:G:269:MET:O	2.66	0.44
2:H:297:ASP:N	2:H:297:ASP:OD1	2.51	0.44
2:I:140:SER:HA	2:I:171:VAL:HB	1.99	0.44
1:D:184:PRO:O	1:D:188:ILE:HG12	2.17	0.43
2:G:320:ARG:O	2:G:373:MET:HA	2.18	0.43
2:H:20:PHE:CB	2:H:235:MET:SD	3.06	0.43
2:H:293:GLN:HG2	2:I:124:LYS:NZ	2.33	0.43
2:I:21:TRP:CE3	2:I:63:PRO:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:LEU:HA	2:I:122:VAL:HG12	1.99	0.43
2:I:232:SER:C	2:I:235:MET:HB2	2.37	0.43
2:I:320:ARG:O	2:I:373:MET:HA	2.18	0.43
2:B:275:LEU:N	2:B:294:GLN:HE22	2.15	0.43
1:D:28:HIS:CE1	1:D:49:PHE:HB3	2.51	0.43
2:H:301:MET:CG	2:H:302:MET:N	2.80	0.43
1:D:177:VAL:HG22	2:I:329:ASP:CG	2.39	0.43
2:G:269:MET:HE1	2:G:270:PRO:O	2.18	0.43
2:G:297:ASP:OD1	2:G:297:ASP:N	2.51	0.43
2:I:19:LYS:HE2	2:I:229:HIS:NE2	2.32	0.43
2:B:297:ASP:OD1	2:B:297:ASP:N	2.51	0.43
2:B:320:ARG:O	2:B:373:MET:HA	2.18	0.43
1:D:18:ASN:O	1:D:22:GLU:HG2	2.17	0.43
1:E:18:ASN:O	1:E:22:GLU:HG2	2.17	0.43
1:E:399:TYR:OH	1:E:415:GLU:HB3	2.18	0.43
1:F:399:TYR:OH	1:F:415:GLU:HB3	2.17	0.43
2:H:323:MET:HE3	2:H:328:VAL:HG23	1.99	0.43
2:B:24:ILE:HG23	2:B:28:HIS:HD2	1.84	0.43
2:B:183:GLU:HA	2:B:186:ASN:HD22	1.84	0.43
2:G:390:ARG:O	2:G:393:GLU:HG3	2.19	0.43
2:H:174:SER:HB2	2:H:206:ASN:HB2	2.00	0.43
2:H:320:ARG:O	2:H:373:MET:HA	2.18	0.43
2:H:390:ARG:O	2:H:393:GLU:HG3	2.19	0.43
2:I:23:ILE:HD13	2:I:23:ILE:HA	1.88	0.43
2:I:297:ASP:OD1	2:I:297:ASP:N	2.51	0.43
2:B:20:PHE:CB	2:B:235:MET:SD	3.06	0.43
2:G:301:MET:HE2	2:G:305:CYS:H	1.83	0.43
2:H:269:MET:HE1	2:H:270:PRO:O	2.18	0.43
2:B:336:GLN:HE21	2:B:336:GLN:CA	1.99	0.43
1:E:427:ALA:HA	1:E:430:LYS:HG2	2.00	0.43
2:I:22:GLU:HG3	2:I:83:PHE:CG	2.54	0.43
2:I:24:ILE:HG23	2:I:28:HIS:HD2	1.84	0.43
2:I:228:ASN:O	2:I:231:VAL:HG12	2.18	0.43
2:B:16:ILE:HG21	2:B:138:THR:HG21	2.01	0.43
2:B:22:GLU:HG3	2:B:83:PHE:CG	2.54	0.43
2:B:62:VAL:HG11	2:G:283:TYR:CG	2.53	0.43
1:E:121:ARG:HD2	1:E:121:ARG:HA	1.37	0.43
2:G:12:CYS:HB2	4:G:501:GSP:C8	2.54	0.43
2:G:22:GLU:HG3	2:G:83:PHE:CG	2.54	0.43
2:G:183:GLU:HA	2:G:186:ASN:HD22	1.84	0.43
2:I:275:LEU:N	2:I:294:GLN:HE22	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ARG:O	2:B:393:GLU:HG3	2.19	0.43
2:B:12:CYS:HB2	4:B:501:GSP:C8	2.54	0.43
2:B:119:LEU:HD12	2:B:123:ARG:NH2	2.34	0.43
2:B:228:ASN:O	2:B:231:VAL:HG12	2.18	0.43
2:B:232:SER:HA	2:B:235:MET:CG	2.29	0.43
1:D:188:ILE:HG23	1:D:425:LEU:HD12	2.00	0.43
2:G:24:ILE:HG23	2:G:28:HIS:HD2	1.84	0.43
2:G:174:SER:HB2	2:G:206:ASN:HB2	2.00	0.43
2:H:12:CYS:HB2	4:H:501:GSP:C8	2.54	0.43
2:H:22:GLU:HG3	2:H:83:PHE:CG	2.54	0.43
2:H:119:LEU:HA	2:H:122:VAL:HG12	1.99	0.43
2:I:12:CYS:HB2	4:I:501:GSP:C8	2.54	0.43
2:I:119:LEU:HD12	2:I:123:ARG:NH2	2.34	0.43
2:I:390:ARG:O	2:I:393:GLU:HG3	2.19	0.43
2:B:401:ARG:HA	2:B:401:ARG:HD2	1.81	0.42
1:D:152:LEU:HD12	1:D:153:LEU:N	2.34	0.42
1:D:314:ALA:O	1:D:379:SER:HB2	2.19	0.42
1:D:332:ILE:HD13	1:D:332:ILE:HA	1.85	0.42
1:F:314:ALA:O	1:F:379:SER:HB2	2.19	0.42
2:B:140:SER:HA	2:B:171:VAL:HB	1.99	0.42
1:D:124:LYS:HA	1:D:127:ASP:OD2	2.18	0.42
1:D:181:VAL:CG2	2:I:350:ASN:HA	2.48	0.42
1:E:152:LEU:HD12	1:E:153:LEU:N	2.35	0.42
1:E:188:ILE:HG23	1:E:425:LEU:HD12	2.00	0.42
1:F:188:ILE:HG23	1:F:425:LEU:HD12	2.00	0.42
1:F:415:GLU:OE1	1:F:415:GLU:N	2.52	0.42
2:I:183:GLU:HA	2:I:186:ASN:HD22	1.84	0.42
1:A:96:LYS:HD2	1:A:96:LYS:HA	1.84	0.42
1:A:152:LEU:HD12	1:A:153:LEU:N	2.34	0.42
1:A:314:ALA:O	1:A:379:SER:HB2	2.19	0.42
2:B:327:GLU:O	2:B:330:GLU:HG3	2.19	0.42
1:D:273:ALA:HA	1:D:274:PRO:HA	1.67	0.42
2:I:20:PHE:CB	2:I:235:MET:SD	3.06	0.42
2:B:41:ASP:HA	2:B:44:LEU:HD23	2.01	0.42
2:B:137:LEU:HG	2:B:166:MET:CE	2.49	0.42
2:B:218:LYS:HD3	2:B:218:LYS:HA	1.82	0.42
1:D:427:ALA:HA	1:D:430:LYS:HG2	2.00	0.42
1:E:155:GLU:OE2	1:E:193:THR:HG22	2.19	0.42
1:F:96:LYS:HD2	1:F:96:LYS:HA	1.84	0.42
2:G:327:GLU:O	2:G:330:GLU:HG3	2.19	0.42
2:H:24:ILE:HG23	2:H:28:HIS:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:275:LEU:N	2:H:294:GLN:HE22	2.15	0.42
2:B:164:ARG:NH1	1:E:97:GLU:OE2	2.49	0.42
1:F:155:GLU:OE2	1:F:193:THR:HG22	2.19	0.42
1:F:186:ASN:OD1	1:F:408:TYR:OH	2.33	0.42
2:G:36:TYR:CZ	2:G:44:LEU:HD22	2.54	0.42
2:G:215:ARG:NH2	2:G:216:THR:OG1	2.51	0.42
2:G:269:MET:C	2:G:269:MET:HE3	2.40	0.42
2:B:36:TYR:CZ	2:B:44:LEU:HD22	2.54	0.42
1:D:121:ARG:HD2	1:D:121:ARG:HA	1.37	0.42
1:D:155:GLU:OE2	1:D:193:THR:HG22	2.19	0.42
1:D:178:SER:HB3	1:D:183:GLU:HG2	2.01	0.42
1:E:23:LEU:C	1:E:23:LEU:HD23	2.40	0.42
1:E:124:LYS:HA	1:E:127:ASP:OD2	2.19	0.42
1:E:178:SER:HB3	1:E:183:GLU:HG2	2.01	0.42
1:F:23:LEU:HD23	1:F:23:LEU:C	2.40	0.42
2:G:313:LEU:HG	2:G:435:TYR:CE2	2.55	0.42
2:H:327:GLU:O	2:H:330:GLU:HG3	2.19	0.42
2:I:259:MET:HE1	2:I:380:ASN:CB	2.45	0.42
2:B:260:VAL:HB	1:E:407:TRP:HE1	1.85	0.42
1:D:186:ASN:OD1	1:D:408:TYR:OH	2.33	0.42
1:D:290:GLU:HA	1:D:293:ASN:ND2	2.34	0.42
1:E:186:ASN:OD1	1:E:408:TYR:OH	2.33	0.42
1:E:314:ALA:O	1:E:379:SER:HB2	2.19	0.42
2:G:137:LEU:HG	2:G:166:MET:CE	2.49	0.42
2:H:119:LEU:HD12	2:H:123:ARG:NH2	2.34	0.42
2:H:137:LEU:HG	2:H:166:MET:CE	2.49	0.42
2:H:183:GLU:HA	2:H:186:ASN:HD22	1.84	0.42
2:H:313:LEU:HG	2:H:435:TYR:CE2	2.55	0.42
2:I:131:CYS:SG	2:I:164:ARG:NH2	2.92	0.42
1:A:178:SER:HB3	1:A:183:GLU:HG2	2.01	0.42
1:A:181:VAL:HG12	2:G:258:ASN:OD1	2.19	0.42
1:D:70:LEU:HG	1:D:145:THR:HG23	2.02	0.42
1:E:290:GLU:HA	1:E:293:ASN:ND2	2.34	0.42
1:F:290:GLU:HA	1:F:293:ASN:ND2	2.34	0.42
2:G:16:ILE:HG21	2:G:138:THR:HG21	2.01	0.42
2:H:218:LYS:HD3	2:H:218:LYS:HA	1.82	0.42
1:A:124:LYS:HA	1:A:127:ASP:OD2	2.19	0.42
1:A:290:GLU:HA	1:A:293:ASN:ND2	2.34	0.42
2:B:260:VAL:HG12	1:E:406:HIS:NE2	2.35	0.42
1:D:96:LYS:HD2	1:D:96:LYS:HA	1.84	0.42
1:E:70:LEU:HG	1:E:145:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:PRO:HB2	1:E:312:TYR:CE1	2.55	0.42
1:F:178:SER:HB3	1:F:183:GLU:HG2	2.01	0.42
2:G:119:LEU:HD12	2:G:123:ARG:NH2	2.34	0.42
2:G:131:CYS:SG	2:G:164:ARG:NH2	2.92	0.42
2:I:36:TYR:CZ	2:I:44:LEU:HD22	2.54	0.42
1:A:186:ASN:OD1	1:A:408:TYR:OH	2.33	0.42
1:A:307:PRO:HB2	1:A:312:TYR:CE1	2.55	0.42
1:E:63:PRO:HG2	1:E:87:PHE:CE1	2.55	0.42
1:F:124:LYS:HA	1:F:127:ASP:OD2	2.19	0.42
2:H:36:TYR:CZ	2:H:44:LEU:HD22	2.54	0.42
2:H:137:LEU:HG	2:H:166:MET:HE1	2.02	0.42
2:I:232:SER:HA	2:I:235:MET:CG	2.29	0.42
