



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:56 AM UTC

PDB ID : 5TWV / pdb_00005twv
EMDB ID : EMD-8470
Title : Cryo-EM structure of the pancreatic ATP-sensitive K⁺ channel SUR1/Kir6.2
in the presence of ATP and glibenclamide
Authors : Martin, G.M.; Yoshioka, C.; Chen, J.Z.; Shyng, S.L.
Deposited on : 2016-11-14
Resolution : 6.30 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

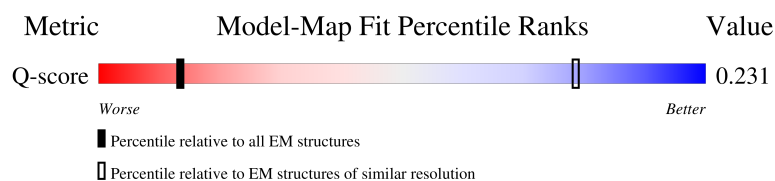
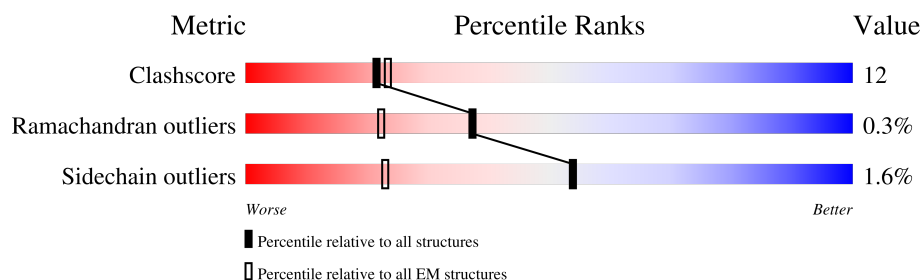
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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

Mol	Chain	Length	Quality of chain
1	A	390	 7% 53% 28% • 17%
1	C	390	 7% 53% 27% • 17%
1	E	390	 7% 53% 27% • 17%
1	G	390	 7% 52% 28% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	1590	19% 75% 12% 14%
2	D	1590	19% 74% 12% 14%
2	F	1590	19% 75% 11% 14%
2	H	1590	19% 74% 12% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41080 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	C	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	E	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		
1	G	325	Total	C	N	O	S	0	0
			2479	1598	422	444	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	D	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	F	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		
2	H	1375	Total	C	N	O	S	0	0
			7760	4866	1450	1439	5		

There are 32 discrepancies between the modelled and reference sequences:

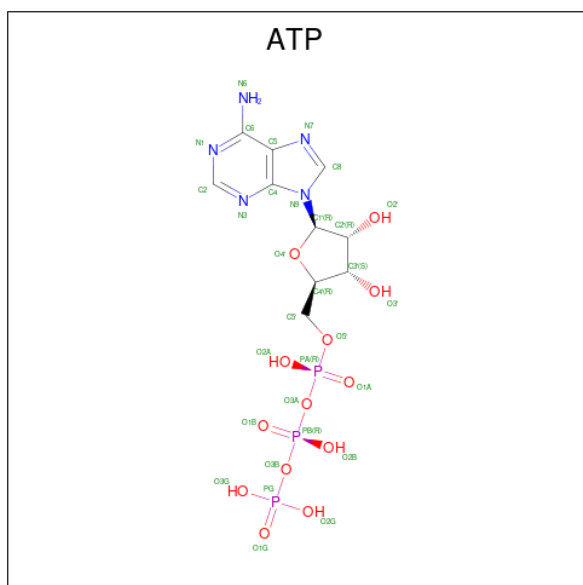
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	ASP	-	expression tag	UNP Q09427
B	-6	TYR	-	expression tag	UNP Q09427
B	-5	LYS	-	expression tag	UNP Q09427
B	-4	ASP	-	expression tag	UNP Q09427
B	-3	ASP	-	expression tag	UNP Q09427
B	-2	ASP	-	expression tag	UNP Q09427
B	-1	ASP	-	expression tag	UNP Q09427
B	0	LYS	-	expression tag	UNP Q09427
D	-7	ASP	-	expression tag	UNP Q09427

Continued on next page...

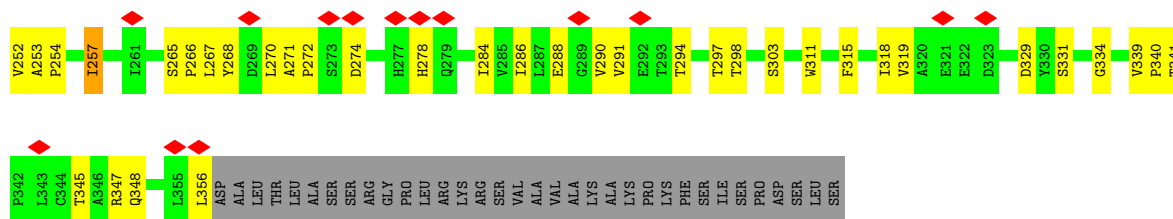
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	TYR	-	expression tag	UNP Q09427
D	-5	LYS	-	expression tag	UNP Q09427
D	-4	ASP	-	expression tag	UNP Q09427
D	-3	ASP	-	expression tag	UNP Q09427
D	-2	ASP	-	expression tag	UNP Q09427
D	-1	ASP	-	expression tag	UNP Q09427
D	0	LYS	-	expression tag	UNP Q09427
F	-7	ASP	-	expression tag	UNP Q09427
F	-6	TYR	-	expression tag	UNP Q09427
F	-5	LYS	-	expression tag	UNP Q09427
F	-4	ASP	-	expression tag	UNP Q09427
F	-3	ASP	-	expression tag	UNP Q09427
F	-2	ASP	-	expression tag	UNP Q09427
F	-1	ASP	-	expression tag	UNP Q09427
F	0	LYS	-	expression tag	UNP Q09427
H	-7	ASP	-	expression tag	UNP Q09427
H	-6	TYR	-	expression tag	UNP Q09427
H	-5	LYS	-	expression tag	UNP Q09427
H	-4	ASP	-	expression tag	UNP Q09427
H	-3	ASP	-	expression tag	UNP Q09427
H	-2	ASP	-	expression tag	UNP Q09427
H	-1	ASP	-	expression tag	UNP Q09427
H	0	LYS	-	expression tag	UNP Q09427

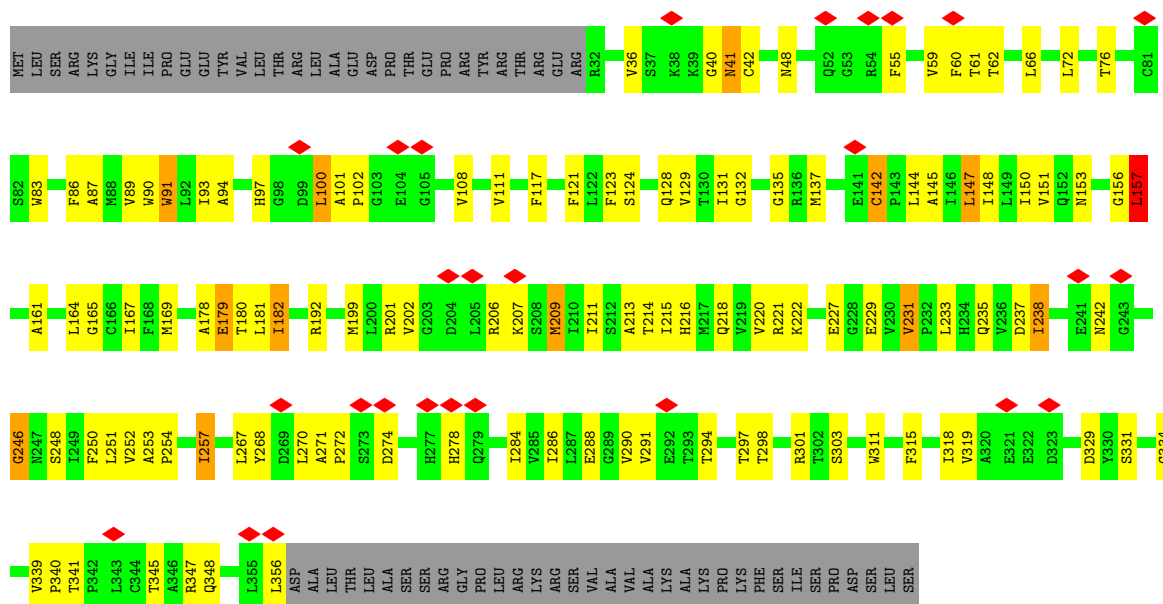
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



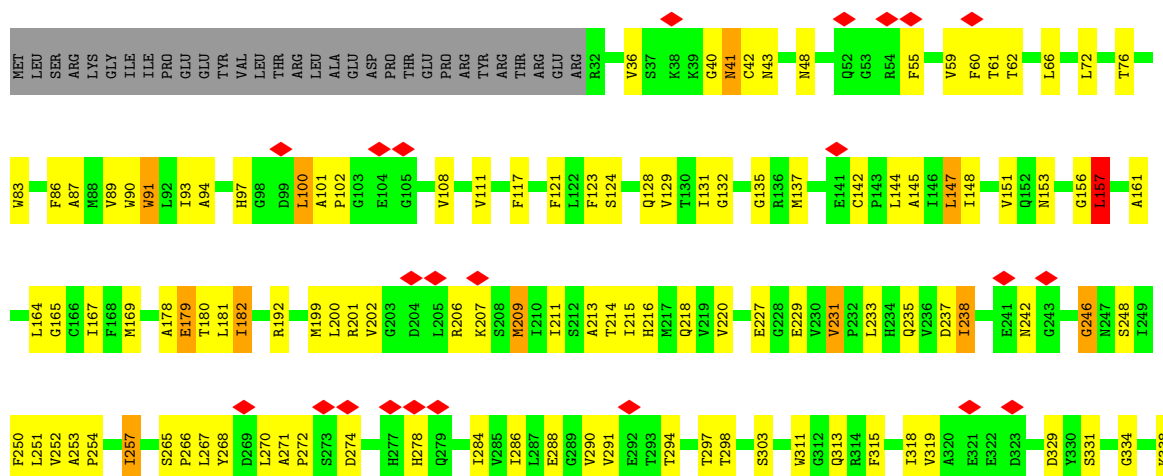
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0



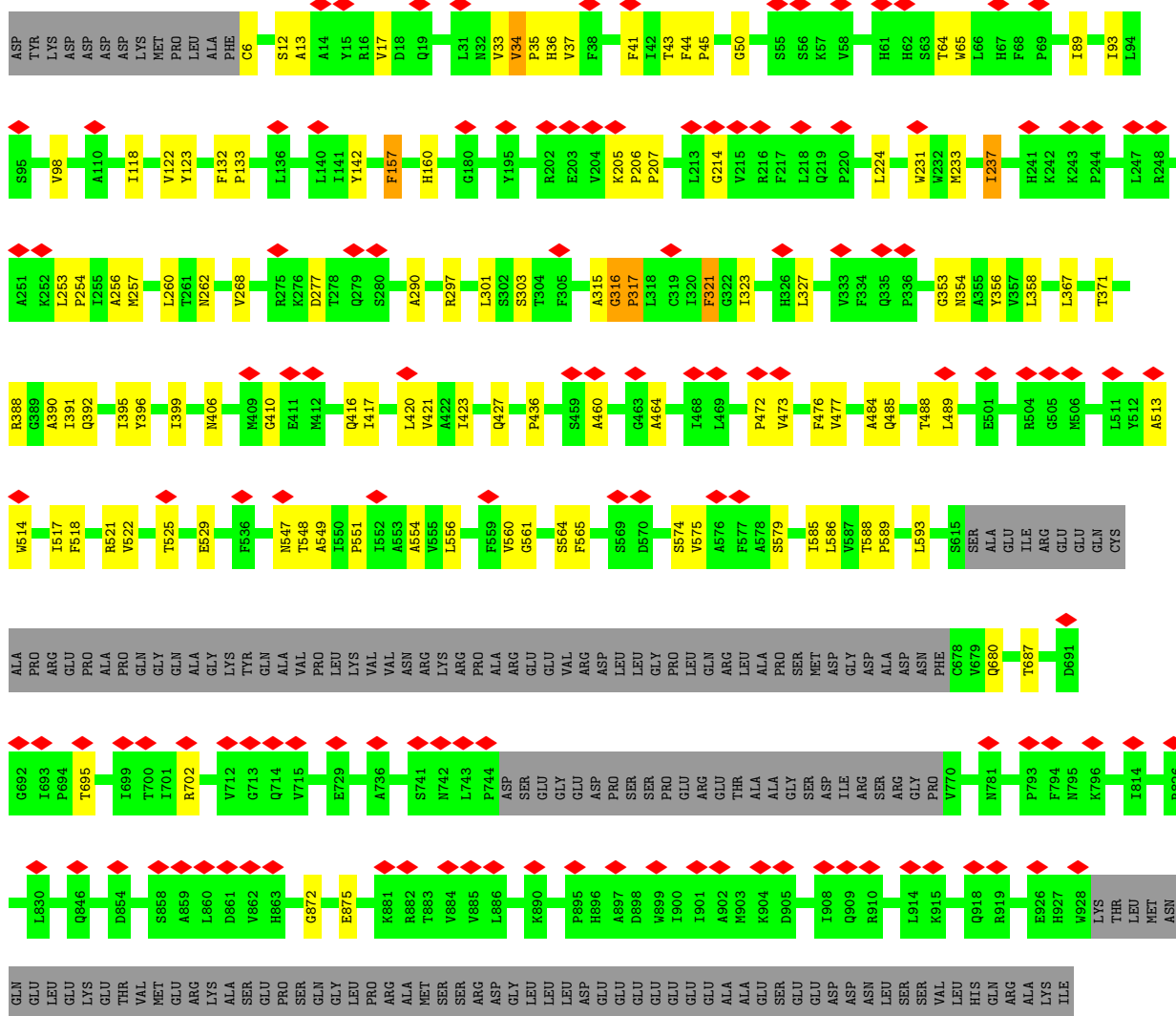
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

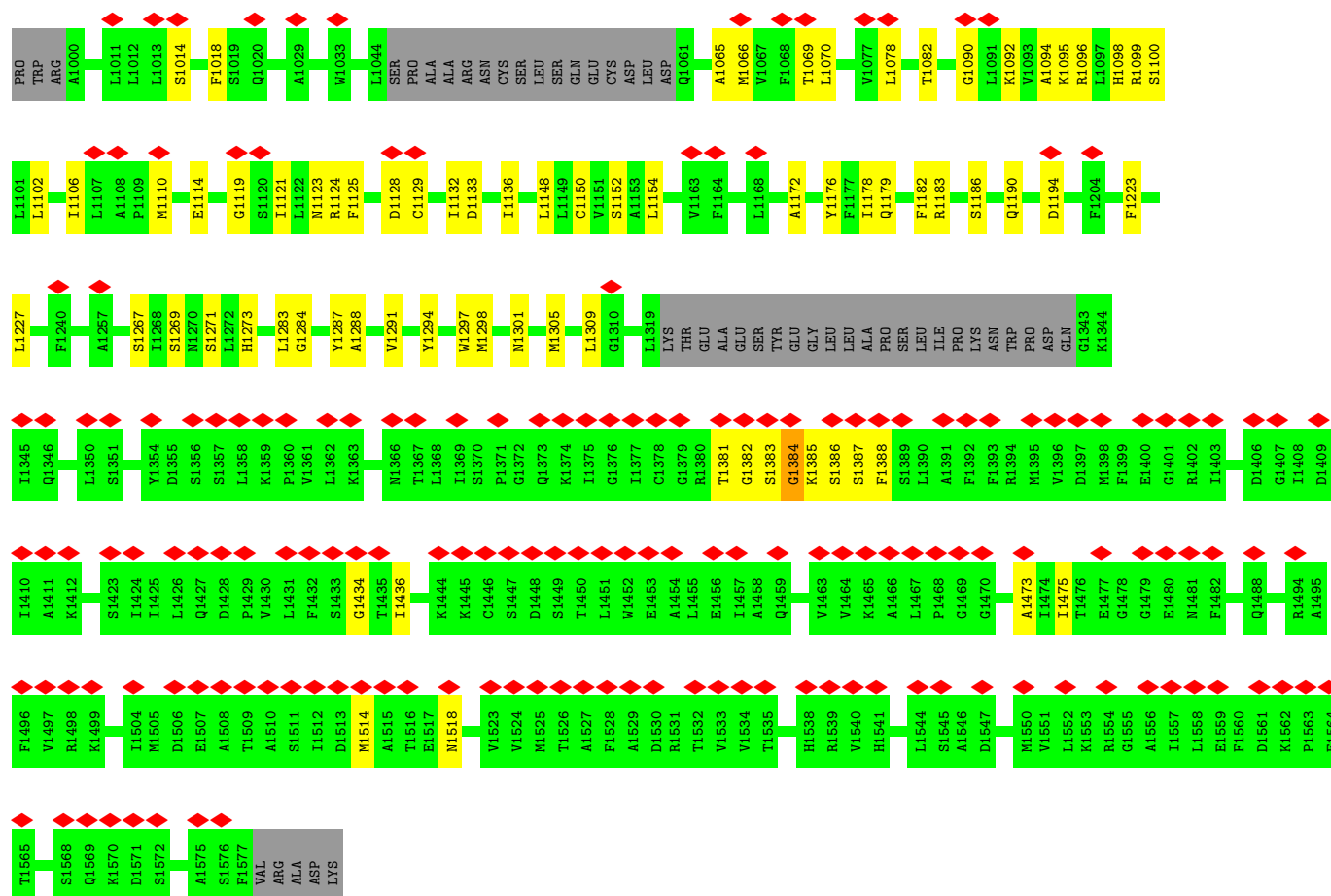


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

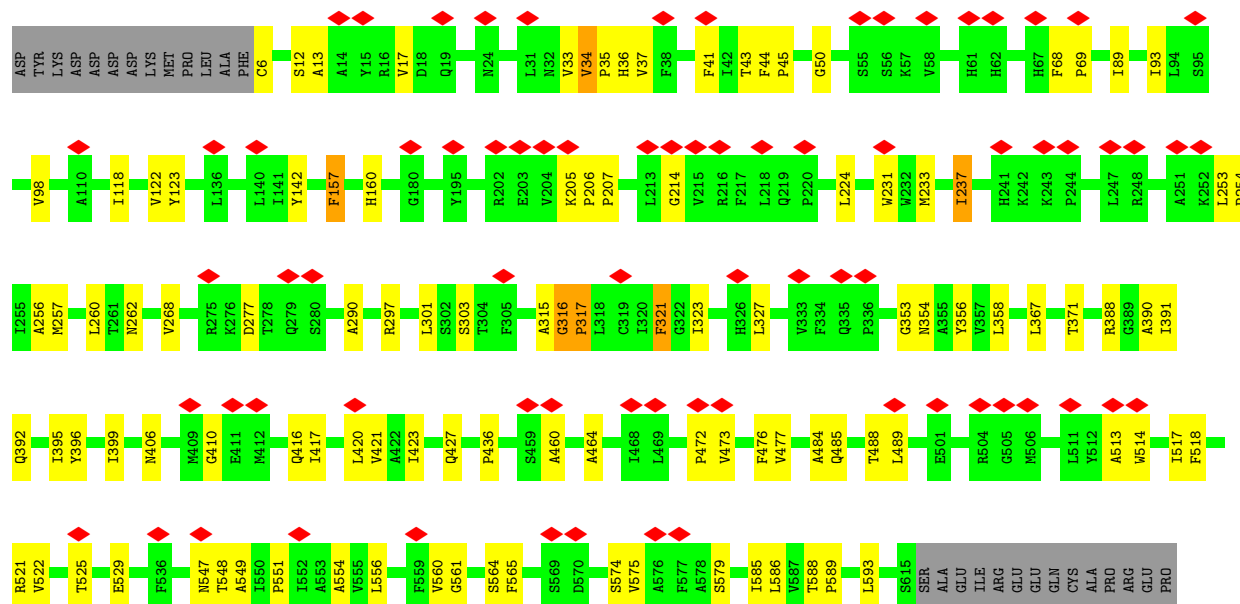
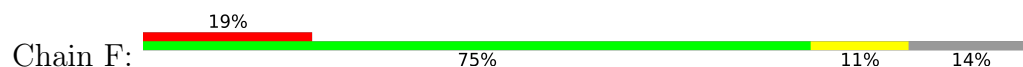








