



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:20 PM UTC

PDB ID : 6RE5 / pdb_00006re5
EMDB ID : EMD-4842
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 2C, composite map
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 3.20 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:

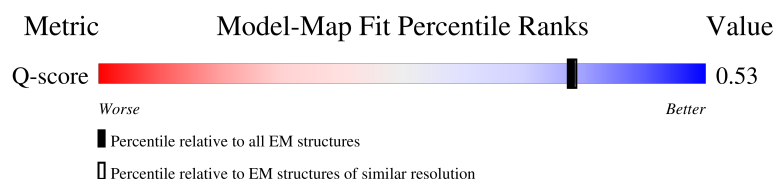
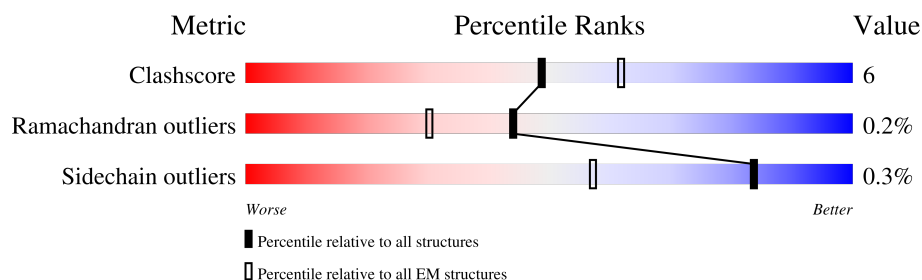
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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.



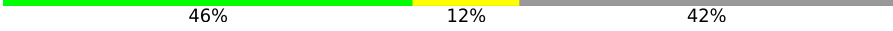
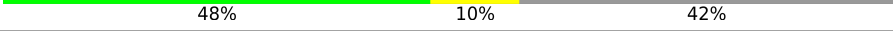
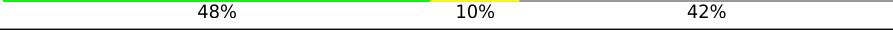
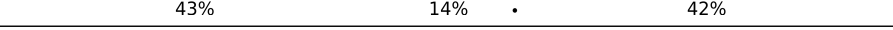
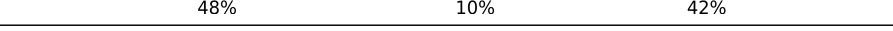
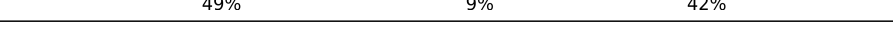
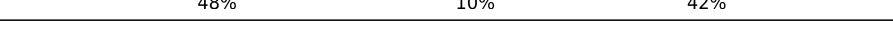
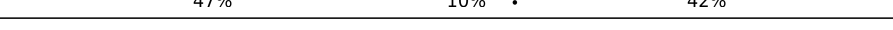
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	0	82	 96%
2	1	618	 86% 10%
3	2	441	 83% 17%
4	3	325	 66% 10% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	4	294	 89% 10%
6	5	123	 80% 20%
7	6	151	 76% 6% 18%
8	7	190	 79% 13% 7%
9	8	89	 89% 10%
10	9	97	 91% 9%
11	A	127	 46% 12% 42%
11	B	127	 48% 10% 42%
11	C	127	 48% 10% 42%
11	D	127	 49% 9% 42%
11	E	127	 43% 14% 42%
11	F	127	 48% 10% 42%
11	G	127	 49% 9% 42%
11	H	127	 49% 9% 42%
11	I	127	 48% 10% 42%
11	J	127	 47% 10% 42%
12	M	327	 61% 6% 34%
13	P	229	 68% 16% 16%
14	Q	74	 82% 15%
15	R	199	 80% 9% 11%
16	S	317	 73% 15% 13%
17	T	562	 79% 14% 7%
17	U	562	 78% 15% 7%
17	V	562	 79% 14% 7%
18	X	574	 80% 13% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	Y	574	 76% 14% 9%
18	Z	574	 80% 13% 6%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 53720 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	441	Total	C	N	O		0	0
			3163	2020	532	611			

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	193	Total	C	N	O	S	0	0
			1532	988	250	290	4		

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

- Molecule 17 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	523	Total	C	N	O	S	0	0
			3979	2537	703	728	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3978	2537	702	728	11		
17	V	520	Total	C	N	O	S	0	0
			3961	2527	700	723	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 18 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		
18	Y	520	Total	C	N	O	S	0	0
			3952	2484	669	786	13		
18	Z	539	Total	C	N	O	S	0	0
			4095	2572	693	817	13		

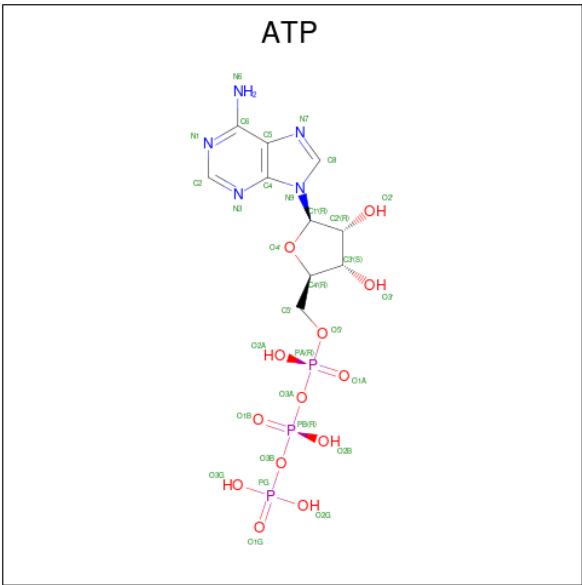
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Zn	0
			1	1	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

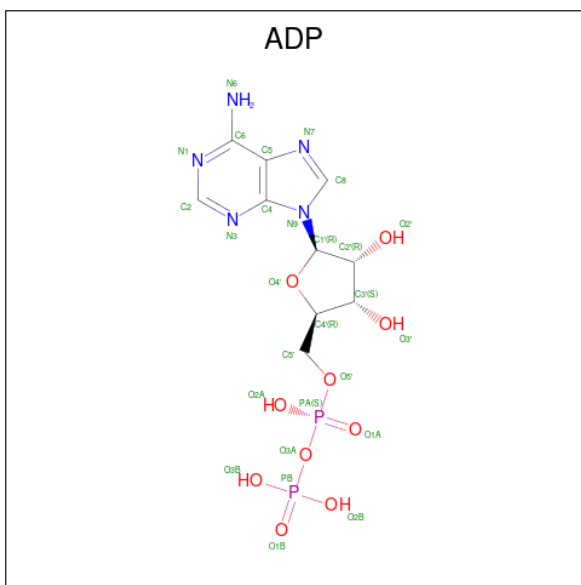


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	T	1	Total	Mg	0
			1	1	
21	U	1	Total	Mg	0
			1	1	
21	V	1	Total	Mg	0
			1	1	
21	Y	1	Total	Mg	0
			1	1	
21	Z	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

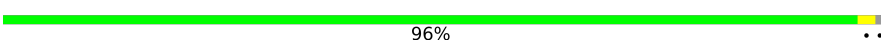


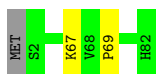
Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total 27	C 10	N 5	O 10	P 2	0
22	Z	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

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

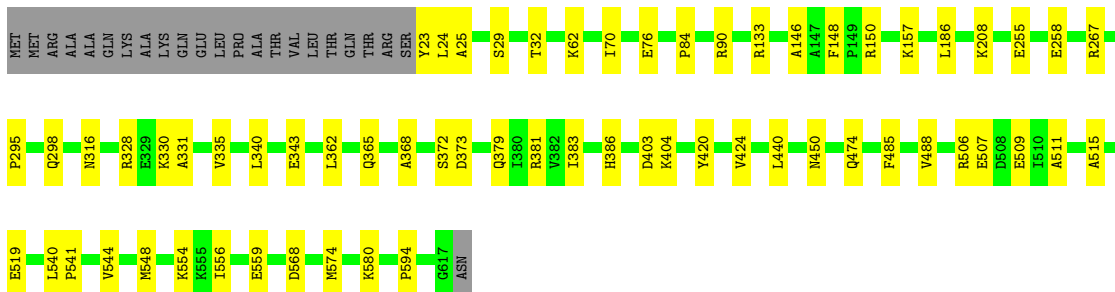
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

Chain 0:  96% ..



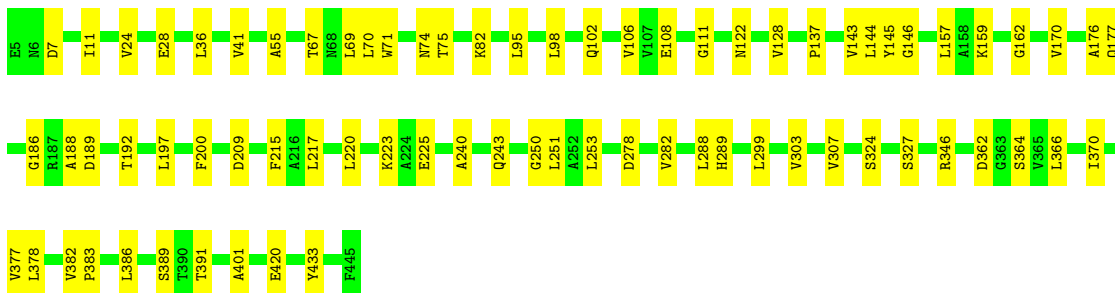
- Molecule 2: ATP synthase associated protein ASA1

Chain 1:  86% 10% .



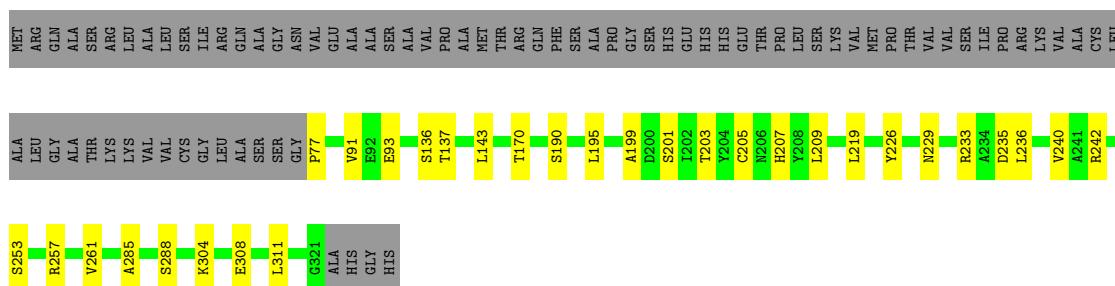
- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

Chain 2:  83% 17%



- Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:  66% 10% 25%



- Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 89% 10%



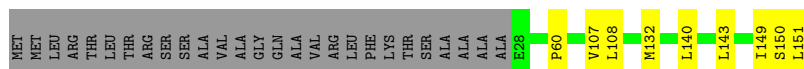
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5: 80% 20%



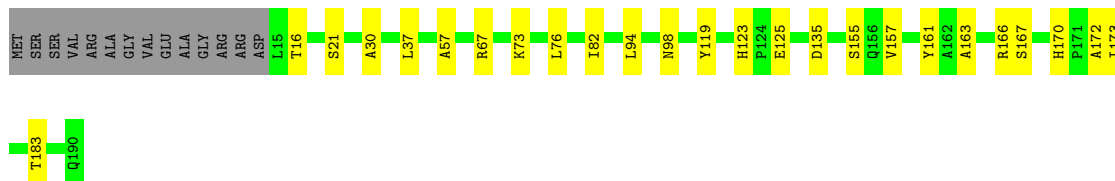
- Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6: 76% 6% 18%



- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7: 79% 13% 7%

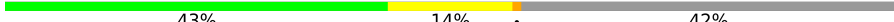


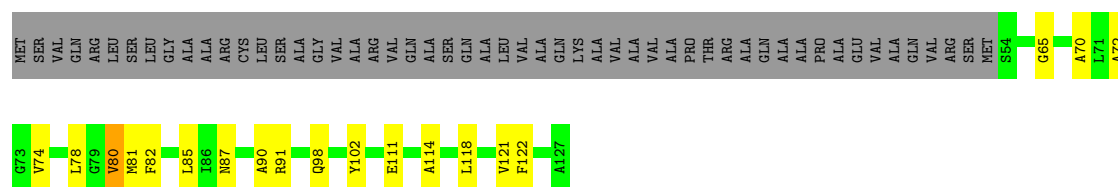
- Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8: 89% 10%



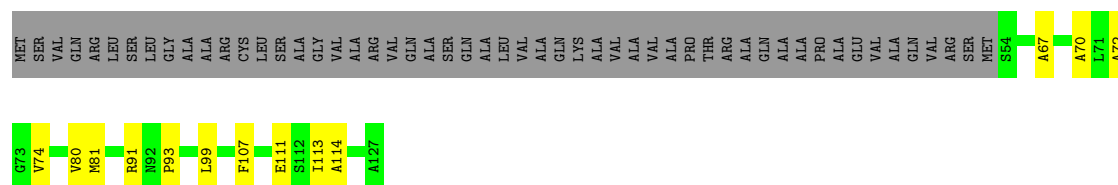
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain E:  43% 14% 42%



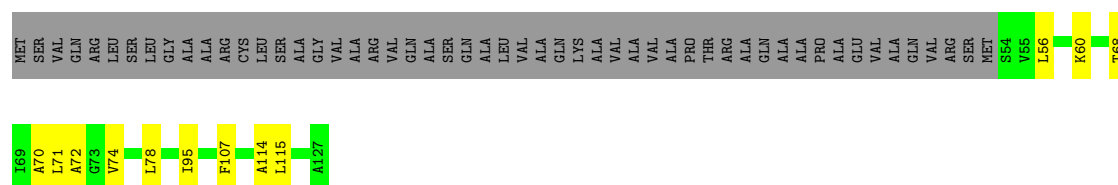
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain F:  48% 10% 42%



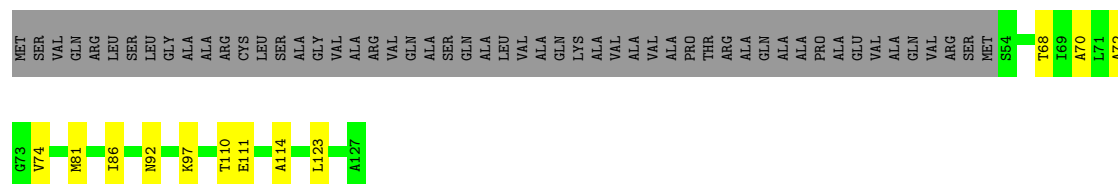
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain G:  49% 9% 42%

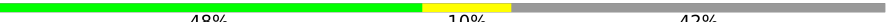


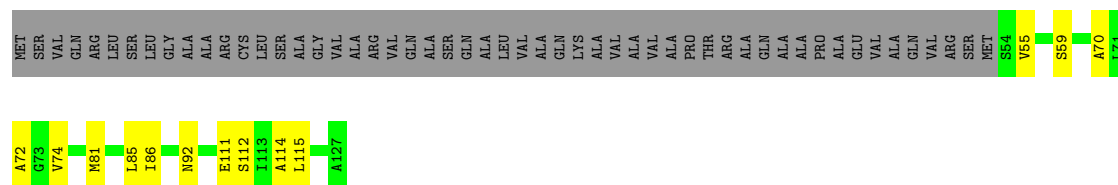
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain H:  49% 9% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

Chain I:  48% 10% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

Met	Ser	Val	Gln	Arg	Leu	Ser	Gly	Ala	Ala	Arg	Cys	Leu	Ser	Gly	Val	Ala	Arg	Val	Gln	Ala	Ser	Gln	Ala	Leu	Val	Ala	Gln	Lys	Ala	Val	Ala	Val	Ala	Ala	Pro	Pro	Thr	Arg	Ala	Gln	Ala	Ala	Pro	Glu	Val	Ala	Gln	Val	Arg	Ser	Met	Met	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

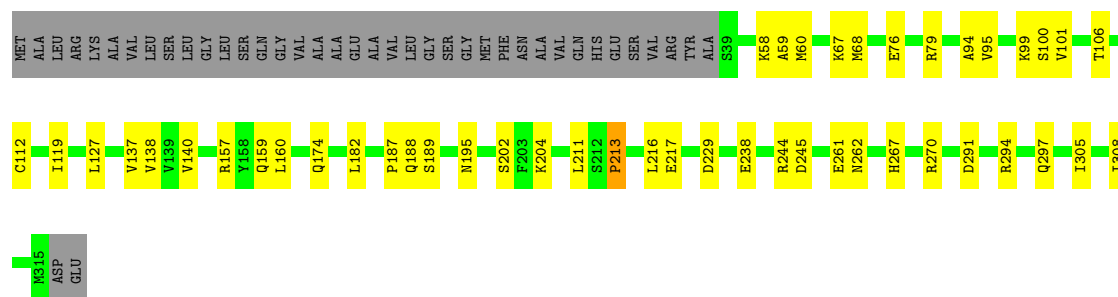
HIS	SER	MET
PHE	PRO	SER
ILE	LEU	VAL
PRO	ASN	LEU
GLY	VAL	SER
GLY	LYS	SER
THR	LEU	VAL
TRP	PRO	PRO
PRO	GLY	MET
PRO	MET	SER
ALA	CYS	SER
F219	SER	ARG
A233	SER	ILE
R239	ILE	GLY
V271	LEU	SER
F275	LEU	LEU
L281	PRO	LEU
L294	LYS	GLY
I322	THR	ARG
V323	THR	SER
K324	ARG	SER
LYS	ILE	ALA
ILE	ALA	TYP
HIS	VAL	LEU
	PRO	ALA
	PHE	GLN
	GLY	CYS
	ASN	GLY
	GLN	PHE
	THR	SER
	MET	THR
	ALA	ARG
	MET	SER
	S95	ASN
	G112	LEU
	N121	GLY
	D132	ILE
	L135	ASP
	D143	THR
	K144	SER
	R145	SER
	M163	VAL
	T175	PHE
	M189	GLN
	K199	ALA
	T200	LEU
	G201	SER
	P205	SER
	C217	ASP
		ASN
		GLU
		ASN
		LYS
		PRO
		ALA
		ALA

ET136	ET137	T138	VI39	NI40		LI46	K150	E151	VI52	Y153	C154	T155	VI56		E166		F182	K183	L184	VI85	M186	Q187		LI94	VI99	T200	E201		N219	V222		I229	ET137	K338	L339	P40		L46	S47	G48	T49		Q69	K69	L74	F77		L109	G113	L134	L135	MET
-------	-------	------	------	------	--	------	------	------	------	------	------	------	------	--	------	--	------	------	------	------	------	------	--	------	------	------	------	--	------	------	--	------	-------	------	------	-----	--	-----	-----	-----	-----	--	-----	-----	-----	-----	--	------	------	------	------	-----

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows the amino acid sequence: MET, CYS, A3, P4, R10, V11, D25, R28, K32, F35, K36, Q43, F47, N67, N74. MET and CYS are in grey boxes, A3 and P4 are in green boxes, and the others are in yellow boxes. MET and CYS have very low information content (near 0). A3 and P4 have high information content (around 0.35 bits). R10, V11, D25, R28, K32, F35, K36, Q43, F47, N67, and N74 have lower information content (around 0.15 bits).