1:A:23:LEU:HD23	1:A:23:LEU:C	2.40	0.41
1:F:152:LEU:HD12	1:F:153:LEU:N	2.35	0.41
2:G:275:LEU:N	2:G:294:GLN:HE22	2.15	0.41
2:H:16:ILE:HG21	2:H:138:THR:HG21	2.01	0.41
2:H:131:CYS:SG	2:H:164:ARG:NH2	2.92	0.41
2:I:16:ILE:HG21	2:I:138:THR:HG21	2.01	0.41
2:I:313:LEU:HG	2:I:435:TYR:CE2	2.55	0.41
1:A:155:GLU:OE2	1:A:193:THR:HG22	2.19	0.41
1:A:360:PRO:HG3	1:A:374:ALA:HB2	2.03	0.41
2:B:323:MET:HE3	2:B:328:VAL:HG23	2.01	0.41
1:A:110:ILE:O	1:A:114:ILE:HG12	2.20	0.41
1:D:63:PRO:HG2	1:D:87:PHE:CE1	2.55	0.41
1:D:110:ILE:O	1:D:114:ILE:HG12	2.20	0.41
1:D:407:TRP:NE1	2:I:257:VAL:HA	2.35	0.41
1:F:307:PRO:HB2	1:F:312:TYR:CE1	2.55	0.41
1:F:360:PRO:HG3	1:F:374:ALA:HB2	2.03	0.41
2:G:123:ARG:NH2	2:G:160:GLU:OE1	2.49	0.41
2:G:218:LYS:HD3	2:G:218:LYS:HA	1.83	0.41
2:H:16:ILE:HG12	2:H:231:VAL:HG11	2.03	0.41
1:A:280:LYS:HB2	1:A:280:LYS:HE2	1.84	0.41
1:A:283:HIS:HA	1:E:60:LYS:CE	2.51	0.41
2:B:202:TYR:HE1	2:B:268:PHE:HD2	1.69	0.41
2:B:313:LEU:HG	2:B:435:TYR:CE2	2.55	0.41
1:E:110:ILE:O	1:E:114:ILE:HG12	2.21	0.41
2:G:259:MET:HE1	2:G:380:ASN:CB	2.46	0.41
2:I:41:ASP:HA	2:I:44:LEU:HD23	2.01	0.41
2:I:137:LEU:HG	2:I:166:MET:CE	2.49	0.41
2:I:202:TYR:HE1	2:I:268:PHE:HD2	1.69	0.41
2:I:327:GLU:O	2:I:330:GLU:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH2	1:A:300:ASN:OD1	2.33	0.41
1:D:177:VAL:HG22	2:I:329:ASP:CB	2.51	0.41
1:F:217:LEU:HD13	1:F:367:ASP:HB2	2.03	0.41
2:H:41:ASP:HA	2:H:44:LEU:HD23	2.01	0.41
2:I:137:LEU:HG	2:I:166:MET:HE1	2.01	0.41
2:I:389:LYS:HE2	2:I:389:LYS:HB3	1.78	0.41
2:B:131:CYS:SG	2:B:164:ARG:NH2	2.92	0.41
1:D:23:LEU:HD23	1:D:23:LEU:C	2.40	0.41
1:F:280:LYS:HE2	1:F:280:LYS:HB2	1.84	0.41
2:G:20:PHE:CB	2:G:235:MET:SD	3.06	0.41
2:G:102:ASN:N	2:G:144:GLY:HA3	2.36	0.41
2:I:259:MET:HB3	2:I:268:PHE:CZ	2.56	0.41
1:A:66:VAL:HG21	1:A:122:ILE:HG13	2.02	0.41
2:B:102:ASN:N	2:B:144:GLY:HA3	2.36	0.41
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.56	0.41
2:H:271:GLY:HA3	2:H:377:PHE:HB3	2.03	0.41
2:I:123:ARG:NH2	2:I:160:GLU:OE1	2.49	0.41
1:A:182:VAL:O	1:A:182:VAL:HG12	2.21	0.41
1:A:217:LEU:HD13	1:A:367:ASP:HB2	2.03	0.41
2:B:247:GLN:HB2	1:E:224:TYR:CE2	2.55	0.41
1:D:181:VAL:HG23	2:I:350:ASN:HA	2.03	0.41
1:F:70:LEU:HG	1:F:145:THR:HG23	2.02	0.41
1:F:182:VAL:O	1:F:182:VAL:HG12	2.21	0.41
2:G:259:MET:HB3	2:G:268:PHE:CZ	2.56	0.41
2:H:259:MET:HB3	2:H:268:PHE:CZ	2.56	0.41
2:I:76:ASP:O	2:I:80:SER:OG	2.31	0.41
2:I:259:MET:HE2	2:I:268:PHE:CD1	2.56	0.41
1:A:5:ILE:HD12	1:A:125:LEU:HD13	2.02	0.41
1:A:63:PRO:HG2	1:A:87:PHE:CE1	2.55	0.41
2:B:269:MET:O	2:B:269:MET:CE	2.66	0.41
2:B:271:GLY:HA3	2:B:377:PHE:HB3	2.03	0.41
1:D:307:PRO:HB2	1:D:312:TYR:CE1	2.55	0.41
1:F:8:HIS:HB3	1:F:13:GLY:O	2.21	0.41
1:F:63:PRO:HG2	1:F:87:PHE:CE1	2.55	0.41
1:F:66:VAL:HG21	1:F:122:ILE:HG13	2.02	0.41
2:G:16:ILE:HG12	2:G:231:VAL:HG11	2.03	0.41
2:G:41:ASP:HA	2:G:44:LEU:HD23	2.01	0.41
2:I:27:GLU:OE2	2:I:320:ARG:NH2	2.40	0.41
2:I:102:ASN:N	2:I:144:GLY:HA3	2.36	0.41
2:I:269:MET:HE1	2:I:270:PRO:O	2.18	0.41
1:A:8:HIS:HB3	1:A:13:GLY:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:MET:HE1	2:B:270:PRO:O	2.19	0.41
2:G:174:SER:HB3	2:G:177:VAL:HG12	2.02	0.41
2:H:102:ASN:N	2:H:144:GLY:HA3	2.36	0.41
2:H:123:ARG:NH2	2:H:160:GLU:OE1	2.49	0.41
2:H:269:MET:HE3	2:H:269:MET:C	2.41	0.41
1:D:8:HIS:HB3	1:D:13:GLY:O	2.21	0.40
1:E:141:PHE:HD2	1:E:172:TYR:HD1	1.69	0.40
1:F:110:ILE:O	1:F:114:ILE:HG12	2.21	0.40
2:G:247:GLN:H	2:G:247:GLN:HG2	1.64	0.40
2:H:215:ARG:NH2	2:H:216:THR:OG1	2.51	0.40
2:H:387:LEU:HD12	2:H:390:ARG:NH1	2.30	0.40
2:I:247:GLN:H	2:I:247:GLN:HG2	1.65	0.40
1:A:151:SER:O	1:A:155:GLU:OE1	2.39	0.40
1:D:100:ALA:HB1	2:I:254:LYS:HA	2.03	0.40
1:D:141:PHE:HD2	1:D:172:TYR:HD1	1.69	0.40
1:E:360:PRO:HG3	1:E:374:ALA:HB2	2.03	0.40
2:G:202:TYR:HE1	2:G:268:PHE:HD2	1.69	0.40
2:G:271:GLY:HA3	2:G:377:PHE:HB3	2.03	0.40
2:H:188:THR:HG23	2:H:425:MET:CE	2.52	0.40
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.95	0.40
1:A:223:THR:HG22	1:A:224:TYR:N	2.36	0.40
2:B:53:TYR:HB3	2:B:61:TYR:HB3	2.04	0.40
1:F:5:ILE:HD12	1:F:125:LEU:HD13	2.02	0.40
1:F:363:VAL:HG13	1:F:366:GLY:HA3	2.04	0.40
2:G:389:LYS:HE2	2:G:389:LYS:HB3	1.78	0.40
2:H:166:MET:HE1	2:H:168:THR:HG22	2.04	0.40
2:H:326:LYS:HG3	2:H:327:GLU:N	2.37	0.40
2:I:188:THR:HG23	2:I:425:MET:CE	2.52	0.40
1:A:363:VAL:HG13	1:A:366:GLY:HA3	2.04	0.40
2:B:76:ASP:O	2:B:80:SER:OG	2.31	0.40
2:B:174:SER:HB3	2:B:177:VAL:HG12	2.02	0.40
1:D:5:ILE:HD12	1:D:125:LEU:HD13	2.02	0.40
1:D:223:THR:HG22	1:D:224:TYR:N	2.37	0.40
1:D:360:PRO:HG3	1:D:374:ALA:HB2	2.03	0.40
1:E:223:THR:HG22	1:E:224:TYR:N	2.36	0.40
1:F:151:SER:O	1:F:155:GLU:OE1	2.40	0.40
2:G:188:THR:HG23	2:G:425:MET:CE	2.52	0.40
2:H:41:ASP:HA	2:H:44:LEU:HD21	2.03	0.40
2:I:53:TYR:HB3	2:I:61:TYR:HB3	2.04	0.40
2:I:269:MET:O	2:I:269:MET:CE	2.66	0.40
2:I:301:MET:HE2	2:I:305:CYS:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HA	1:A:144:GLY:N	2.37	0.40
2:B:137:LEU:HG	2:B:166:MET:HE1	2.02	0.40
2:B:240:THR:HG21	2:B:320:ARG:HD2	2.03	0.40
2:B:301:MET:HE2	2:B:305:CYS:H	1.86	0.40
2:B:326:LYS:HG3	2:B:327:GLU:N	2.37	0.40
2:B:333:LEU:HD12	2:B:333:LEU:HA	1.96	0.40
1:D:66:VAL:HG21	1:D:122:ILE:HG13	2.02	0.40
1:E:8:HIS:HB3	1:E:13:GLY:O	2.21	0.40
1:E:182:VAL:HG12	1:E:182:VAL:O	2.21	0.40
1:E:363:VAL:CG1	1:E:366:GLY:HA3	2.52	0.40
1:F:363:VAL:CG1	1:F:366:GLY:HA3	2.52	0.40
2:H:202:TYR:HE1	2:H:268:PHE:HD2	1.69	0.40
2:I:115:VAL:HA	2:I:118:VAL:HG22	2.04	0.40
2:I:219:LEU:HD12	2:I:219:LEU:HA	1.98	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	418/450 (93%)	404 (97%)	13 (3%)	1 (0%)	47	81
1	D	418/450 (93%)	404 (97%)	13 (3%)	1 (0%)	47	81
1	E	418/450 (93%)	404 (97%)	13 (3%)	1 (0%)	47	81
1	F	418/450 (93%)	403 (96%)	14 (3%)	1 (0%)	47	81
2	B	424/447 (95%)	409 (96%)	14 (3%)	1 (0%)	47	81
2	G	424/447 (95%)	409 (96%)	14 (3%)	1 (0%)	47	81
2	H	424/447 (95%)	409 (96%)	14 (3%)	1 (0%)	47	81
2	I	424/447 (95%)	409 (96%)	14 (3%)	1 (0%)	47	81
All	All	3368/3588 (94%)	3251 (96%)	109 (3%)	8 (0%)	50	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	235	MET
2	G	235	MET
2	H	235	MET
2	I	235	MET
1	A	414	GLU
1	D	414	GLU
1	E	414	GLU
1	F	414	GLU