• Molecule 2: ATP-binding cassette sub-family C member 8





E1559	F1560	D1561	K1562	P1563	E1564	T1565	S1568	Q1569	K1570	D1571	S1572	A1575	S1576	F1577	VAL	ARG	ALA	ASP	LYS
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.027736	Depositor
Map size (Å)	233.92, 233.92, 233.92	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/2536	1.15	28/3459 (0.8%)
1	C	0.42	0/2536	1.15	28/3459 (0.8%)
1	E	0.41	0/2536	1.15	31/3459 (0.9%)
1	G	0.41	0/2536	1.15	28/3459 (0.8%)
2	B	0.28	0/7912	0.81	16/10995 (0.1%)
2	D	0.29	0/7912	0.81	16/10995 (0.1%)
2	F	0.29	0/7912	0.81	16/10995 (0.1%)
2	H	0.29	0/7912	0.81	16/10995 (0.1%)
All	All	0.32	0/41792	0.90	179/57816 (0.3%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLY	N-CA-C	12.56	126.05	111.36
1	C	246	GLY	N-CA-C	12.56	126.05	111.36
1	E	246	GLY	N-CA-C	12.56	126.05	111.36
1	G	246	GLY	N-CA-C	12.56	126.05	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	VAL	N-CA-C	11.98	122.82	110.72
1	C	59	VAL	N-CA-C	11.98	122.82	110.72
1	E	59	VAL	N-CA-C	11.98	122.82	110.72
1	G	59	VAL	N-CA-C	11.98	122.82	110.72
2	B	321	PHE	CA-C-N	9.69	132.34	120.13
2	B	321	PHE	C-N-CA	9.69	132.34	120.13
2	F	321	PHE	CA-C-N	9.69	132.34	120.13
2	F	321	PHE	C-N-CA	9.69	132.34	120.13
2	H	321	PHE	CA-C-N	9.69	132.34	120.13
2	H	321	PHE	C-N-CA	9.69	132.34	120.13
2	D	321	PHE	CA-C-N	9.68	132.32	120.13
2	D	321	PHE	C-N-CA	9.68	132.32	120.13
2	F	17	VAL	N-CA-C	9.05	119.85	110.62
2	H	17	VAL	N-CA-C	9.05	119.85	110.62
2	B	17	VAL	N-CA-C	9.02	119.82	110.62
2	D	17	VAL	N-CA-C	9.00	119.80	110.62
2	B	43	THR	N-CA-C	8.12	120.13	111.28
2	D	43	THR	N-CA-C	8.12	120.13	111.28
2	F	43	THR	N-CA-C	8.12	120.13	111.28
2	H	43	THR	N-CA-C	8.12	120.13	111.28
2	B	549	ALA	CA-C-N	-7.84	115.30	120.24
2	B	549	ALA	C-N-CA	-7.84	115.30	120.24
2	D	549	ALA	CA-C-N	-7.84	115.30	120.24
2	D	549	ALA	C-N-CA	-7.84	115.30	120.24
2	F	549	ALA	CA-C-N	-7.84	115.30	120.24
2	F	549	ALA	C-N-CA	-7.84	115.30	120.24
2	H	549	ALA	CA-C-N	-7.84	115.30	120.24
2	H	549	ALA	C-N-CA	-7.84	115.30	120.24
1	C	100	LEU	N-CA-C	7.49	120.51	111.82
1	G	100	LEU	N-CA-C	7.49	120.51	111.82
1	A	100	LEU	N-CA-C	7.47	120.48	111.82
1	E	100	LEU	N-CA-C	7.47	120.48	111.82
1	E	207	LYS	N-CA-C	-7.40	104.25	113.28
1	A	207	LYS	N-CA-C	-7.37	104.29	113.28
1	C	207	LYS	N-CA-C	-7.37	104.29	113.28
1	G	207	LYS	N-CA-C	-7.37	104.29	113.28
1	E	91	TRP	N-CA-C	-6.71	105.10	113.28
1	G	91	TRP	N-CA-C	-6.71	105.10	113.28
1	A	91	TRP	N-CA-C	-6.71	105.10	113.28
1	C	91	TRP	N-CA-C	-6.71	105.10	113.28
1	C	231	VAL	CA-C-N	6.45	126.20	119.05
1	C	231	VAL	C-N-CA	6.45	126.20	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	VAL	CA-C-N	6.43	126.18	119.05
1	A	231	VAL	C-N-CA	6.43	126.18	119.05
1	G	231	VAL	CA-C-N	6.43	126.18	119.05
1	G	231	VAL	C-N-CA	6.43	126.18	119.05
1	E	231	VAL	CA-C-N	6.42	126.17	119.05
1	E	231	VAL	C-N-CA	6.42	126.17	119.05
2	F	33	VAL	N-CA-C	6.41	117.16	110.62
1	A	157	LEU	N-CA-C	-6.38	105.32	113.23
1	C	157	LEU	N-CA-C	-6.38	105.32	113.23
1	G	157	LEU	N-CA-C	-6.38	105.32	113.23
1	E	157	LEU	N-CA-C	-6.37	105.33	113.23
2	B	33	VAL	N-CA-C	6.37	117.11	110.62
2	D	33	VAL	N-CA-C	6.37	117.11	110.62
2	H	33	VAL	N-CA-C	6.36	117.10	110.62
2	B	317	PRO	N-CA-C	6.24	121.75	113.57
2	F	317	PRO	N-CA-C	6.24	121.75	113.57
2	H	317	PRO	N-CA-C	6.24	121.75	113.57
2	D	317	PRO	N-CA-C	6.21	121.70	113.57
1	E	238	ILE	CA-C-N	6.15	126.10	119.76
1	E	238	ILE	C-N-CA	6.15	126.10	119.76
1	G	238	ILE	CA-C-N	6.14	126.09	119.76
1	G	238	ILE	C-N-CA	6.14	126.09	119.76
1	C	66	LEU	N-CA-C	6.14	119.13	110.23
1	A	66	LEU	N-CA-C	6.13	119.12	110.23
1	G	66	LEU	N-CA-C	6.13	119.12	110.23
1	A	238	ILE	CA-C-N	6.11	126.06	119.76
1	A	238	ILE	C-N-CA	6.11	126.06	119.76
1	C	238	ILE	CA-C-N	6.11	126.06	119.76
1	C	238	ILE	C-N-CA	6.11	126.06	119.76
1	E	66	LEU	N-CA-C	6.11	119.09	110.23
1	C	41	ASN	N-CA-C	6.10	119.77	111.17
1	A	41	ASN	N-CA-C	6.08	119.74	111.17
1	E	41	ASN	N-CA-C	6.08	119.74	111.17
1	G	41	ASN	N-CA-C	6.08	119.74	111.17
1	E	108	VAL	CA-C-N	5.97	125.88	119.85
1	E	108	VAL	C-N-CA	5.97	125.88	119.85
1	A	108	VAL	CA-C-N	5.96	125.87	119.85
1	A	108	VAL	C-N-CA	5.96	125.87	119.85
1	C	108	VAL	CA-C-N	5.96	125.87	119.85
1	C	108	VAL	C-N-CA	5.96	125.87	119.85
1	G	108	VAL	CA-C-N	5.96	125.87	119.85
1	G	108	VAL	C-N-CA	5.96	125.87	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LEU	N-CA-C	5.95	119.34	107.62
1	E	251	LEU	N-CA-C	5.95	119.34	107.62
1	G	251	LEU	N-CA-C	5.95	119.34	107.62
1	C	209	MET	N-CA-C	5.95	118.52	109.95
1	A	209	MET	N-CA-C	5.95	118.51	109.95
1	E	209	MET	N-CA-C	5.95	118.51	109.95
1	G	209	MET	N-CA-C	5.95	118.51	109.95
1	C	251	LEU	N-CA-C	5.93	119.31	107.62
2	F	214	GLY	N-CA-C	5.91	121.29	113.37
2	D	214	GLY	N-CA-C	5.91	121.29	113.37
2	B	214	GLY	N-CA-C	5.89	121.27	113.37
2	H	214	GLY	N-CA-C	5.87	121.24	113.37
1	C	97	HIS	N-CA-C	-5.87	104.29	112.45
1	A	97	HIS	N-CA-C	-5.87	104.29	112.45
1	E	97	HIS	N-CA-C	-5.87	104.29	112.45
1	G	97	HIS	N-CA-C	-5.87	104.29	112.45
2	H	875	GLU	N-CA-C	-5.79	105.23	112.93
2	B	875	GLU	N-CA-C	-5.79	105.23	112.93
2	D	875	GLU	N-CA-C	-5.79	105.23	112.93
2	F	875	GLU	N-CA-C	-5.79	105.23	112.93
1	C	284	ILE	N-CA-C	5.70	117.21	108.71
1	A	284	ILE	N-CA-C	5.68	117.17	108.71
1	E	284	ILE	N-CA-C	5.68	117.17	108.71
1	G	284	ILE	N-CA-C	5.68	117.17	108.71
2	H	157	PHE	N-CA-C	5.61	117.39	111.28
2	F	157	PHE	N-CA-C	5.59	117.38	111.28
2	B	157	PHE	N-CA-C	5.58	117.36	111.28
1	A	271	ALA	CA-C-N	5.56	124.75	118.97
1	A	271	ALA	C-N-CA	5.56	124.75	118.97
1	C	271	ALA	CA-C-N	5.56	124.75	118.97
1	C	271	ALA	C-N-CA	5.56	124.75	118.97
1	E	271	ALA	CA-C-N	5.56	124.75	118.97
1	E	271	ALA	C-N-CA	5.56	124.75	118.97
1	G	271	ALA	CA-C-N	5.55	124.74	118.97
1	G	271	ALA	C-N-CA	5.55	124.74	118.97
2	D	157	PHE	N-CA-C	5.55	117.33	111.28
1	A	331	SER	N-CA-C	-5.49	106.42	113.23
1	E	331	SER	N-CA-C	-5.49	106.42	113.23
1	A	182	ILE	N-CA-C	5.49	116.89	108.71
1	E	182	ILE	N-CA-C	5.49	116.89	108.71
1	G	182	ILE	N-CA-C	5.48	116.88	108.71
1	C	182	ILE	N-CA-C	5.47	116.86	108.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	SER	N-CA-C	-5.46	106.45	113.23
1	G	331	SER	N-CA-C	-5.45	106.47	113.23
2	D	290	ALA	N-CA-C	-5.45	105.42	111.36
2	B	290	ALA	N-CA-C	-5.42	105.45	111.36
2	H	290	ALA	N-CA-C	-5.41	105.46	111.36
2	F	290	ALA	N-CA-C	-5.39	105.49	111.36
2	F	34	VAL	CB-CA-C	-5.36	108.67	114.35
2	B	34	VAL	CB-CA-C	-5.33	108.70	114.35
2	F	872	GLY	N-CA-C	-5.33	105.95	112.77
2	H	34	VAL	CB-CA-C	-5.33	108.70	114.35
1	A	179	GLU	N-CA-C	5.33	116.77	111.07
1	C	179	GLU	N-CA-C	5.33	116.77	111.07
1	G	179	GLU	N-CA-C	5.33	116.77	111.07
2	B	872	GLY	N-CA-C	-5.31	105.97	112.77
2	D	872	GLY	N-CA-C	-5.31	105.97	112.77
1	E	179	GLU	N-CA-C	5.31	116.75	111.07
2	H	872	GLY	N-CA-C	-5.31	105.97	112.77
2	D	34	VAL	CB-CA-C	-5.30	108.73	114.35
1	C	199	MET	N-CA-C	5.23	117.49	109.07
1	E	199	MET	N-CA-C	5.23	117.49	109.07
1	A	199	MET	N-CA-C	5.21	117.46	109.07
1	G	199	MET	N-CA-C	5.21	117.46	109.07
2	H	50	GLY	N-CA-C	-5.16	108.56	115.32
2	B	50	GLY	N-CA-C	-5.16	108.57	115.32
2	D	50	GLY	N-CA-C	-5.16	108.57	115.32
2	F	50	GLY	N-CA-C	-5.16	108.57	115.32
1	A	60	PHE	N-CA-C	5.10	116.84	111.28
1	E	60	PHE	N-CA-C	5.10	116.84	111.28
2	H	237	ILE	N-CA-C	5.09	115.82	110.62
1	G	60	PHE	N-CA-C	5.08	116.82	111.28
2	B	237	ILE	N-CA-C	5.07	115.79	110.62
1	C	60	PHE	N-CA-C	5.07	116.80	111.28
2	D	237	ILE	N-CA-C	5.07	115.79	110.62
2	F	237	ILE	N-CA-C	5.07	115.79	110.62
1	G	147	LEU	N-CA-C	-5.05	106.62	112.89
1	A	341	THR	CA-C-N	5.04	124.80	119.76
1	A	341	THR	C-N-CA	5.04	124.80	119.76
1	C	341	THR	CA-C-N	5.04	124.80	119.76
1	C	341	THR	C-N-CA	5.04	124.80	119.76
1	E	341	THR	CA-C-N	5.04	124.80	119.76
1	E	341	THR	C-N-CA	5.04	124.80	119.76
1	G	341	THR	CA-C-N	5.04	124.80	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	341	THR	C-N-CA	5.04	124.80	119.76
1	A	147	LEU	N-CA-C	-5.04	106.64	112.89
1	C	147	LEU	N-CA-C	-5.04	106.64	112.89
1	E	147	LEU	N-CA-C	-5.04	106.64	112.89
1	E	142	CYS	CA-C-N	5.01	126.10	119.84
1	E	142	CYS	C-N-CA	5.01	126.10	119.84
1	E	301	ARG	N-CA-C	5.01	117.41	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1384	GLY	Peptide
2	D	1384	GLY	Peptide
2	F	1384	GLY	Peptide
2	H	1384	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2479	0	2442	94	0
1	C	2479	0	2442	96	0
1	E	2479	0	2442	95	0
1	G	2479	0	2442	98	0
2	B	7760	0	4559	117	0
2	D	7760	0	4559	117	0
2	F	7760	0	4559	116	0
2	H	7760	0	4559	120	0
3	A	31	0	12	8	0
3	C	31	0	12	8	0
3	E	31	0	12	8	0
3	G	31	0	12	7	0
All	All	41080	0	28052	806	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 12.