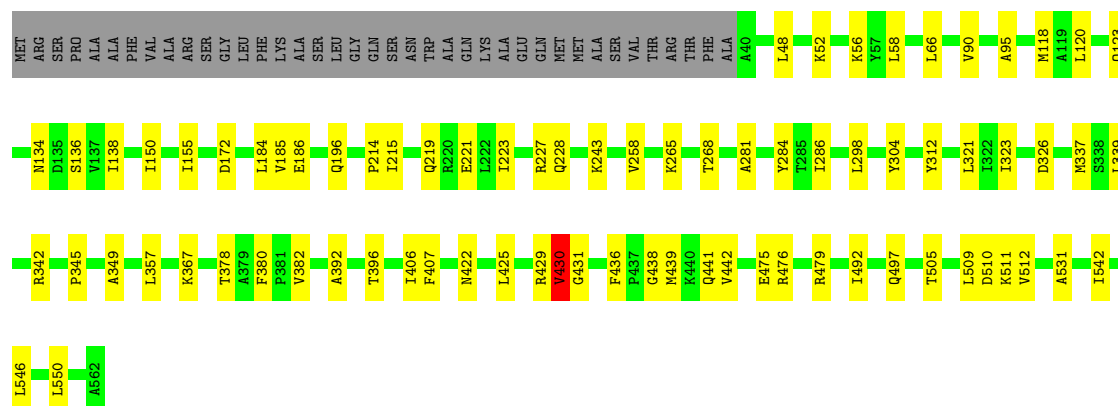
MET	PHE	GLY	LEU	LYS	ARG	ALA	VAL	THR	VAL	GLY	ARG	ARG	PHE	ILE	SER	THR	SER	ALA	ALA	ARG	MET	E23	F33	W37	A41	Q64	P71	K86	G96	G99	H104	E125	V136	N139	G140	V141	E148	V160	K161	V195	F200
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------

Chain S: 73% 15% 13%



- Molecule 17: ATP synthase subunit alpha

Chain T: 79% 14% 7%



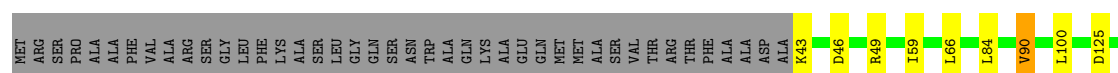
- Molecule 17: ATP synthase subunit alpha

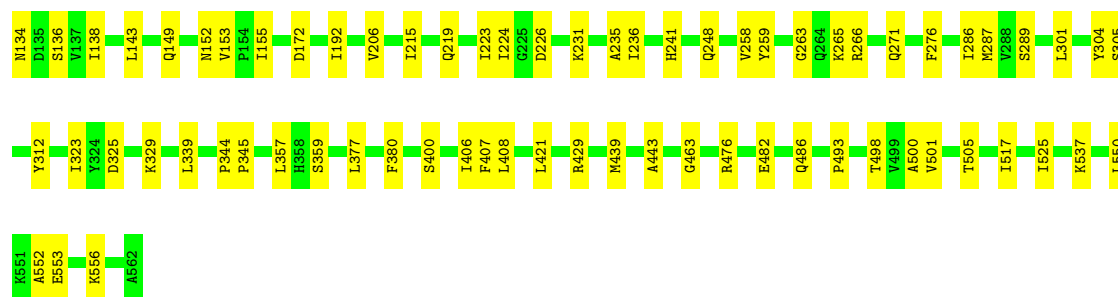
Chain U: 78% 15% 7%



- Molecule 17: ATP synthase subunit alpha

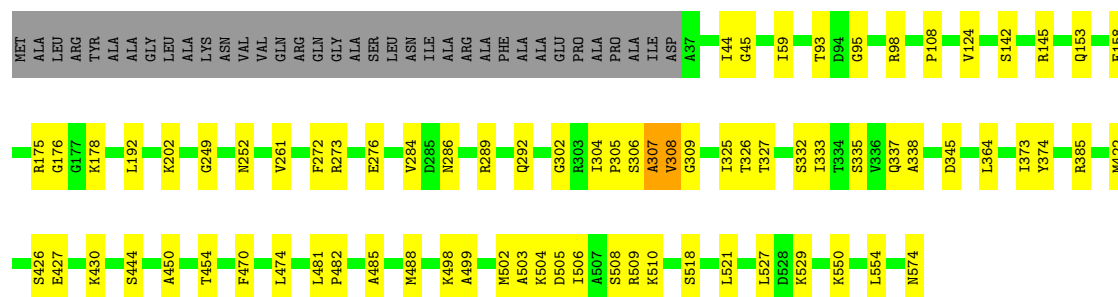
Chain V: 79% 14% 7%





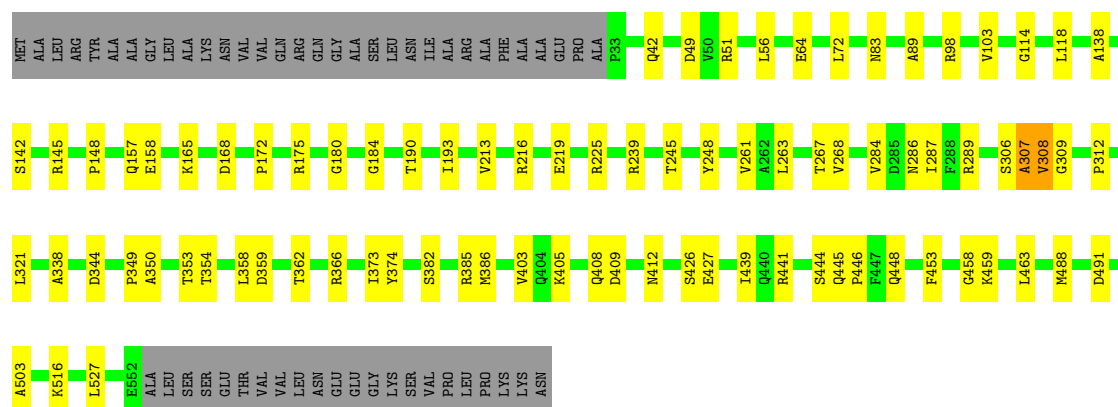
• Molecule 18: ATP synthase subunit beta

Chain X: 80% 13% 6%



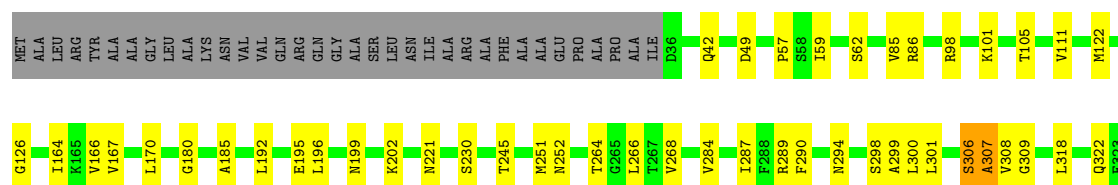
• Molecule 18: ATP synthase subunit beta

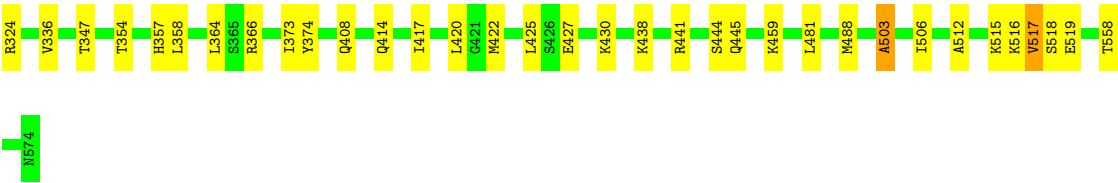
Chain Y: 76% 14% 9%



• Molecule 18: ATP synthase subunit beta

Chain Z: 80% 13% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60429	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.918	Depositor
Minimum map value	-21.137	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.037	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	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, ADP, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.37	0/628	0.46	0/856
2	1	0.40	0/4750	0.48	0/6434
3	2	0.31	0/3212	0.52	2/4371 (0.0%)
4	3	0.35	0/1911	0.52	1/2601 (0.0%)
5	4	0.34	0/2216	0.50	1/3000 (0.0%)
6	5	0.50	0/1011	0.58	0/1376
7	6	0.43	0/946	0.55	0/1287
8	7	0.42	0/1374	0.51	1/1865 (0.1%)
9	8	0.44	0/715	0.52	0/974
10	9	0.27	0/802	0.48	0/1084
11	A	0.26	0/520	0.45	0/704
11	B	0.34	0/520	0.52	0/704
11	C	0.28	0/519	0.48	0/701
11	D	0.28	0/520	0.46	0/704
11	E	0.28	0/520	0.49	0/704
11	F	0.37	0/520	0.53	0/704
11	G	0.40	0/520	0.52	0/704
11	H	0.38	0/520	0.48	0/704
11	I	0.33	0/520	0.46	0/704
11	J	0.29	0/520	0.56	1/704 (0.1%)
12	M	0.45	0/1683	0.59	0/2295
13	P	0.40	0/1553	0.61	2/2093 (0.1%)
14	Q	0.29	0/574	0.49	0/774
15	R	0.35	0/1336	0.56	0/1827
16	S	0.37	0/2153	0.51	0/2901
17	T	0.50	0/4048	0.57	0/5481
17	U	0.47	0/4047	0.55	0/5479
17	V	0.46	0/4030	0.52	0/5456
18	X	0.46	0/4147	0.55	1/5619 (0.0%)
18	Y	0.48	0/4011	0.57	1/5435 (0.0%)
18	Z	0.43	0/4155	0.56	0/5630
All	All	0.42	0/54501	0.53	10/73875 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	X	0	1
18	Y	0	2
18	Z	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	77	PRO	N-CA-CB	6.75	110.42	103.00
13	P	48	GLY	CA-C-N	6.26	133.49	121.54
13	P	48	GLY	C-N-CA	6.26	133.49	121.54
18	Y	308	VAL	N-CA-C	5.81	121.43	109.34
5	4	62	VAL	N-CA-C	-5.61	107.35	112.96
8	7	157	VAL	N-CA-C	-5.55	107.41	112.96
3	2	225	GLU	CA-C-N	5.49	132.02	121.54
3	2	225	GLU	C-N-CA	5.49	132.02	121.54
18	X	308	VAL	N-CA-C	5.20	120.16	109.34
11	J	95	ILE	N-CA-C	-5.11	106.46	111.77

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	503	ALA	Mainchain
18	Z	503	ALA	Mainchain

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	0	607	0	584	2	0
2	1	4661	0	4695	46	0
3	2	3163	0	3262	46	0
4	3	1874	0	1826	21	0
5	4	2177	0	2169	23	0
6	5	986	0	1021	22	0
7	6	926	0	941	9	0
8	7	1347	0	1345	24	0
9	8	692	0	694	7	0
10	9	776	0	757	7	0
11	A	514	0	554	12	0
11	B	514	0	554	12	0
11	C	514	0	553	11	0
11	D	514	0	554	10	0
11	E	514	0	554	20	0
11	F	514	0	554	13	0
11	G	514	0	554	11	0
11	H	514	0	554	11	0
11	I	514	0	554	10	0
11	J	514	0	554	13	0
12	M	1640	0	1665	14	0
13	P	1532	0	1603	31	0
14	Q	561	0	565	8	0
15	R	1303	0	1266	10	0
16	S	2130	0	2180	32	0
17	T	3979	0	4119	68	0
17	U	3978	0	4116	55	0
17	V	3961	0	4105	51	0
18	X	4087	0	4110	52	0
18	Y	3952	0	3964	63	0
18	Z	4095	0	4114	52	0
19	M	1	0	0	0	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
20	V	31	0	12	0	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	Y	1	0	0	0	0
21	Z	1	0	0	0	0
22	Y	27	0	12	4	0
22	Z	27	0	12	1	0
All	All	53720	0	54700	629	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 6.