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	356/375 (95%)	341 (96%)	15 (4%)	30	54
1	D	356/375 (95%)	341 (96%)	15 (4%)	30	54
1	E	356/375 (95%)	341 (96%)	15 (4%)	30	54
1	F	356/375 (95%)	341 (96%)	15 (4%)	30	54
2	B	365/382 (96%)	351 (96%)	14 (4%)	33	57
2	G	365/382 (96%)	351 (96%)	14 (4%)	33	57
2	H	365/382 (96%)	351 (96%)	14 (4%)	33	57
2	I	365/382 (96%)	350 (96%)	15 (4%)	30	55
All	All	2884/3028 (95%)	2767 (96%)	117 (4%)	34	55

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	33	ASP
1	A	47	ASP
1	A	82	THR
1	A	122	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	LYS
1	A	203	MET
1	A	230	LEU
1	A	337	THR
1	A	339	ARG
1	A	377	MET
1	A	378	LEU
1	A	413	MET
1	A	414	GLU
2	B	26	ASP
2	B	44	LEU
2	B	93	VAL
2	B	149	MET
2	B	166	MET
2	B	176	LYS
2	B	231	VAL
2	B	269	MET
2	B	301	MET
2	B	302	MET
2	B	336	GLN
2	B	349	ASN
2	B	413	MET
2	B	416	MET
1	D	1	MET
1	D	2	ARG
1	D	33	ASP
1	D	47	ASP
1	D	82	THR
1	D	122	ILE
1	D	124	LYS
1	D	203	MET
1	D	230	LEU
1	D	337	THR
1	D	339	ARG
1	D	377	MET
1	D	378	LEU
1	D	413	MET
1	D	414	GLU
1	E	1	MET
1	E	2	ARG
1	E	33	ASP
1	E	47	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	82	THR
1	E	122	ILE
1	E	124	LYS
1	E	203	MET
1	E	230	LEU
1	E	337	THR
1	E	339	ARG
1	E	377	MET
1	E	378	LEU
1	E	413	MET
1	E	414	GLU
1	F	1	MET
1	F	2	ARG
1	F	33	ASP
1	F	47	ASP
1	F	82	THR
1	F	122	ILE
1	F	124	LYS
1	F	203	MET
1	F	230	LEU
1	F	337	THR
1	F	339	ARG
1	F	377	MET
1	F	378	LEU
1	F	413	MET
1	F	414	GLU
2	G	26	ASP
2	G	44	LEU
2	G	93	VAL
2	G	149	MET
2	G	166	MET
2	G	176	LYS
2	G	231	VAL
2	G	269	MET
2	G	301	MET
2	G	302	MET
2	G	325	MET
2	G	336	GLN
2	G	413	MET
2	G	416	MET
2	H	26	ASP
2	H	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	93	VAL
2	H	149	MET
2	H	166	MET
2	H	176	LYS
2	H	231	VAL
2	H	269	MET
2	H	301	MET
2	H	302	MET
2	H	325	MET
2	H	336	GLN
2	H	413	MET
2	H	416	MET
2	I	26	ASP
2	I	44	LEU
2	I	93	VAL
2	I	149	MET
2	I	166	MET
2	I	176	LYS
2	I	231	VAL
2	I	269	MET
2	I	301	MET
2	I	302	MET
2	I	325	MET
2	I	336	GLN
2	I	349	ASN
2	I	413	MET
2	I	416	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
2	B	6	HIS
2	B	15	GLN
2	B	247	GLN
2	B	294	GLN
2	B	300	ASN
2	B	336	GLN
2	B	349	ASN
1	D	128	GLN
1	E	128	GLN
1	F	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	6	HIS
2	G	15	GLN
2	G	247	GLN
2	G	294	GLN
2	G	300	ASN
2	G	336	GLN
2	H	6	HIS
2	H	15	GLN
2	H	247	GLN
2	H	294	GLN
2	H	300	ASN
2	H	336	GLN
2	I	6	HIS
2	I	15	GLN
2	I	247	GLN
2	I	294	GLN
2	I	300	ASN
2	I	336	GLN
2	I	349	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 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	$\#\|Z\| > 2$
3	GTP	A	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
3	GTP	D	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.61	7 (21%)
4	GSP	B	501	-	26,34,34	2.17	3 (11%)	27,54,54	1.53	6 (22%)
3	GTP	E	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
4	GSP	G	501	-	26,34,34	2.17	3 (11%)	27,54,54	1.53	6 (22%)
4	GSP	H	501	-	26,34,34	2.16	3 (11%)	27,54,54	1.52	6 (22%)
4	GSP	I	501	-	26,34,34	2.16	3 (11%)	27,54,54	1.53	6 (22%)
3	GTP	F	501	-	26,34,34	1.12	2 (7%)	32,54,54	1.60	7 (21%)

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
3	GTP	A	501	-	-	4/18/38/38	0/3/3/3
3	GTP	D	501	-	-	4/18/38/38	0/3/3/3
4	GSP	B	501	-	-	0/17/38/38	0/3/3/3
3	GTP	E	501	-	-	4/18/38/38	0/3/3/3
4	GSP	G	501	-	-	0/17/38/38	0/3/3/3
4	GSP	H	501	-	-	0/17/38/38	0/3/3/3
4	GSP	I	501	-	-	0/17/38/38	0/3/3/3
3	GTP	F	501	-	-	4/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	501	GSP	PG-S1G	-9.35	1.70	1.90
4	B	501	GSP	PG-S1G	-9.32	1.70	1.90
4	I	501	GSP	PG-S1G	-9.31	1.70	1.90
4	H	501	GSP	PG-S1G	-9.28	1.70	1.90
3	E	501	GTP	C5-C6	-4.01	1.39	1.47
4	B	501	GSP	C5-C6	-4.00	1.39	1.47
4	H	501	GSP	C5-C6	-3.97	1.39	1.47
3	A	501	GTP	C5-C6	-3.96	1.39	1.47
4	G	501	GSP	C5-C6	-3.96	1.39	1.47
4	I	501	GSP	C5-C6	-3.95	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	GTP	C5-C6	-3.93	1.39	1.47
3	F	501	GTP	C5-C6	-3.93	1.39	1.47
4	I	501	GSP	C2-N3	2.20	1.38	1.33
4	B	501	GSP	C2-N3	2.20	1.38	1.33
3	D	501	GTP	C2-N3	2.18	1.38	1.33
4	H	501	GSP	C2-N3	2.17	1.38	1.33
3	F	501	GTP	C2-N3	2.17	1.38	1.33
3	E	501	GTP	C2-N3	2.16	1.38	1.33
3	A	501	GTP	C2-N3	2.16	1.38	1.33
4	G	501	GSP	C2-N3	2.16	1.38	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	GTP	PB-O3B-PG	-3.91	119.39	132.83
3	A	501	GTP	PB-O3B-PG	-3.91	119.41	132.83
3	E	501	GTP	PB-O3B-PG	-3.91	119.41	132.83
3	D	501	GTP	PB-O3B-PG	-3.91	119.42	132.83
3	A	501	GTP	PA-O3A-PB	-3.32	121.42	132.83
3	E	501	GTP	PA-O3A-PB	-3.32	121.42	132.83
3	D	501	GTP	PA-O3A-PB	-3.32	121.43	132.83
3	F	501	GTP	PA-O3A-PB	-3.31	121.45	132.83
4	G	501	GSP	C5-C6-N1	3.25	119.69	113.95
4	B	501	GSP	C5-C6-N1	3.24	119.68	113.95
4	I	501	GSP	C5-C6-N1	3.22	119.64	113.95
3	D	501	GTP	C5-C6-N1	3.22	119.63	113.95
3	A	501	GTP	C5-C6-N1	3.21	119.62	113.95
3	F	501	GTP	C5-C6-N1	3.21	119.62	113.95
3	E	501	GTP	C5-C6-N1	3.20	119.61	113.95
4	H	501	GSP	C5-C6-N1	3.20	119.60	113.95
4	G	501	GSP	C8-N7-C5	3.03	108.77	102.99
4	I	501	GSP	C8-N7-C5	3.03	108.76	102.99
4	I	501	GSP	PA-O3A-PB	-3.03	122.44	132.83
3	D	501	GTP	C3'-C2'-C1'	3.03	105.53	100.98
4	B	501	GSP	PA-O3A-PB	-3.02	122.45	132.83
4	G	501	GSP	PA-O3A-PB	-3.02	122.45	132.83
4	H	501	GSP	PA-O3A-PB	-3.02	122.47	132.83
3	F	501	GTP	C3'-C2'-C1'	3.01	105.51	100.98
4	B	501	GSP	C8-N7-C5	3.01	108.72	102.99
3	E	501	GTP	C8-N7-C5	3.00	108.70	102.99
3	A	501	GTP	C3'-C2'-C1'	3.00	105.49	100.98
4	H	501	GSP	C8-N7-C5	3.00	108.70	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	GTP	C8-N7-C5	3.00	108.70	102.99
3	F	501	GTP	C8-N7-C5	2.99	108.68	102.99
3	D	501	GTP	C8-N7-C5	2.98	108.66	102.99
3	E	501	GTP	C3'-C2'-C1'	2.97	105.45	100.98
3	D	501	GTP	C2-N1-C6	-2.87	119.81	125.10
3	A	501	GTP	C2-N1-C6	-2.87	119.81	125.10
3	F	501	GTP	C2-N1-C6	-2.87	119.82	125.10
3	E	501	GTP	C2-N1-C6	-2.87	119.82	125.10
4	G	501	GSP	C2-N1-C6	-2.85	119.86	125.10
4	H	501	GSP	C2-N1-C6	-2.84	119.87	125.10
4	B	501	GSP	C2-N1-C6	-2.83	119.88	125.10
4	I	501	GSP	C2-N1-C6	-2.83	119.89	125.10
4	G	501	GSP	C3'-C2'-C1'	2.46	104.67	100.98
4	B	501	GSP	C3'-C2'-C1'	2.45	104.67	100.98
4	H	501	GSP	C3'-C2'-C1'	2.45	104.66	100.98
4	I	501	GSP	C3'-C2'-C1'	2.43	104.64	100.98
3	D	501	GTP	O6-C6-C5	-2.17	120.14	124.37
3	F	501	GTP	O6-C6-C5	-2.15	120.17	124.37
3	A	501	GTP	O6-C6-C5	-2.15	120.18	124.37
4	B	501	GSP	O6-C6-C5	-2.14	120.19	124.37
4	G	501	GSP	O6-C6-C5	-2.13	120.21	124.37
3	E	501	GTP	O6-C6-C5	-2.12	120.23	124.37
4	I	501	GSP	O6-C6-C5	-2.11	120.25	124.37
4	H	501	GSP	O6-C6-C5	-2.10	120.27	124.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	C4'-C5'-O5'-PA
3	D	501	GTP	C4'-C5'-O5'-PA
3	E	501	GTP	C4'-C5'-O5'-PA
3	F	501	GTP	C4'-C5'-O5'-PA
3	F	501	GTP	C3'-C4'-C5'-O5'
3	A	501	GTP	C3'-C4'-C5'-O5'
3	D	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	D	501	GTP	O4'-C4'-C5'-O5'
3	E	501	GTP	O4'-C4'-C5'-O5'
3	F	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	C5'-O5'-PA-O3A
3	D	501	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	501	GTP	C5'-O5'-PA-O3A
3	F	501	GTP	C5'-O5'-PA-O3A
3	A	501	GTP	O4'-C4'-C5'-O5'

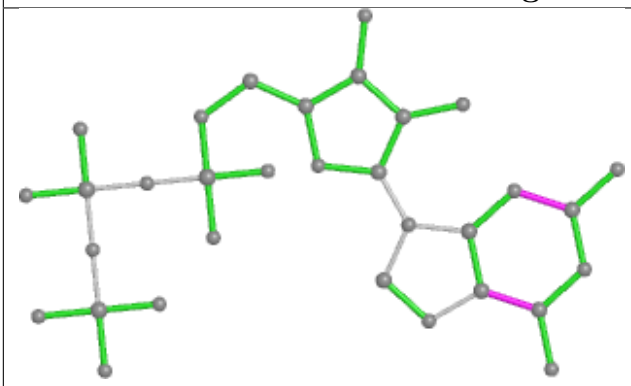
There are no ring outliers.