All (806) 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:E:137:MET:HE2	1:G:135:GLY:HA3	1.63	0.81
1:C:137:MET:HE2	1:E:135:GLY:HA3	1.63	0.80
1:A:137:MET:HE2	1:C:135:GLY:HA3	1.64	0.80
2:F:206:PRO:HB2	2:F:207:PRO:HD3	1.64	0.80
2:H:206:PRO:HB2	2:H:207:PRO:HD3	1.64	0.80
1:A:135:GLY:HA3	1:G:137:MET:HE2	1.64	0.79
2:B:206:PRO:HB2	2:B:207:PRO:HD3	1.64	0.78
2:D:206:PRO:HB2	2:D:207:PRO:HD3	1.64	0.78
2:F:233:MET:O	2:F:237:ILE:CB	2.37	0.73
2:D:233:MET:O	2:D:237:ILE:CB	2.37	0.72
1:E:213:ALA:HB1	1:E:288:GLU:O	1.89	0.72
2:H:233:MET:O	2:H:237:ILE:CB	2.37	0.72
2:B:233:MET:O	2:B:237:ILE:CB	2.37	0.71
1:C:213:ALA:HB1	1:C:288:GLU:O	1.89	0.71
1:G:213:ALA:HB1	1:G:288:GLU:O	1.89	0.71
1:A:213:ALA:HB1	1:A:288:GLU:O	1.89	0.71
1:E:48:ASN:O	3:E:401:ATP:N6	2.26	0.69
1:C:48:ASN:O	3:C:401:ATP:N6	2.26	0.69
1:A:48:ASN:O	3:A:401:ATP:N6	2.26	0.68
1:G:48:ASN:O	3:G:401:ATP:N6	2.26	0.68
2:H:44:PHE:HB2	2:H:45:PRO:HD3	1.77	0.67
1:G:257:ILE:N	1:G:257:ILE:HD12	2.10	0.66
1:E:257:ILE:N	1:E:257:ILE:HD12	2.10	0.66
2:B:44:PHE:HB2	2:B:45:PRO:HD3	1.77	0.66
2:F:44:PHE:HB2	2:F:45:PRO:HD3	1.77	0.66
1:G:220:VAL:HG13	1:G:220:VAL:O	1.96	0.66
2:D:44:PHE:HB2	2:D:45:PRO:HD3	1.77	0.66
2:B:1172:ALA:O	2:B:1176:TYR:HB2	1.96	0.65
1:G:339:VAL:HG13	1:G:340:PRO:HD2	1.78	0.65
1:A:257:ILE:HD12	1:A:257:ILE:N	2.10	0.65
1:A:220:VAL:O	1:A:220:VAL:HG13	1.96	0.65
1:C:257:ILE:HD12	1:C:257:ILE:N	2.10	0.65
2:D:1172:ALA:O	2:D:1176:TYR:HB2	1.96	0.65
1:A:339:VAL:HG13	1:A:340:PRO:HD2	1.78	0.65
2:F:1119:GLY:O	2:F:1123:ASN:HB2	1.97	0.65
1:E:220:VAL:HG13	1:E:220:VAL:O	1.96	0.65
2:H:1172:ALA:O	2:H:1176:TYR:HB2	1.96	0.65
1:C:339:VAL:HG13	1:C:340:PRO:HD2	1.78	0.65
2:B:1119:GLY:O	2:B:1123:ASN:HB2	1.97	0.65
1:C:220:VAL:O	1:C:220:VAL:HG13	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:HB	1:E:42:CYS:HB3	1.79	0.64
2:H:1119:GLY:O	2:H:1123:ASN:HB2	1.97	0.64
2:D:585:ILE:O	2:D:589:PRO:CD	2.45	0.64
2:F:1172:ALA:O	2:F:1176:TYR:HB2	1.96	0.64
2:H:585:ILE:O	2:H:589:PRO:CD	2.45	0.64
2:D:1119:GLY:O	2:D:1123:ASN:HB2	1.97	0.64
1:E:101:ALA:CB	2:F:12:SER:CB	2.76	0.64
2:F:585:ILE:O	2:F:589:PRO:CD	2.45	0.64
3:E:401:ATP:H3'	3:E:401:ATP:O3A	1.99	0.63
1:G:36:VAL:HB	1:G:42:CYS:HB3	1.79	0.63
1:A:36:VAL:HB	1:A:42:CYS:HB3	1.79	0.63
2:B:585:ILE:O	2:B:589:PRO:CD	2.45	0.63
2:B:1094:ALA:O	2:B:1098:HIS:HB3	1.99	0.63
1:C:90:TRP:CE2	1:C:123:PHE:CE2	2.86	0.63
1:E:339:VAL:HG13	1:E:340:PRO:HD2	1.78	0.63
1:A:101:ALA:CB	2:B:12:SER:CB	2.76	0.63
1:G:101:ALA:CB	2:H:12:SER:CB	2.76	0.63
1:E:90:TRP:CE2	1:E:123:PHE:CE2	2.86	0.63
1:C:101:ALA:CB	2:D:12:SER:CB	2.76	0.63
3:A:401:ATP:H3'	3:A:401:ATP:O3A	1.99	0.63
1:C:36:VAL:HB	1:C:42:CYS:HB3	1.79	0.63
3:C:401:ATP:H3'	3:C:401:ATP:O3A	1.99	0.63
1:A:90:TRP:CE2	1:A:123:PHE:CE2	2.86	0.62
1:G:90:TRP:CE2	1:G:123:PHE:CE2	2.86	0.62
2:H:1094:ALA:O	2:H:1098:HIS:HB3	1.99	0.62
1:C:101:ALA:HB3	2:D:12:SER:CB	2.30	0.62
3:G:401:ATP:H3'	3:G:401:ATP:O3A	1.99	0.62
1:A:101:ALA:HB3	2:B:12:SER:CB	2.30	0.62
1:C:220:VAL:HG22	1:C:233:LEU:HD22	1.82	0.62
2:D:1094:ALA:O	2:D:1098:HIS:HB3	1.99	0.62
1:E:101:ALA:HB3	2:F:12:SER:CB	2.30	0.62
2:F:1094:ALA:O	2:F:1098:HIS:HB3	1.99	0.62
2:D:157:PHE:O	2:D:160:HIS:C	2.43	0.61
1:E:91:TRP:CE2	1:E:117:PHE:HD1	2.19	0.61
1:G:101:ALA:HB3	2:H:12:SER:CB	2.30	0.61
2:H:157:PHE:O	2:H:160:HIS:C	2.43	0.61
1:A:91:TRP:CE2	1:A:117:PHE:HD1	2.19	0.61
1:G:91:TRP:CE2	1:G:117:PHE:HD1	2.19	0.61
1:A:220:VAL:HG22	1:A:233:LEU:HD22	1.82	0.61
1:G:220:VAL:HG22	1:G:233:LEU:HD22	1.82	0.61
2:F:157:PHE:O	2:F:160:HIS:C	2.43	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TRP:CE2	1:C:117:PHE:HD1	2.19	0.61
2:B:157:PHE:O	2:B:160:HIS:C	2.43	0.60
1:E:220:VAL:HG22	1:E:233:LEU:HD22	1.82	0.60
1:A:129:VAL:HG12	1:A:129:VAL:O	2.02	0.60
2:F:585:ILE:O	2:F:589:PRO:HD2	2.02	0.60
2:B:1223:PHE:O	2:B:1227:LEU:HB2	2.02	0.60
2:D:1223:PHE:O	2:D:1227:LEU:HB2	2.02	0.60
2:H:1223:PHE:O	2:H:1227:LEU:HB2	2.02	0.60
1:C:40:GLY:O	1:C:41:ASN:OD1	2.20	0.59
2:B:585:ILE:O	2:B:589:PRO:HD2	2.02	0.59
1:A:40:GLY:O	1:A:41:ASN:OD1	2.20	0.59
1:C:36:VAL:CG1	1:C:303:SER:HB2	2.33	0.59
1:E:36:VAL:CG1	1:E:303:SER:HB2	2.33	0.59
1:G:129:VAL:HG12	1:G:129:VAL:O	2.02	0.59
1:A:36:VAL:CG1	1:A:303:SER:HB2	2.33	0.59
2:D:89:ILE:O	2:D:93:ILE:HG12	2.03	0.59
2:D:585:ILE:O	2:D:589:PRO:HD2	2.02	0.59
1:E:40:GLY:O	1:E:41:ASN:OD1	2.20	0.59
1:G:36:VAL:CG1	1:G:303:SER:HB2	2.33	0.59
1:E:129:VAL:O	1:E:129:VAL:HG12	2.02	0.59
2:B:89:ILE:O	2:B:93:ILE:HG12	2.03	0.59
1:G:40:GLY:O	1:G:41:ASN:OD1	2.20	0.59
1:C:169:MET:CE	1:E:294:THR:HG22	2.33	0.58
2:F:588:THR:CB	2:F:589:PRO:HD3	2.33	0.58
2:H:89:ILE:O	2:H:93:ILE:HG12	2.03	0.58
2:F:89:ILE:O	2:F:93:ILE:HG12	2.03	0.58
1:A:169:MET:CE	1:C:294:THR:HG22	2.33	0.58
2:D:588:THR:CB	2:D:589:PRO:HD3	2.33	0.58
1:E:169:MET:CE	1:G:294:THR:HG22	2.33	0.58
2:F:1223:PHE:O	2:F:1227:LEU:HB2	2.02	0.58
1:G:237:ASP:OD1	1:G:238:ILE:N	2.37	0.58
2:H:585:ILE:O	2:H:589:PRO:HD2	2.02	0.58
1:C:237:ASP:OD1	1:C:238:ILE:N	2.37	0.58
1:E:36:VAL:CB	1:E:42:CYS:HB3	2.34	0.58
1:E:237:ASP:OD1	1:E:238:ILE:N	2.37	0.58
1:C:36:VAL:CB	1:C:42:CYS:HB3	2.34	0.58
2:D:315:ALA:O	2:D:317:PRO:N	2.37	0.58
2:H:588:THR:CB	2:H:589:PRO:HD3	2.33	0.58
1:A:294:THR:HG22	1:G:169:MET:CE	2.33	0.57
2:F:315:ALA:O	2:F:317:PRO:N	2.37	0.57
1:G:128:GLN:OE1	1:G:156:GLY:HA3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:315:ALA:O	2:H:317:PRO:N	2.37	0.57
1:A:128:GLN:OE1	1:A:156:GLY:HA3	2.04	0.57
2:B:556:LEU:O	2:B:560:VAL:N	2.38	0.57
1:C:129:VAL:HG12	1:C:129:VAL:O	2.02	0.57
2:B:588:THR:CB	2:B:589:PRO:HD3	2.33	0.57
1:E:102:PRO:HB3	2:F:13:ALA:CB	2.35	0.57
1:A:334:GLY:HA3	3:G:401:ATP:O1A	2.05	0.57
1:A:36:VAL:CB	1:A:42:CYS:HB3	2.34	0.57
1:G:36:VAL:CB	1:G:42:CYS:HB3	2.34	0.57
1:G:102:PRO:HB3	2:H:13:ALA:CB	2.35	0.57
1:A:102:PRO:HB3	2:B:13:ALA:HB1	1.87	0.57
1:A:237:ASP:OD1	1:A:238:ILE:N	2.37	0.57
1:C:102:PRO:HB3	2:D:13:ALA:HB1	1.87	0.56
1:E:102:PRO:HB3	2:F:13:ALA:HB1	1.87	0.56
3:C:401:ATP:O1A	1:E:334:GLY:HA3	2.04	0.56
2:H:556:LEU:O	2:H:560:VAL:N	2.38	0.56
1:A:290:VAL:HB	1:A:297:THR:HG22	1.88	0.56
2:D:556:LEU:O	2:D:560:VAL:N	2.38	0.56
2:H:1284:GLY:O	2:H:1288:ALA:HB2	2.06	0.56
1:C:128:GLN:OE1	1:C:156:GLY:HA3	2.04	0.56
1:C:290:VAL:HB	1:C:297:THR:HG22	1.88	0.56
2:F:1284:GLY:O	2:F:1288:ALA:HB2	2.06	0.56
2:B:315:ALA:O	2:B:317:PRO:N	2.37	0.56
1:G:102:PRO:HB3	2:H:13:ALA:HB1	1.87	0.56
1:A:102:PRO:HB3	2:B:13:ALA:CB	2.35	0.56
1:E:128:GLN:OE1	1:E:156:GLY:HA3	2.04	0.56
1:E:290:VAL:HB	1:E:297:THR:HG22	1.88	0.56
1:C:102:PRO:HB3	2:D:13:ALA:CB	2.35	0.56
1:G:290:VAL:HB	1:G:297:THR:HG22	1.88	0.56
2:F:1090:GLY:O	2:F:1094:ALA:HB2	2.06	0.56
2:B:1090:GLY:O	2:B:1094:ALA:HB2	2.06	0.55
2:B:1284:GLY:O	2:B:1288:ALA:HB2	2.06	0.55
2:D:1284:GLY:O	2:D:1288:ALA:HB2	2.06	0.55
2:F:556:LEU:O	2:F:560:VAL:N	2.38	0.55
2:B:472:PRO:O	2:B:476:PHE:HB3	2.07	0.55
3:E:401:ATP:O1A	1:G:334:GLY:HA3	2.06	0.55
2:H:206:PRO:CB	2:H:207:PRO:HD3	2.36	0.55
3:A:401:ATP:O1A	1:C:334:GLY:HA3	2.06	0.55
2:F:472:PRO:O	2:F:476:PHE:HB3	2.07	0.55
2:D:1090:GLY:O	2:D:1094:ALA:HB2	2.06	0.55
2:H:1090:GLY:O	2:H:1094:ALA:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1294:TYR:O	2:H:1298:MET:CB	2.55	0.55
2:D:1294:TYR:O	2:D:1298:MET:CB	2.55	0.55
2:D:472:PRO:O	2:D:476:PHE:HB3	2.07	0.55
2:F:206:PRO:CB	2:F:207:PRO:HD3	2.36	0.55
2:F:1294:TYR:O	2:F:1298:MET:CB	2.55	0.55
1:A:137:MET:HE2	1:C:135:GLY:CA	2.37	0.54
1:C:137:MET:CE	1:E:135:GLY:HA3	2.37	0.54
2:D:206:PRO:CB	2:D:207:PRO:HD3	2.36	0.54
2:H:268:VAL:HG12	2:H:390:ALA:HB2	1.89	0.54
2:B:1223:PHE:O	2:B:1227:LEU:CB	2.56	0.54
2:D:1223:PHE:O	2:D:1227:LEU:CB	2.56	0.54
2:B:268:VAL:HG12	2:B:390:ALA:HB2	1.89	0.54
2:B:1294:TYR:O	2:B:1298:MET:CB	2.55	0.54
1:E:272:PRO:HB3	1:E:311:TRP:CE2	2.43	0.54
2:H:472:PRO:O	2:H:476:PHE:HB3	2.07	0.54
1:G:290:VAL:HG22	1:G:291:VAL:N	2.23	0.54
2:H:1223:PHE:O	2:H:1227:LEU:CB	2.56	0.54
1:E:137:MET:CE	1:G:135:GLY:HA3	2.36	0.54
2:D:1383:SER:O	2:D:1387:SER:CB	2.56	0.54
2:F:1182:PHE:O	2:F:1186:SER:CB	2.56	0.54
2:F:1223:PHE:O	2:F:1227:LEU:CB	2.56	0.54
2:H:1182:PHE:O	2:H:1186:SER:CB	2.56	0.54
2:D:268:VAL:HG12	2:D:390:ALA:HB2	1.89	0.53
1:G:48:ASN:O	3:G:401:ATP:C6	2.61	0.53
1:A:290:VAL:HG22	1:A:291:VAL:N	2.23	0.53
2:B:1383:SER:O	2:B:1387:SER:CB	2.56	0.53
1:A:48:ASN:O	3:A:401:ATP:C6	2.61	0.53
1:C:272:PRO:HB3	1:C:311:TRP:CE2	2.43	0.53
2:D:315:ALA:O	2:D:316:GLY:C	2.51	0.53
2:F:315:ALA:O	2:F:316:GLY:C	2.51	0.53
2:B:575:VAL:O	2:B:579:SER:CB	2.57	0.53
1:C:290:VAL:HG22	1:C:291:VAL:N	2.23	0.53
2:D:575:VAL:O	2:D:579:SER:CB	2.57	0.53
1:G:272:PRO:HB3	1:G:311:TRP:CE2	2.43	0.53
2:H:575:VAL:O	2:H:579:SER:CB	2.57	0.53
2:H:1383:SER:O	2:H:1387:SER:CB	2.56	0.53
1:A:242:ASN:HB2	1:A:246:GLY:H	1.73	0.53
2:F:1383:SER:O	2:F:1387:SER:CB	2.56	0.53
3:G:401:ATP:O1G	3:G:401:ATP:H8	1.92	0.53
1:A:272:PRO:HB3	1:A:311:TRP:CE2	2.43	0.53
2:F:268:VAL:HG12	2:F:390:ALA:HB2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:575:VAL:O	2:F:579:SER:CB	2.57	0.53
2:H:315:ALA:O	2:H:316:GLY:C	2.51	0.53
1:A:90:TRP:NE1	1:A:123:PHE:CE2	2.77	0.53
3:A:401:ATP:O1G	3:A:401:ATP:H8	1.92	0.53
2:B:1182:PHE:O	2:B:1186:SER:CB	2.56	0.53
1:C:90:TRP:NE1	1:C:123:PHE:CE2	2.77	0.53
3:C:401:ATP:O1G	3:C:401:ATP:H8	1.92	0.53
2:D:1182:PHE:O	2:D:1186:SER:CB	2.57	0.53
1:E:290:VAL:HG22	1:E:291:VAL:N	2.23	0.53
1:A:137:MET:CE	1:C:135:GLY:HA3	2.37	0.52
1:C:242:ASN:HB2	1:C:246:GLY:H	1.73	0.52
1:E:90:TRP:NE1	1:E:123:PHE:CE2	2.77	0.52
1:A:135:GLY:CA	1:G:137:MET:HE2	2.38	0.52
2:D:253:LEU:O	2:D:257:MET:N	2.36	0.52
2:D:1287:TYR:O	2:D:1291:VAL:CB	2.58	0.52
2:F:513:ALA:O	2:F:517:ILE:CB	2.58	0.52
1:G:90:TRP:NE1	1:G:123:PHE:CE2	2.77	0.52
1:G:242:ASN:HB2	1:G:246:GLY:H	1.73	0.52
2:B:1287:TYR:O	2:B:1291:VAL:CB	2.58	0.52
2:D:513:ALA:O	2:D:517:ILE:CB	2.58	0.52
2:B:315:ALA:O	2:B:316:GLY:C	2.51	0.52
1:E:137:MET:HE2	1:G:135:GLY:CA	2.36	0.52
2:H:1096:ARG:O	2:H:1100:SER:CB	2.58	0.52
2:H:1119:GLY:O	2:H:1123:ASN:CB	2.58	0.52
2:B:1119:GLY:O	2:B:1123:ASN:CB	2.58	0.52
1:C:48:ASN:O	3:C:401:ATP:C6	2.61	0.52
1:E:242:ASN:HB2	1:E:246:GLY:H	1.73	0.52
2:B:514:TRP:O	2:B:518:PHE:CB	2.58	0.52
2:B:1096:ARG:O	2:B:1100:SER:CB	2.58	0.52
2:D:514:TRP:O	2:D:518:PHE:CB	2.58	0.52
1:E:48:ASN:O	3:E:401:ATP:C6	2.61	0.52
1:G:86:PHE:HB2	1:G:124:SER:OG	2.10	0.52
2:H:513:ALA:O	2:H:517:ILE:CB	2.58	0.52
2:D:1382:GLY:O	2:D:1386:SER:CB	2.58	0.52
3:E:401:ATP:O1G	3:E:401:ATP:H8	1.92	0.52
1:A:201:ARG:CZ	1:A:315:PHE:HB3	2.40	0.52
2:B:1382:GLY:O	2:B:1386:SER:CB	2.58	0.52
2:D:1096:ARG:O	2:D:1100:SER:CB	2.58	0.52
2:F:1382:GLY:O	2:F:1386:SER:CB	2.58	0.52
2:H:1287:TYR:O	2:H:1291:VAL:CB	2.58	0.52
2:F:1096:ARG:O	2:F:1100:SER:CB	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:GLU:HB2	1:G:229:GLU:OE1	2.10	0.52
1:C:216:HIS:O	1:C:286:ILE:HB	2.10	0.52
2:H:1123:ASN:O	2:H:1127:SER:OG	2.26	0.52
1:A:86:PHE:HB2	1:A:124:SER:OG	2.10	0.51
2:B:513:ALA:O	2:B:517:ILE:CB	2.58	0.51
1:C:86:PHE:HB2	1:C:124:SER:OG	2.10	0.51
1:C:227:GLU:HB2	1:C:229:GLU:OE1	2.10	0.51
2:F:1119:GLY:O	2:F:1123:ASN:CB	2.58	0.51
1:G:201:ARG:CZ	1:G:315:PHE:HB3	2.40	0.51
2:F:514:TRP:O	2:F:518:PHE:CB	2.58	0.51
2:F:1287:TYR:O	2:F:1291:VAL:CB	2.58	0.51
2:H:514:TRP:O	2:H:518:PHE:CB	2.58	0.51
1:A:89:VAL:O	1:A:93:ILE:HG23	2.10	0.51
2:D:1119:GLY:O	2:D:1123:ASN:CB	2.58	0.51
1:A:216:HIS:O	1:A:286:ILE:HB	2.10	0.51
1:C:89:VAL:O	1:C:93:ILE:HG23	2.11	0.51
1:C:117:PHE:C	1:C:117:PHE:CD2	2.89	0.51
2:D:1095:LYS:O	2:D:1099:ARG:CB	2.59	0.51
1:E:86:PHE:HB2	1:E:124:SER:OG	2.10	0.51
2:F:1095:LYS:O	2:F:1099:ARG:CB	2.59	0.51
1:G:111:VAL:HA	1:G:137:MET:O	2.11	0.51
2:H:1382:GLY:O	2:H:1386:SER:CB	2.58	0.51
2:B:1095:LYS:O	2:B:1099:ARG:CB	2.59	0.51
1:C:201:ARG:CZ	1:C:315:PHE:HB3	2.40	0.51
1:E:48:ASN:O	3:E:401:ATP:N1	2.44	0.51
1:E:218:GLN:HG2	1:E:235:GLN:HB3	1.93	0.51
1:E:267:LEU:HA	1:E:270:LEU:HD13	1.93	0.51
1:A:135:GLY:HA3	1:G:137:MET:CE	2.38	0.51
1:A:227:GLU:HB2	1:A:229:GLU:OE1	2.10	0.51
2:B:460:ALA:O	2:B:464:ALA:HB3	2.11	0.51
1:C:48:ASN:O	3:C:401:ATP:N1	2.44	0.51
2:D:1436:ILE:N	2:D:1473:ALA:O	2.41	0.51
1:E:89:VAL:O	1:E:93:ILE:HG23	2.11	0.51
1:E:227:GLU:HB2	1:E:229:GLU:OE1	2.10	0.51
2:F:253:LEU:O	2:F:257:MET:N	2.36	0.51
2:F:460:ALA:O	2:F:464:ALA:HB3	2.11	0.51
2:H:1095:LYS:O	2:H:1099:ARG:CB	2.59	0.51
1:A:267:LEU:HA	1:A:270:LEU:HD13	1.93	0.51
2:D:1381:THR:O	2:D:1385:LYS:CB	2.59	0.51
1:E:201:ARG:CZ	1:E:315:PHE:HB3	2.40	0.51
1:G:216:HIS:O	1:G:286:ILE:HB	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:GLN:HG2	1:G:235:GLN:HB3	1.93	0.51
1:E:111:VAL:HA	1:E:137:MET:O	2.11	0.50
1:E:117:PHE:C	1:E:117:PHE:CD2	2.89	0.50
2:H:1436:ILE:N	2:H:1473:ALA:O	2.41	0.50
1:A:111:VAL:HA	1:A:137:MET:O	2.11	0.50
1:A:218:GLN:HG2	1:A:235:GLN:HB3	1.93	0.50
1:A:117:PHE:C	1:A:117:PHE:CD2	2.89	0.50
1:C:55:PHE:CE1	1:E:206:ARG:HD3	2.47	0.50
1:C:218:GLN:HG2	1:C:235:GLN:HB3	1.93	0.50
1:E:216:HIS:O	1:E:286:ILE:HB	2.10	0.50
2:H:1381:THR:O	2:H:1385:LYS:CB	2.59	0.50
1:G:267:LEU:HA	1:G:270:LEU:HD13	1.93	0.50
2:B:1381:THR:O	2:B:1385:LYS:CB	2.59	0.50
1:C:111:VAL:HA	1:C:137:MET:O	2.11	0.50
1:G:48:ASN:O	3:G:401:ATP:N1	2.44	0.50
1:G:89:VAL:O	1:G:93:ILE:HG23	2.10	0.50
1:G:117:PHE:C	1:G:117:PHE:CD2	2.89	0.50
2:B:1190:GLN:O	2:B:1194:ASP:CB	2.60	0.50
1:C:267:LEU:HA	1:C:270:LEU:HD13	1.93	0.50
2:D:460:ALA:O	2:D:464:ALA:HB3	2.11	0.50
2:H:1190:GLN:O	2:H:1194:ASP:CB	2.60	0.50
2:D:525:THR:O	2:D:529:GLU:CB	2.60	0.50
2:F:1381:THR:O	2:F:1385:LYS:CB	2.59	0.50
1:A:48:ASN:O	3:A:401:ATP:N1	2.44	0.50
2:B:1178:ILE:O	2:B:1182:PHE:HB3	2.12	0.50
2:D:321:PHE:HE1	2:D:574:SER:CB	2.25	0.50
2:F:525:THR:O	2:F:529:GLU:CB	2.60	0.50
2:H:460:ALA:O	2:H:464:ALA:HB3	2.11	0.50
1:A:165:GLY:O	1:A:169:MET:HG2	2.12	0.49
2:B:321:PHE:HE1	2:B:574:SER:CB	2.25	0.49
2:B:1436:ILE:N	2:B:1473:ALA:O	2.41	0.49
1:C:179:GLU:C	1:C:181:LEU:H	2.20	0.49
2:D:561:GLY:O	2:D:565:PHE:HB2	2.12	0.49
2:H:1178:ILE:O	2:H:1182:PHE:HB3	2.12	0.49
1:A:55:PHE:CE1	1:C:206:ARG:HD3	2.47	0.49
1:A:179:GLU:C	1:A:181:LEU:H	2.20	0.49
2:D:1305:MET:O	2:D:1309:LEU:CB	2.60	0.49
2:F:321:PHE:HE1	2:F:574:SER:CB	2.25	0.49
1:G:36:VAL:HG13	1:G:303:SER:HB2	1.94	0.49
2:H:1305:MET:O	2:H:1309:LEU:CB	2.61	0.49
1:E:101:ALA:N	1:E:102:PRO:HD2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:GLU:C	1:E:181:LEU:H	2.20	0.49
1:G:211:ILE:O	1:G:290:VAL:HG12	2.12	0.49
2:H:353:GLY:HA2	2:H:356:TYR:HD2	1.77	0.49
2:F:1305:MET:O	2:F:1309:LEU:CB	2.61	0.49
2:H:321:PHE:HE1	2:H:574:SER:CB	2.25	0.49
1:E:211:ILE:O	1:E:290:VAL:HG12	2.12	0.49
2:B:353:GLY:HA2	2:B:356:TYR:HD2	1.77	0.49
1:C:137:MET:HE2	1:E:135:GLY:CA	2.37	0.49
1:C:211:ILE:O	1:C:290:VAL:HG12	2.12	0.49
2:D:1190:GLN:O	2:D:1194:ASP:CB	2.60	0.49
2:F:1190:GLN:O	2:F:1194:ASP:CB	2.60	0.49
1:G:165:GLY:O	1:G:169:MET:HG2	2.12	0.49
2:H:525:THR:O	2:H:529:GLU:CB	2.60	0.49
2:D:1178:ILE:O	2:D:1182:PHE:HB3	2.12	0.49
1:G:101:ALA:N	1:G:102:PRO:HD2	2.28	0.49
2:F:561:GLY:O	2:F:565:PHE:HB2	2.13	0.49
1:C:165:GLY:O	1:C:169:MET:HG2	2.12	0.49
2:F:353:GLY:HA2	2:F:356:TYR:HD2	1.77	0.49
2:F:354:ASN:O	2:F:358:LEU:CB	2.61	0.49
2:F:1178:ILE:O	2:F:1182:PHE:HB3	2.12	0.49
2:H:354:ASN:O	2:H:358:LEU:CB	2.61	0.49
1:A:36:VAL:HG13	1:A:303:SER:HB2	1.94	0.49
2:B:525:THR:O	2:B:529:GLU:CB	2.60	0.49
2:D:548:THR:O	2:D:551:PRO:HD2	2.13	0.49
1:G:179:GLU:C	1:G:181:LEU:H	2.20	0.49
1:C:201:ARG:NH1	1:C:315:PHE:HB3	2.28	0.48
1:E:165:GLY:O	1:E:169:MET:HG2	2.13	0.48
2:B:1172:ALA:O	2:B:1176:TYR:CB	2.62	0.48
1:G:201:ARG:NH1	1:G:315:PHE:HB3	2.28	0.48
2:H:253:LEU:O	2:H:257:MET:N	2.36	0.48
1:A:201:ARG:NH1	1:A:315:PHE:HB3	2.28	0.48
1:A:211:ILE:O	1:A:290:VAL:HG12	2.12	0.48
2:B:37:VAL:CB	2:B:41:PHE:CE2	2.96	0.48
2:H:551:PRO:HA	2:H:554:ALA:HB3	1.95	0.48
1:A:101:ALA:N	1:A:102:PRO:HD2	2.27	0.48
1:A:206:ARG:HD3	1:G:55:PHE:CE1	2.47	0.48
2:B:548:THR:O	2:B:551:PRO:HD2	2.13	0.48
1:C:101:ALA:N	1:C:102:PRO:HD2	2.27	0.48
3:C:401:ATP:O4'	1:E:182:ILE:HG21	2.13	0.48
2:D:37:VAL:CB	2:D:41:PHE:CE2	2.96	0.48
2:D:353:GLY:HA2	2:D:356:TYR:HD2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:548:THR:O	2:F:551:PRO:HD2	2.13	0.48
2:H:37:VAL:CB	2:H:41:PHE:CE2	2.96	0.48
2:H:548:THR:O	2:H:551:PRO:HD2	2.13	0.48
2:D:551:PRO:HA	2:D:554:ALA:HB3	1.95	0.48
2:D:1172:ALA:O	2:D:1176:TYR:CB	2.62	0.48
1:E:55:PHE:CE1	1:G:206:ARG:HD3	2.47	0.48
2:F:1436:ILE:N	2:F:1473:ALA:O	2.41	0.48
2:H:561:GLY:O	2:H:565:PHE:HB2	2.13	0.48
2:B:354:ASN:O	2:B:358:LEU:CB	2.61	0.48
2:B:548:THR:C	2:B:551:PRO:HD2	2.39	0.48
2:D:1124:ARG:O	2:D:1128:ASP:CB	2.62	0.48
1:E:36:VAL:HG13	1:E:303:SER:HB2	1.94	0.48
2:B:253:LEU:O	2:B:257:MET:N	2.36	0.48
2:B:1305:MET:O	2:B:1309:LEU:CB	2.61	0.48
1:G:94:ALA:HB1	1:G:100:LEU:HD23	1.96	0.48
3:E:401:ATP:O4'	1:G:182:ILE:HG21	2.14	0.48
2:F:37:VAL:CB	2:F:41:PHE:CE2	2.96	0.48
2:F:551:PRO:HA	2:F:554:ALA:HB3	1.95	0.48
2:H:323:ILE:O	2:H:327:LEU:CB	2.62	0.48
2:H:548:THR:C	2:H:551:PRO:HD2	2.39	0.48
2:B:1124:ARG:O	2:B:1128:ASP:CB	2.62	0.48
2:D:323:ILE:O	2:D:327:LEU:CB	2.62	0.48
2:D:589:PRO:O	2:D:593:LEU:CB	2.62	0.48
1:A:94:ALA:HB1	1:A:100:LEU:HD23	1.96	0.48
1:A:182:ILE:HG21	3:G:401:ATP:O4'	2.14	0.48
2:B:561:GLY:O	2:B:565:PHE:HB2	2.13	0.48
2:B:589:PRO:O	2:B:593:LEU:CB	2.62	0.48
2:D:354:ASN:O	2:D:358:LEU:CB	2.61	0.48
2:F:367:LEU:O	2:F:371:THR:CB	2.62	0.48
2:H:367:LEU:O	2:H:371:THR:CB	2.62	0.48
2:H:1124:ARG:O	2:H:1128:ASP:CB	2.62	0.48
3:A:401:ATP:O4'	1:C:182:ILE:HG21	2.14	0.47
1:C:36:VAL:HG13	1:C:303:SER:HB2	1.94	0.47
2:D:548:THR:C	2:D:551:PRO:HD2	2.39	0.47
1:E:201:ARG:NH1	1:E:315:PHE:HB3	2.28	0.47
2:B:323:ILE:O	2:B:327:LEU:CB	2.62	0.47
2:F:548:THR:C	2:F:551:PRO:HD2	2.39	0.47
2:B:551:PRO:HA	2:B:554:ALA:HB3	1.95	0.47
2:F:323:ILE:O	2:F:327:LEU:CB	2.62	0.47
2:F:1269:SER:O	2:F:1273:HIS:CB	2.62	0.47
2:D:1269:SER:O	2:D:1273:HIS:CB	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:517:ILE:O	2:D:521:ARG:CB	2.63	0.47
1:E:257:ILE:N	1:E:257:ILE:CD1	2.77	0.47
2:F:1124:ARG:O	2:F:1128:ASP:CB	2.62	0.47
2:H:1269:SER:O	2:H:1273:HIS:CB	2.62	0.47
2:H:423:ILE:O	2:H:427:GLN:CB	2.63	0.47
2:H:1297:TRP:O	2:H:1301:ASN:CB	2.63	0.47
1:A:214:THR:HA	1:A:248:SER:HB3	1.97	0.47
1:A:318:ILE:HG23	1:A:329:ASP:O	2.15	0.47
2:B:423:ILE:O	2:B:427:GLN:CB	2.63	0.47
1:C:318:ILE:HG23	1:C:329:ASP:O	2.15	0.47
2:F:517:ILE:O	2:F:521:ARG:CB	2.63	0.47
2:F:1172:ALA:O	2:F:1176:TYR:CB	2.62	0.47
2:F:1267:SER:O	2:F:1271:SER:CB	2.63	0.47
2:H:517:ILE:O	2:H:521:ARG:CB	2.63	0.47
2:B:1129:CYS:O	2:B:1133:ASP:CB	2.63	0.47
2:B:1267:SER:O	2:B:1271:SER:CB	2.63	0.47
2:B:1269:SER:O	2:B:1273:HIS:CB	2.62	0.47
1:E:94:ALA:HB1	1:E:100:LEU:HD23	1.96	0.47
2:F:589:PRO:O	2:F:593:LEU:CB	2.62	0.47
1:G:318:ILE:HG23	1:G:329:ASP:O	2.15	0.47
2:H:417:ILE:O	2:H:421:VAL:CB	2.63	0.47
2:H:589:PRO:O	2:H:593:LEU:CB	2.62	0.47
2:B:367:LEU:O	2:B:371:THR:CB	2.62	0.47
2:B:517:ILE:O	2:B:521:ARG:CB	2.63	0.47
1:C:214:THR:HA	1:C:248:SER:HB3	1.97	0.47
2:D:1129:CYS:O	2:D:1133:ASP:CB	2.63	0.47
2:F:423:ILE:O	2:F:427:GLN:CB	2.63	0.47
2:B:1297:TRP:O	2:B:1301:ASN:CB	2.63	0.47
2:D:253:LEU:HA	2:D:256:ALA:HB3	1.97	0.47
2:D:367:LEU:O	2:D:371:THR:CB	2.62	0.47
2:D:1102:LEU:O	2:D:1106:ILE:CB	2.63	0.47
2:F:1102:LEU:O	2:F:1106:ILE:CB	2.63	0.47
2:B:417:ILE:O	2:B:421:VAL:CB	2.63	0.46
2:D:1267:SER:O	2:D:1271:SER:CB	2.63	0.46
2:D:1297:TRP:O	2:D:1301:ASN:CB	2.63	0.46
1:E:214:THR:HA	1:E:248:SER:HB3	1.97	0.46
1:A:257:ILE:N	1:A:257:ILE:CD1	2.77	0.46
1:C:94:ALA:HB1	1:C:100:LEU:HD23	1.96	0.46
2:H:1129:CYS:O	2:H:1133:ASP:CB	2.63	0.46
2:B:206:PRO:CB	2:B:207:PRO:HD3	2.36	0.46
2:D:423:ILE:O	2:D:427:GLN:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:LEU:HA	2:F:256:ALA:HB3	1.97	0.46
2:F:417:ILE:O	2:F:421:VAL:CB	2.63	0.46
2:F:1065:ALA:O	2:F:1069:THR:CB	2.63	0.46
2:H:1065:ALA:O	2:H:1069:THR:CB	2.63	0.46
2:H:1172:ALA:O	2:H:1176:TYR:CB	2.62	0.46
2:D:1150:CYS:O	2:D:1154:LEU:CB	2.64	0.46
2:F:1297:TRP:O	2:F:1301:ASN:CB	2.63	0.46
2:H:1267:SER:O	2:H:1271:SER:CB	2.63	0.46
2:B:1065:ALA:O	2:B:1069:THR:CB	2.63	0.46
2:B:1102:LEU:O	2:B:1106:ILE:CB	2.63	0.46
1:E:318:ILE:HG23	1:E:329:ASP:O	2.15	0.46
1:G:87:ALA:CB	1:G:121:PHE:HA	2.46	0.46
2:B:253:LEU:HA	2:B:256:ALA:HB3	1.97	0.46
2:B:1150:CYS:O	2:B:1154:LEU:CB	2.64	0.46
2:D:1121:ILE:O	2:D:1125:PHE:HB2	2.16	0.46
2:F:1129:CYS:O	2:F:1133:ASP:CB	2.63	0.46
2:H:1102:LEU:O	2:H:1106:ILE:CB	2.63	0.46
2:H:1150:CYS:O	2:H:1154:LEU:CB	2.64	0.46
1:C:257:ILE:N	1:C:257:ILE:CD1	2.77	0.46
1:E:87:ALA:CB	1:E:121:PHE:HA	2.46	0.46
1:G:214:THR:HA	1:G:248:SER:HB3	1.97	0.46
2:H:560:VAL:O	2:H:564:SER:CB	2.64	0.46
2:B:1078:LEU:O	2:B:1082:THR:CB	2.64	0.46
2:D:560:VAL:O	2:D:564:SER:CB	2.64	0.46
2:D:1065:ALA:O	2:D:1069:THR:CB	2.63	0.46
2:D:1078:LEU:O	2:D:1082:THR:CB	2.64	0.46
2:D:37:VAL:O	2:D:41:PHE:CG	2.69	0.45
2:D:417:ILE:O	2:D:421:VAL:CB	2.63	0.45
1:E:142:CYS:SG	1:E:145:ALA:HB3	2.56	0.45
2:F:1150:CYS:O	2:F:1154:LEU:CB	2.64	0.45
2:D:1384:GLY:O	2:D:1388:PHE:CB	2.65	0.45
2:F:560:VAL:O	2:F:564:SER:CB	2.64	0.45
2:F:1121:ILE:O	2:F:1125:PHE:HB2	2.16	0.45
2:H:521:ARG:O	2:H:525:THR:CB	2.65	0.45
2:F:37:VAL:O	2:F:41:PHE:CG	2.69	0.45
2:H:37:VAL:O	2:H:41:PHE:CG	2.70	0.45
2:H:253:LEU:HA	2:H:256:ALA:HB3	1.97	0.45
2:B:1384:GLY:O	2:B:1388:PHE:CB	2.65	0.45
1:C:87:ALA:CB	1:C:121:PHE:HA	2.46	0.45
2:D:1092:LYS:O	2:D:1096:ARG:CB	2.65	0.45
2:F:396:TYR:HA	2:F:399:ILE:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:O	2:B:41:PHE:CG	2.69	0.45
2:D:321:PHE:CE1	2:D:574:SER:CB	3.00	0.45
2:F:1078:LEU:O	2:F:1082:THR:CB	2.64	0.45
2:F:1384:GLY:O	2:F:1388:PHE:CB	2.64	0.45
2:H:1092:LYS:O	2:H:1096:ARG:CB	2.65	0.45
2:H:1384:GLY:O	2:H:1388:PHE:CB	2.65	0.45
2:B:560:VAL:O	2:B:564:SER:CB	2.64	0.45
2:B:1110:MET:O	2:B:1114:GLU:CB	2.65	0.45
2:F:1092:LYS:O	2:F:1096:ARG:CB	2.65	0.45
2:F:1110:MET:O	2:F:1114:GLU:CB	2.65	0.45
2:H:396:TYR:HA	2:H:399:ILE:HG22	1.99	0.45
1:A:142:CYS:SG	1:A:145:ALA:HB3	2.56	0.45
2:B:521:ARG:O	2:B:525:THR:CB	2.65	0.45
1:C:178:ALA:HB2	1:C:298:THR:OG1	2.17	0.45
1:E:220:VAL:CG2	1:E:233:LEU:HD22	2.47	0.45
2:F:1121:ILE:O	2:F:1125:PHE:CB	2.65	0.45
1:G:142:CYS:SG	1:G:145:ALA:HB3	2.56	0.45
1:G:144:LEU:O	1:G:147:LEU:HG	2.17	0.45
2:B:396:TYR:HA	2:B:399:ILE:HG22	1.99	0.45
2:B:556:LEU:O	2:B:560:VAL:CB	2.65	0.45
2:B:1121:ILE:O	2:B:1125:PHE:HB2	2.16	0.45
1:E:161:ALA:HB1	1:G:164:LEU:HD23	1.99	0.45
1:G:43:ASN:OD1	1:G:43:ASN:N	2.44	0.45
1:G:178:ALA:HB2	1:G:298:THR:OG1	2.17	0.45
2:H:1078:LEU:O	2:H:1082:THR:CB	2.64	0.45
2:B:1014:SER:O	2:B:1018:PHE:HB2	2.17	0.45
2:B:1092:LYS:O	2:B:1096:ARG:CB	2.65	0.45
2:D:396:TYR:HA	2:D:399:ILE:HG22	1.99	0.45
2:H:1110:MET:O	2:H:1114:GLU:CB	2.65	0.45
2:H:1121:ILE:O	2:H:1125:PHE:HB2	2.16	0.45
1:A:87:ALA:CB	1:A:121:PHE:HA	2.46	0.45
2:D:231:TRP:O	2:D:231:TRP:CE3	2.70	0.45
2:F:260:LEU:C	2:F:262:ASN:H	2.25	0.45
2:H:586:LEU:C	2:H:589:PRO:HD2	2.42	0.45
2:B:260:LEU:C	2:B:262:ASN:H	2.25	0.44
2:B:1121:ILE:O	2:B:1125:PHE:CB	2.65	0.44
2:D:1014:SER:O	2:D:1018:PHE:HB2	2.17	0.44
2:D:1110:MET:O	2:D:1114:GLU:CB	2.65	0.44
1:E:144:LEU:O	1:E:147:LEU:HG	2.17	0.44
1:E:274:ASP:O	1:E:278:HIS:HB2	2.17	0.44
2:F:231:TRP:CE3	2:F:231:TRP:O	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1434:GLY:O	2:F:1475:ILE:N	2.44	0.44
1:G:220:VAL:CG2	1:G:233:LEU:HD22	2.47	0.44
1:G:345:THR:CG2	1:G:348:GLN:HB2	2.47	0.44
2:H:260:LEU:C	2:H:262:ASN:H	2.25	0.44
2:H:556:LEU:O	2:H:560:VAL:CB	2.65	0.44
2:H:1121:ILE:O	2:H:1125:PHE:CB	2.65	0.44
2:B:406:ASN:O	2:B:410:GLY:N	2.51	0.44
1:C:142:CYS:SG	1:C:145:ALA:HB3	2.56	0.44
2:D:521:ARG:O	2:D:525:THR:CB	2.65	0.44
1:E:144:LEU:O	1:E:148:ILE:HG12	2.17	0.44
2:F:321:PHE:CE1	2:F:574:SER:CB	3.00	0.44
2:H:321:PHE:CE1	2:H:574:SER:CB	3.00	0.44
1:C:144:LEU:O	1:C:147:LEU:HG	2.17	0.44
2:D:556:LEU:O	2:D:560:VAL:CB	2.65	0.44
2:D:1121:ILE:O	2:D:1125:PHE:CB	2.65	0.44
1:E:345:THR:CG2	1:E:348:GLN:HB2	2.47	0.44
2:F:521:ARG:O	2:F:525:THR:CB	2.65	0.44
2:F:556:LEU:O	2:F:560:VAL:CB	2.65	0.44
1:G:61:THR:HG23	1:G:62:THR:N	2.32	0.44
1:G:144:LEU:O	1:G:148:ILE:HG12	2.17	0.44
1:G:274:ASP:O	1:G:278:HIS:HB2	2.17	0.44
1:A:161:ALA:HB1	1:C:164:LEU:HD23	1.99	0.44
1:A:178:ALA:HB2	1:A:298:THR:OG1	2.17	0.44
1:C:144:LEU:O	1:C:148:ILE:HG12	2.17	0.44
1:G:252:VAL:HG23	1:G:253:ALA:N	2.33	0.44
2:B:388:ARG:O	2:B:392:GLN:CB	2.66	0.44
2:F:68:PHE:HA	2:F:69:PRO:HD3	1.86	0.44
2:H:1014:SER:O	2:H:1018:PHE:HB2	2.17	0.44
1:A:144:LEU:O	1:A:148:ILE:HG12	2.17	0.44
1:C:274:ASP:O	1:C:278:HIS:HB2	2.18	0.44
2:D:1283:LEU:O	2:D:1287:TYR:HB2	2.18	0.44
2:H:547:ASN:O	2:H:551:PRO:HD2	2.18	0.44
1:A:144:LEU:O	1:A:147:LEU:HG	2.17	0.44
2:B:231:TRP:O	2:B:231:TRP:CE3	2.70	0.44
2:B:321:PHE:CE1	2:B:574:SER:CB	3.00	0.44
2:B:1283:LEU:O	2:B:1287:TYR:HB2	2.18	0.44
2:F:547:ASN:O	2:F:551:PRO:HD2	2.18	0.44
2:F:1179:GLN:O	2:F:1183:ARG:CB	2.66	0.44
1:A:164:LEU:HD23	1:G:161:ALA:HB1	2.00	0.44
1:C:61:THR:HG23	1:C:62:THR:N	2.33	0.44
1:C:202:VAL:O	1:C:254:PRO:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:CG2	1:C:348:GLN:HB2	2.47	0.44
2:D:586:LEU:C	2:D:589:PRO:HD2	2.42	0.44
1:E:61:THR:HG23	1:E:62:THR:N	2.33	0.44
1:E:178:ALA:HB2	1:E:298:THR:OG1	2.17	0.44
2:F:586:LEU:C	2:F:589:PRO:HD2	2.42	0.44
1:A:252:VAL:HG23	1:A:253:ALA:N	2.33	0.44
2:B:547:ASN:O	2:B:551:PRO:HD2	2.18	0.44
2:B:586:LEU:C	2:B:589:PRO:HD2	2.42	0.44
2:H:231:TRP:O	2:H:231:TRP:CE3	2.70	0.44
2:B:118:ILE:O	2:B:122:VAL:HG23	2.18	0.43
1:C:265:SER:HA	1:C:266:PRO:HD3	1.84	0.43
2:D:1179:GLN:O	2:D:1183:ARG:CB	2.66	0.43
1:E:252:VAL:HG23	1:E:253:ALA:N	2.33	0.43
2:F:406:ASN:O	2:F:410:GLY:N	2.51	0.43
2:F:1014:SER:O	2:F:1018:PHE:HB2	2.17	0.43
2:H:388:ARG:O	2:H:392:GLN:CB	2.66	0.43
2:H:1179:GLN:O	2:H:1183:ARG:CB	2.66	0.43
1:A:274:ASP:O	1:A:278:HIS:HB2	2.18	0.43
1:A:345:THR:CG2	1:A:348:GLN:HB2	2.47	0.43
2:B:36:HIS:HA	2:B:142:TYR:HE1	1.83	0.43
2:D:260:LEU:C	2:D:262:ASN:H	2.25	0.43
2:H:406:ASN:O	2:H:410:GLY:N	2.51	0.43
2:D:118:ILE:O	2:D:122:VAL:HG23	2.18	0.43
2:D:205:LYS:N	2:D:206:PRO:CD	2.82	0.43
2:D:388:ARG:O	2:D:392:GLN:CB	2.66	0.43
1:E:179:GLU:C	1:E:181:LEU:N	2.76	0.43
2:F:1283:LEU:O	2:F:1287:TYR:HB2	2.18	0.43
1:G:231:VAL:HG13	1:G:231:VAL:O	2.19	0.43
1:A:202:VAL:O	1:A:254:PRO:HA	2.18	0.43
2:B:1351:SER:O	2:B:1399:PHE:N	2.47	0.43
1:C:55:PHE:HE1	1:E:206:ARG:CD	2.31	0.43
2:D:547:ASN:O	2:D:551:PRO:HD2	2.18	0.43
1:G:179:GLU:C	1:G:181:LEU:N	2.76	0.43
2:H:473:VAL:O	2:H:477:VAL:CB	2.67	0.43
1:A:153:ASN:O	1:A:157:LEU:HB2	2.19	0.43
1:A:178:ALA:HA	1:A:181:LEU:HD12	2.01	0.43
2:B:473:VAL:O	2:B:477:VAL:CB	2.67	0.43
2:D:547:ASN:O	2:D:551:PRO:CD	2.67	0.43
1:A:61:THR:HG23	1:A:62:THR:N	2.33	0.43
1:C:178:ALA:HA	1:C:181:LEU:HD12	2.01	0.43
2:D:303:SER:HA	2:D:436:PRO:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:473:VAL:O	2:D:477:VAL:CB	2.67	0.43
2:F:303:SER:HA	2:F:436:PRO:HB3	2.01	0.43
1:A:231:VAL:HG13	1:A:231:VAL:O	2.19	0.43
2:B:37:VAL:O	2:B:41:PHE:CD2	2.72	0.43
2:B:1179:GLN:O	2:B:1183:ARG:CB	2.66	0.43
1:C:161:ALA:HB1	1:E:164:LEU:HD23	1.99	0.43
2:F:388:ARG:O	2:F:392:GLN:CB	2.66	0.43
2:H:118:ILE:O	2:H:122:VAL:HG23	2.18	0.43
2:B:205:LYS:N	2:B:206:PRO:CD	2.82	0.43
1:C:179:GLU:C	1:C:181:LEU:N	2.76	0.43
2:F:118:ILE:O	2:F:122:VAL:HG23	2.18	0.43
2:H:36:HIS:HA	2:H:142:TYR:HE1	1.83	0.43
2:H:1351:SER:O	2:H:1399:PHE:N	2.47	0.43
1:C:220:VAL:O	1:C:220:VAL:CG1	2.66	0.43
1:E:178:ALA:HA	1:E:181:LEU:HD12	2.01	0.43
1:E:202:VAL:O	1:E:254:PRO:HA	2.18	0.43
2:F:473:VAL:O	2:F:477:VAL:CB	2.67	0.43
1:G:202:VAL:O	1:G:254:PRO:HA	2.18	0.43
1:A:36:VAL:HG23	1:A:42:CYS:HB3	2.01	0.43
2:D:253:LEU:N	2:D:254:PRO:CD	2.82	0.43
1:E:55:PHE:HE1	1:G:206:ARG:CD	2.32	0.43
1:E:231:VAL:O	1:E:231:VAL:HG13	2.19	0.43
1:G:36:VAL:CG2	1:G:42:CYS:HB3	2.49	0.43
2:H:1132:ILE:O	2:H:1136:ILE:CB	2.67	0.43
2:H:1283:LEU:O	2:H:1287:TYR:HB2	2.18	0.43
2:D:37:VAL:O	2:D:41:PHE:CD2	2.72	0.42
2:H:37:VAL:O	2:H:41:PHE:CD2	2.72	0.42
1:A:132:GLY:HA3	1:C:131:ILE:O	2.19	0.42
1:A:206:ARG:CD	1:G:55:PHE:HE1	2.32	0.42
2:B:253:LEU:N	2:B:254:PRO:CD	2.82	0.42
1:C:36:VAL:CG2	1:C:42:CYS:HB3	2.49	0.42
2:D:36:HIS:HA	2:D:142:TYR:HE1	1.83	0.42
2:D:1434:GLY:O	2:D:1475:ILE:N	2.44	0.42
1:E:36:VAL:CG2	1:E:42:CYS:HB3	2.49	0.42
2:F:547:ASN:O	2:F:551:PRO:CD	2.67	0.42
1:G:40:GLY:C	1:G:41:ASN:OD1	2.62	0.42
1:G:153:ASN:O	1:G:157:LEU:HB2	2.19	0.42
1:G:178:ALA:HA	1:G:181:LEU:HD12	2.00	0.42
2:B:303:SER:HA	2:B:436:PRO:HB3	2.01	0.42
2:B:588:THR:N	2:B:589:PRO:CD	2.82	0.42
1:E:40:GLY:C	1:E:41:ASN:OD1	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:HIS:HA	2:F:142:TYR:HE1	1.83	0.42
2:F:588:THR:N	2:F:589:PRO:CD	2.82	0.42
2:H:132:PHE:HA	2:H:133:PRO:HD3	1.81	0.42
2:H:687:THR:HA	2:H:695:THR:H	1.85	0.42
1:A:265:SER:HA	1:A:266:PRO:HD3	1.84	0.42
2:B:1132:ILE:O	2:B:1136:ILE:CB	2.67	0.42
1:C:40:GLY:C	1:C:41:ASN:OD1	2.62	0.42
1:C:153:ASN:O	1:C:157:LEU:HB2	2.19	0.42
2:D:406:ASN:O	2:D:410:GLY:N	2.51	0.42
2:D:687:THR:HA	2:D:695:THR:H	1.85	0.42
2:D:1132:ILE:O	2:D:1136:ILE:CB	2.67	0.42
2:F:205:LYS:N	2:F:206:PRO:CD	2.82	0.42
2:F:687:THR:HA	2:F:695:THR:H	1.84	0.42
2:H:547:ASN:O	2:H:551:PRO:CD	2.67	0.42
1:C:36:VAL:HG23	1:C:42:CYS:HB3	2.01	0.42
1:C:231:VAL:O	1:C:231:VAL:HG13	2.19	0.42
2:F:253:LEU:N	2:F:254:PRO:CD	2.82	0.42
1:A:36:VAL:CG2	1:A:42:CYS:HB3	2.49	0.42
1:A:142:CYS:SG	1:A:142:CYS:O	2.78	0.42
1:A:220:VAL:O	1:A:220:VAL:CG1	2.66	0.42
2:B:1514:MET:O	2:B:1518:ASN:CB	2.67	0.42
1:C:252:VAL:HG23	1:C:253:ALA:N	2.33	0.42
1:E:227:GLU:OE2	1:G:192:ARG:HA	2.20	0.42
2:F:37:VAL:O	2:F:41:PHE:CD2	2.72	0.42
2:F:1132:ILE:O	2:F:1136:ILE:CB	2.67	0.42
2:H:588:THR:N	2:H:589:PRO:CD	2.82	0.42
1:A:227:GLU:OE2	1:C:192:ARG:HA	2.18	0.42
1:C:268:TYR:CE2	1:C:347:ARG:HG2	2.55	0.42
2:D:1514:MET:O	2:D:1518:ASN:CB	2.67	0.42
1:E:153:ASN:O	1:E:157:LEU:HB2	2.19	0.42
2:F:1514:MET:O	2:F:1518:ASN:CB	2.67	0.42
2:H:518:PHE:O	2:H:522:VAL:CB	2.68	0.42
2:H:1514:MET:O	2:H:1518:ASN:CB	2.68	0.42
1:A:55:PHE:HE1	1:C:206:ARG:CD	2.32	0.42
2:B:547:ASN:O	2:B:551:PRO:CD	2.67	0.42
1:C:220:VAL:CG2	1:C:233:LEU:HD22	2.47	0.42
1:E:48:ASN:C	3:E:401:ATP:HN62	2.27	0.42
1:G:142:CYS:SG	1:G:142:CYS:O	2.78	0.42
1:G:257:ILE:N	1:G:257:ILE:CD1	2.77	0.42
1:G:341:THR:HA	1:G:342:PRO:HD3	1.88	0.42
2:H:253:LEU:N	2:H:254:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HA	1:G:227:GLU:OE2	2.20	0.42
1:C:132:GLY:HA3	1:E:131:ILE:O	2.20	0.42
2:D:132:PHE:HA	2:D:133:PRO:HD3	1.81	0.42
1:E:132:GLY:HA3	1:G:131:ILE:O	2.20	0.42
2:H:1434:GLY:O	2:H:1475:ILE:N	2.44	0.42
1:A:40:GLY:C	1:A:41:ASN:OD1	2.62	0.42
1:A:268:TYR:CE2	1:A:347:ARG:HG2	2.55	0.42
2:B:518:PHE:O	2:B:522:VAL:CB	2.68	0.42
2:B:687:THR:HA	2:B:695:THR:H	1.85	0.42
2:B:1066:MET:O	2:B:1070:LEU:CB	2.68	0.42
1:E:268:TYR:CE2	1:E:347:ARG:HG2	2.55	0.42
2:F:518:PHE:O	2:F:522:VAL:CB	2.68	0.42
1:G:36:VAL:HG23	1:G:42:CYS:HB3	2.01	0.42
2:H:205:LYS:N	2:H:206:PRO:CD	2.82	0.42
1:C:48:ASN:C	3:C:401:ATP:HN62	2.27	0.41
2:D:588:THR:N	2:D:589:PRO:CD	2.82	0.41
1:E:147:LEU:O	1:E:151:VAL:HG23	2.20	0.41
2:H:303:SER:HA	2:H:436:PRO:HB3	2.01	0.41
2:H:1066:MET:O	2:H:1070:LEU:CB	2.68	0.41
2:B:132:PHE:HA	2:B:133:PRO:HD3	1.81	0.41
1:C:339:VAL:HG13	1:C:340:PRO:CD	2.49	0.41
2:D:1066:MET:O	2:D:1070:LEU:CB	2.68	0.41
2:B:206:PRO:HB2	2:B:207:PRO:CD	2.44	0.41
1:C:72:LEU:O	1:C:76:THR:HG23	2.21	0.41
2:D:391:ILE:O	2:D:395:ILE:CB	2.69	0.41
1:E:142:CYS:SG	1:E:142:CYS:O	2.78	0.41
1:A:179:GLU:C	1:A:181:LEU:N	2.76	0.41
2:B:485:GLN:O	2:B:489:LEU:CB	2.69	0.41
2:D:34:VAL:CB	2:D:35:PRO:CD	2.98	0.41
2:D:518:PHE:O	2:D:522:VAL:CB	2.68	0.41
1:E:36:VAL:HG23	1:E:42:CYS:HB3	2.01	0.41
1:G:345:THR:HG23	1:G:348:GLN:H	1.86	0.41
1:A:220:VAL:CG2	1:A:233:LEU:HD22	2.47	0.41
1:C:345:THR:HG23	1:C:348:GLN:H	1.86	0.41
2:D:416:GLN:O	2:D:420:LEU:HB2	2.21	0.41
1:A:131:ILE:O	1:G:132:GLY:HA3	2.20	0.41
2:B:391:ILE:O	2:B:395:ILE:CB	2.69	0.41
1:C:142:CYS:SG	1:C:142:CYS:O	2.78	0.41
2:F:391:ILE:O	2:F:395:ILE:CB	2.69	0.41
2:F:561:GLY:O	2:F:565:PHE:CB	2.69	0.41
1:G:72:LEU:O	1:G:76:THR:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:LEU:O	1:G:151:VAL:HG23	2.20	0.41
1:A:345:THR:HG23	1:A:348:GLN:H	1.86	0.41
1:C:147:LEU:O	1:C:151:VAL:HG23	2.20	0.41
1:G:268:TYR:CE2	1:G:347:ARG:HG2	2.55	0.41
2:H:44:PHE:N	2:H:45:PRO:CD	2.83	0.41
2:H:472:PRO:O	2:H:476:PHE:CB	2.69	0.41
1:A:72:LEU:O	1:A:76:THR:HG23	2.21	0.41
2:D:297:ARG:O	2:D:301:LEU:HB2	2.21	0.41
1:A:48:ASN:C	3:A:401:ATP:HN62	2.27	0.41
2:B:34:VAL:CB	2:B:35:PRO:CD	2.98	0.41
2:B:44:PHE:N	2:B:45:PRO:CD	2.83	0.41
2:B:561:GLY:O	2:B:565:PHE:CB	2.69	0.41
1:C:227:GLU:OE2	1:E:192:ARG:HA	2.20	0.41
1:C:238:ILE:O	1:C:238:ILE:HG13	2.21	0.41
2:D:44:PHE:N	2:D:45:PRO:CD	2.83	0.41
2:D:64:THR:O	2:D:65:TRP:CG	2.74	0.41
2:D:1148:LEU:O	2:D:1152:SER:CB	2.69	0.41
1:E:268:TYR:CD2	1:E:347:ARG:HG2	2.56	0.41
2:F:34:VAL:CB	2:F:35:PRO:CD	2.98	0.41
2:F:297:ARG:O	2:F:301:LEU:HB2	2.21	0.41
2:F:1148:LEU:O	2:F:1152:SER:CB	2.69	0.41
1:G:268:TYR:CD2	1:G:347:ARG:HG2	2.56	0.41
2:H:391:ILE:O	2:H:395:ILE:CB	2.69	0.41
2:H:561:GLY:O	2:H:565:PHE:CB	2.69	0.41
2:B:1123:ASN:O	2:B:1127:SER:OG	2.26	0.41
2:D:680:GLN:HA	2:D:702:ARG:HG2	2.03	0.41
2:F:485:GLN:O	2:F:489:LEU:CB	2.69	0.41
1:G:200:LEU:HD23	1:G:200:LEU:HA	1.96	0.41
1:G:209:MET:HE1	1:G:250:PHE:CE1	2.56	0.41
1:G:238:ILE:O	1:G:238:ILE:HG13	2.21	0.41
2:H:297:ARG:O	2:H:301:LEU:HB2	2.21	0.41
2:H:485:GLN:O	2:H:489:LEU:CB	2.69	0.41
2:B:484:ALA:O	2:B:488:THR:CB	2.69	0.40
2:B:1434:GLY:O	2:B:1475:ILE:N	2.44	0.40
1:E:345:THR:HG23	1:E:348:GLN:H	1.86	0.40
2:F:416:GLN:O	2:F:420:LEU:HB2	2.21	0.40
2:F:472:PRO:O	2:F:476:PHE:CB	2.69	0.40
2:F:1066:MET:O	2:F:1070:LEU:CB	2.68	0.40
1:G:265:SER:HA	1:G:266:PRO:HD3	1.84	0.40
1:G:313:GLN:HA	1:G:338:LYS:HA	2.03	0.40
2:H:416:GLN:O	2:H:420:LEU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG12	1:A:282:GLU:O	2.22	0.40
1:A:313:GLN:HA	1:A:338:LYS:HA	2.03	0.40
2:B:64:THR:O	2:B:65:TRP:CG	2.74	0.40
1:C:150:ILE:HG23	1:E:83:TRP:HZ3	1.85	0.40
1:C:209:MET:HE1	1:C:250:PHE:CE1	2.56	0.40
1:E:209:MET:HE1	1:E:250:PHE:CE1	2.56	0.40
2:F:484:ALA:O	2:F:488:THR:CB	2.69	0.40
2:H:460:ALA:O	2:H:464:ALA:CB	2.70	0.40
2:H:484:ALA:O	2:H:488:THR:CB	2.69	0.40
1:A:268:TYR:CD2	1:A:347:ARG:HG2	2.56	0.40
1:C:268:TYR:CD2	1:C:347:ARG:HG2	2.56	0.40
2:D:472:PRO:O	2:D:476:PHE:CB	2.69	0.40
1:E:72:LEU:O	1:E:76:THR:HG23	2.21	0.40
1:E:150:ILE:HG23	1:G:83:TRP:HZ3	1.85	0.40
1:E:221:ARG:HG2	1:E:222:LYS:N	2.37	0.40
2:F:44:PHE:N	2:F:45:PRO:CD	2.83	0.40
2:H:718:GLY:O	2:H:722:LEU:N	2.48	0.40
1:A:147:LEU:O	1:A:151:VAL:HG23	2.20	0.40
2:B:297:ARG:O	2:B:301:LEU:HB2	2.21	0.40
2:B:1148:LEU:O	2:B:1152:SER:CB	2.69	0.40
2:D:485:GLN:O	2:D:489:LEU:CB	2.69	0.40
2:D:561:GLY:O	2:D:565:PHE:CB	2.69	0.40
2:H:34:VAL:CB	2:H:35:PRO:CD	2.98	0.40
2:D:484:ALA:O	2:D:488:THR:CB	2.69	0.40
1:E:55:PHE:HE1	1:G:206:ARG:HD3	1.87	0.40
2:F:1277:SER:OG	2:F:1279:GLY:O	2.32	0.40
2:H:146:ALA:HB1	2:H:179:TYR:CZ	2.56	0.40
2:H:1148:LEU:O	2:H:1152:SER:CB	2.69	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	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	36	72
1	C	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	36	72
1	E	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	36	72
1	G	323/390 (83%)	310 (96%)	12 (4%)	1 (0%)	36	72
2	B	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	36	72
2	D	1363/1590 (86%)	1302 (96%)	57 (4%)	4 (0%)	36	72
2	F	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	36	72
2	H	1363/1590 (86%)	1303 (96%)	56 (4%)	4 (0%)	36	72
All	All	6744/7920 (85%)	6451 (96%)	273 (4%)	20 (0%)	37	72