All (629) 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)
11:A:78:LEU:HD11	11:A:111:GLU:OE2	1.33	1.27
18:X:503:ALA:O	18:X:506:ILE:HG12	1.32	1.25
11:J:107:PHE:O	11:J:111:GLU:HG2	1.56	1.02
17:T:219:GLN:HG3	17:T:430:VAL:HG11	1.45	0.99
17:T:429:ARG:HG2	22:Y:601:ADP:O3'	1.74	0.88
17:T:429:ARG:HD2	18:Y:453:PHE:CG	2.09	0.87
18:Y:157:GLN:NE2	18:Y:385:ARG:HH12	1.74	0.86
17:T:407:PHE:CD2	17:T:425:LEU:HD22	2.11	0.85
17:T:510:ASP:O	17:T:511:LYS:HG2	1.77	0.84
17:T:429:ARG:NE	18:Y:453:PHE:CD2	2.47	0.82
18:Z:516:LYS:HA	18:Z:519:GLU:HG2	1.65	0.78
11:E:111:GLU:OE1	11:F:113:ILE:HD11	1.84	0.77
2:1:316:ASN:HD21	2:1:331:ALA:H	1.31	0.77
17:T:429:ARG:HD2	18:Y:453:PHE:CB	2.15	0.77
17:T:219:GLN:CG	17:T:430:VAL:HG11	2.16	0.75
18:X:485:ALA:HB2	18:X:502:MET:HE1	1.68	0.75
17:T:546:LEU:O	17:T:550:LEU:HB2	1.87	0.74
17:V:400:SER:HB2	18:Z:289:ARG:HH22	1.52	0.74
17:T:429:ARG:CG	22:Y:601:ADP:O3'	2.36	0.73
17:T:219:GLN:OE1	17:T:430:VAL:HG12	1.88	0.72
18:X:482:PRO:HG2	18:X:502:MET:HE3	1.71	0.71
18:X:485:ALA:HB2	18:X:502:MET:CE	2.22	0.70
13:P:146:LEU:O	13:P:146:LEU:HG	1.93	0.69
11:E:111:GLU:CD	11:F:113:ILE:HD11	2.18	0.69
11:J:107:PHE:CE1	11:J:111:GLU:OE2	2.46	0.69
17:T:422:ASN:OD1	17:T:425:LEU:HD13	1.93	0.68
18:Z:515:LYS:O	18:Z:517:VAL:N	2.23	0.68
11:B:113:ILE:HA	11:B:116:PHE:HB2	1.75	0.67
17:T:407:PHE:HD2	17:T:425:LEU:HD22	1.58	0.67
17:T:214:PRO:O	17:T:431:GLY:HA3	1.94	0.66
11:E:78:LEU:CD2	11:E:111:GLU:OE2	2.44	0.66
14:Q:47:PHE:HB3	16:S:174:GLN:HE21	1.61	0.65
18:X:325:ILE:HG21	18:X:335:SER:HB2	1.77	0.65
17:V:550:LEU:HA	17:V:553:GLU:HB2	1.78	0.65
13:P:151:GLU:O	13:P:152:VAL:HG23	1.97	0.64
11:I:74:VAL:HG11	11:I:114:ALA:HB2	1.80	0.64
17:U:67:ILE:HG13	17:U:68:PRO:HD3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:523:ALA:O	17:U:527:GLN:HB2	1.99	0.63
11:A:78:LEU:CD1	11:A:111:GLU:OE2	2.28	0.63
17:T:407:PHE:CD2	17:T:425:LEU:CD2	2.81	0.62
16:S:213:PRO:O	16:S:217:GLU:HB3	1.98	0.62
18:Z:515:LYS:O	18:Z:517:VAL:HG22	2.00	0.62
11:H:74:VAL:HG11	11:H:114:ALA:HB2	1.81	0.62
14:Q:4:PRO:HG2	14:Q:11:VAL:HA	1.82	0.62
13:P:150:LYS:O	13:P:182:PHE:HA	2.00	0.61
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.33	0.61
18:Z:307:ALA:O	18:Z:309:GLY:N	2.32	0.61
8:7:170:HIS:HD2	8:7:172:ALA:H	1.48	0.61
17:U:151:VAL:HG11	17:U:301:LEU:HD21	1.80	0.61
7:6:107:VAL:HG11	10:9:48:GLY:HA3	1.82	0.61
8:7:123:HIS:HD2	8:7:125:GLU:H	1.49	0.61
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.82	0.61
17:U:314:ARG:NH2	17:U:364:ARG:O	2.34	0.60
17:T:407:PHE:CE2	17:T:425:LEU:HD22	2.36	0.60
18:X:518:SER:HB2	18:X:521:LEU:HB2	1.82	0.60
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.83	0.60
17:V:271:GLN:HG3	18:Y:385:ARG:NH1	2.16	0.60
11:E:111:GLU:OE2	11:F:113:ILE:HD11	2.01	0.60
17:T:219:GLN:CD	17:T:430:VAL:CG1	2.75	0.60
14:Q:25:ASP:OD1	14:Q:28:ARG:NH1	2.35	0.59
2:1:295:PRO:HA	2:1:298:GLN:HG2	1.85	0.59
4:3:203:THR:HG21	4:3:235:ASP:HB2	1.85	0.59
17:T:219:GLN:CD	17:T:430:VAL:HG12	2.27	0.59
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.84	0.59
11:D:74:VAL:HG11	11:D:114:ALA:HB2	1.85	0.59
13:P:184:LEU:HD12	13:P:184:LEU:O	2.01	0.59
11:G:72:ALA:HB2	11:H:70:ALA:HA	1.85	0.58
18:Z:42:GLN:HB3	18:Z:49:ASP:HB2	1.85	0.58
17:U:246:ASN:HD21	17:U:255:VAL:H	1.50	0.58
17:T:342:ARG:NH1	18:X:302:GLY:O	2.37	0.58
18:Z:516:LYS:O	18:Z:518:SER:N	2.36	0.58
17:U:407:PHE:H	17:U:426:SER:HB3	1.68	0.57
18:Y:306:SER:OG	18:Y:307:ALA:N	2.36	0.57
18:Z:86:ARG:NH2	18:Z:300:LEU:O	2.37	0.57
17:T:429:ARG:CD	18:Y:453:PHE:CG	2.84	0.57
18:Y:157:GLN:NE2	18:Y:385:ARG:NH1	2.49	0.57
2:1:544:VAL:HG12	2:1:548:MET:HE2	1.86	0.57
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:160:VAL:HG23	15:R:161:LYS:HD3	1.86	0.57
12:M:163:ASN:ND2	12:M:175:THR:OG1	2.37	0.57
13:P:155:THR:HB	13:P:201:GLU:HB2	1.87	0.57
18:Y:373:ILE:HG23	18:Y:444:SER:HB3	1.87	0.57
17:T:219:GLN:NE2	17:T:221:GLU:OE1	2.37	0.57
17:T:476:ARG:NH2	17:T:505:THR:O	2.37	0.57
17:V:476:ARG:NH1	17:V:505:THR:O	2.37	0.57
18:Y:405:LYS:NZ	18:Y:409:ASP:OD1	2.37	0.57
3:2:288:LEU:HD23	3:2:307:VAL:HG11	1.87	0.57
11:B:93:PRO:HB3	11:C:95:ILE:HD12	1.85	0.57
18:Y:287:ILE:HD11	18:Y:321:LEU:HD21	1.86	0.57
16:S:297:GLN:NE2	18:X:345:ASP:OD2	2.38	0.56
17:V:206:VAL:HA	17:V:486:GLN:HE22	1.69	0.56
2:1:328:ARG:NH1	10:9:12:GLU:OE1	2.37	0.56
3:2:36:LEU:HD22	3:2:41:VAL:HG21	1.87	0.56
17:T:492:ILE:O	17:T:497:GLN:NE2	2.38	0.56
17:V:226:ASP:O	17:V:231:LYS:NZ	2.37	0.56
11:F:107:PHE:CZ	11:F:111:GLU:OE1	2.58	0.56
13:P:135:LEU:HG	17:U:45:LEU:HD11	1.87	0.56
5:4:254:LYS:HA	5:4:257:GLU:HB2	1.86	0.56
11:E:118:LEU:HA	11:E:121:VAL:HG12	1.85	0.56
13:P:184:LEU:HD12	13:P:184:LEU:C	2.30	0.56
18:Y:385:ARG:NH2	18:Y:385:ARG:HB3	2.21	0.56
18:Y:145:ARG:HH12	18:Y:267:THR:HG23	1.71	0.56
18:Z:445:GLN:NE2	18:Z:459:LYS:O	2.39	0.56
18:Z:195:GLU:O	18:Z:199:ASN:HB2	2.06	0.56
4:3:311:LEU:HD12	12:M:322:ILE:HD12	1.88	0.56
9:8:36:ALA:HA	9:8:40:LEU:HB3	1.88	0.56
18:X:426:SER:OG	18:X:427:GLU:N	2.38	0.56
18:Y:114:GLY:HA3	18:Y:138:ALA:HB3	1.87	0.56
13:P:40:PRO:O	13:P:59:GLN:NE2	2.36	0.56
20:T:1001:ATP:O3G	18:X:385:ARG:NH1	2.37	0.56
3:2:324:SER:HA	3:2:327:SER:HB2	1.88	0.55
18:X:249:GLY:HA3	18:X:261:VAL:HG21	1.87	0.55
18:Y:491:ASP:N	18:Y:491:ASP:OD2	2.39	0.55
13:P:151:GLU:OE2	13:P:183:LYS:HE3	2.06	0.55
17:T:134:ASN:ND2	17:T:136:SER:OG	2.39	0.55
18:Y:286:ASN:H	18:Y:338:ALA:HB3	1.72	0.55
11:D:86:ILE:HG21	11:E:85:LEU:HA	1.89	0.55
11:H:111:GLU:OE2	11:I:112:SER:OG	2.24	0.55
12:M:121:ASN:O	12:M:145:ARG:NH1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:76:GLU:OE2	16:S:79:ARG:NH1	2.39	0.55
4:3:261:VAL:HG11	4:3:285:ALA:HB2	1.88	0.55
11:D:72:ALA:HB2	11:E:70:ALA:HA	1.89	0.55
14:Q:10:ARG:NH2	16:S:245:ASP:OD1	2.38	0.55
18:X:306:SER:OG	18:X:307:ALA:N	2.39	0.55
4:3:304:LYS:NZ	4:3:308:GLU:OE2	2.39	0.55
17:V:265:LYS:NZ	18:Y:359:ASP:OD1	2.40	0.55
13:P:184:LEU:CD1	13:P:186:MET:SD	2.95	0.55
18:Y:184:GLY:O	18:Y:366:ARG:NH2	2.40	0.55
13:P:183:LYS:HG3	13:P:183:LYS:O	2.07	0.55
2:1:267:ARG:NH2	7:6:150:SER:OG	2.40	0.54
11:J:107:PHE:CE1	11:J:111:GLU:CD	2.85	0.54
18:X:284:VAL:HB	18:X:337:GLN:HG2	1.89	0.54
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.40	0.54
3:2:240:ALA:H	3:2:243:GLN:HE21	1.55	0.54
17:V:463:GLY:H	18:Y:426:SER:HB2	1.72	0.54
18:Y:172:PRO:HG2	18:Y:386:MET:HB2	1.90	0.54
17:T:439:MET:HA	17:T:442:VAL:HG12	1.90	0.54
2:1:90:ARG:NH2	2:1:507:GLU:OE1	2.40	0.54
11:D:107:PHE:O	11:D:111:GLU:HG2	2.07	0.54
18:X:153:GLN:HE22	18:X:326:THR:HG21	1.73	0.54
2:1:76:GLU:OE2	2:1:133:ARG:NH2	2.40	0.54
18:Y:286:ASN:HB3	18:Y:289:ARG:HG2	1.89	0.54
18:Z:516:LYS:HA	18:Z:519:GLU:CG	2.35	0.54
2:1:511:ALA:HB2	6:5:68:LEU:HD21	1.90	0.53
11:B:72:ALA:HB2	11:C:70:ALA:HA	1.90	0.53
17:U:240:ILE:HD12	17:U:279:THR:HG21	1.90	0.53
17:V:259:TYR:OH	17:V:325:ASP:OD2	2.26	0.53
11:I:92:ASN:HB3	16:S:229:ASP:HB3	1.90	0.53
2:1:559:GLU:OE1	6:5:39:LYS:NZ	2.37	0.53
5:4:181:ASP:OD1	5:4:181:ASP:N	2.40	0.53
10:9:80:GLN:HB3	10:9:86:ALA:HB2	1.89	0.53
2:1:186:LEU:HD13	2:1:440:LEU:HB2	1.91	0.53
3:2:145:TYR:HH	8:7:16:THR:HG1	1.57	0.53
8:7:170:HIS:CD2	8:7:172:ALA:H	2.27	0.53
18:X:307:ALA:O	18:X:309:GLY:N	2.38	0.53
6:5:3:LEU:HD11	11:H:123:LEU:HD11	1.91	0.53
11:B:86:ILE:HG21	11:C:85:LEU:HA	1.91	0.53
18:Z:185:ALA:O	18:Z:366:ARG:NH2	2.41	0.53
7:6:149:ILE:HD12	7:6:151:LEU:HD11	1.91	0.53
2:1:157:LYS:O	8:7:98:ASN:ND2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.91	0.53
13:P:184:LEU:HD13	13:P:186:MET:SD	2.48	0.53
17:T:123:GLN:O	18:Y:98:ARG:NH1	2.41	0.53
18:Y:403:VAL:HG13	18:Y:439:ILE:HD12	1.91	0.53
18:Z:306:SER:OG	18:Z:307:ALA:N	2.40	0.53
18:X:176:GLY:HA3	18:X:327:THR:HG23	1.90	0.52
3:2:7:ASP:N	3:2:7:ASP:OD2	2.40	0.52
17:T:323:ILE:HG13	17:T:380:PHE:HB2	1.91	0.52
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.91	0.52
17:V:223:ILE:HD11	17:V:380:PHE:HD2	1.74	0.52
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.92	0.52
11:G:74:VAL:HG21	11:G:114:ALA:HB2	1.91	0.52
15:R:64:GLN:HE21	15:R:139:ASN:HD22	1.57	0.52
3:2:159:LYS:NZ	5:4:194:ASP:OD1	2.42	0.52
13:P:194:LEU:HD21	13:P:199:VAL:HG23	1.91	0.52
17:T:150:ILE:HB	17:T:184:LEU:HD22	1.92	0.52
2:1:404:LYS:NZ	6:5:74:ASN:OD1	2.39	0.52
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.91	0.52
17:U:189:ALA:HB3	18:X:252:ASN:HD22	1.75	0.52
17:V:149:GLN:HE21	17:V:152:ASN:HD21	1.58	0.52
2:1:485:PHE:HB2	2:1:488:VAL:HG12	1.90	0.52
17:T:219:GLN:OE1	17:T:430:VAL:CG1	2.57	0.52
17:T:339:LEU:HD21	17:T:345:PRO:HB3	1.92	0.52
18:X:286:ASN:H	18:X:338:ALA:HB3	1.75	0.52
18:X:470:PHE:O	18:X:474:LEU:HB2	2.09	0.52
18:Y:190:THR:OG1	22:Y:601:ADP:O3B	2.28	0.52
3:2:74:ASN:ND2	8:7:21:SER:OG	2.43	0.51
18:Z:322:GLN:HG2	18:Z:357:HIS:HB3	1.92	0.51
17:T:155:ILE:HD12	17:T:312:TYR:HB2	1.91	0.51
17:U:84:LEU:HD23	17:U:143:LEU:HD22	1.92	0.51
16:S:202:SER:HB2	16:S:204:LYS:HE3	1.92	0.51
17:T:185:VAL:HG23	17:T:186:GLU:HG2	1.92	0.51
17:V:215:ILE:HG23	17:V:219:GLN:HE21	1.75	0.51
16:S:95:VAL:HG11	16:S:211:LEU:HD21	1.92	0.51
17:T:326:ASP:H	17:T:382:VAL:HB	1.74	0.51
17:U:414:TYR:HB2	18:Z:408:GLN:HE21	1.76	0.51
18:Y:374:TYR:HB2	18:Y:488:MET:HE1	1.91	0.51
3:2:122:ASN:OD1	5:4:201:LYS:NZ	2.44	0.51
18:Y:216:ARG:NH1	18:Y:219:GLU:OE2	2.44	0.51
11:H:72:ALA:HB2	11:I:70:ALA:HA	1.91	0.51
1:0:67:LYS:O	10:9:60:ASN:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:125:ASP:OD2	17:V:125:ASP:N	2.42	0.51
11:C:74:VAL:HG11	11:C:114:ALA:HB2	1.92	0.51
11:G:74:VAL:O	11:G:78:LEU:HB2	2.10	0.51
18:Y:142:SER:O	18:Y:145:ARG:NH2	2.44	0.51
18:Z:373:ILE:HG23	18:Z:444:SER:HB3	1.92	0.51
3:2:137:PRO:HB3	3:2:170:VAL:HG12	1.93	0.51
5:4:74:LEU:HD23	5:4:219:VAL:HG13	1.93	0.51
18:X:158:GLU:OE2	18:X:175:ARG:NH1	2.44	0.51
2:1:372:SER:OG	2:1:373:ASP:N	2.44	0.51
6:5:118:VAL:HG21	8:7:94:LEU:HD22	1.93	0.51
18:Z:427:GLU:HA	18:Z:430:LYS:HB2	1.91	0.51
3:2:188:ALA:HB2	3:2:220:LEU:HD22	1.93	0.50
11:E:78:LEU:HD21	11:E:111:GLU:OE2	2.10	0.50
13:P:136:GLU:O	13:P:140:ASN:ND2	2.43	0.50
17:V:46:ASP:OD1	17:V:49:ARG:NH1	2.45	0.50
17:V:482:GLU:HB3	17:V:517:ILE:HD12	1.92	0.50
18:Z:266:LEU:HD21	18:Z:324:ARG:HB2	1.93	0.50
17:U:154:PRO:HD2	17:U:168:GLY:HA3	1.92	0.50
6:5:5:PRO:O	9:8:65:ARG:NH1	2.45	0.50
8:7:16:THR:O	8:7:73:LYS:NZ	2.43	0.50
8:7:167:SER:OG	8:7:170:HIS:O	2.29	0.50
11:E:87:ASN:OD1	11:E:91:ARG:NH1	2.45	0.50
14:Q:43:GLN:NE2	14:Q:67:ASN:O	2.44	0.50
18:Y:64:GLU:HB2	18:Y:103:VAL:HG12	1.92	0.50
18:Z:516:LYS:C	18:Z:518:SER:H	2.20	0.50
3:2:382:VAL:HG13	3:2:386:LEU:HB2	1.94	0.50
5:4:17:SER:OG	5:4:19:ASP:OD1	2.28	0.50
11:G:68:THR:O	11:G:68:THR:OG1	2.30	0.50
13:P:185:VAL:HG12	13:P:185:VAL:O	2.11	0.50
18:Y:42:GLN:HG2	18:Y:49:ASP:HB2	1.94	0.50
2:1:506:ARG:NH1	2:1:509:GLU:OE1	2.45	0.50
6:5:83:THR:O	8:7:119:TYR:OH	2.28	0.50
17:U:219:GLN:NE2	17:U:221:GLU:OE1	2.45	0.50
18:Z:374:TYR:HB2	18:Z:488:MET:HE1	1.94	0.50
17:U:516:ASP:O	17:U:520:ALA:N	2.38	0.50
17:V:134:ASN:ND2	17:V:136:SER:OG	2.43	0.50
17:V:339:LEU:HD21	17:V:345:PRO:HB3	1.92	0.50
18:Z:318:LEU:HD21	18:Z:354:THR:HB	1.93	0.50
17:T:438:GLY:HA2	17:T:441:GLN:HE21	1.76	0.50
18:Z:284:VAL:HG11	18:Z:287:ILE:HD13	1.94	0.50
3:2:366:LEU:HD22	3:2:378:LEU:HD11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:156:VAL:HG21	13:P:186:MET:HE1	1.94	0.50
16:S:60:MET:HE1	18:Z:420:LEU:HD21	1.93	0.50
17:U:41:ASP:OD1	17:U:41:ASP:N	2.43	0.50
17:U:198:VAL:HB	17:U:430:VAL:HG21	1.94	0.50
17:V:304:TYR:OH	17:V:357:LEU:O	2.25	0.50
17:V:552:ALA:O	17:V:556:LYS:NZ	2.44	0.50
4:3:199:ALA:HA	4:3:236:LEU:HD13	1.94	0.49
17:T:304:TYR:OH	17:T:357:LEU:O	2.29	0.49
17:U:241:HIS:HE1	17:U:493:PRO:HA	1.76	0.49
18:X:504:LYS:O	18:X:508:SER:OG	2.27	0.49
17:T:510:ASP:O	17:T:511:LYS:CG	2.54	0.49
17:V:84:LEU:HD23	17:V:143:LEU:HD22	1.93	0.49
17:V:248:GLN:OE1	17:V:537:LYS:NZ	2.41	0.49
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	1.94	0.49
6:5:41:HIS:HA	7:6:140:LEU:HD21	1.93	0.49
11:A:64:ALA:HB1	11:A:121:VAL:HG13	1.95	0.49
11:A:86:ILE:HG21	11:B:85:LEU:HA	1.94	0.49
11:E:80:VAL:HG12	11:F:80:VAL:HG11	1.93	0.49
17:T:219:GLN:CD	17:T:430:VAL:HG11	2.38	0.49
17:T:223:ILE:HD11	17:T:380:PHE:HD2	1.77	0.49
3:2:362:ASP:OD1	3:2:364:SER:OG	2.28	0.49
16:S:308:ILE:HD13	18:X:304:ILE:HG23	1.93	0.49
17:U:113:SER:OG	18:X:574:ASN:ND2	2.45	0.49
17:V:192:ILE:O	18:Z:221:ASN:ND2	2.44	0.49
17:T:136:SER:HA	18:X:59:ILE:HB	1.93	0.49
17:U:323:ILE:HG13	17:U:380:PHE:HB2	1.94	0.49
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.39	0.49
11:E:98:GLN:NE2	11:E:102:TYR:OH	2.40	0.49
11:I:86:ILE:HG21	11:J:85:LEU:HA	1.95	0.49
12:M:200:THR:OG1	12:M:201:GLY:N	2.45	0.49
18:X:273:ARG:HD3	18:X:333:ILE:HG13	1.93	0.49
18:Z:122:MET:HE3	18:Z:126:GLY:HA2	1.94	0.49
4:3:136:SER:OG	4:3:137:THR:N	2.46	0.49
12:M:271:VAL:O	12:M:275:PHE:HB2	2.13	0.49
2:1:267:ARG:NH2	2:1:515:ALA:O	2.46	0.49
10:9:19:SER:OG	10:9:20:ALA:N	2.44	0.49
11:B:57:ALA:HA	11:B:60:LYS:HD3	1.95	0.49
15:R:71:PRO:HG2	15:R:141:VAL:HG12	1.95	0.49
17:U:62:VAL:O	17:U:66:LEU:N	2.45	0.49
17:U:125:ASP:OD2	17:U:125:ASP:N	2.46	0.49
17:V:172:ASP:OD1	17:V:172:ASP:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:438:LYS:NZ	18:Z:481:LEU:O	2.41	0.49
3:2:108:GLU:OE2	3:2:177:GLN:NE2	2.42	0.48
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.94	0.48
16:S:58:LYS:HB3	17:U:459:PHE:HE1	1.78	0.48
17:U:259:TYR:OH	17:U:325:ASP:OD2	2.28	0.48
18:Y:307:ALA:O	18:Y:309:GLY:N	2.37	0.48
18:Z:427:GLU:HG3	18:Z:430:LYS:HD2	1.94	0.48
16:S:79:ARG:NE	16:S:261:GLU:OE2	2.43	0.48
16:S:127:LEU:HD23	16:S:157:ARG:HH11	1.78	0.48
17:U:202:LEU:HD13	17:U:378:THR:HG21	1.93	0.48
4:3:219:LEU:HD22	4:3:240:VAL:HG13	1.95	0.48
3:2:55:ALA:HB1	3:2:69:LEU:HD21	1.94	0.48
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.95	0.48
18:Y:385:ARG:CB	18:Y:385:ARG:HH21	2.26	0.48
18:Z:166:VAL:HG23	18:Z:170:LEU:HD12	1.95	0.48
18:Z:202:LYS:HE3	18:Z:230:SER:HB3	1.94	0.48
17:T:243:LYS:HG3	17:T:281:ALA:HA	1.96	0.48
17:T:429:ARG:HD2	18:Y:453:PHE:HB2	1.95	0.48
18:Y:118:LEU:O	18:Y:239:ARG:NH2	2.44	0.48
2:1:29:SER:HB3	17:T:58:LEU:HB3	1.96	0.48
2:1:84:PRO:HG3	6:5:79:ASN:HD22	1.79	0.48
16:S:106:THR:HG22	16:S:119:ILE:HD11	1.96	0.48
2:1:148:PHE:O	2:1:150:ARG:NH2	2.47	0.48
11:D:75:GLY:HA3	11:E:74:VAL:HG12	1.95	0.48
17:T:531:ALA:HB3	18:Y:527:LEU:HD13	1.96	0.48
11:J:78:LEU:HD11	11:J:111:GLU:OE2	2.12	0.48
18:Z:180:GLY:HA3	18:Z:358:LEU:HD13	1.96	0.48
7:6:60:PRO:HB3	9:8:15:PRO:HB2	1.96	0.48
11:F:91:ARG:O	15:R:99:GLY:N	2.42	0.48
18:Z:516:LYS:C	18:Z:518:SER:N	2.69	0.48
4:3:235:ASP:OD1	4:3:235:ASP:N	2.44	0.48
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.96	0.48
6:5:110:SER:HB3	6:5:113:VAL:HG22	1.95	0.48
17:T:258:VAL:HG22	17:T:286:ILE:HD12	1.96	0.48
17:U:108:LEU:HG	17:U:151:VAL:HG22	1.96	0.48
2:1:540:LEU:HD12	2:1:541:PRO:HD2	1.94	0.47
3:2:209:ASP:OD1	8:7:67:ARG:NH2	2.47	0.47
18:Z:62:SER:O	18:Z:105:THR:OG1	2.32	0.47
11:A:56:LEU:HG	11:A:60:LYS:HE2	1.96	0.47
11:J:68:THR:HG23	11:J:121:VAL:HG21	1.96	0.47
16:S:188:GLN:HB3	16:S:216:LEU:HD23	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:529:ASN:HD22	18:X:527:LEU:HD23	1.78	0.47
1:O:69:PRO:HD2	10:9:60:ASN:HD22	1.79	0.47
11:J:74:VAL:HG11	11:J:114:ALA:HB2	1.95	0.47
17:U:220:ARG:NH1	17:U:363:GLU:OE2	2.48	0.47
18:Y:426:SER:OG	18:Y:427:GLU:N	2.47	0.47