8 monomers are involved in 16 short contacts:

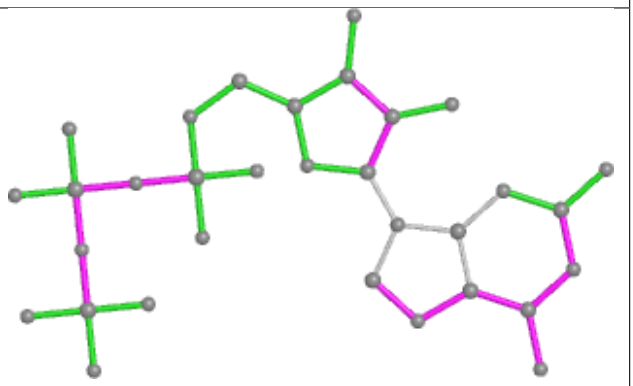
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	1	0
3	D	501	GTP	1	0
4	B	501	GSP	3	0
3	E	501	GTP	1	0
4	G	501	GSP	3	0
4	H	501	GSP	3	0
4	I	501	GSP	3	0
3	F	501	GTP	1	0

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.

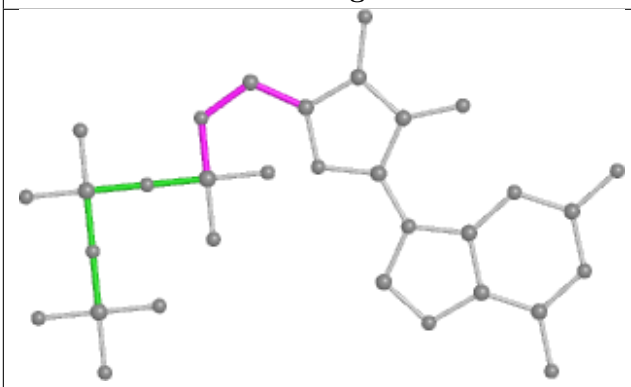
Ligand GTP A 501



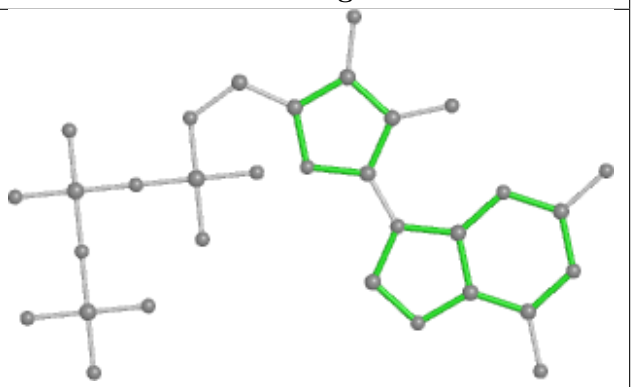
Bond lengths



Bond angles

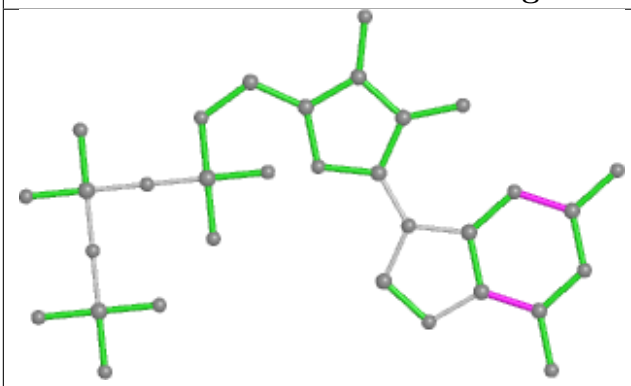


Torsions

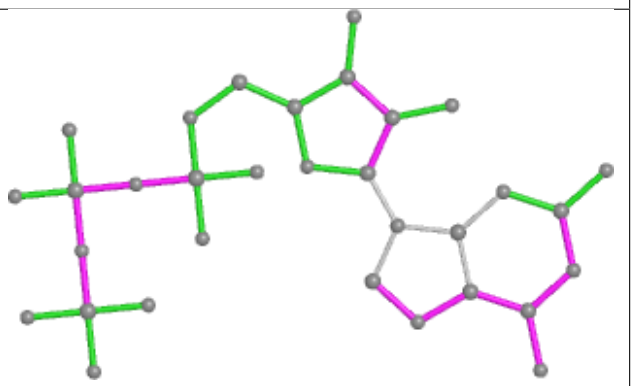


Rings

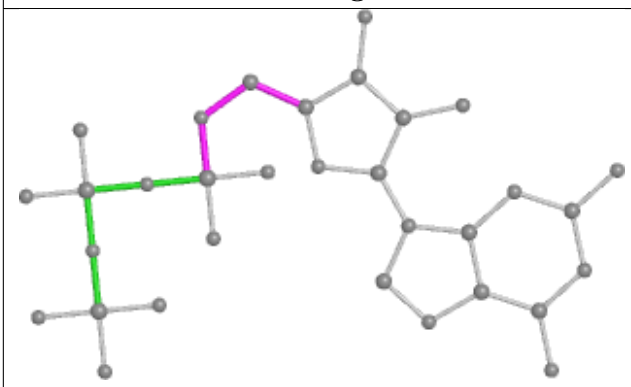
Ligand GTP D 501



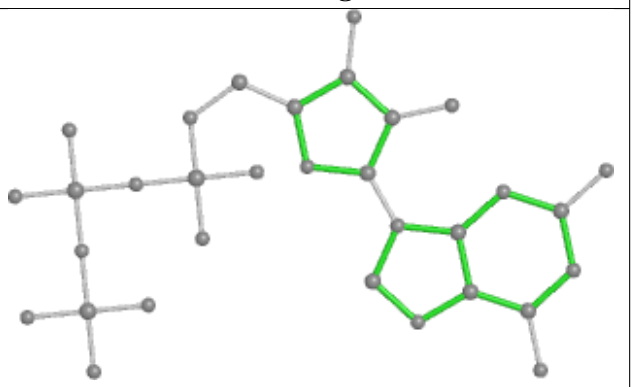
Bond lengths



Bond angles

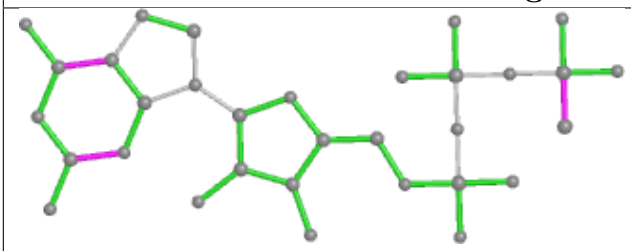


Torsions

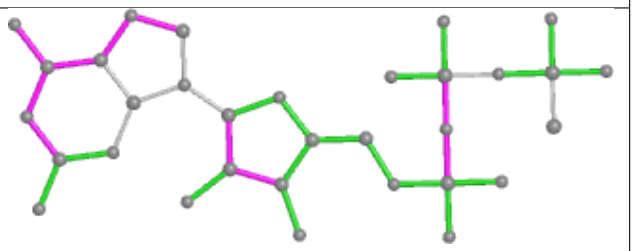


Rings

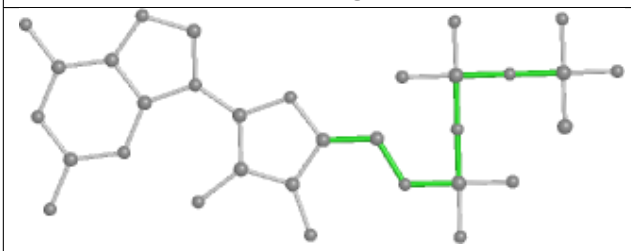
Ligand GSP B 501



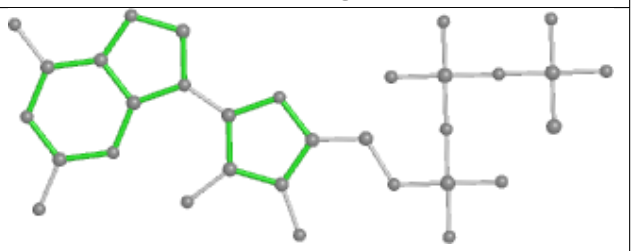
Bond lengths



Bond angles

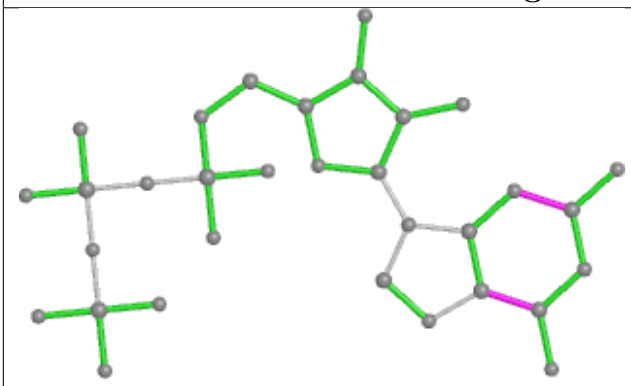


Torsions

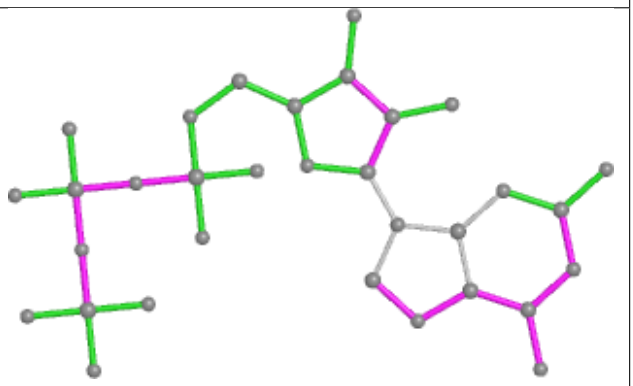


Rings

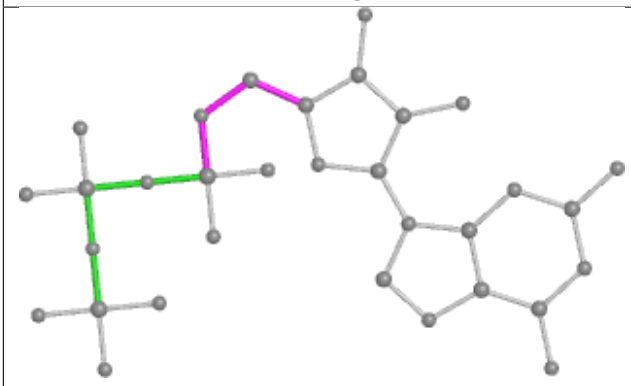