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	VAL
2	B	277	ASP
2	B	316	GLY
2	D	98	VAL
2	D	277	ASP
2	D	316	GLY
2	F	98	VAL
2	F	277	ASP
2	F	316	GLY
2	H	98	VAL
2	H	277	ASP
2	H	316	GLY
1	A	180	THR
1	C	180	THR
1	E	180	THR
1	G	180	THR
2	B	224	LEU
2	D	224	LEU
2	F	224	LEU
2	H	224	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/341 (77%)	258 (98%)	6 (2%)	44	64
1	C	264/341 (77%)	258 (98%)	6 (2%)	44	64
1	E	264/341 (77%)	258 (98%)	6 (2%)	44	64
1	G	264/341 (77%)	258 (98%)	6 (2%)	44	64
2	B	224/1381 (16%)	222 (99%)	2 (1%)	70	79
2	D	224/1381 (16%)	222 (99%)	2 (1%)	70	79
2	F	224/1381 (16%)	222 (99%)	2 (1%)	70	79
2	H	224/1381 (16%)	222 (99%)	2 (1%)	70	79
All	All	1952/6888 (28%)	1920 (98%)	32 (2%)	54	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LEU
1	A	167	ILE
1	A	215	ILE
1	A	257	ILE
1	A	319	VAL
1	A	356	LEU
2	B	6	CYS
2	B	123	TYR
1	C	157	LEU
1	C	167	ILE
1	C	215	ILE
1	C	257	ILE
1	C	319	VAL
1	C	356	LEU
2	D	6	CYS
2	D	123	TYR
1	E	157	LEU
1	E	167	ILE
1	E	215	ILE
1	E	257	ILE
1	E	319	VAL
1	E	356	LEU
2	F	6	CYS
2	F	123	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	157	LEU
1	G	167	ILE
1	G	215	ILE
1	G	257	ILE
1	G	319	VAL
1	G	356	LEU
2	H	6	CYS
2	H	123	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	97	HIS
1	A	193	HIS
1	A	235	GLN
1	A	264	ASN
1	A	278	HIS
1	A	279	GLN
1	C	46	HIS
1	C	97	HIS
1	C	193	HIS
1	C	235	GLN
1	C	264	ASN
1	C	278	HIS
1	C	279	GLN
1	E	46	HIS
1	E	97	HIS
1	E	193	HIS
1	E	235	GLN
1	E	264	ASN
1	E	278	HIS
1	E	279	GLN
1	G	97	HIS
1	G	193	HIS
1	G	235	GLN
1	G	264	ASN
1	G	278	HIS
1	G	279	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	ATP	A	401	-	32,33,33	1.34	5 (15%)	48,52,52	1.69	8 (16%)
3	ATP	G	401	-	32,33,33	1.34	5 (15%)	48,52,52	1.68	8 (16%)
3	ATP	C	401	-	32,33,33	1.34	5 (15%)	48,52,52	1.69	8 (16%)
3	ATP	E	401	-	32,33,33	1.34	5 (15%)	48,52,52	1.69	8 (16%)