2:1:559:GLU:OE2	4:3:207:HIS:NE2	2.44	0.47
17:V:266:ARG:NH2	18:Y:148:PRO:O	2.44	0.47
18:Y:445:GLN:NE2	18:Y:459:LYS:O	2.48	0.47
18:Z:441:ARG:O	18:Z:444:SER:OG	2.31	0.47
17:U:172:ASP:OD1	17:U:172:ASP:N	2.45	0.47
17:U:512:VAL:HB	17:U:516:ASP:HB2	1.95	0.47
18:Z:196:LEU:HD13	18:Z:336:VAL:HG11	1.95	0.47
2:1:90:ARG:NH1	6:5:67:SER:O	2.48	0.47
16:S:100:SER:OG	16:S:189:SER:OG	2.32	0.47
17:T:475:GLU:HG3	17:T:479:ARG:HH12	1.80	0.47
17:V:153:VAL:HG11	17:V:305:SER:HB3	1.97	0.47
17:V:231:LYS:HG2	17:V:408:LEU:HD12	1.97	0.47
17:V:287:MET:HE2	17:V:287:MET:HB2	1.78	0.47
14:Q:32:LYS:HB2	14:Q:35:PHE:HD2	1.80	0.47
17:U:122:LEU:HB3	18:X:98:ARG:HD3	1.96	0.47
18:X:509:ARG:HE	18:X:510:LYS:HZ1	1.62	0.47
2:1:450:ASN:HB3	2:1:474:GLN:HE21	1.80	0.47
4:3:242:ARG:NH2	12:M:132:ASP:OD1	2.41	0.47
11:C:56:LEU:O	11:C:60:LYS:NZ	2.47	0.47
6:5:51:TYR:HE2	7:6:143:LEU:HD13	1.80	0.47
11:F:74:VAL:HG21	11:F:114:ALA:HB2	1.97	0.47
2:1:70:ILE:HG13	2:1:133:ARG:HH11	1.80	0.46
17:V:100:LEU:O	18:Z:98:ARG:NH2	2.45	0.46
18:Y:306:SER:HB2	18:Y:312:PRO:HA	1.97	0.46
18:Z:57:PRO:HD2	18:Z:85:VAL:HG11	1.97	0.46
4:3:91:VAL:HG13	4:3:93:GLU:H	1.79	0.46
11:G:78:LEU:HD23	11:H:110:THR:HA	1.97	0.46
11:I:81:MET:HE2	11:I:81:MET:HB3	1.83	0.46
16:S:101:VAL:HG22	16:S:138:VAL:HB	1.97	0.46
4:3:201:SER:HA	4:3:205:CYS:HB2	1.98	0.46
17:U:154:PRO:HB3	17:U:180:VAL:HG11	1.97	0.46
18:Z:245:THR:HG21	18:Z:268:VAL:HG11	1.98	0.46
11:C:86:ILE:HG21	11:D:85:LEU:HA	1.97	0.46
13:P:134:LEU:HA	13:P:137:VAL:HG12	1.97	0.46
16:S:140:VAL:HG13	16:S:160:LEU:HB3	1.97	0.46
16:S:195:ASN:HD22	16:S:262:ASN:HD22	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:305:ILE:HG12	17:T:345:PRO:HG2	1.97	0.46
18:Y:158:GLU:HG3	18:Y:175:ARG:HB3	1.96	0.46
18:X:485:ALA:CB	18:X:502:MET:HE1	2.42	0.46
18:Y:362:THR:HA	18:Y:382:SER:HB2	1.97	0.46
3:2:346:ARG:NH1	13:P:166:GLU:OE1	2.48	0.46
15:R:104:HIS:HB3	15:R:136:VAL:HG11	1.98	0.46
2:1:32:THR:OG1	8:7:163:ALA:O	2.28	0.46
11:E:65:GLY:HA2	11:F:67:ALA:HB2	1.98	0.46
13:P:154:CYS:O	13:P:187:GLN:HB3	2.16	0.46
13:P:222:VAL:HG23	17:T:66:LEU:HD11	1.98	0.46
17:V:359:SER:OG	18:Z:251:MET:O	2.31	0.46
3:2:282:VAL:HG21	5:4:15:LEU:HD22	1.97	0.46
4:3:288:SER:O	4:3:288:SER:OG	2.32	0.46
10:9:65:THR:HG23	10:9:67:GLY:H	1.81	0.46
11:A:59:SER:HA	11:A:62:VAL:HG12	1.98	0.46
17:V:500:ALA:HB2	17:V:525:ILE:HD11	1.97	0.46
18:Y:168:ASP:HB3	18:Y:463:LEU:HD13	1.97	0.46
17:V:236:ILE:HD12	17:V:276:PHE:HZ	1.81	0.46
17:U:201:PRO:HB3	17:U:435:GLN:HA	1.97	0.46
11:G:115:LEU:HD11	12:M:239:ARG:HB2	1.97	0.45
13:P:46:LEU:O	18:Y:51:ARG:NH2	2.46	0.45
13:P:74:LEU:HD13	13:P:138:THR:HG22	1.98	0.45
16:S:59:ALA:HB2	17:U:459:PHE:HD1	1.81	0.45
17:T:509:LEU:HD13	17:T:512:VAL:HG21	1.98	0.45
17:V:406:ILE:HG23	17:V:421:LEU:HD12	1.97	0.45
18:Y:408:GLN:HE21	18:Y:412:ASN:HD21	1.63	0.45
18:Z:192:LEU:HD22	18:Z:364:LEU:HD11	1.98	0.45
4:3:253:SER:O	4:3:257:ARG:N	2.41	0.45
11:H:68:THR:O	11:H:68:THR:OG1	2.34	0.45
18:X:481:LEU:HD23	18:X:499:ALA:CB	2.47	0.45
18:Y:408:GLN:O	18:Y:412:ASN:ND2	2.36	0.45
3:2:128:VAL:HG21	3:2:143:VAL:HG11	1.99	0.45
2:1:381:ARG:NH2	2:1:403:ASP:OD1	2.36	0.45
18:X:550:LYS:HD2	18:X:550:LYS:HA	1.74	0.45
2:1:554:LYS:NZ	4:3:170:THR:O	2.43	0.45
11:H:92:ASN:N	11:H:92:ASN:OD1	2.48	0.45
16:S:137:VAL:HB	16:S:157:ARG:HD2	1.99	0.45
4:3:209:LEU:HD21	12:M:135:LEU:HD13	1.98	0.45
17:U:303:PRO:HG2	17:U:330:GLN:HG3	1.98	0.45
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.98	0.45
18:Y:213:VAL:HG22	18:Y:261:VAL:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:233:ARG:HE	4:3:233:ARG:HB3	1.60	0.45
11:F:93:PRO:HB3	11:G:95:ILE:HD13	1.99	0.45
17:U:207:LYS:NZ	17:U:483:MET:O	2.38	0.45
18:Y:344:ASP:OD2	18:Y:366:ARG:NE	2.43	0.45
2:1:568:ASP:OD1	2:1:568:ASP:N	2.50	0.44
3:2:24:VAL:HG23	3:2:28:GLU:HB2	1.98	0.44
11:G:78:LEU:HD11	11:G:107:PHE:HD1	1.82	0.44
15:R:86:LYS:NZ	15:R:125:GLU:OE2	2.39	0.44
2:1:368:ALA:O	2:1:379:GLN:NE2	2.41	0.44
3:2:67:THR:HG21	3:2:102:GLN:HG2	1.99	0.44
3:2:95:LEU:HD12	3:2:98:LEU:HD12	2.00	0.44
5:4:72:LEU:HB3	5:4:74:LEU:HG	1.98	0.44
5:4:292:VAL:HG22	17:T:48:LEU:HD12	1.99	0.44
2:1:574:MET:HE2	2:1:574:MET:HB3	1.85	0.44
17:U:90:VAL:HG13	18:Z:59:ILE:HD11	1.98	0.44
18:X:202:LYS:HB3	18:X:202:LYS:HE2	1.78	0.44
3:2:11:ILE:HG21	8:7:57:ALA:HB2	1.99	0.44
7:6:132:MET:HE2	12:M:112:GLY:HA3	1.99	0.44
17:T:90:VAL:HG21	17:T:138:ILE:HB	2.00	0.44
18:Z:252:ASN:OD1	18:Z:252:ASN:N	2.50	0.44
3:2:82:LYS:HA	5:4:84:ARG:HD3	1.99	0.44
4:3:195:LEU:O	4:3:226:TYR:OH	2.29	0.44
5:4:271:ASP:HB3	17:T:52:LYS:HB3	1.99	0.44
11:H:81:MET:HE2	11:H:81:MET:HB3	1.86	0.44
17:U:121:ASN:HB2	18:X:44:ILE:HG12	2.00	0.44
18:X:45:GLY:O	18:X:93:THR:OG1	2.31	0.44
18:X:498:LYS:O	18:X:502:MET:HB2	2.18	0.44
18:Y:349:PRO:O	18:Y:353:THR:OG1	2.31	0.44
17:U:104:GLN:HB3	18:X:95:GLY:HA2	1.99	0.44
17:V:258:VAL:HG22	17:V:286:ILE:HD12	2.00	0.44
17:V:344:PRO:HG2	18:Z:299:ALA:HB1	2.00	0.44
18:Y:72:LEU:HD11	18:Y:89:ALA:HB1	2.00	0.44
11:E:81:MET:HE2	11:E:81:MET:HB3	1.79	0.44
2:1:208:LYS:HD3	2:1:208:LYS:HA	1.78	0.44
11:E:74:VAL:HG21	11:E:114:ALA:HB2	1.99	0.44
16:S:308:ILE:HD11	18:X:305:PRO:HG2	2.00	0.44
18:X:422:MET:O	18:X:430:LYS:NZ	2.37	0.44
18:Y:350:ALA:O	18:Y:354:THR:OG1	2.33	0.44
11:A:61:MET:HG3	11:B:124:ILE:HD12	2.00	0.43
8:7:30:ALA:HB2	8:7:37:LEU:HB3	2.00	0.43
13:P:184:LEU:HD11	13:P:186:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:112:CYS:SG	16:S:270:ARG:NH2	2.92	0.43
17:T:196:GLN:HE21	17:T:367:LYS:HE3	1.82	0.43
18:X:373:ILE:HG23	18:X:444:SER:HB2	2.00	0.43
3:2:176:ALA:HB2	3:2:200:PHE:HZ	1.83	0.43
5:4:118:THR:HG23	5:4:121:ASP:H	1.82	0.43
11:D:81:MET:HE2	11:D:81:MET:HB3	1.85	0.43
15:R:37:TRP:O	15:R:41:ALA:N	2.50	0.43
17:T:227:ARG:HG2	17:T:228:GLN:HG3	1.99	0.43
17:V:271:GLN:NE2	18:Y:157:GLN:NE2	2.66	0.43
5:4:119:VAL:HG22	5:4:155:PHE:HD1	1.84	0.43
13:P:77:PHE:HZ	13:P:109:LEU:HD11	1.83	0.43
17:U:112:ASP:N	17:U:112:ASP:OD1	2.51	0.43
18:Y:446:PRO:HG3	18:Y:488:MET:HB3	2.00	0.43
18:Z:290:PHE:O	18:Z:294:ASN:ND2	2.52	0.43
3:2:189:ASP:O	3:2:192:THR:OG1	2.29	0.43
11:A:82:PHE:HB3	11:B:81:MET:HE3	2.01	0.43
17:T:337:MET:HE2	17:T:337:MET:HB3	1.84	0.43
17:T:429:ARG:HG3	22:Y:601:ADP:O3'	2.18	0.43
9:8:43:ARG:NH1	12:M:143:ASP:O	2.50	0.43
11:B:81:MET:HE2	11:B:103:ALA:HA	2.01	0.43
11:C:86:ILE:HG23	11:D:99:LEU:HD22	2.00	0.43
2:1:23:TYR:HB2	8:7:82:ILE:HD11	2.01	0.43
11:B:90:ALA:HB2	11:C:99:LEU:HD11	2.00	0.43
18:Y:441:ARG:O	18:Y:444:SER:OG	2.32	0.43
18:Z:414:GLN:HA	18:Z:417:ILE:HG12	2.00	0.43
2:1:362:LEU:O	2:1:386:HIS:NE2	2.52	0.43
3:2:70:LEU:HD23	3:2:70:LEU:HA	1.91	0.43
13:P:151:GLU:O	13:P:152:VAL:CG2	2.66	0.43
16:S:138:VAL:HG13	16:S:159:GLN:HB2	2.00	0.43
2:1:556:ILE:HG21	6:5:36:ARG:HA	2.00	0.43
5:4:85:TYR:OH	8:7:161:TYR:OH	2.36	0.43
17:T:345:PRO:HB2	17:T:349:ALA:HA	2.01	0.43
2:1:365:GLN:HG2	2:1:383:ILE:HD12	2.00	0.43
6:5:111:LYS:HD3	6:5:111:LYS:HA	1.76	0.43
6:5:122:LEU:HD22	8:7:76:LEU:HB3	2.00	0.43
17:T:172:ASP:OD2	17:T:172:ASP:N	2.49	0.43
17:U:243:LYS:HG3	17:U:281:ALA:HA	2.00	0.43
17:U:300:PHE:HE1	17:U:357:LEU:HD11	1.83	0.43
18:Y:225:ARG:HA	18:Y:225:ARG:HD3	1.78	0.43
18:Z:503:ALA:HA	18:Z:506:ILE:HG12	2.00	0.43
2:1:25:ALA:HB2	8:7:155:SER:HB3	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:89:LEU:HB3	8:7:172:ALA:HB2	2.00	0.42
5:4:267:LYS:HD3	5:4:267:LYS:HA	1.91	0.42
11:F:72:ALA:HB2	11:G:70:ALA:HA	2.00	0.42
14:Q:32:LYS:O	14:Q:36:LYS:N	2.39	0.42
17:T:298:LEU:HD23	17:T:298:LEU:HA	1.87	0.42
18:X:142:SER:O	18:X:145:ARG:NH2	2.51	0.42
3:2:70:LEU:HD12	3:2:106:VAL:HG22	2.02	0.42
11:I:55:VAL:O	11:I:59:SER:HB2	2.19	0.42
18:X:178:LYS:HG3	18:X:335:SER:HB3	2.00	0.42
18:X:374:TYR:HB2	18:X:488:MET:HE1	2.01	0.42
11:G:71:LEU:HA	11:G:74:VAL:HG22	2.01	0.42
18:Y:284:VAL:HG11	18:Y:287:ILE:HD13	2.00	0.42
3:2:159:LYS:NZ	5:4:193:GLU:OE1	2.44	0.42
5:4:64:GLU:OE2	8:7:166:ARG:NH2	2.52	0.42
6:5:92:LEU:O	6:5:96:VAL:HB	2.19	0.42
13:P:152:VAL:O	13:P:184:LEU:HA	2.18	0.42
18:X:450:ALA:O	18:X:454:THR:OG1	2.38	0.42
3:2:144:LEU:HD12	3:2:144:LEU:HA	1.88	0.42
11:C:93:PRO:HB3	11:D:95:ILE:HD13	2.01	0.42
11:H:86:ILE:HG21	11:I:85:LEU:HA	2.01	0.42
9:8:26:HIS:HD2	9:8:28:PHE:HB2	1.83	0.42
17:T:265:LYS:HB2	17:T:268:THR:HG23	2.02	0.42
17:V:241:HIS:HE1	17:V:493:PRO:HA	1.83	0.42
17:V:498:THR:HA	17:V:501:VAL:HG12	2.01	0.42
18:Y:245:THR:HG21	18:Y:268:VAL:HG11	2.01	0.42
18:Z:422:MET:HA	18:Z:425:LEU:HD13	2.01	0.42
13:P:49:THR:HA	17:V:59:ILE:HD11	2.01	0.42
18:Y:516:LYS:HE3	18:Y:516:LYS:HB3	1.80	0.42
3:2:197:LEU:HD21	3:2:217:LEU:HD11	2.02	0.42
5:4:118:THR:HA	5:4:154:LEU:HA	2.01	0.42
18:X:108:PRO:HB2	18:X:142:SER:HB2	2.02	0.42
18:X:192:LEU:HD22	18:X:364:LEU:HD21	2.01	0.42
3:2:278:ASP:HB2	5:4:27:LYS:HG2	2.01	0.42
3:2:420:GLU:OE2	3:2:433:TYR:OH	2.33	0.42
4:3:233:ARG:NH1	4:3:235:ASP:OD2	2.41	0.42
13:P:69:LYS:NZ	13:P:113:GLY:O	2.50	0.42
16:S:101:VAL:HG11	16:S:182:LEU:HD22	2.02	0.42
3:2:162:GLY:HA3	3:2:192:THR:HG22	2.02	0.42
11:I:111:GLU:O	11:I:115:LEU:HB2	2.20	0.42
17:U:258:VAL:HG22	17:U:286:ILE:HD12	2.02	0.42
18:Z:298:SER:HA	18:Z:301:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:186:GLY:O	3:2:389:SER:OG	2.33	0.41
4:3:143:LEU:HD23	4:3:143:LEU:HA	1.90	0.41
11:D:113:ILE:HD13	11:D:113:ILE:HA	1.91	0.41
11:E:82:PHE:HB2	11:F:81:MET:HE2	2.02	0.41
16:S:99:LYS:HB3	16:S:187:PRO:HA	2.03	0.41
17:T:58:LEU:HD23	17:T:58:LEU:HA	1.93	0.41
17:U:161:GLY:HA2	17:U:282:MET:HG2	2.01	0.41
17:U:453:TYR:O	17:U:457:ALA:HB2	2.19	0.41
17:U:456:VAL:HA	17:U:459:PHE:HD2	1.85	0.41
18:Z:101:LYS:HD3	18:Z:101:LYS:HA	1.76	0.41
2:1:330:LYS:HD3	2:1:330:LYS:HA	1.89	0.41
11:C:119:LEU:O	11:C:123:LEU:HB2	2.20	0.41
11:E:90:ALA:HB2	11:F:99:LEU:HD11	2.02	0.41
12:M:199:LYS:HA	12:M:199:LYS:HD3	1.76	0.41
17:U:389:ASP:OD1	17:U:391:SER:OG	2.38	0.41
17:V:66:LEU:HA	17:V:66:LEU:HD23	1.83	0.41
3:2:299:LEU:HD13	3:2:303:VAL:HG12	2.02	0.41
5:4:113:THR:O	5:4:113:THR:OG1	2.38	0.41
15:R:33:PHE:HD2	16:S:94:ALA:HB2	1.84	0.41
17:T:321:LEU:HD12	17:T:378:THR:HB	2.02	0.41
18:Z:318:LEU:O	18:Z:322:GLN:HB2	2.19	0.41
2:1:404:LYS:HZ1	6:5:78:GLU:HB3	1.85	0.41
3:2:143:VAL:HG12	3:2:157:LEU:HD21	2.02	0.41
6:5:115:ILE:HD12	6:5:115:ILE:HA	1.94	0.41
7:6:143:LEU:HA	7:6:143:LEU:HD12	1.77	0.41
11:C:123:LEU:O	11:C:127:ALA:N	2.53	0.41
11:E:91:ARG:HD2	15:R:96:GLY:HA3	2.01	0.41
17:V:429:ARG:NH2	22:Z:601:ADP:O2B	2.53	0.41
17:V:439:MET:O	17:V:443:ALA:CB	2.69	0.41
18:X:529:LYS:HA	18:X:529:LYS:HD2	1.88	0.41
18:Z:164:ILE:HB	18:Z:167:VAL:HB	2.01	0.41
3:2:251:LEU:HD23	3:2:251:LEU:HA	1.93	0.41
11:J:81:MET:HE2	11:J:81:MET:HB3	1.87	0.41
16:S:213:PRO:HG3	16:S:244:ARG:HA	2.02	0.41
3:2:71:TRP:O	3:2:75:THR:OG1	2.32	0.41
6:5:122:LEU:HD23	6:5:122:LEU:HA	1.93	0.41
8:7:170:HIS:HB3	8:7:173:ILE:HB	2.02	0.41
11:E:118:LEU:O	11:E:122:PHE:HB2	2.21	0.41
11:H:97:LYS:HD3	11:H:97:LYS:HA	1.81	0.41
17:U:203:PHE:O	17:U:242:GLN:NE2	2.54	0.41
17:V:224:ILE:HG23	17:V:407:PHE:HD1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:503:ALA:C	18:X:505:ASP:N	2.76	0.41
2:1:340:LEU:HA	2:1:343:GLU:HG2	2.02	0.41
2:1:594:PRO:HG2	9:8:8:LEU:HD23	2.02	0.41
16:S:291:ASP:OD1	16:S:294:ARG:NH2	2.37	0.41
17:T:436:PHE:HB3	17:T:439:MET:HB3	2.01	0.41
17:V:556:LYS:H	17:V:556:LYS:HG2	1.72	0.41
18:Y:448:GLN:HG2	18:Y:458:GLY:HA3	2.02	0.41
3:2:111:GLY:HA3	3:2:146:GLY:HA2	2.03	0.41
11:B:60:LYS:NZ	11:B:124:ILE:O	2.38	0.41
13:P:219:ASN:HA	13:P:222:VAL:HG12	2.02	0.41
17:T:215:ILE:HD11	17:T:406:ILE:HD11	2.03	0.41
17:T:542:ILE:HD13	17:T:546:LEU:HD23	2.03	0.41
17:U:132:PHE:CE1	17:U:297:PRO:HB2	2.55	0.41
18:X:554:LEU:HD23	18:X:554:LEU:HA	1.86	0.41
18:Y:56:LEU:HD11	18:Y:83:ASN:HA	2.03	0.41
18:Y:190:THR:HA	18:Y:193:ILE:HG22	2.02	0.41
2:1:420:TYR:HB2	2:1:424:VAL:HG13	2.02	0.41
3:2:223:LYS:HA	3:2:223:LYS:HD3	1.89	0.41
11:J:107:PHE:CD1	11:J:111:GLU:OE2	2.74	0.41
17:U:386:GLN:HB3	18:Z:347:THR:HB	2.03	0.41
18:X:272:PHE:HD1	18:X:276:GLU:HG3	1.85	0.41
18:X:289:ARG:HA	18:X:292:GLN:HG2	2.03	0.41
18:X:499:ALA:HA	18:X:502:MET:HB3	2.03	0.41
2:1:568:ASP:HB2	2:1:580:LYS:HE3	2.03	0.40
3:2:289:HIS:HD2	3:2:307:VAL:HG23	1.86	0.40
3:2:370:ILE:HB	3:2:377:VAL:HG12	2.04	0.40
7:6:108:LEU:HD11	12:M:281:LEU:HD13	2.03	0.40
13:P:37:LEU:HD12	13:P:37:LEU:HA	1.93	0.40
17:V:301:LEU:HD23	17:V:301:LEU:HA	1.94	0.40
18:X:327:THR:HG22	18:X:332:SER:HB2	2.03	0.40
17:T:90:VAL:HG23	17:T:95:ALA:HB2	2.03	0.40
17:U:49:ARG:HB3	17:V:43:LYS:HE3	2.02	0.40
17:U:94:ILE:HG13	17:U:340:LEU:HB3	2.03	0.40
17:U:483:MET:HE3	17:U:483:MET:HB3	1.93	0.40
17:V:263:GLY:HA3	17:V:329:LYS:HD3	2.04	0.40
3:2:253:LEU:HD11	3:2:401:ALA:HB2	2.03	0.40
13:P:38:LYS:HB2	13:P:38:LYS:HE2	1.89	0.40
14:Q:28:ARG:NE	15:R:148:GLU:OE2	2.41	0.40
16:S:67:LYS:HB3	16:S:267:HIS:CD2	2.55	0.40
17:V:289:SER:O	17:V:289:SER:OG	2.33	0.40
18:Y:248:TYR:HD1	18:Y:248:TYR:HA	1.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:263:LEU:O	18:Y:267:THR:OG1	2.37	0.40
2:1:255:GLU:HA	2:1:258:GLU:HG3	2.03	0.40
11:A:70:ALA:HA	11:J:72:ALA:HB2	2.02	0.40
11:G:60:LYS:HB3	11:G:60:LYS:HE2	1.78	0.40
12:M:294:LEU:HD23	12:M:294:LEU:HA	1.95	0.40
17:T:392:ALA:O	17:T:396:THR:OG1	2.27	0.40
17:U:135:ASP:OD1	17:U:135:ASP:N	2.52	0.40
17:U:443:ALA:HA	17:U:446:LEU:HB3	2.03	0.40
17:V:90:VAL:HG11	17:V:138:ILE:HB	2.03	0.40
4:3:190:SER:OG	4:3:229:ASN:ND2	2.42	0.40
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.56	0.40
11:A:95:ILE:HD11	11:J:90:ALA:HA	2.04	0.40
12:M:189:TRP:CD2	12:M:233:ALA:HB2	2.57	0.40
16:S:68:MET:HE2	16:S:68:MET:HB3	2.00	0.40
17:T:118:MET:HE3	17:T:120:LEU:HD13	2.04	0.40
17:T:243:LYS:HG2	17:T:284:TYR:HE1	1.86	0.40
17:V:377:LEU:HD12	17:V:377:LEU:HA	1.89	0.40
18:Y:165:LYS:HB2	18:Y:165:LYS:HE3	1.91	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	0	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
2	1	593/618 (96%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	416 (95%)	22 (5%)	1 (0%)	43	73
4	3	243/325 (75%)	234 (96%)	9 (4%)	0	100	100
5	4	288/294 (98%)	274 (95%)	14 (5%)	0	100	100
6	5	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	16	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	6	122/151 (81%)	110 (90%)	12 (10%)	0	100	100
8	7	174/190 (92%)	165 (95%)	9 (5%)	0	100	100
9	8	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	72 (100%)	0	0	100	100
11	B	72/127 (57%)	72 (100%)	0	0	100	100
11	C	71/127 (56%)	71 (100%)	0	0	100	100
11	D	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	E	72/127 (57%)	72 (100%)	0	0	100	100
11	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	G	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	H	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	205 (96%)	8 (4%)	0	100	100
13	P	191/229 (83%)	179 (94%)	12 (6%)	0	100	100
14	Q	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
15	R	175/199 (88%)	160 (91%)	15 (9%)	0	100	100
16	S	275/317 (87%)	265 (96%)	9 (3%)	1 (0%)	30	62
17	T	521/562 (93%)	493 (95%)	26 (5%)	2 (0%)	30	62
17	U	521/562 (93%)	499 (96%)	21 (4%)	1 (0%)	43	73
17	V	518/562 (92%)	497 (96%)	21 (4%)	0	100	100
18	X	536/574 (93%)	509 (95%)	26 (5%)	1 (0%)	43	73
18	Y	518/574 (90%)	478 (92%)	39 (8%)	1 (0%)	43	73
18	Z	537/574 (94%)	498 (93%)	34 (6%)	5 (1%)	14	47
All	All	7034/8234 (85%)	6680 (95%)	341 (5%)	13 (0%)	44	73