Ligand GTP E 501



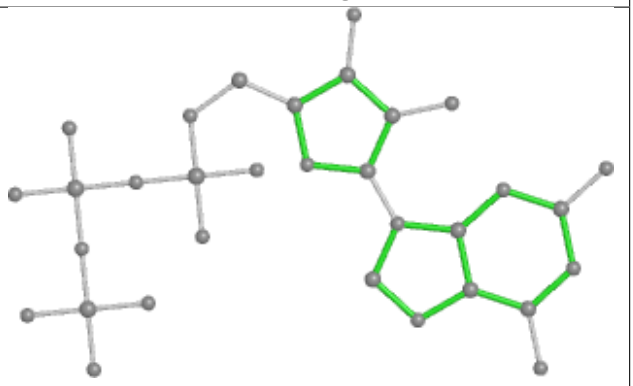
Bond lengths



Bond angles

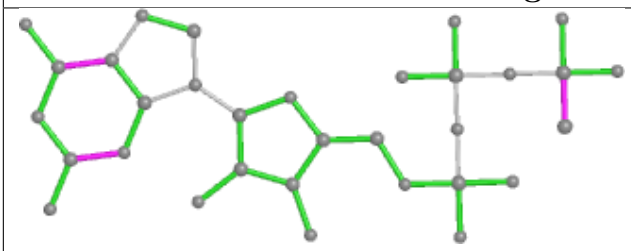


Torsions

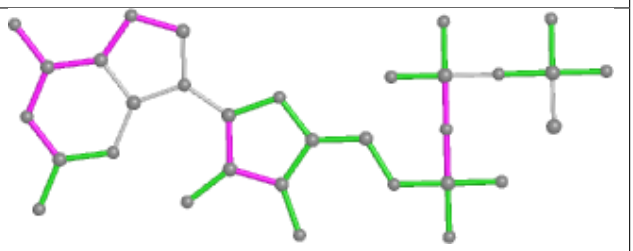


Rings

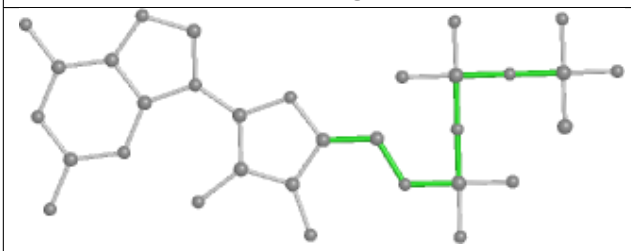
Ligand GSP G 501



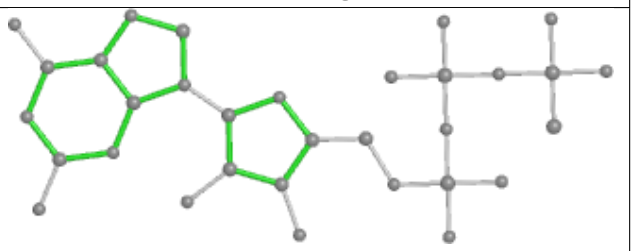
Bond lengths



Bond angles

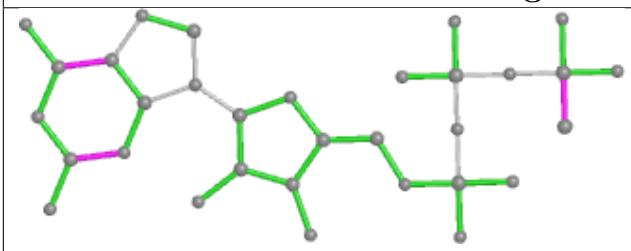


Torsions

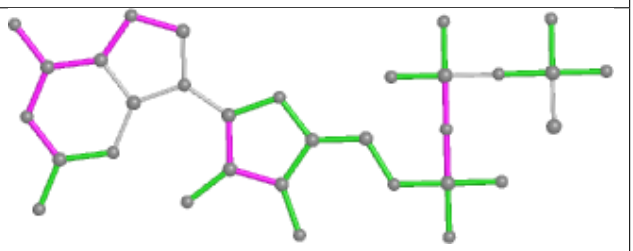


Rings

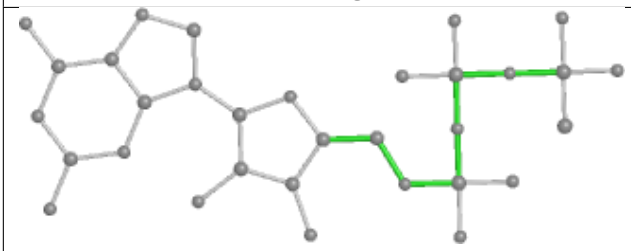
Ligand GSP H 501



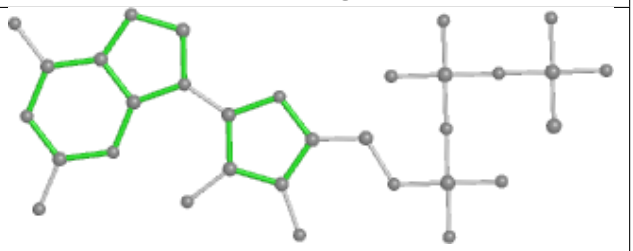
Bond lengths



Bond angles

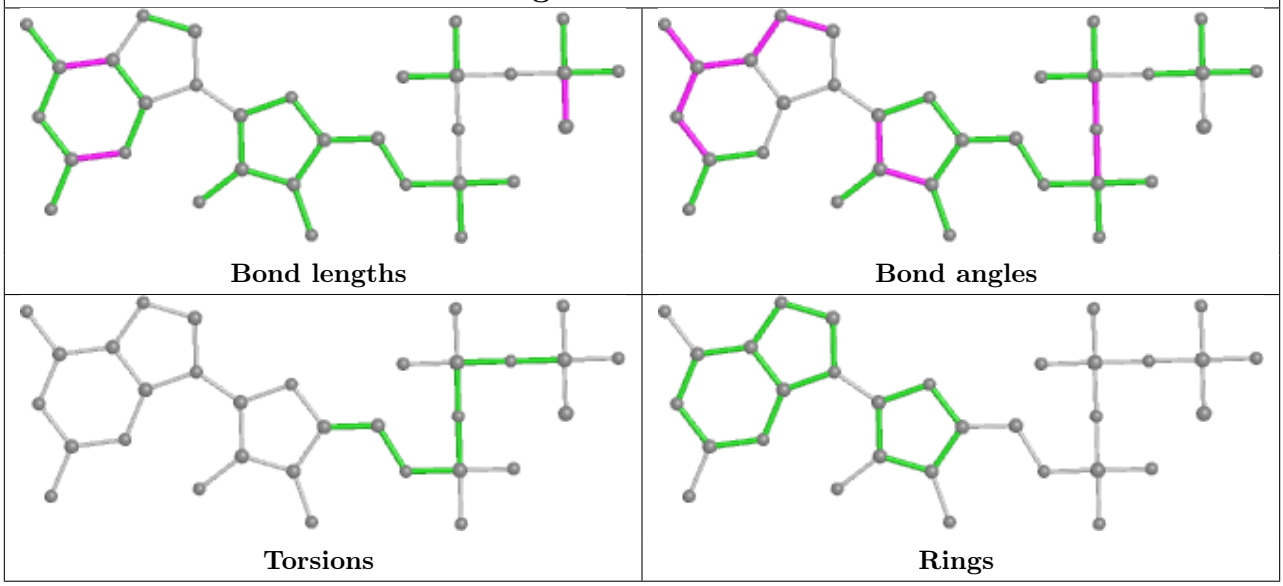


Torsions

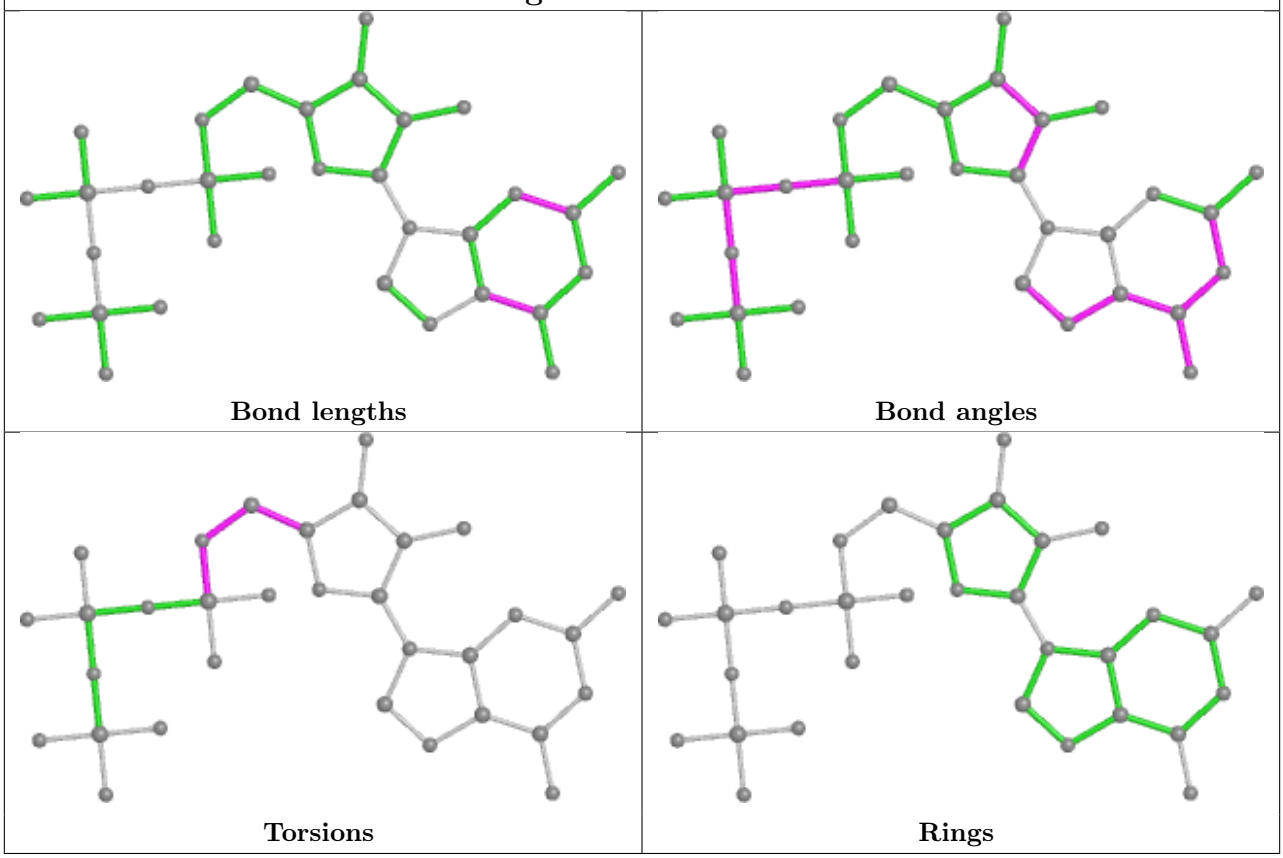


Rings

Ligand GSP I 501



Ligand GTP F 501



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.

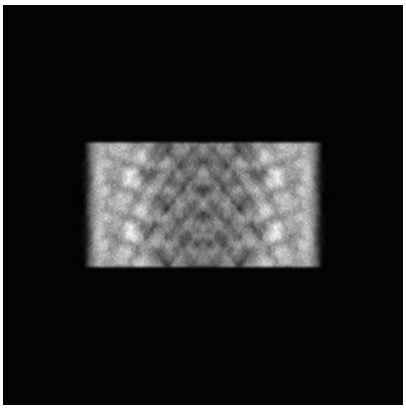
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34080. These allow visual inspection of the internal detail of the map and identification of artifacts.

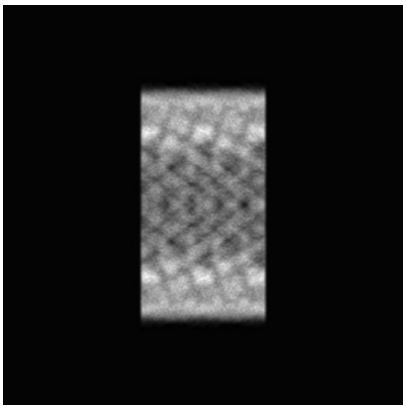
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