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	ATP	A	401	-	-	10/22/38/38	0/3/3/3
3	ATP	G	401	-	-	10/22/38/38	0/3/3/3
3	ATP	C	401	-	-	10/22/38/38	0/3/3/3
3	ATP	E	401	-	-	10/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ATP	C5-C4	3.88	1.46	1.39
3	A	401	ATP	C5-C4	3.87	1.46	1.39
3	E	401	ATP	C5-C4	3.87	1.46	1.39
3	G	401	ATP	C5-C4	3.87	1.46	1.39
3	A	401	ATP	C5-C6	2.74	1.48	1.41
3	C	401	ATP	C5-C6	2.74	1.48	1.41
3	E	401	ATP	C5-C6	2.74	1.48	1.41
3	G	401	ATP	C5-C6	2.74	1.48	1.41
3	C	401	ATP	C8-N7	2.42	1.36	1.31
3	A	401	ATP	C8-N7	2.40	1.36	1.31
3	E	401	ATP	C8-N7	2.40	1.36	1.31
3	G	401	ATP	C8-N7	2.40	1.36	1.31
3	E	401	ATP	C4-N9	-2.31	1.32	1.37
3	A	401	ATP	C4-N9	-2.29	1.32	1.37
3	C	401	ATP	C4-N9	-2.29	1.32	1.37
3	G	401	ATP	C4-N9	-2.29	1.32	1.37
3	A	401	ATP	C5-N7	-2.28	1.34	1.39
3	C	401	ATP	C5-N7	-2.28	1.34	1.39
3	E	401	ATP	C5-N7	-2.28	1.34	1.39
3	G	401	ATP	C5-N7	-2.28	1.34	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ATP	C5-C4-N3	-5.40	119.29	126.72
3	A	401	ATP	C5-C4-N3	-5.39	119.30	126.72
3	E	401	ATP	C5-C4-N3	-5.39	119.30	126.72
3	G	401	ATP	C5-C4-N3	-5.36	119.34	126.72
3	E	401	ATP	N3-C4-N9	4.55	134.90	127.17
3	A	401	ATP	N3-C4-N9	4.53	134.86	127.17
3	C	401	ATP	N3-C4-N9	4.53	134.86	127.17
3	G	401	ATP	N3-C4-N9	4.50	134.82	127.17
3	C	401	ATP	C2-N3-C4	3.49	120.36	111.83
3	A	401	ATP	C2-N3-C4	3.49	120.36	111.83
3	E	401	ATP	C2-N3-C4	3.49	120.36	111.83
3	G	401	ATP	C2-N3-C4	3.48	120.32	111.83
3	E	401	ATP	C4-N9-C8	3.03	108.92	105.74
3	A	401	ATP	C4-N9-C8	2.96	108.85	105.74
3	C	401	ATP	C4-N9-C8	2.96	108.85	105.74
3	G	401	ATP	C4-N9-C8	2.96	108.85	105.74
3	C	401	ATP	N3-C2-N1	-2.92	124.16	128.58
3	A	401	ATP	N3-C2-N1	-2.92	124.16	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	ATP	N3-C2-N1	-2.92	124.16	128.58
3	G	401	ATP	N3-C2-N1	-2.92	124.16	128.58
3	E	401	ATP	C3'-C2'-C1'	2.34	105.89	101.46
3	A	401	ATP	C3'-C2'-C1'	2.32	105.85	101.46
3	G	401	ATP	C3'-C2'-C1'	2.32	105.85	101.46
3	C	401	ATP	C3'-C2'-C1'	2.31	105.84	101.46
3	C	401	ATP	C4-C5-N7	-2.31	107.94	110.58
3	A	401	ATP	C4-C5-N7	-2.30	107.96	110.58
3	E	401	ATP	C4-C5-N7	-2.30	107.96	110.58
3	G	401	ATP	C4-C5-N7	-2.30	107.96	110.58
3	A	401	ATP	N6-C6-N1	2.07	123.00	118.38
3	C	401	ATP	N6-C6-N1	2.07	123.00	118.38
3	G	401	ATP	N6-C6-N1	2.07	123.00	118.38
3	E	401	ATP	N6-C6-N1	2.07	122.98	118.38