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	T	430	VAL
18	X	308	VAL
18	Y	308	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Z	308	VAL
3	2	383	PRO
17	T	56	LYS
18	Z	307	ALA
18	Z	517	VAL
18	Z	512	ALA
16	S	213	PRO
17	U	513	ARG
18	Z	306	SER
6	5	120	PRO

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	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	491 (100%)	2 (0%)	84	86
3	2	312/312 (100%)	311 (100%)	1 (0%)	86	88
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	A	50/86 (58%)	50 (100%)	0	100	100
11	B	50/86 (58%)	50 (100%)	0	100	100
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	50 (100%)	0	100	100
11	E	50/86 (58%)	49 (98%)	1 (2%)	48	72
11	F	50/86 (58%)	50 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	G	50/86 (58%)	49 (98%)	1 (2%)	48	72
11	H	50/86 (58%)	50 (100%)	0	100	100
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	49 (98%)	1 (2%)	48	72
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	171 (100%)	0	100	100
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	133 (99%)	1 (1%)	76	83
16	S	235/265 (89%)	234 (100%)	1 (0%)	84	86
17	T	419/448 (94%)	418 (100%)	1 (0%)	87	89
17	U	419/448 (94%)	416 (99%)	3 (1%)	76	83
17	V	418/448 (93%)	417 (100%)	1 (0%)	87	89
18	X	446/469 (95%)	445 (100%)	1 (0%)	87	89
18	Y	429/469 (92%)	429 (100%)	0	100	100
18	Z	447/469 (95%)	446 (100%)	1 (0%)	87	89
All	All	5628/6445 (87%)	5613 (100%)	15 (0%)	84	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	24	LEU
2	1	335	VAL
3	2	391	THR
11	E	80	VAL
11	G	56	LEU
11	J	68	THR
15	R	195	VAL
16	S	238	GLU
17	T	430	VAL
17	U	67	ILE
17	U	180	VAL
17	U	514	VAL
17	V	90	VAL
18	X	124	VAL
18	Z	558	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109)

such sidechains are listed below:

Mol	Chain	Res	Type
1	0	60	GLN
2	1	65	GLN
2	1	82	HIS
2	1	100	GLN
2	1	101	ASN
2	1	285	GLN
2	1	298	GLN
2	1	316	ASN
2	1	365	GLN
2	1	438	GLN
2	1	482	ASN
2	1	527	GLN
2	1	606	ASN
3	2	59	GLN
3	2	68	ASN
3	2	74	ASN
3	2	243	GLN
3	2	289	HIS
3	2	432	GLN
4	3	94	ASN
4	3	151	ASN
4	3	179	GLN
4	3	206	ASN
4	3	229	ASN
4	3	309	ASN
4	3	319	GLN
5	4	38	GLN
5	4	240	GLN
6	5	25	HIS
6	5	79	ASN
7	6	40	ASN
7	6	74	GLN
8	7	38	ASN
8	7	86	HIS
8	7	106	GLN
8	7	123	HIS
8	7	170	HIS
9	8	26	HIS
10	9	35	GLN
10	9	60	ASN
11	B	92	ASN
11	E	98	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	94	ASN
11	J	94	ASN
12	M	120	GLN
12	M	121	ASN
12	M	163	ASN
12	M	295	GLN
13	P	148	HIS
13	P	223	ASN
15	R	64	GLN
15	R	171	GLN
16	S	52	ASN
16	S	98	ASN
16	S	174	GLN
16	S	262	ASN
16	S	267	HIS
17	T	60	GLN
17	T	61	HIS
17	T	64	GLN
17	T	134	ASN
17	T	140	GLN
17	T	228	GLN
17	T	241	HIS
17	T	549	HIS
17	U	149	GLN
17	U	152	ASN
17	U	242	GLN
17	U	246	ASN
17	U	248	GLN
17	U	264	GLN
17	U	271	GLN
17	U	319	HIS
17	U	386	GLN
17	U	486	GLN
17	V	121	ASN
17	V	134	ASN
17	V	139	HIS
17	V	149	GLN
17	V	179	ASN
17	V	219	GLN
17	V	242	GLN
17	V	244	ASN
17	V	264	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	V	271	GLN
17	V	278	GLN
17	V	486	GLN
17	V	488	GLN
17	V	497	GLN
18	X	144	HIS
18	X	174	GLN
18	X	199	ASN
18	X	250	GLN
18	X	294	ASN
18	X	404	GLN
18	X	574	ASN
18	Y	68	HIS
18	Y	157	GLN
18	Y	174	GLN
18	Y	198	ASN
18	Y	199	ASN
18	Y	204	HIS
18	Y	390	ASN
18	Y	408	GLN
18	Y	414	GLN
18	Y	445	GLN
18	Z	174	GLN
18	Z	408	GLN
18	Z	412	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	ADP	Y	601	21	28,29,29	1.43	4 (14%)	43,45,45	1.90	9 (20%)
20	ATP	V	1001	21	32,33,33	1.35	6 (18%)	48,52,52	1.73	8 (16%)
20	ATP	U	1001	21	32,33,33	1.30	6 (18%)	48,52,52	1.77	10 (20%)
20	ATP	T	1001	21	32,33,33	1.30	5 (15%)	48,52,52	1.82	9 (18%)
22	ADP	Z	601	21	28,29,29	1.38	6 (21%)	43,45,45	1.85	10 (23%)

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
22	ADP	Y	601	21	-	5/16/32/32	0/3/3/3
20	ATP	V	1001	21	-	6/22/38/38	0/3/3/3
20	ATP	U	1001	21	-	0/22/38/38	0/3/3/3
20	ATP	T	1001	21	-	2/22/38/38	0/3/3/3
22	ADP	Z	601	21	-	5/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	601	ADP	C5-C4	4.33	1.46	1.39
22	Y	601	ADP	C5-C4	4.19	1.46	1.39
20	T	1001	ATP	C5-C4	4.12	1.46	1.39
20	V	1001	ATP	C5-C4	4.09	1.46	1.39
20	U	1001	ATP	C5-C4	4.00	1.46	1.39
22	Y	601	ADP	C5-N7	-2.92	1.33	1.39
20	T	1001	ATP	C5-N7	-2.85	1.33	1.39
20	U	1001	ATP	C5-N7	-2.71	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	1001	ATP	C5-N7	-2.63	1.34	1.39
22	Z	601	ADP	C5-N7	-2.58	1.34	1.39
22	Y	601	ADP	C8-N9	-2.55	1.33	1.37
22	Y	601	ADP	C5-C6	2.49	1.47	1.41
22	Z	601	ADP	C5-C6	2.45	1.47	1.41
20	U	1001	ATP	C4-N9	-2.38	1.32	1.37
20	V	1001	ATP	C4-N9	-2.36	1.32	1.37
20	U	1001	ATP	C5-C6	2.31	1.47	1.41
22	Z	601	ADP	C4-N9	-2.27	1.33	1.37
20	V	1001	ATP	C8-N9	-2.24	1.33	1.37
20	V	1001	ATP	C5-C6	2.24	1.47	1.41
20	T	1001	ATP	C8-N9	-2.22	1.33	1.37
20	T	1001	ATP	C4-N9	-2.13	1.33	1.37
20	T	1001	ATP	C5-C6	2.09	1.46	1.41
20	V	1001	ATP	C8-N7	2.07	1.35	1.31
20	U	1001	ATP	C8-N9	-2.06	1.34	1.37
22	Z	601	ADP	C8-N9	-2.05	1.34	1.37
20	U	1001	ATP	C8-N7	2.02	1.35	1.31
22	Z	601	ADP	C8-N7	2.01	1.35	1.31

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	601	ADP	C5-C4-N3	-6.49	117.78	126.72
20	T	1001	ATP	C5-C4-N3	-5.83	118.69	126.72
20	V	1001	ATP	C5-C4-N3	-5.82	118.70	126.72
22	Z	601	ADP	C5-C4-N3	-5.63	118.97	126.72
20	U	1001	ATP	C5-C4-N3	-5.56	119.06	126.72
22	Y	601	ADP	N3-C4-N9	5.07	135.80	127.17
20	T	1001	ATP	N3-C4-N9	4.99	135.66	127.17
22	Z	601	ADP	N3-C4-N9	4.61	135.00	127.17
20	V	1001	ATP	N3-C4-N9	4.58	134.96	127.17
20	U	1001	ATP	N3-C4-N9	4.50	134.81	127.17
22	Y	601	ADP	C2-N3-C4	3.78	121.05	111.83
20	U	1001	ATP	C2-N3-C4	3.69	120.84	111.83
20	T	1001	ATP	C2-N3-C4	3.63	120.71	111.83
20	V	1001	ATP	C2-N3-C4	3.63	120.70	111.83
22	Z	601	ADP	C2-N3-C4	3.54	120.48	111.83
22	Y	601	ADP	C4-C5-N7	-3.52	106.56	110.58
20	V	1001	ATP	C4-C5-N7	-3.44	106.65	110.58
20	U	1001	ATP	N3-C2-N1	-3.43	123.39	128.58
20	T	1001	ATP	N3-C2-N1	-3.38	123.47	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	601	ADP	C4-C5-N7	-3.34	106.76	110.58
20	V	1001	ATP	N3-C2-N1	-3.22	123.70	128.58
22	Z	601	ADP	N3-C2-N1	-3.16	123.80	128.58
20	U	1001	ATP	C4-C5-N7	-3.06	107.08	110.58
22	Z	601	ADP	C4-N9-C8	2.97	108.86	105.74
20	T	1001	ATP	C4-C5-N7	-2.88	107.29	110.58
22	Y	601	ADP	N3-C2-N1	-2.86	124.26	128.58
20	T	1001	ATP	C4-N9-C8	2.79	108.67	105.74
20	V	1001	ATP	C4-N9-C8	2.79	108.67	105.74
20	U	1001	ATP	C4-N9-C8	2.79	108.66	105.74
20	U	1001	ATP	C2'-C1'-N9	-2.58	106.89	113.30
22	Y	601	ADP	C3'-C2'-C1'	2.57	106.32	101.46
22	Z	601	ADP	C2'-C1'-N9	-2.53	107.03	113.30
22	Z	601	ADP	C5-N7-C8	2.42	107.25	103.45
22	Z	601	ADP	C3'-C2'-C1'	2.37	105.95	101.46
20	V	1001	ATP	C5-N7-C8	2.36	107.17	103.45
22	Y	601	ADP	C5-N7-C8	2.35	107.14	103.45
20	V	1001	ATP	O2A-PA-O1A	2.31	123.18	112.44
20	T	1001	ATP	C3'-C2'-C1'	2.29	105.80	101.46
20	U	1001	ATP	C3'-C2'-C1'	2.29	105.80	101.46
22	Y	601	ADP	C2'-C1'-N9	-2.25	107.71	113.30
20	U	1001	ATP	C5-N7-C8	2.20	106.90	103.45
20	T	1001	ATP	C5-N7-C8	2.20	106.90	103.45
20	T	1001	ATP	O3A-PB-O1B	-2.14	104.26	110.70
20	U	1001	ATP	C6-C5-N7	2.04	136.02	132.09
22	Y	601	ADP	C4-N9-C8	2.04	107.88	105.74
22	Z	601	ADP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	V	1001	ATP	C5'-O5'-PA-O2A
22	Y	601	ADP	C5'-O5'-PA-O1A
22	Y	601	ADP	C5'-O5'-PA-O2A
22	Y	601	ADP	C5'-O5'-PA-O3A
22	Y	601	ADP	O4'-C4'-C5'-O5'
22	Z	601	ADP	C5'-O5'-PA-O2A
22	Z	601	ADP	C5'-O5'-PA-O3A
22	Y	601	ADP	C3'-C4'-C5'-O5'
22	Z	601	ADP	O4'-C4'-C5'-O5'
20	V	1001	ATP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

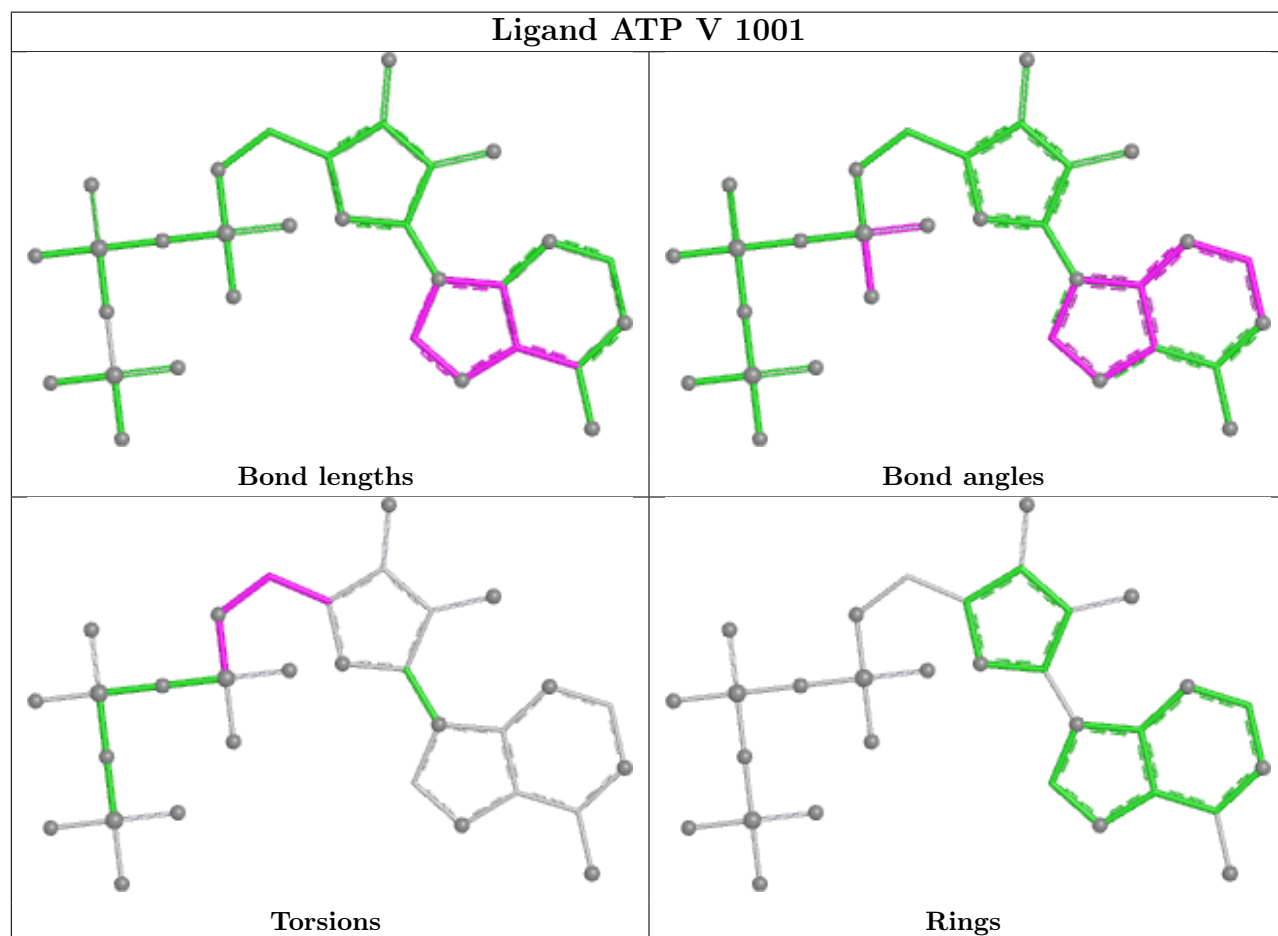
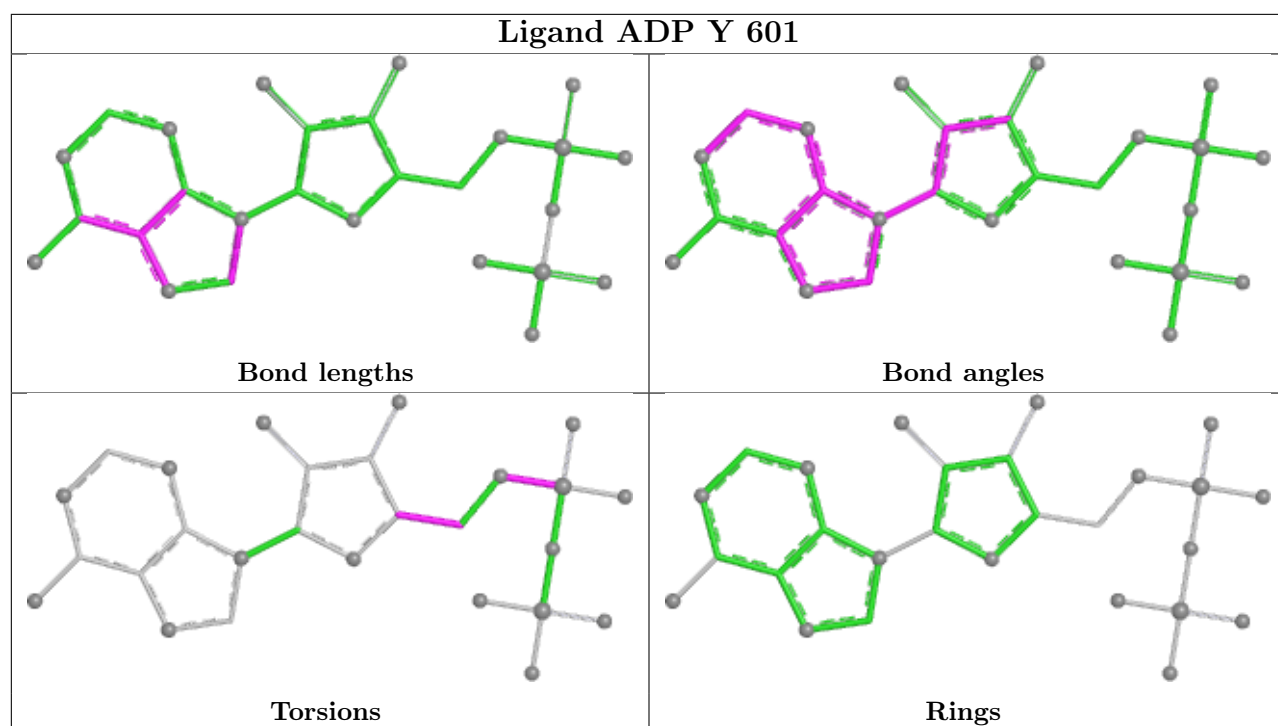
Mol	Chain	Res	Type	Atoms
20	V	1001	ATP	C5'-O5'-PA-O3A
22	Z	601	ADP	C5'-O5'-PA-O1A
22	Z	601	ADP	C3'-C4'-C5'-O5'
20	V	1001	ATP	C4'-C5'-O5'-PA
20	V	1001	ATP	C3'-C4'-C5'-O5'
20	T	1001	ATP	PG-O3B-PB-O2B
20	V	1001	ATP	O4'-C4'-C5'-O5'
20	T	1001	ATP	PG-O3B-PB-O1B