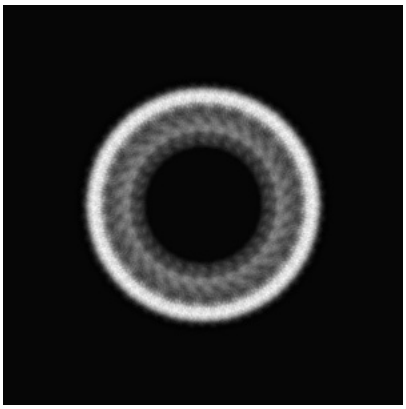
6.1.1 Primary map



X

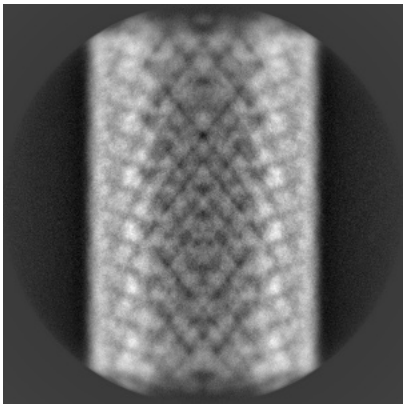


Y

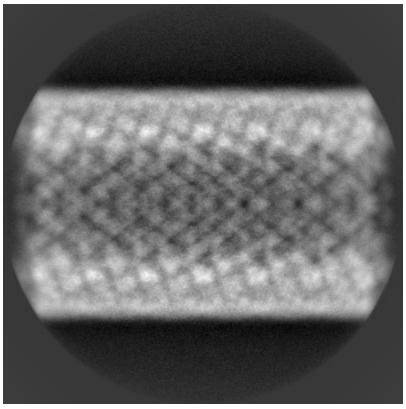


Z

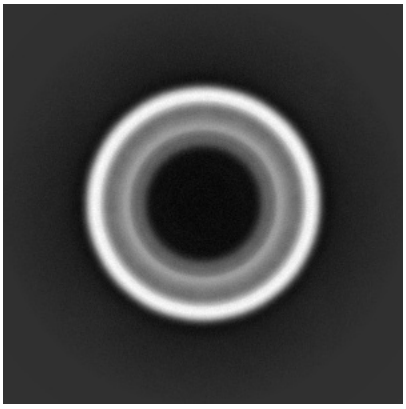
6.1.2 Raw map



X



Y

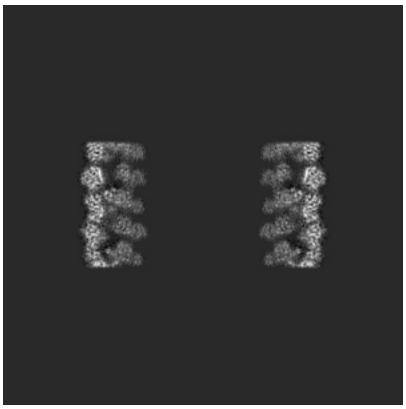


Z

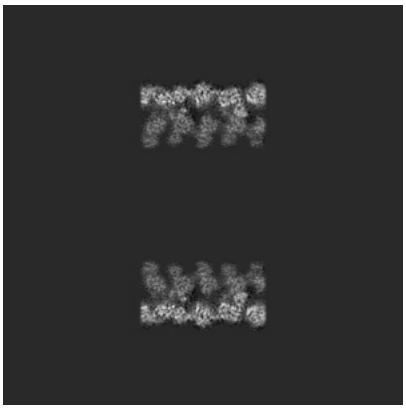
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

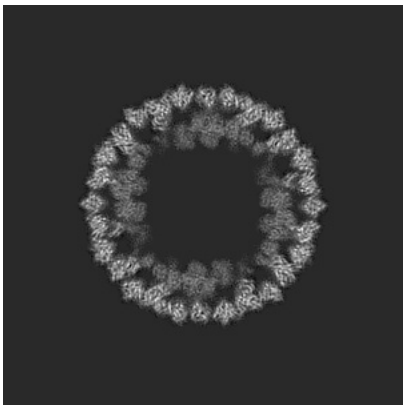
6.2.1 Primary map



X Index: 400

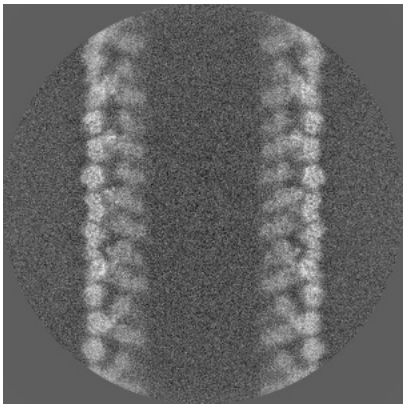


Y Index: 400

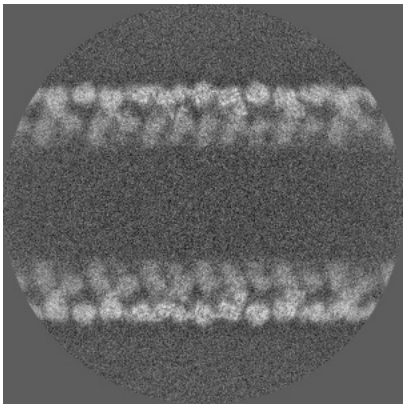


Z Index: 400

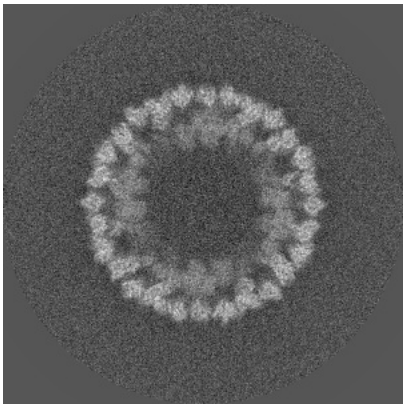
6.2.2 Raw map



X Index: 400



Y Index: 400

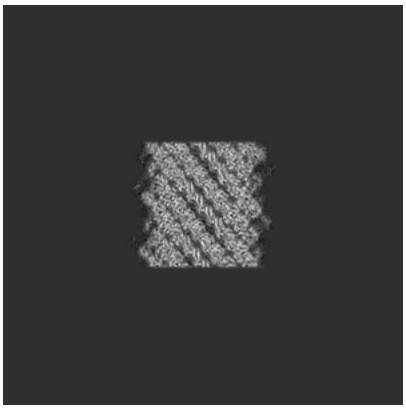


Z Index: 400

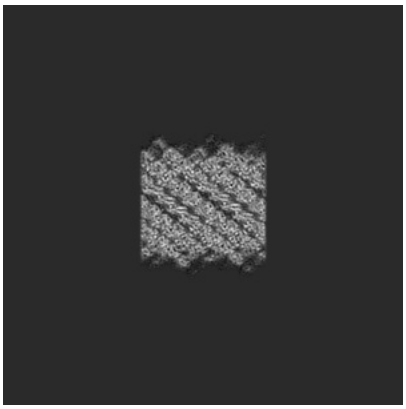
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

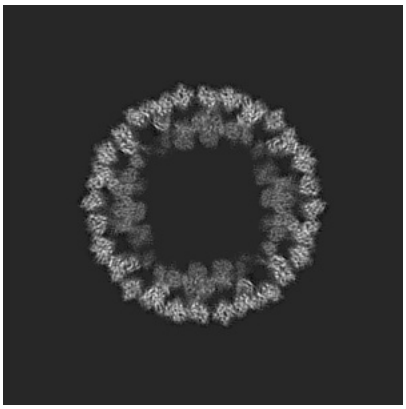
6.3.1 Primary map



X Index: 606

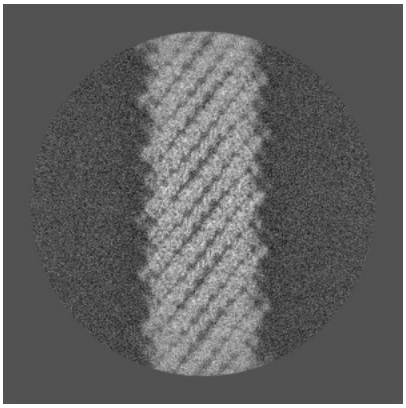


Y Index: 193

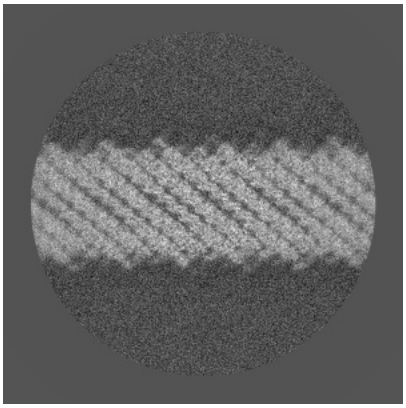


Z Index: 404

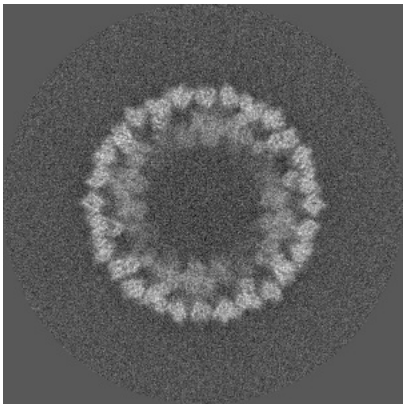
6.3.2 Raw map



X Index: 194



Y Index: 194

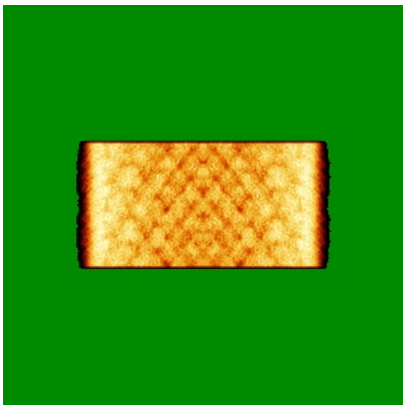


Z Index: 398

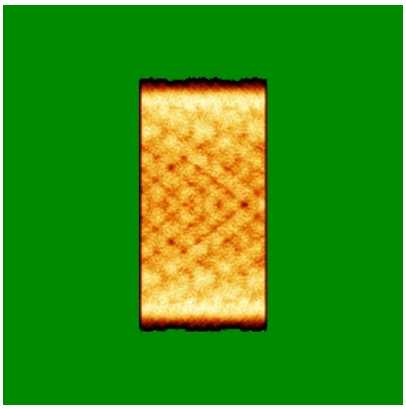
The images above show the largest variance slices of the map in three orthogonal directions.

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

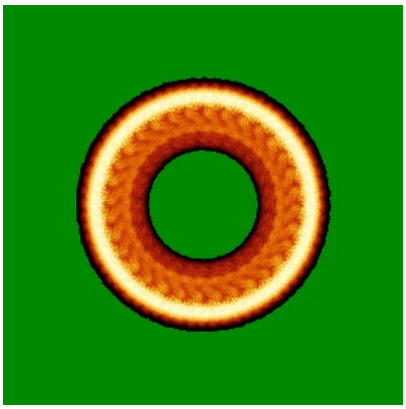
6.4.1 Primary map



X

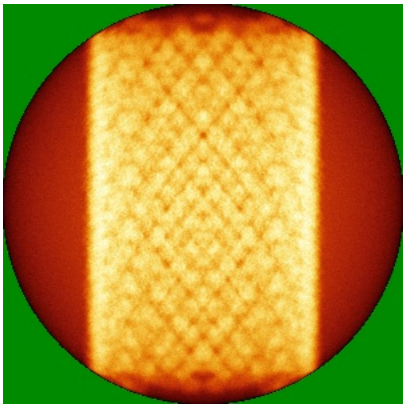


Y

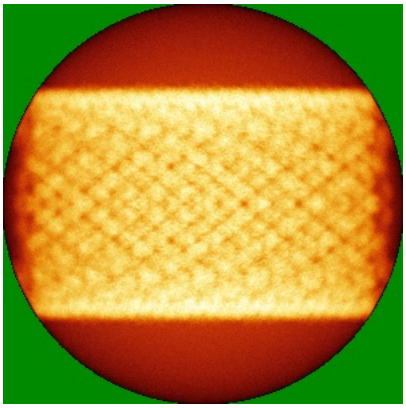


Z

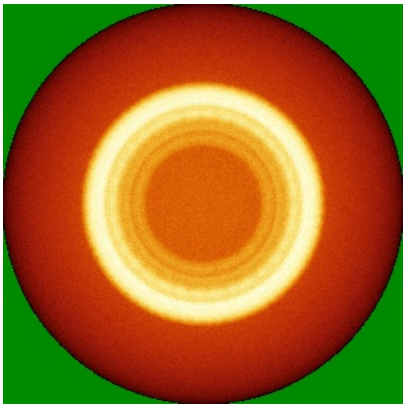
6.4.2 Raw map



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 0.005. 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.