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O2A
3	E	401	ATP	C5'-O5'-PA-O2A
3	G	401	ATP	C5'-O5'-PA-O2A
3	A	401	ATP	O4'-C4'-C5'-O5'
3	C	401	ATP	O4'-C4'-C5'-O5'
3	E	401	ATP	O4'-C4'-C5'-O5'
3	G	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	C2'-C1'-N9-C8
3	C	401	ATP	C2'-C1'-N9-C8
3	E	401	ATP	C2'-C1'-N9-C8
3	G	401	ATP	C2'-C1'-N9-C8
3	A	401	ATP	C3'-C4'-C5'-O5'
3	C	401	ATP	C3'-C4'-C5'-O5'
3	E	401	ATP	C3'-C4'-C5'-O5'
3	G	401	ATP	C3'-C4'-C5'-O5'
3	A	401	ATP	C5'-O5'-PA-O1A
3	A	401	ATP	C5'-O5'-PA-O3A
3	C	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O3A
3	E	401	ATP	C5'-O5'-PA-O1A
3	E	401	ATP	C5'-O5'-PA-O3A
3	G	401	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

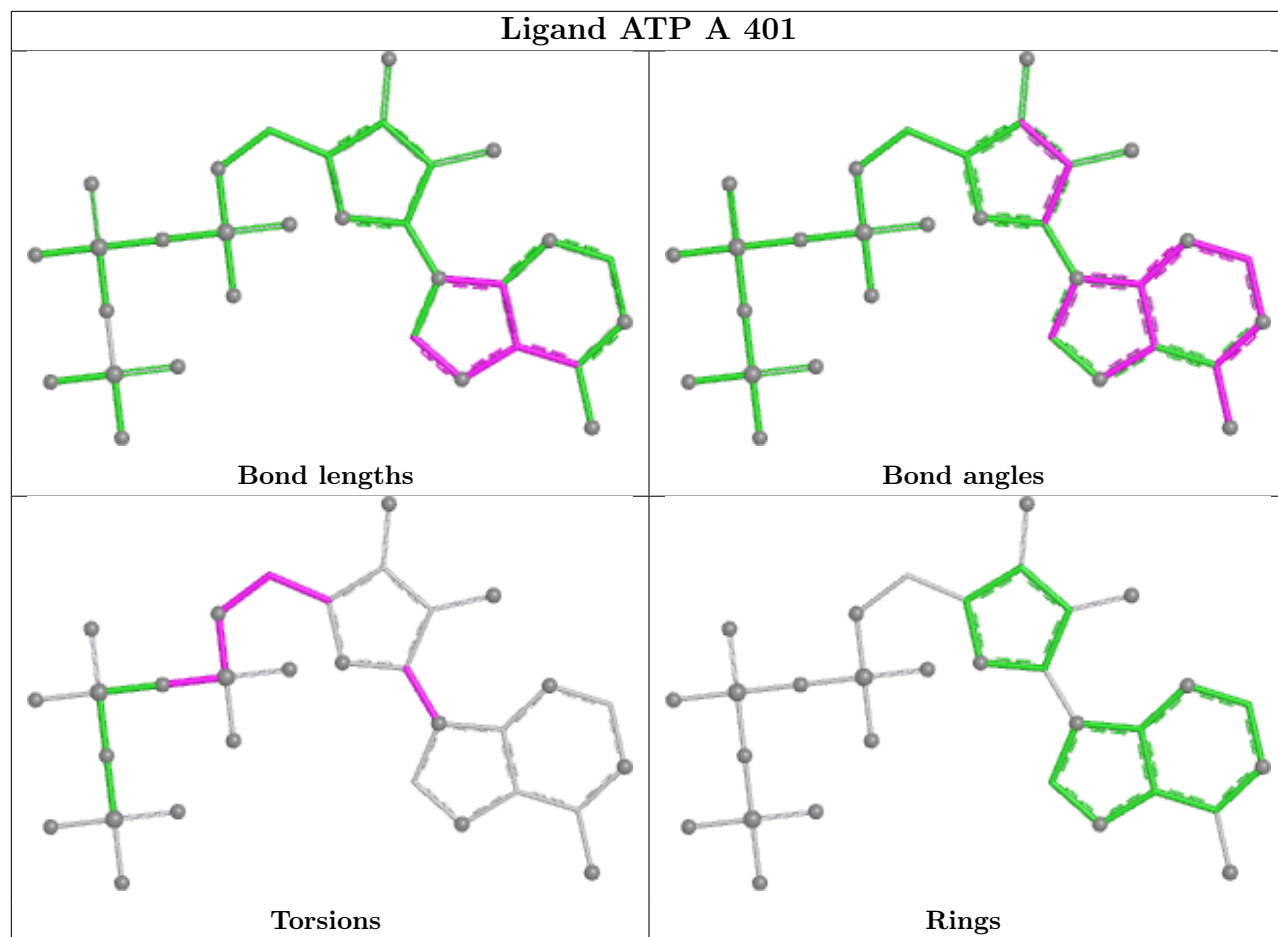
Mol	Chain	Res	Type	Atoms
3	G	401	ATP	C5'-O5'-PA-O3A
3	A	401	ATP	C2'-C1'-N9-C4
3	C	401	ATP	C2'-C1'-N9-C4
3	E	401	ATP	C2'-C1'-N9-C4
3	G	401	ATP	C2'-C1'-N9-C4
3	A	401	ATP	C4'-C5'-O5'-PA
3	C	401	ATP	C4'-C5'-O5'-PA
3	E	401	ATP	C4'-C5'-O5'-PA
3	G	401	ATP	C4'-C5'-O5'-PA
3	A	401	ATP	O4'-C1'-N9-C8
3	C	401	ATP	O4'-C1'-N9-C8
3	E	401	ATP	O4'-C1'-N9-C8
3	G	401	ATP	O4'-C1'-N9-C8
3	A	401	ATP	PB-O3A-PA-O2A
3	C	401	ATP	PB-O3A-PA-O2A
3	E	401	ATP	PB-O3A-PA-O2A
3	G	401	ATP	PB-O3A-PA-O2A

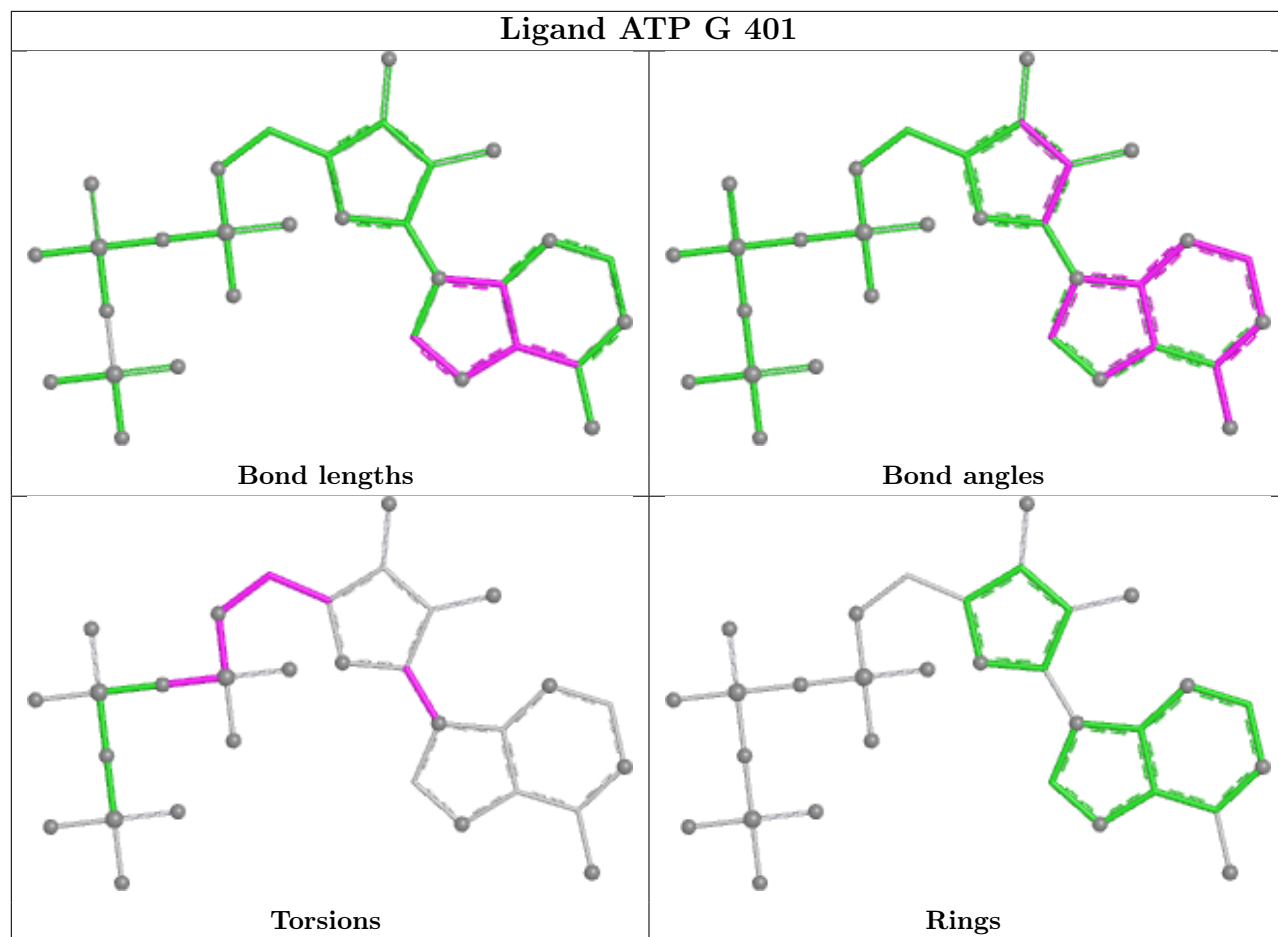
There are no ring outliers.