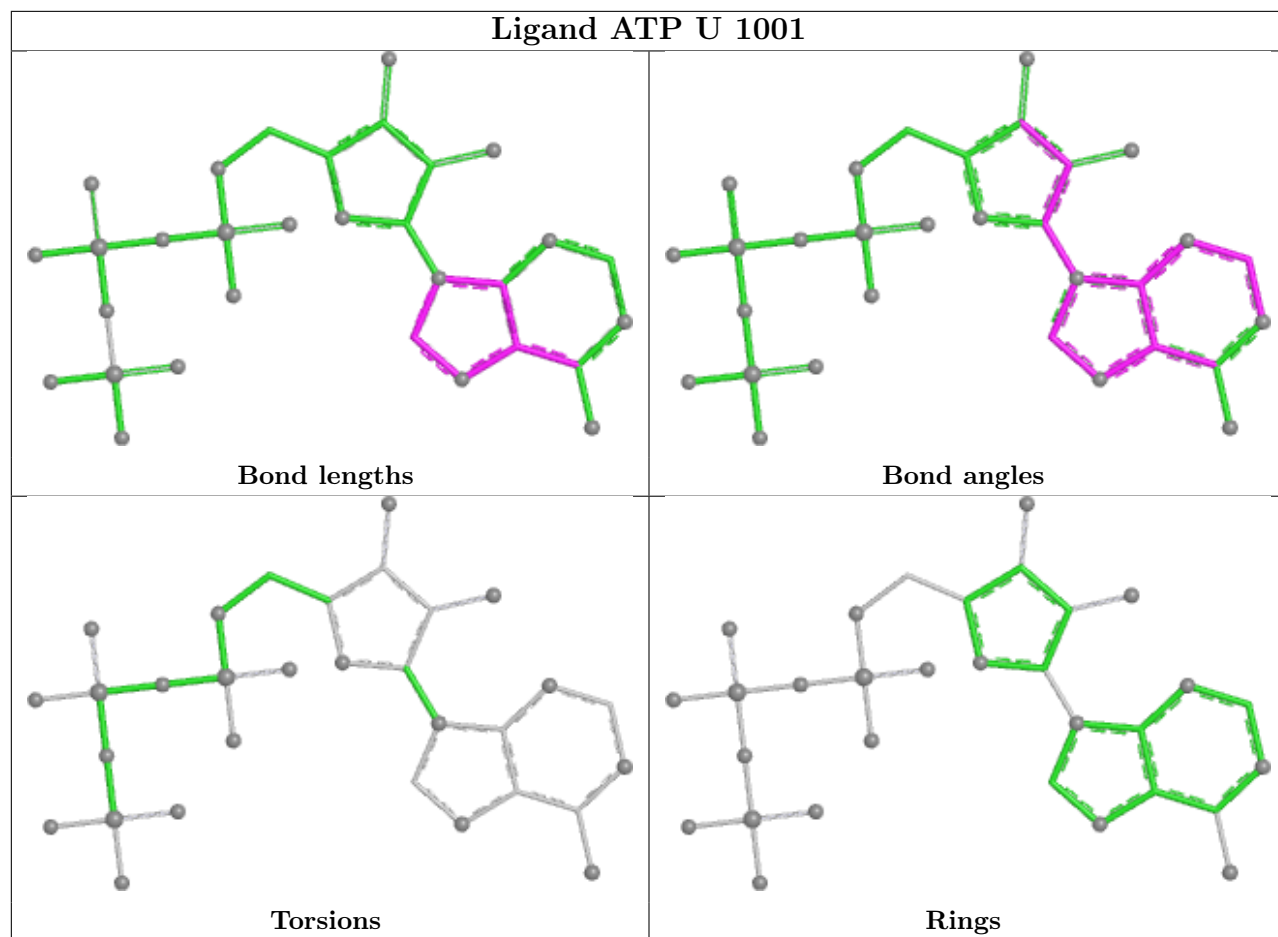
There are no ring outliers.

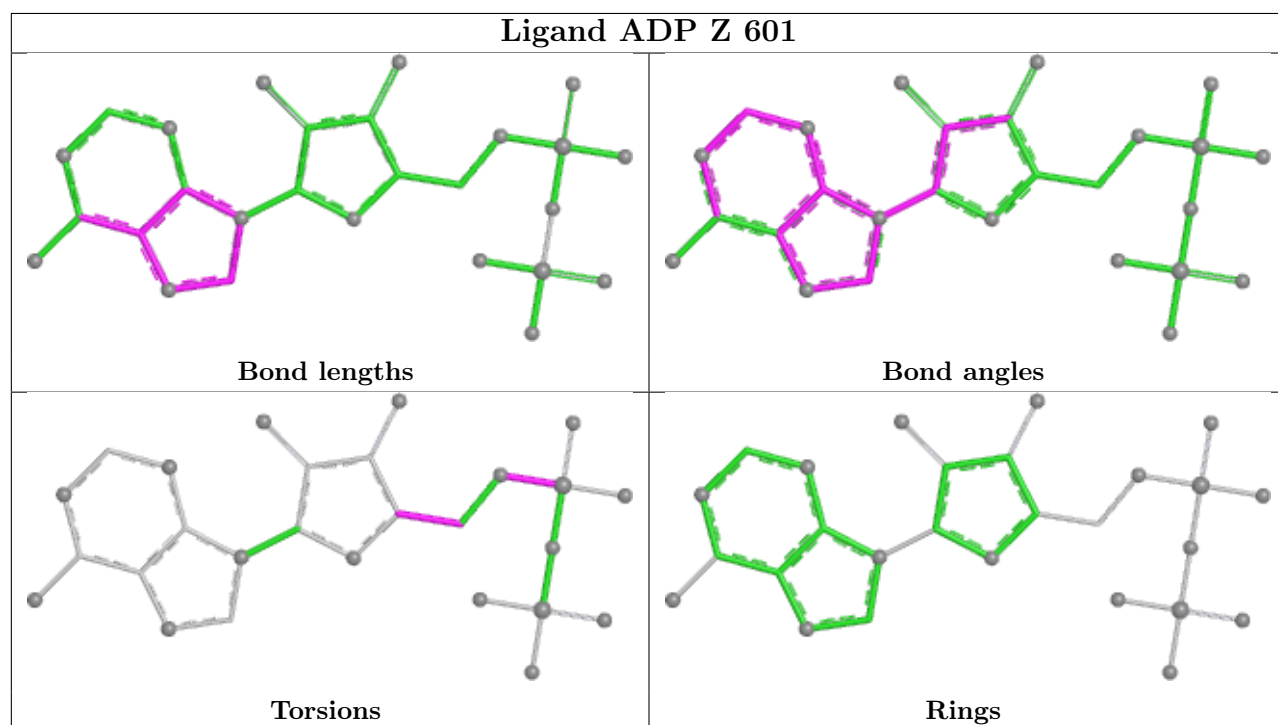
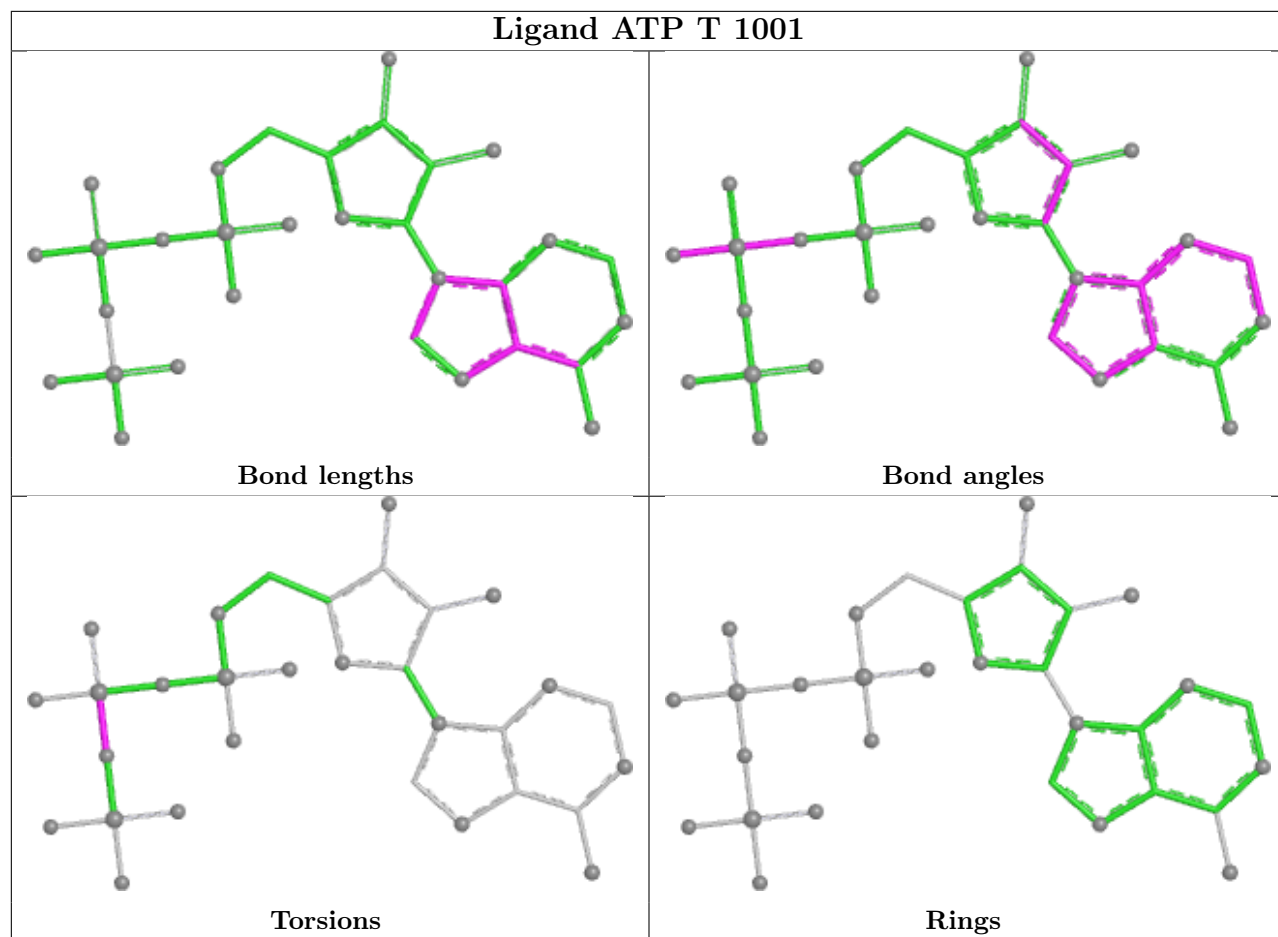
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Y	601	ADP	4	0
20	T	1001	ATP	1	0
22	Z	601	ADP	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.23

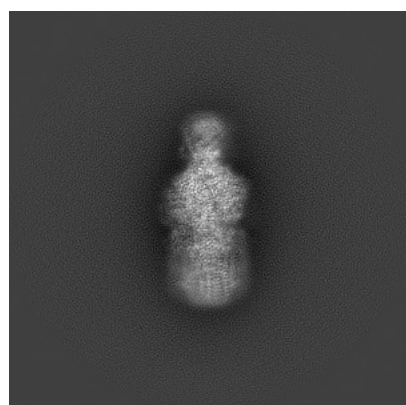
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4842. These allow visual inspection of the internal detail of the map and identification of artifacts.

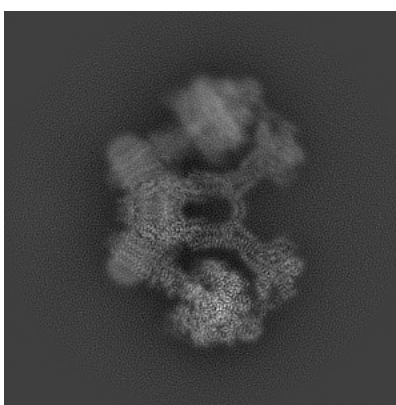
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

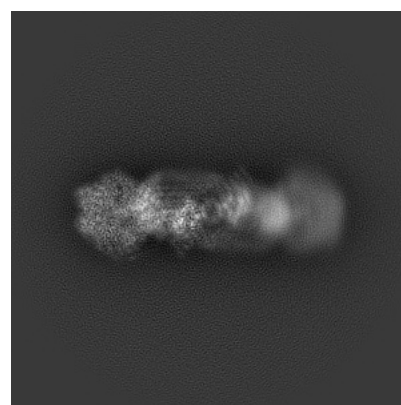
6.1.1 Primary map



X



Y

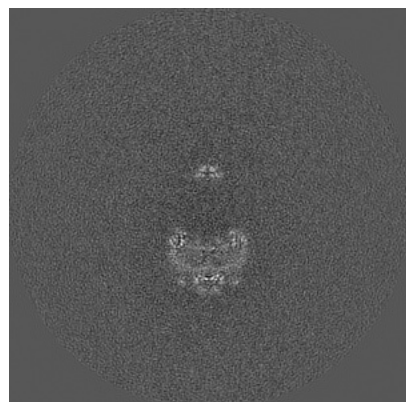


Z

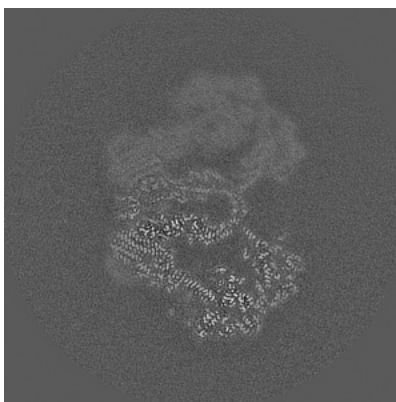
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

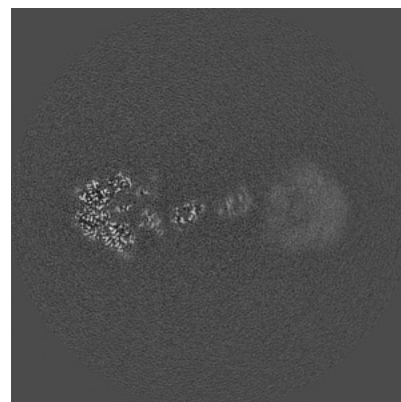
6.2.1 Primary map



X Index: 240



Y Index: 240

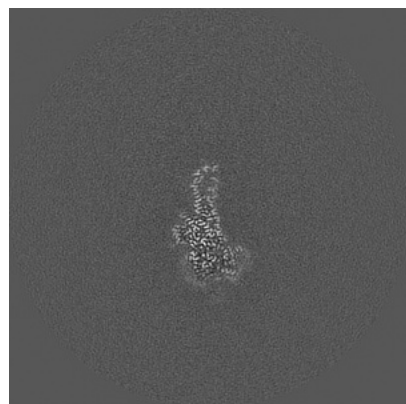


Z Index: 240

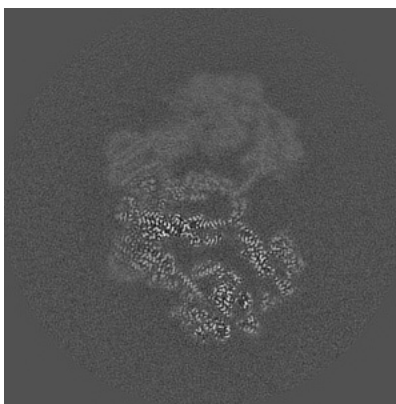
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 216



Y Index: 234

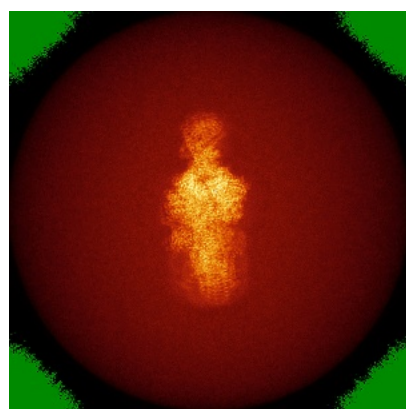


Z Index: 264

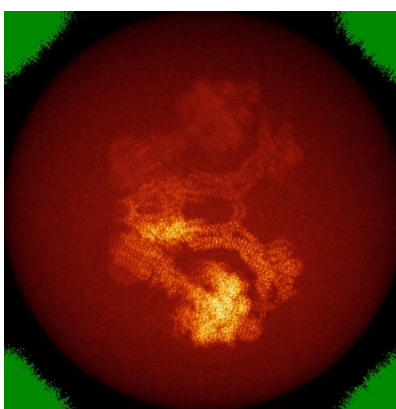
The images above show the largest variance slices of the map in three orthogonal directions.