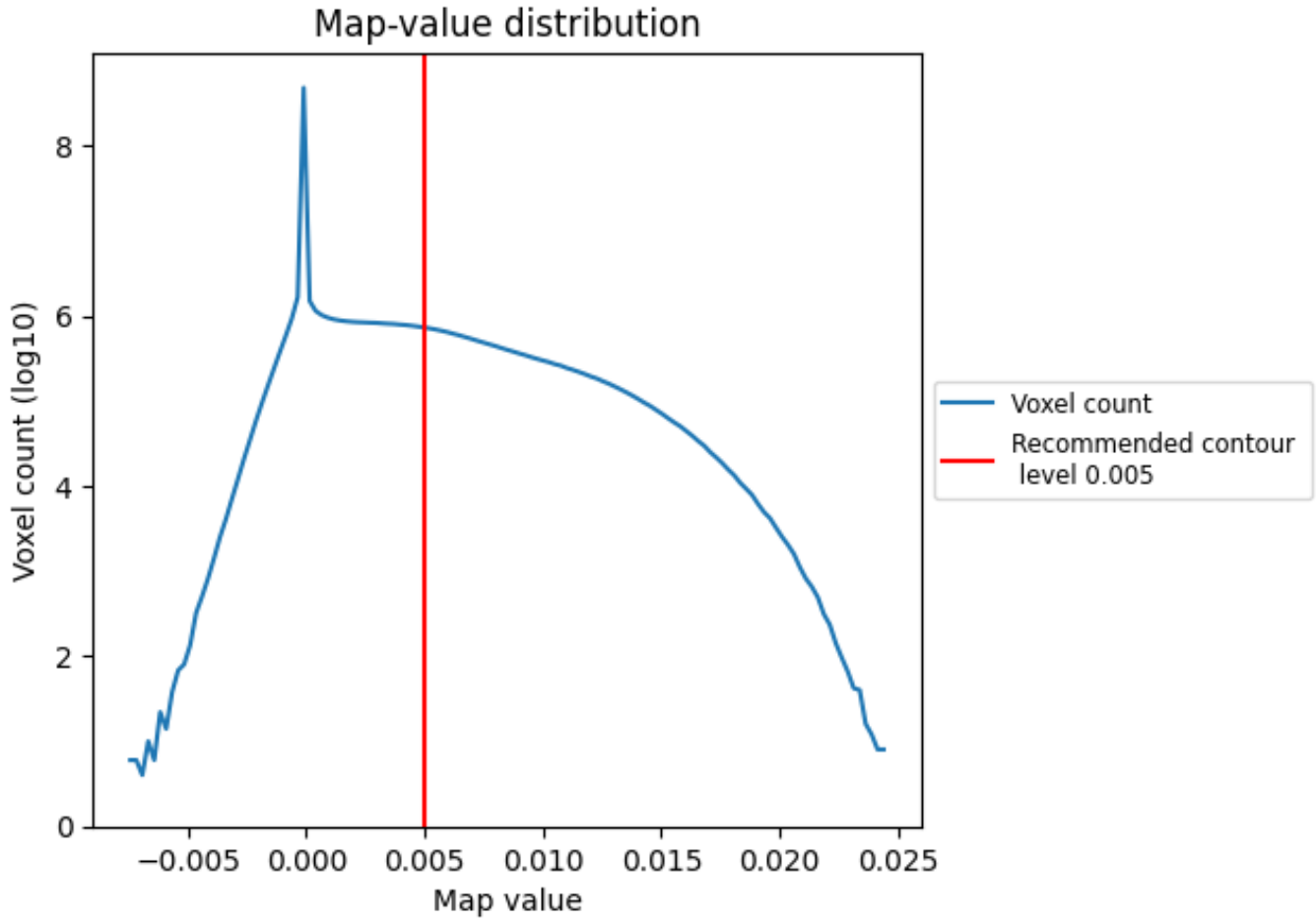
6.6 Mask visualisation (i)

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

7 Map analysis

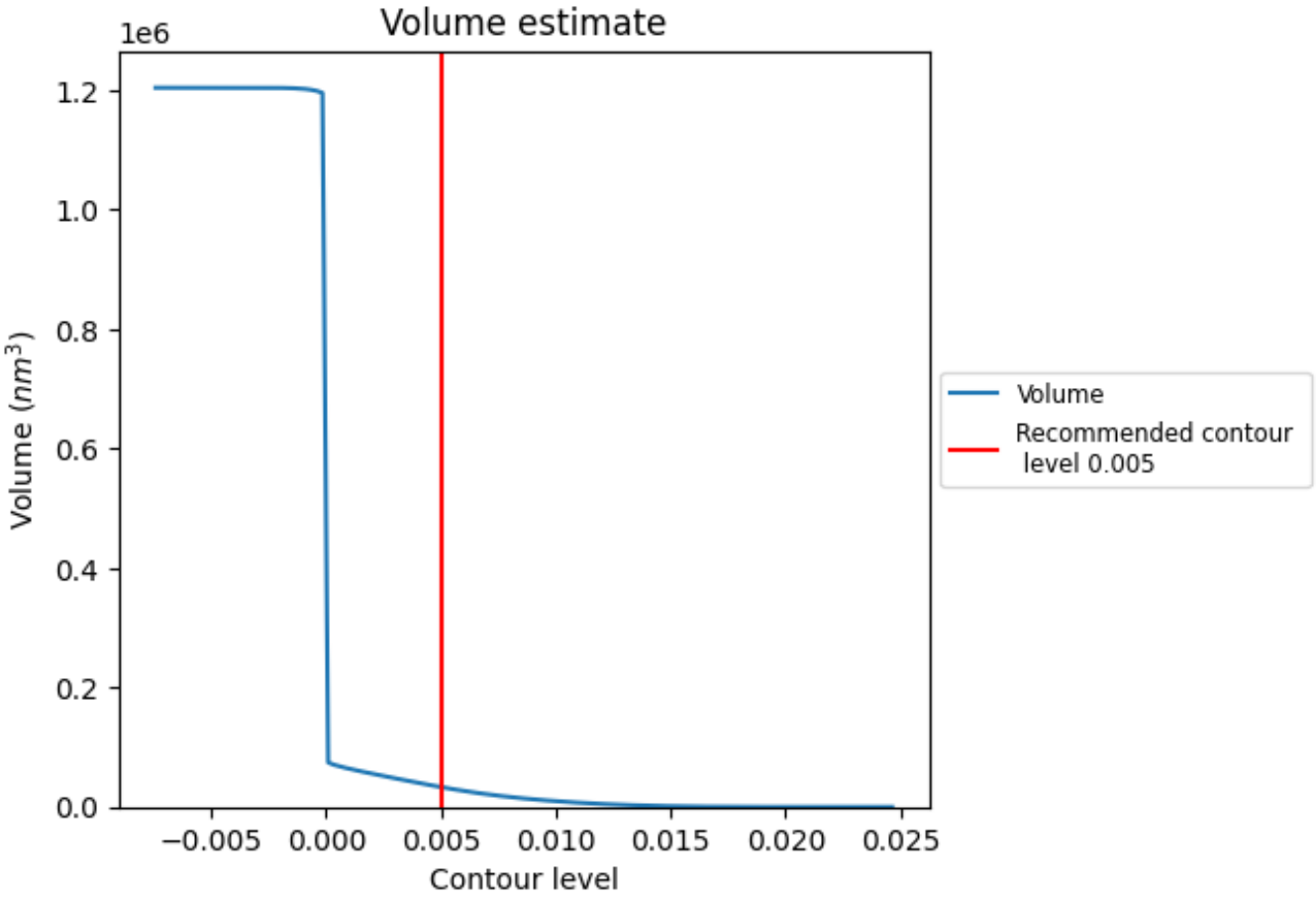
This section contains the results of statistical analysis of the map.

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.

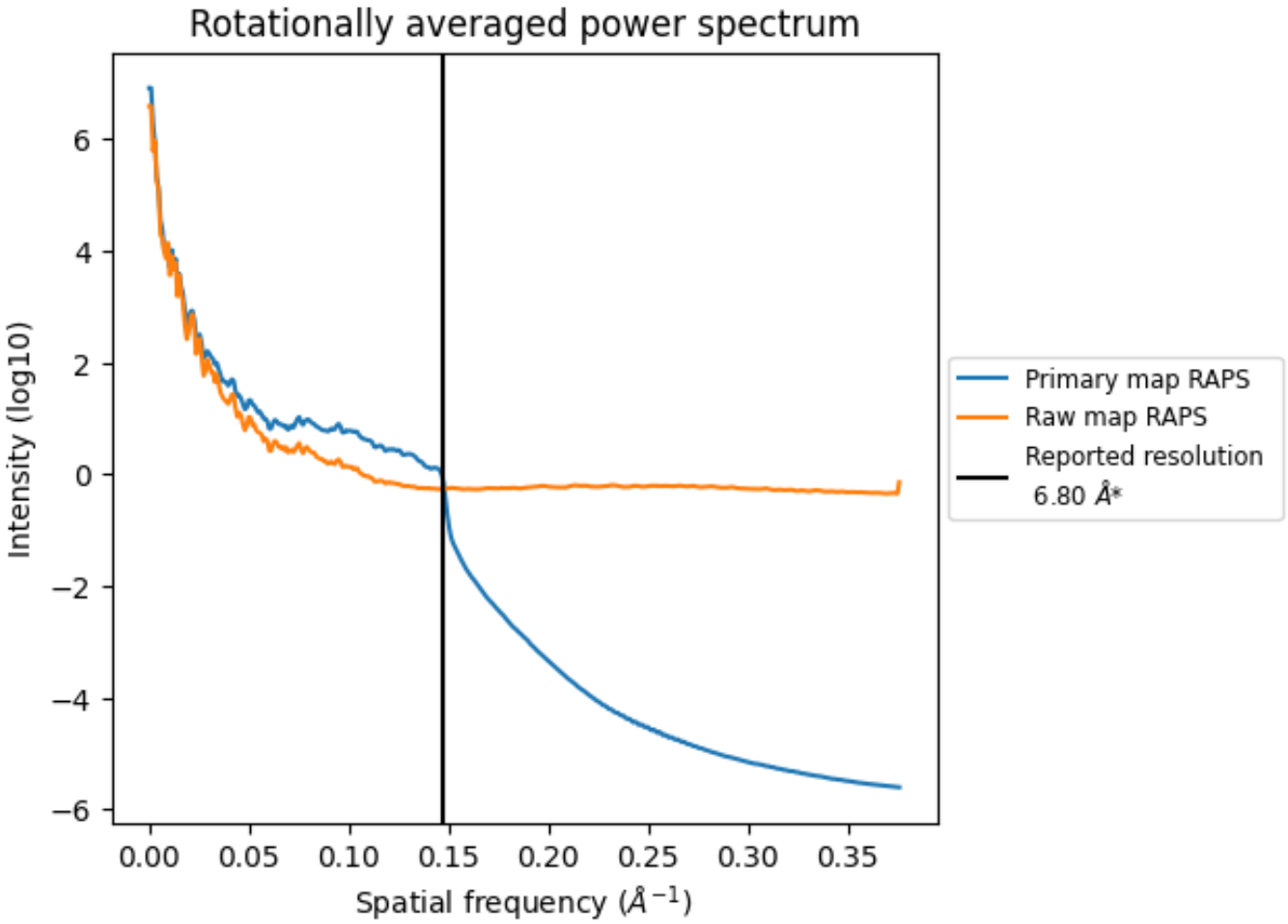
7.2 Volume estimate



The volume at the recommended contour level is 33306 nm^3; this corresponds to an approximate mass of 30086 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)