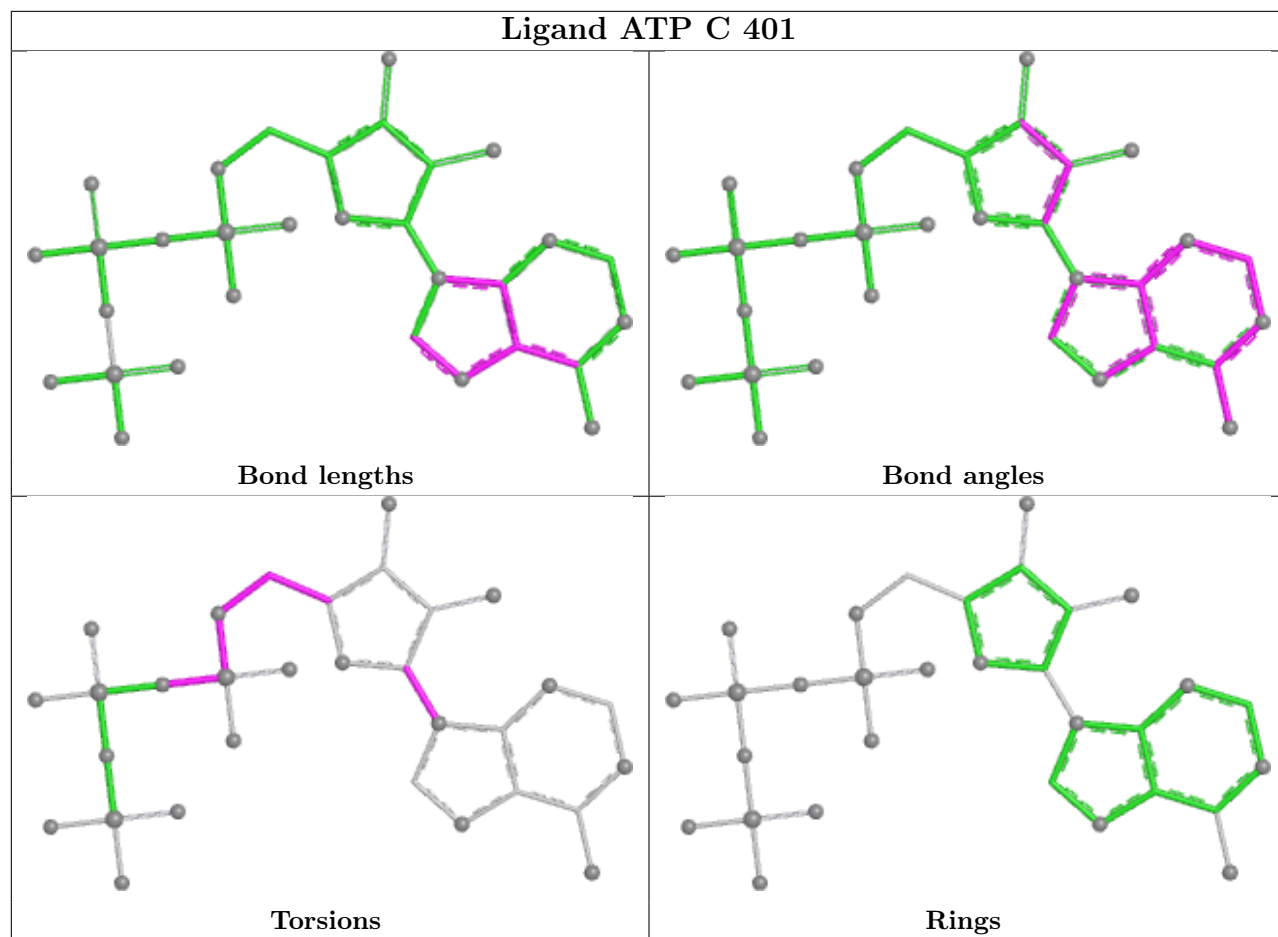
4 monomers are involved in 31 short contacts:

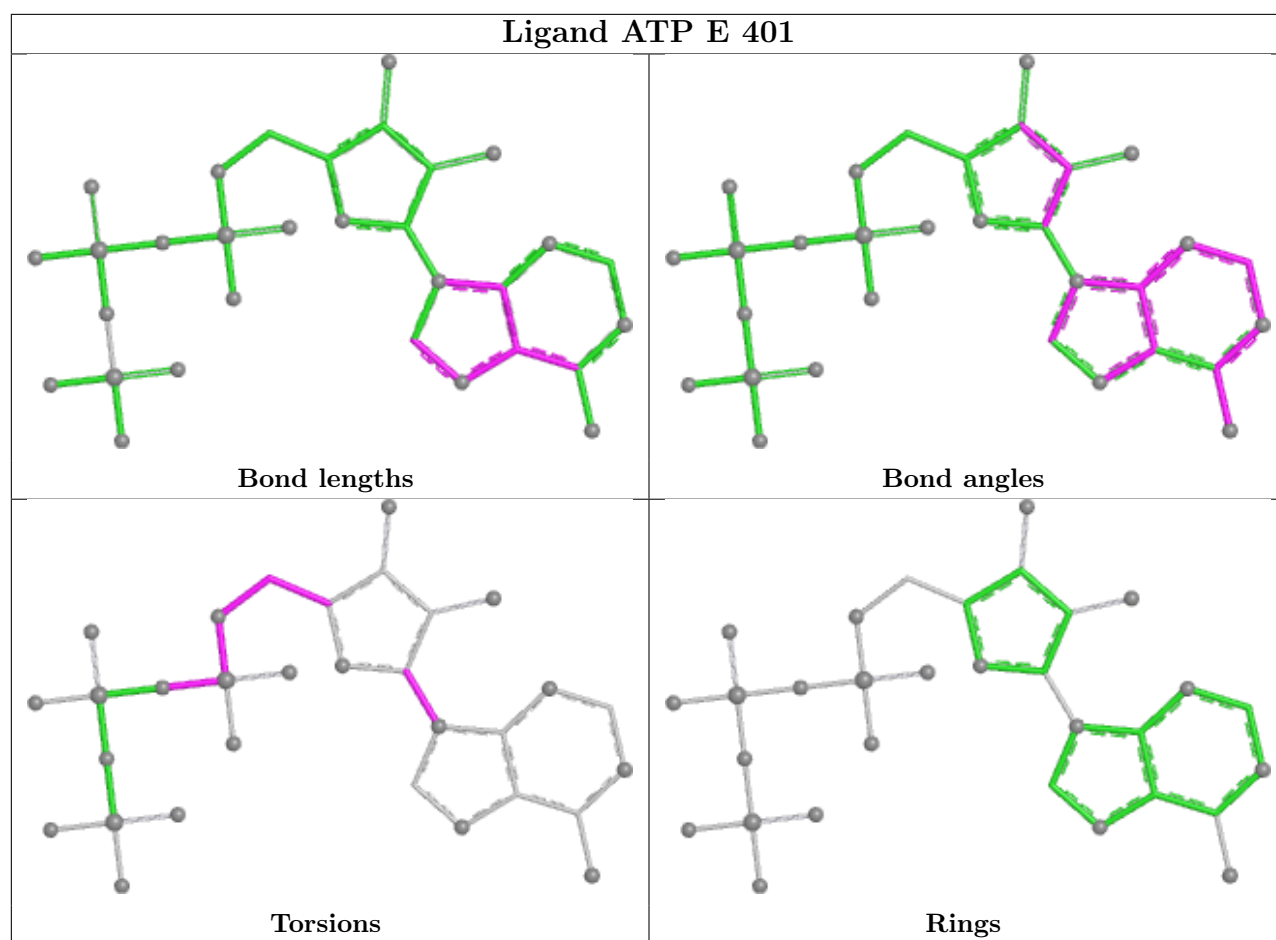
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	8	0
3	G	401	ATP	7	0
3	C	401	ATP	8	0
3	E	401	ATP	8	0

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 than 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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

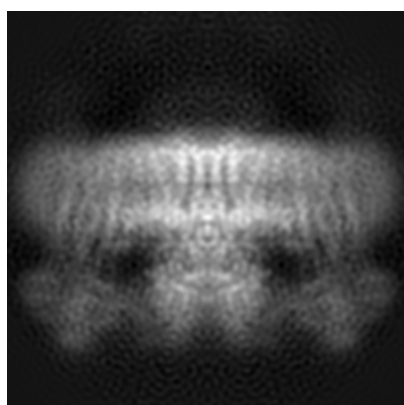
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8470. These allow visual inspection of the internal detail of the map and identification of artifacts.

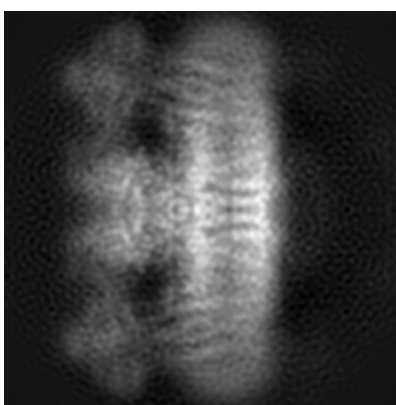
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

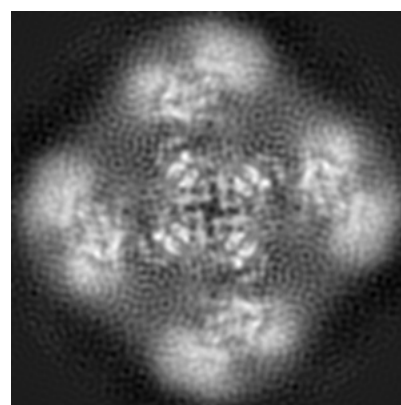
6.1.1 Primary map



X



Y

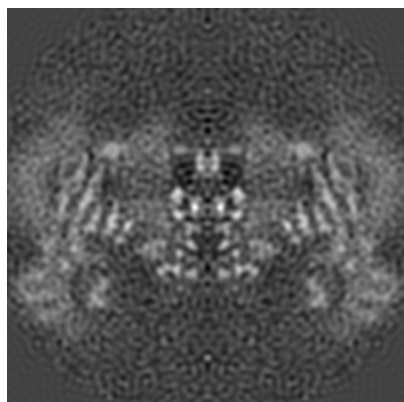


Z

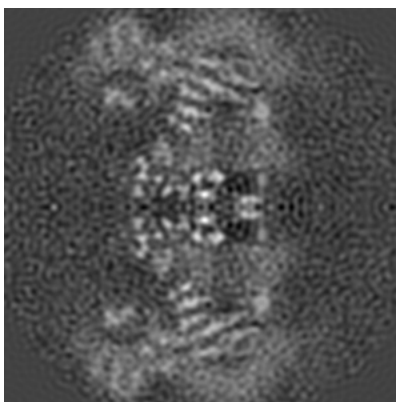
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

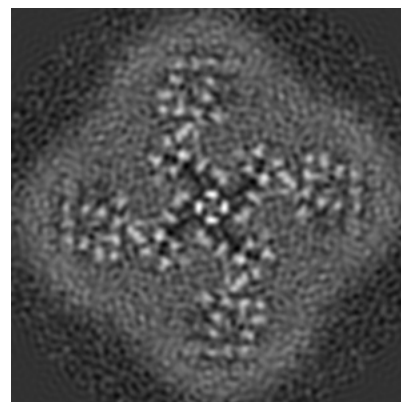
6.2.1 Primary map



X Index: 136



Y Index: 136

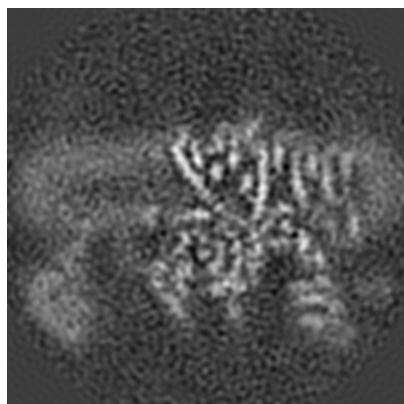


Z Index: 136

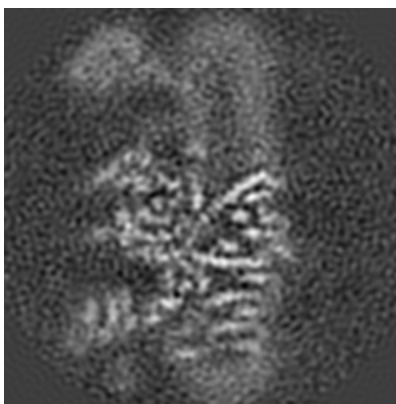
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

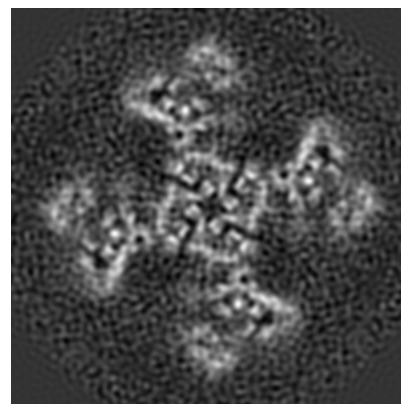
6.3.1 Primary map



X Index: 118



Y Index: 118

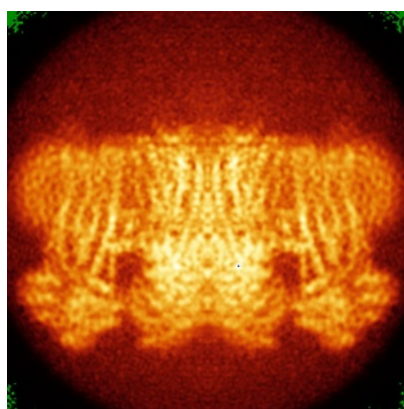


Z Index: 112

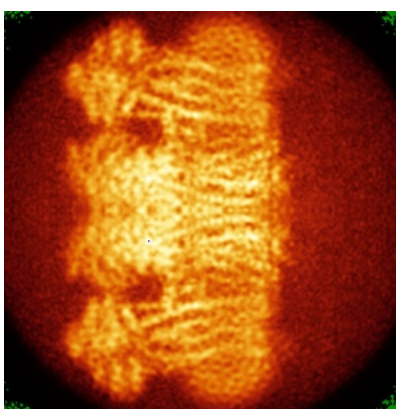
The images above show the largest variance slices of the map in three orthogonal directions.

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

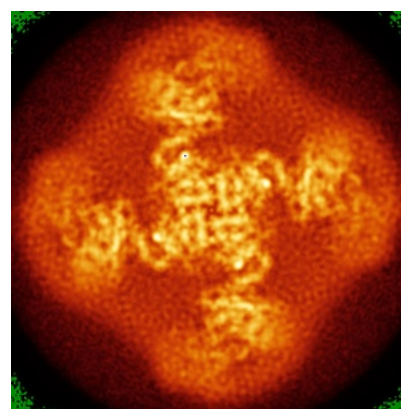
6.4.1 Primary map



X



Y

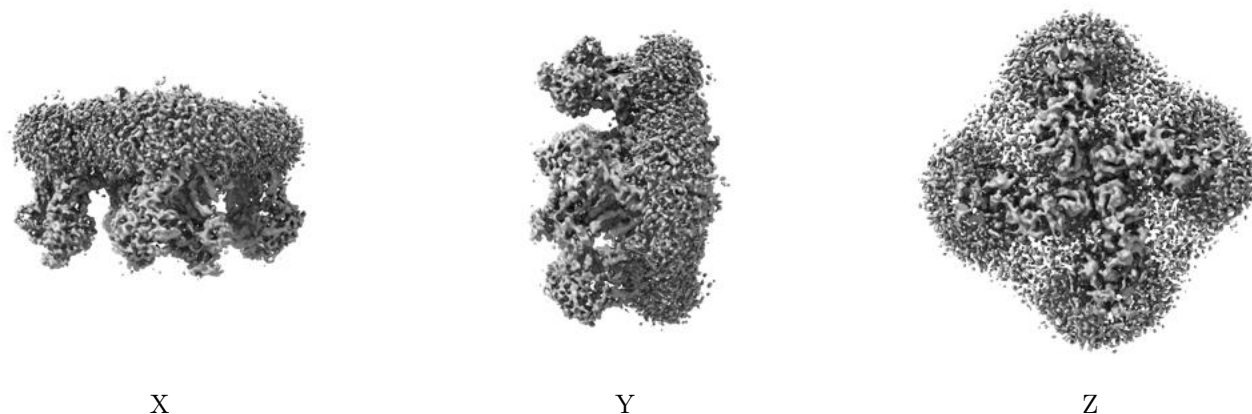


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027736. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

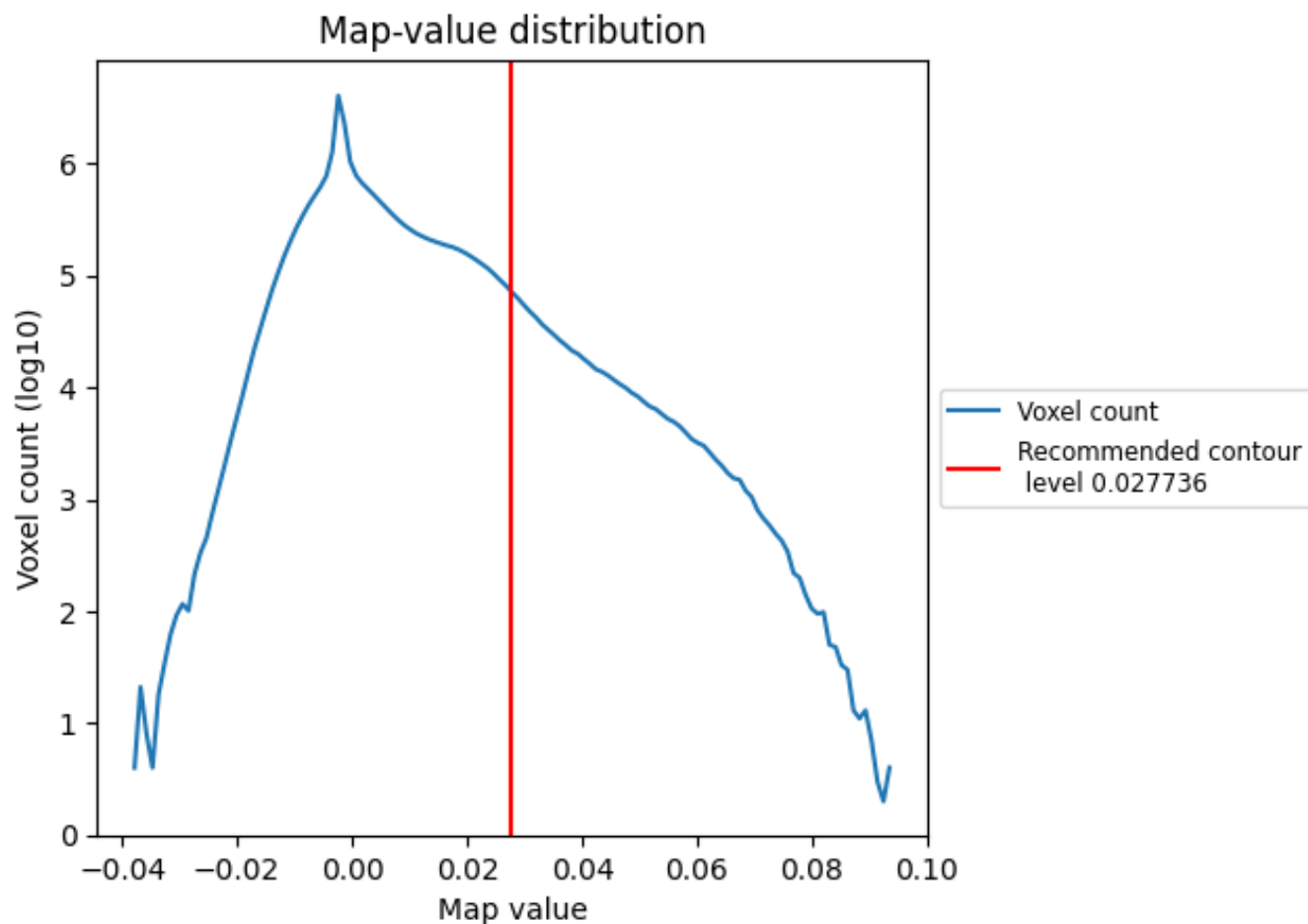
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