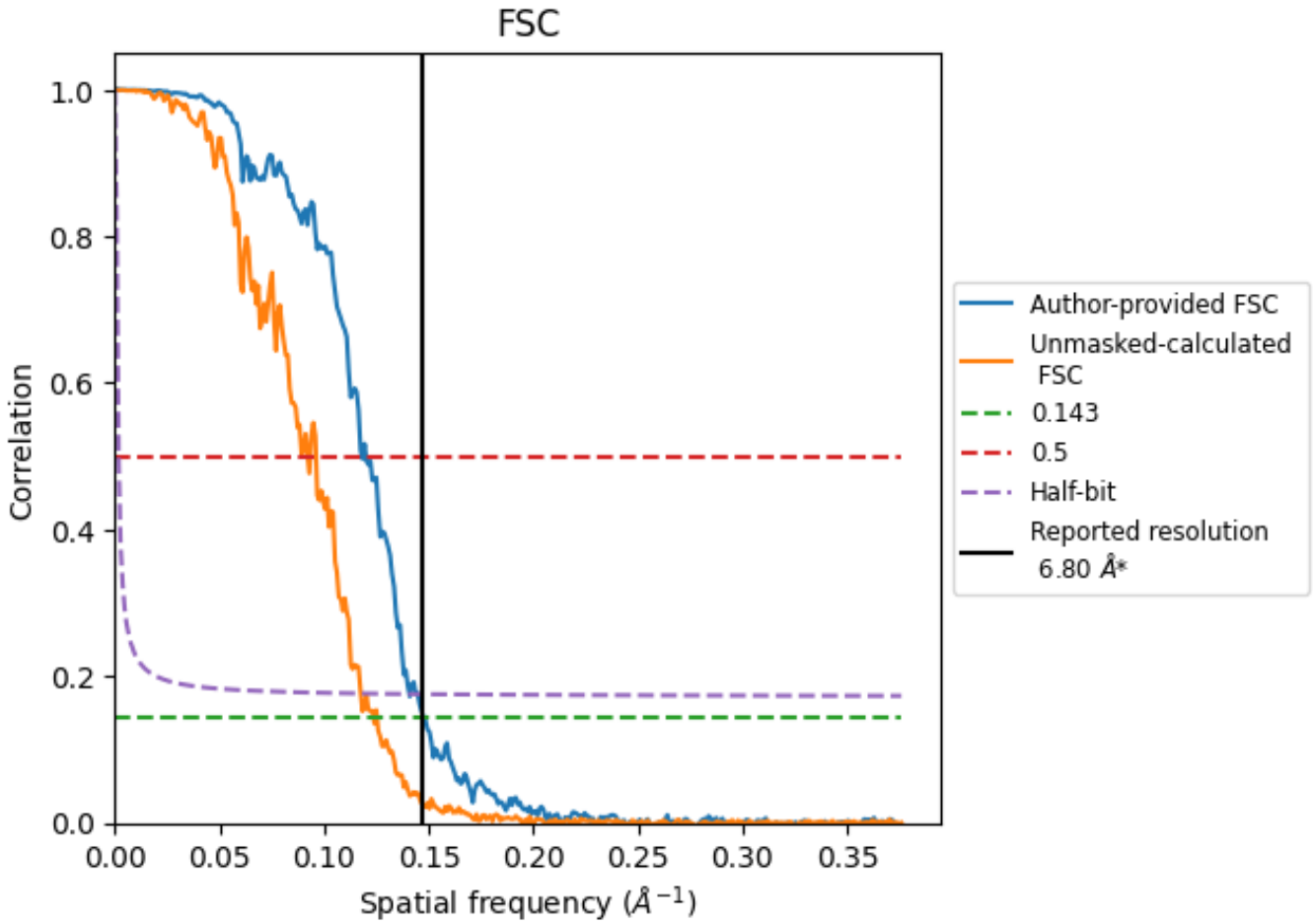


*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

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 0.147 Å^{-1}

8.2 Resolution estimates (i)

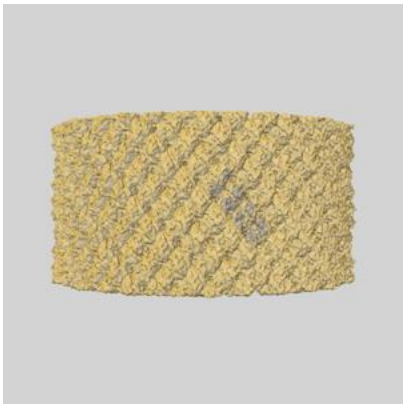
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.77	8.47	7.10
Unmasked-calculated*	8.09	10.83	8.50

*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 8.09 differs from the reported value 6.8 by more than 10 %

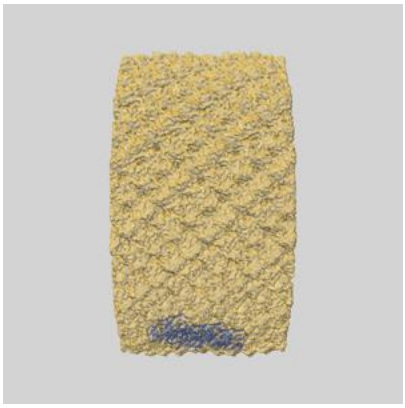
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34080 and PDB model 7YSQ. Per-residue inclusion information can be found in section 3 on page 6.

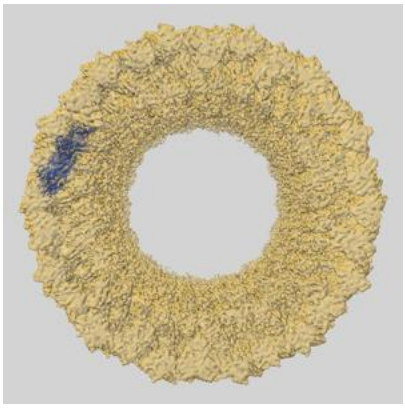
9.1 Map-model overlay



X



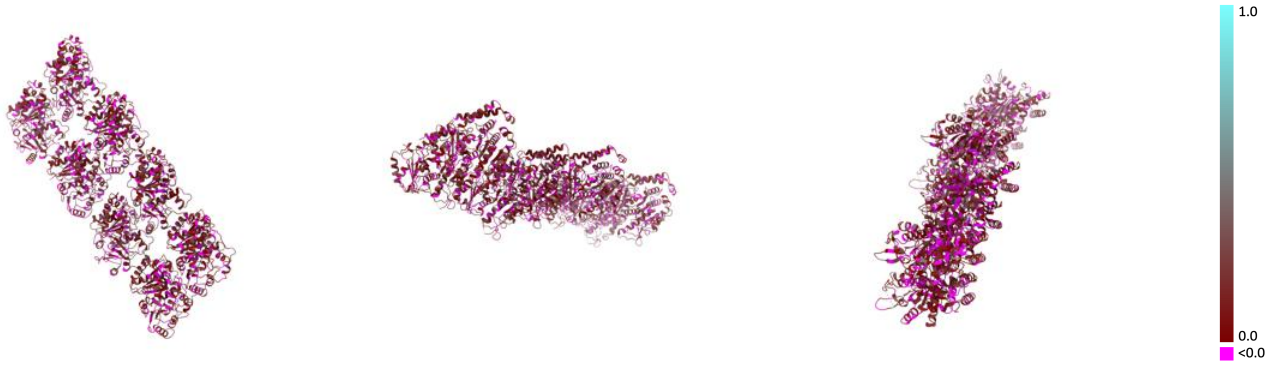
Y



Z

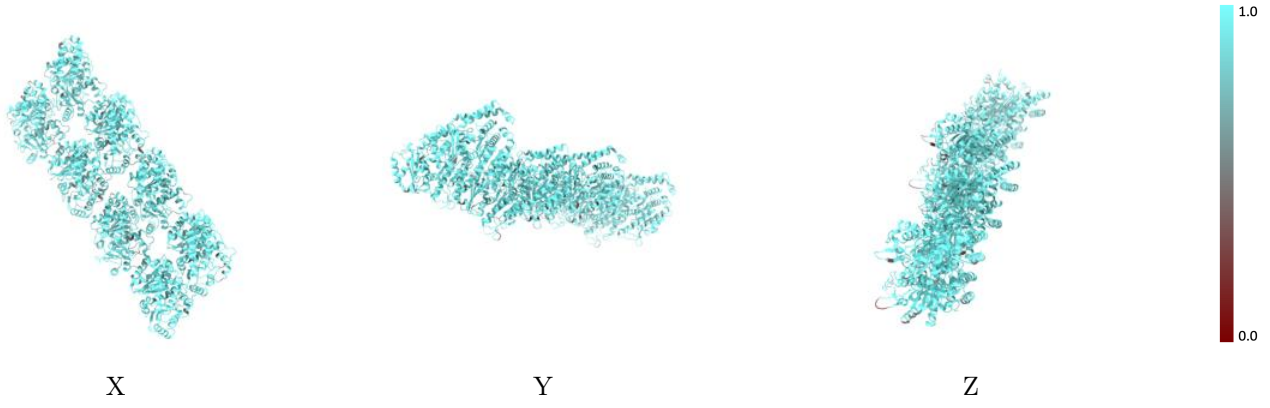
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



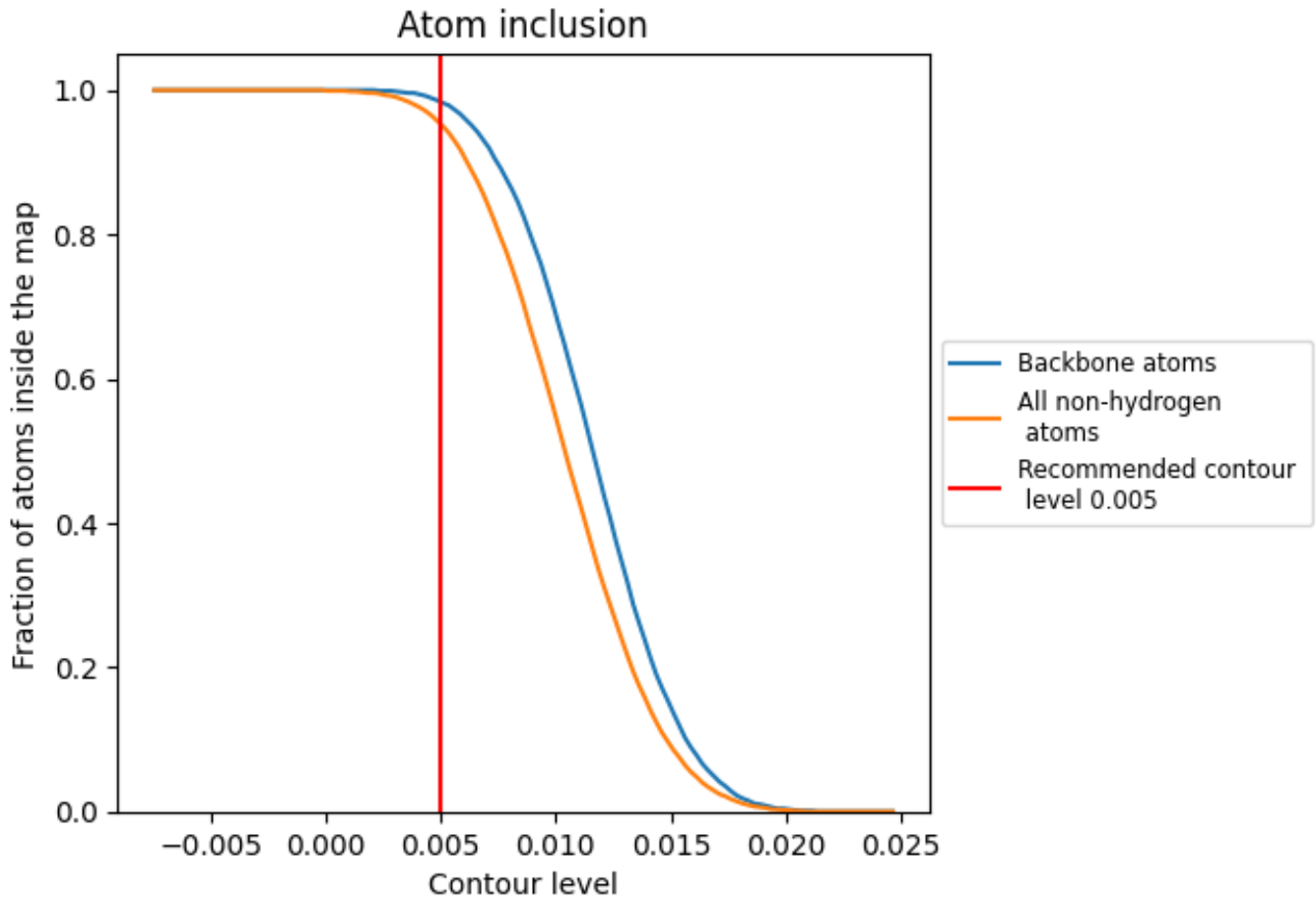
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.1080
A	0.9410	0.0980
B	0.9530	0.1000
D	0.9580	0.1220
E	0.9480	0.1050
F	0.9470	0.1130
G	0.9600	0.0990
H	0.9580	0.1200
I	0.9580	0.1090