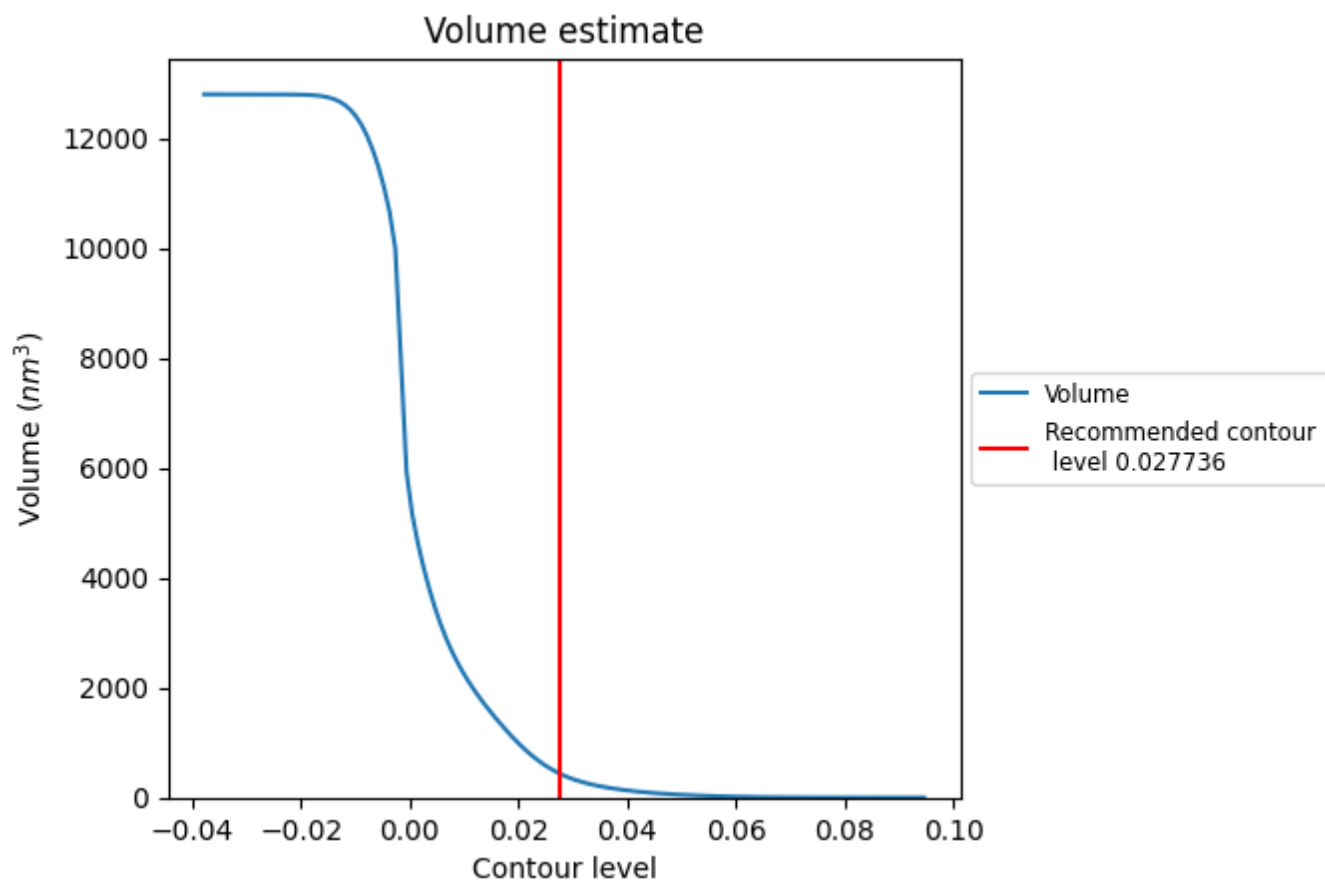
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

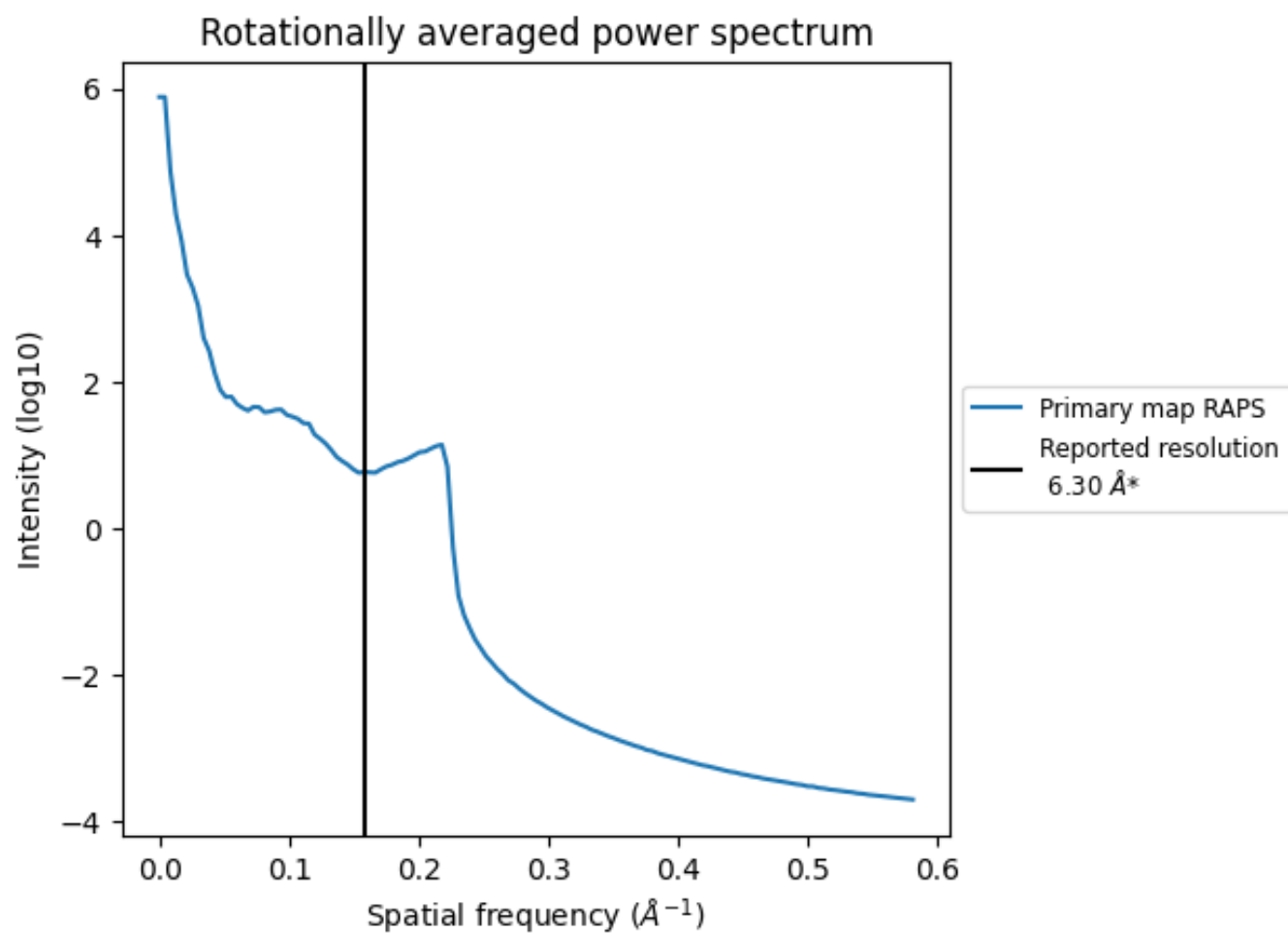
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm^3 ; this corresponds to an approximate mass of 387 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

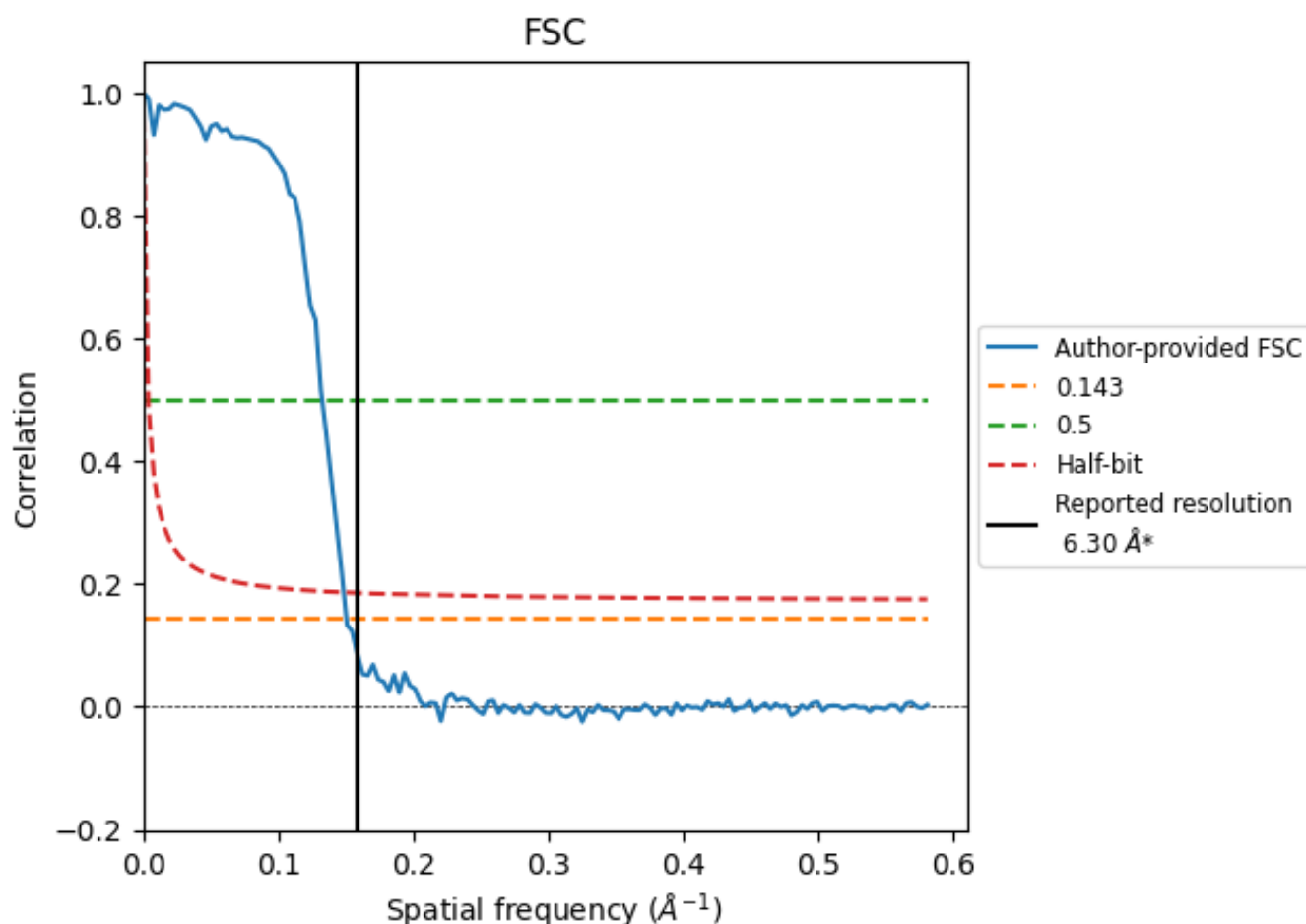


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

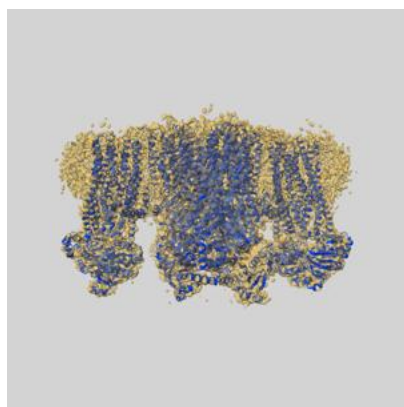
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.64	7.54	6.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

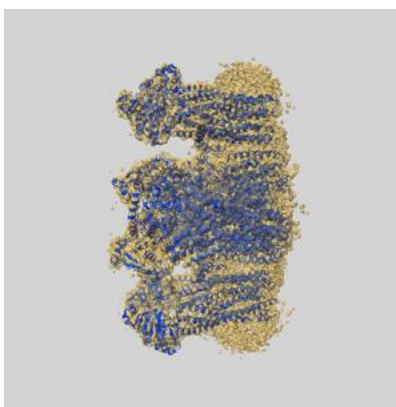
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8470 and PDB model 5TWV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

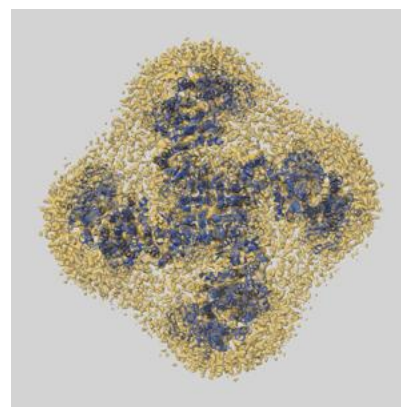
9.1 Map-model overlay [i](#)



X



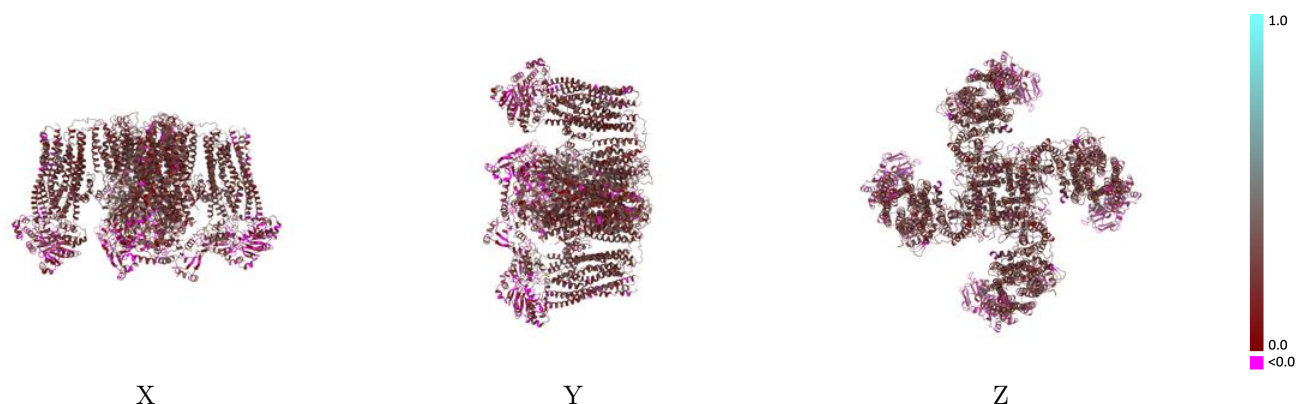
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027736 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

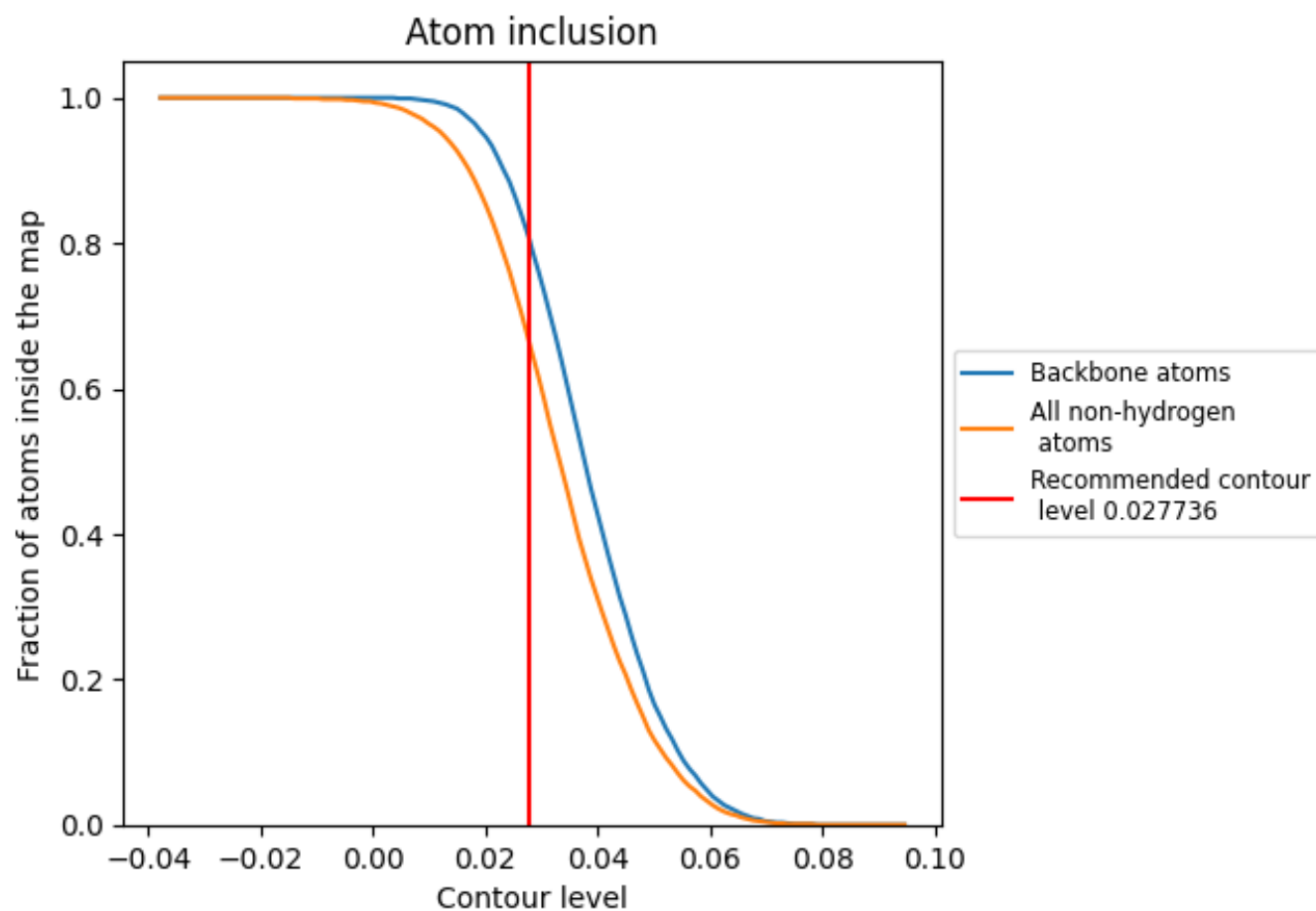


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 66% 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 (0.027736) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.2310
A	0.6480	0.2570
B	0.6710	0.2220
C	0.6480	0.2550
D	0.6690	0.2230
E	0.6490	0.2560
F	0.6730	0.2230
G	0.6490	0.2570
H	0.6680	0.2230

1.0

0.0

<0.0