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

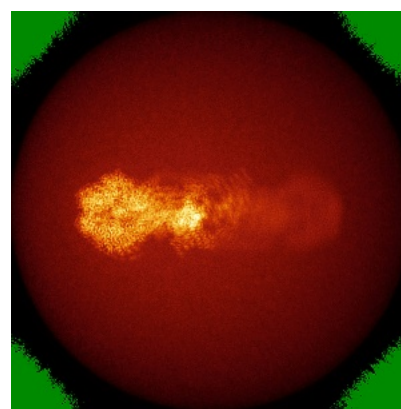
6.4.1 Primary map



X



Y

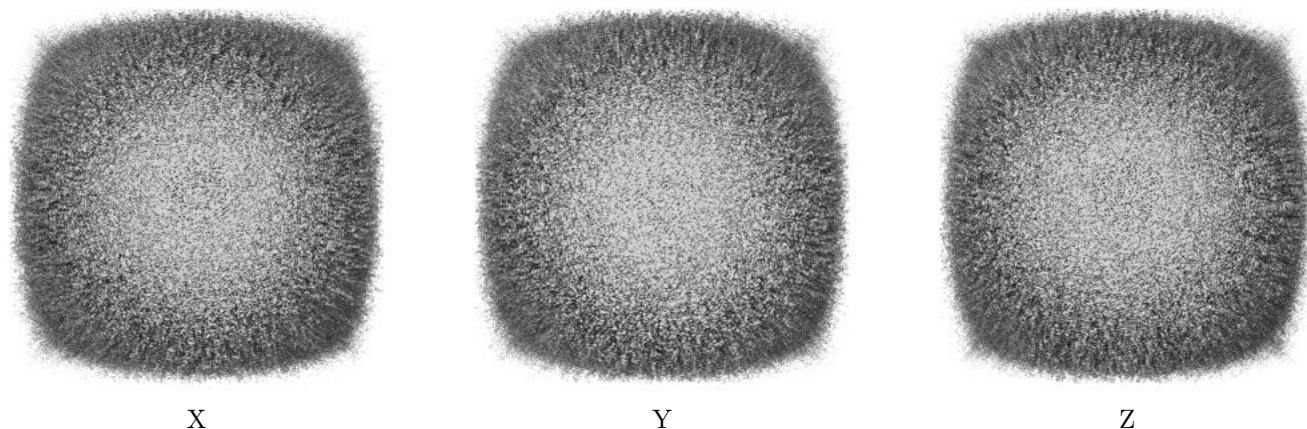


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

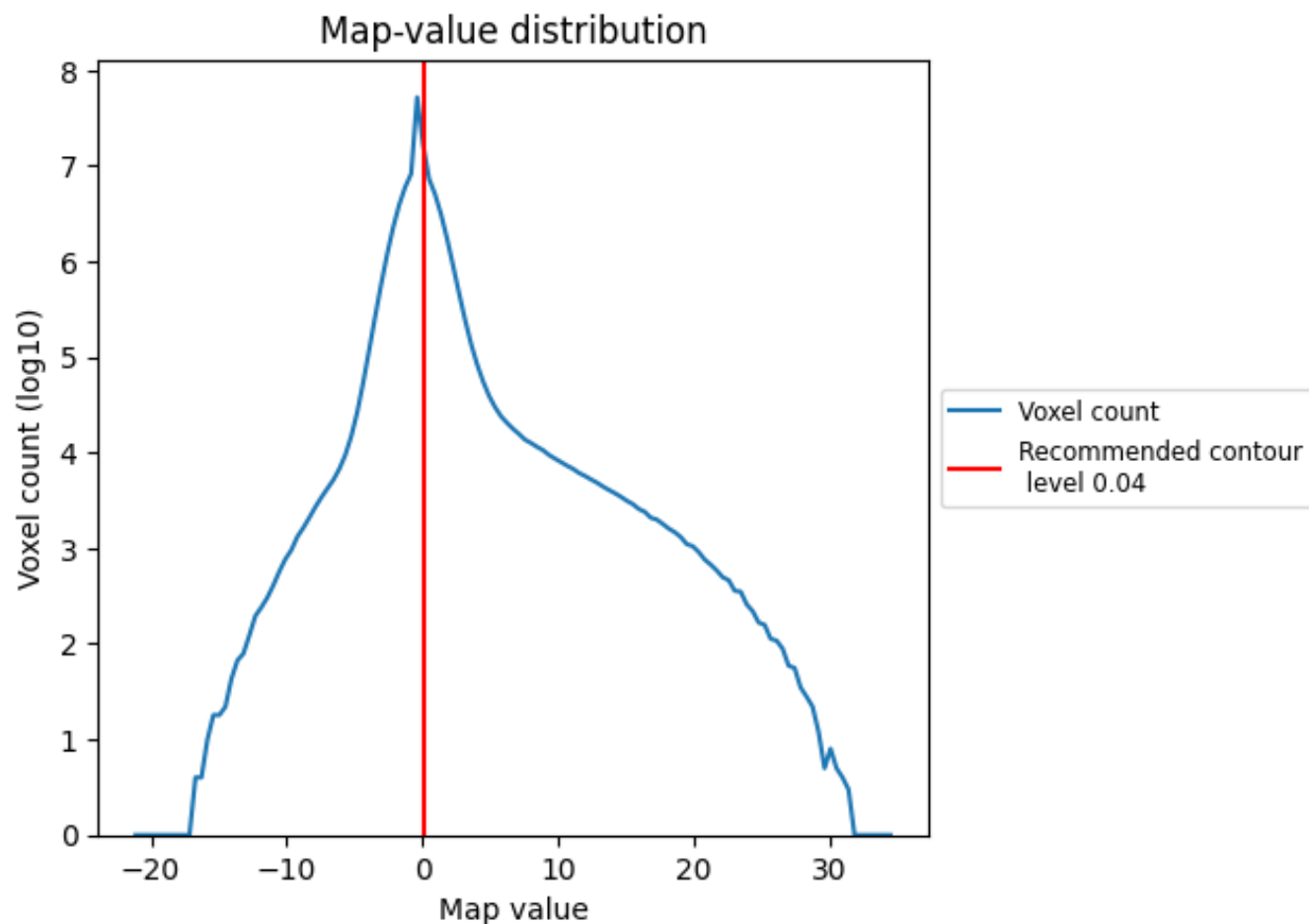
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

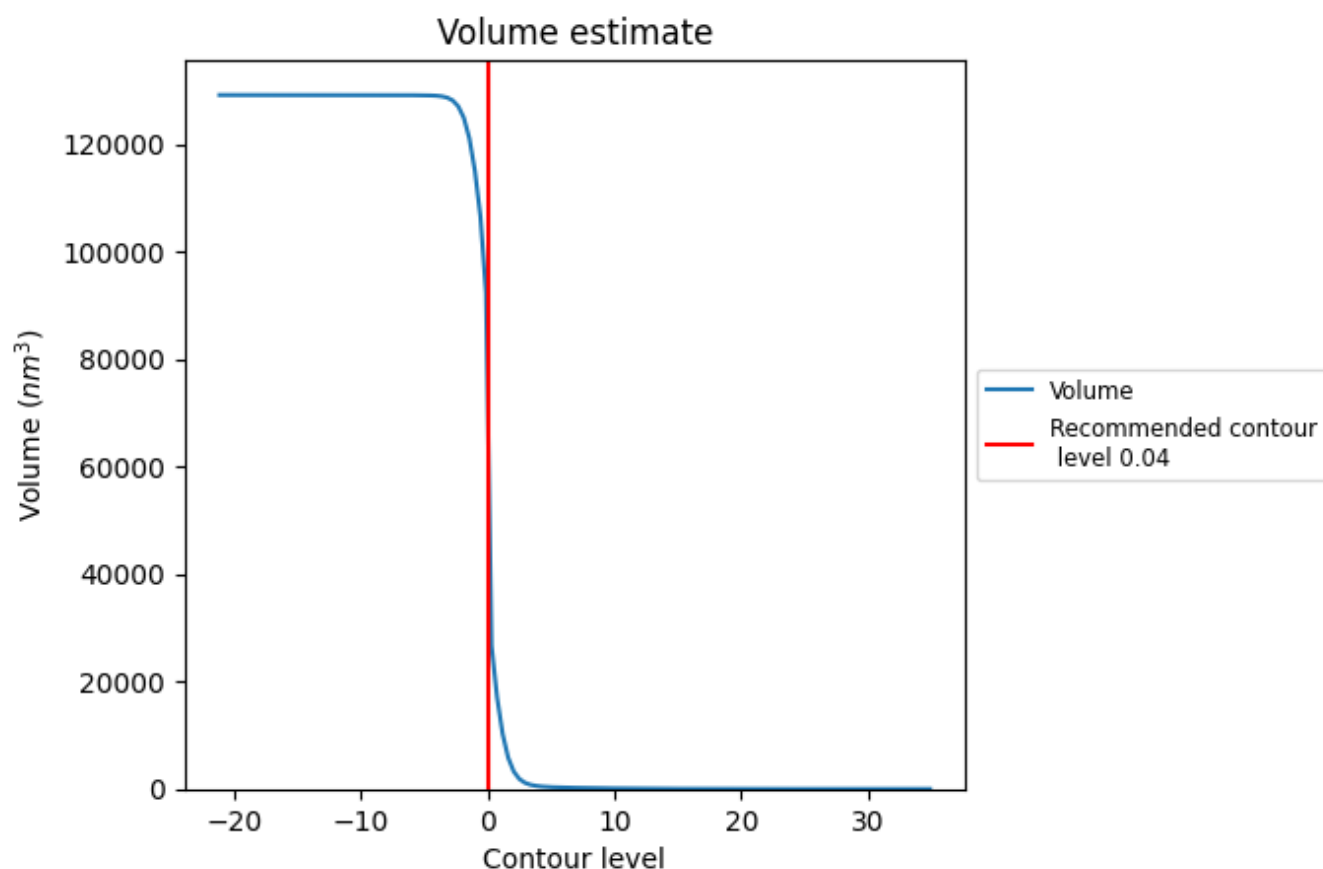
This section contains the results of statistical analysis of the map.

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.

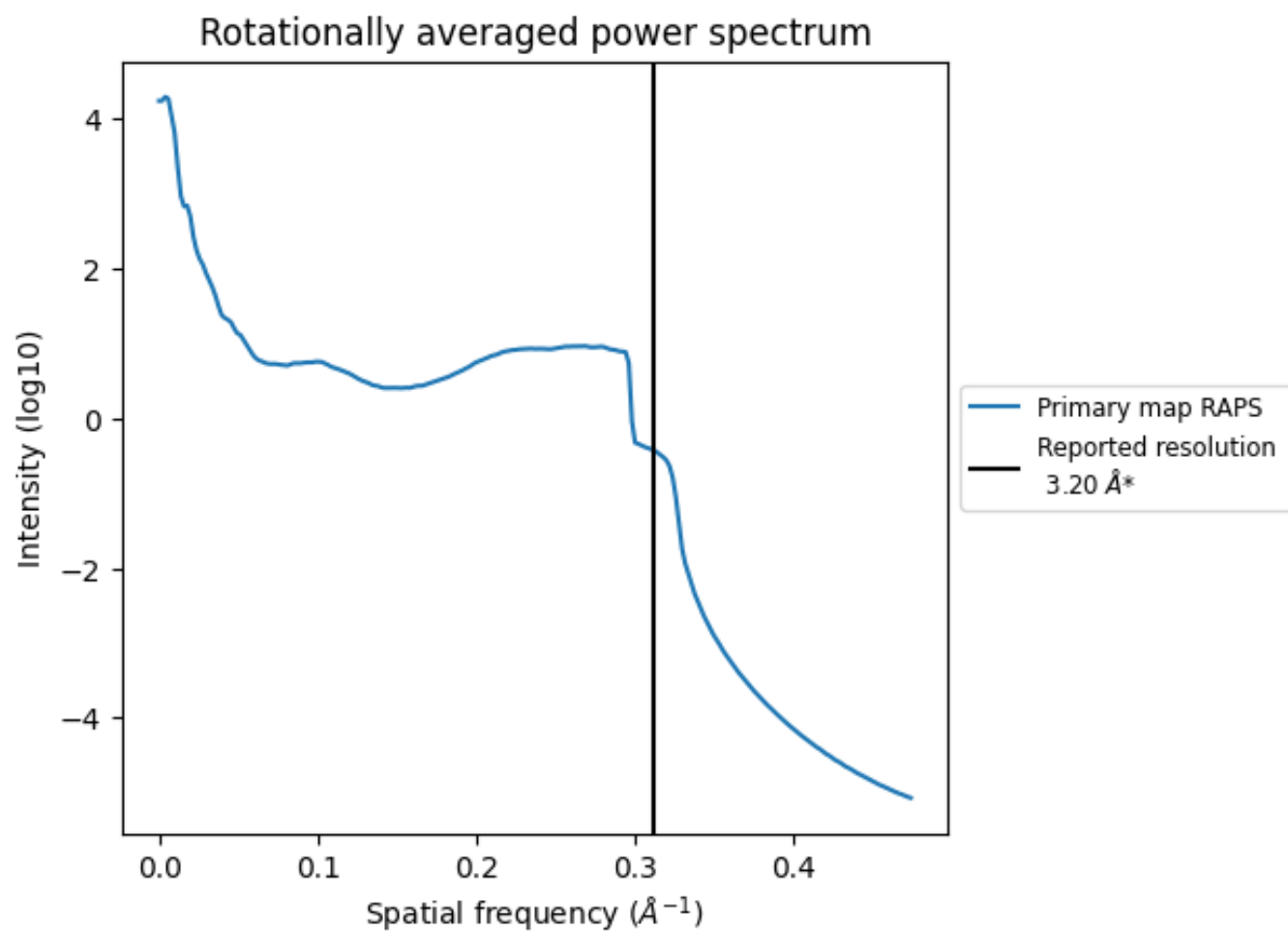
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68898 nm^3 ; this corresponds to an approximate mass of 62237 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 0.312 Å⁻¹

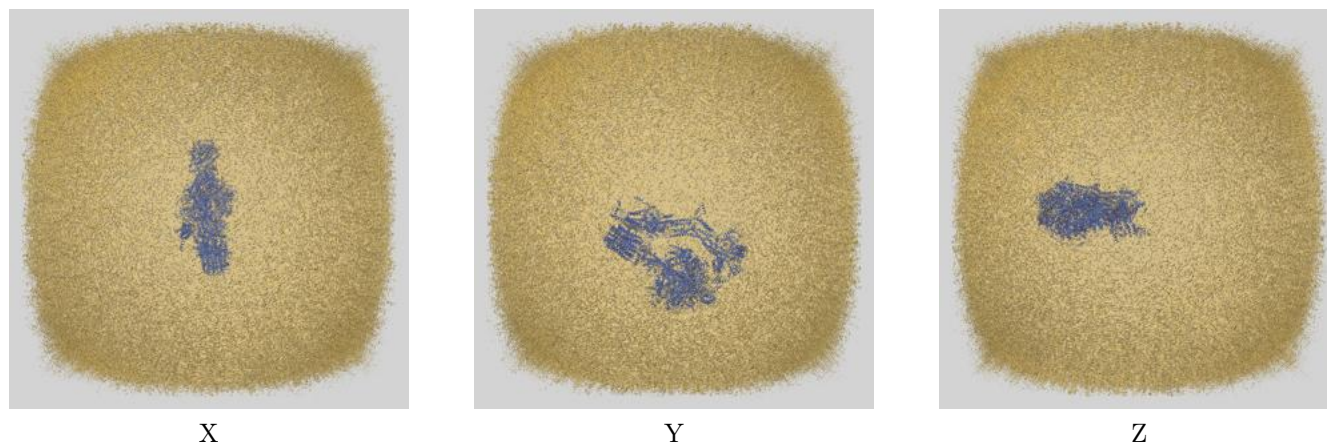
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

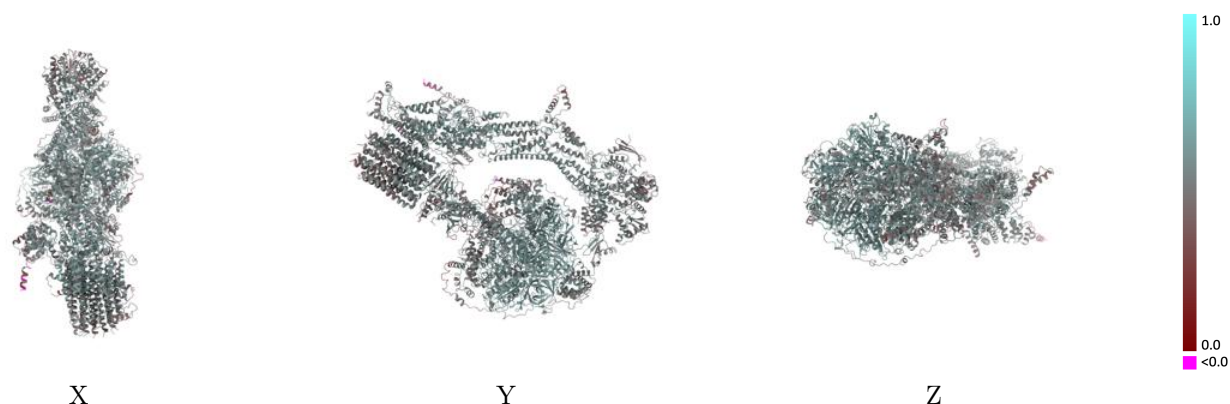
This section contains information regarding the fit between EMDB map EMD-4842 and PDB model 6RE5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



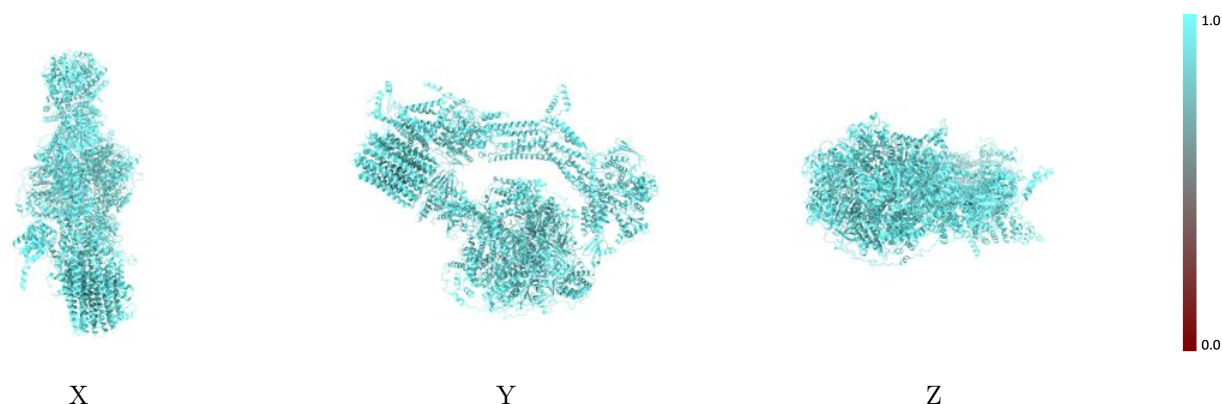
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



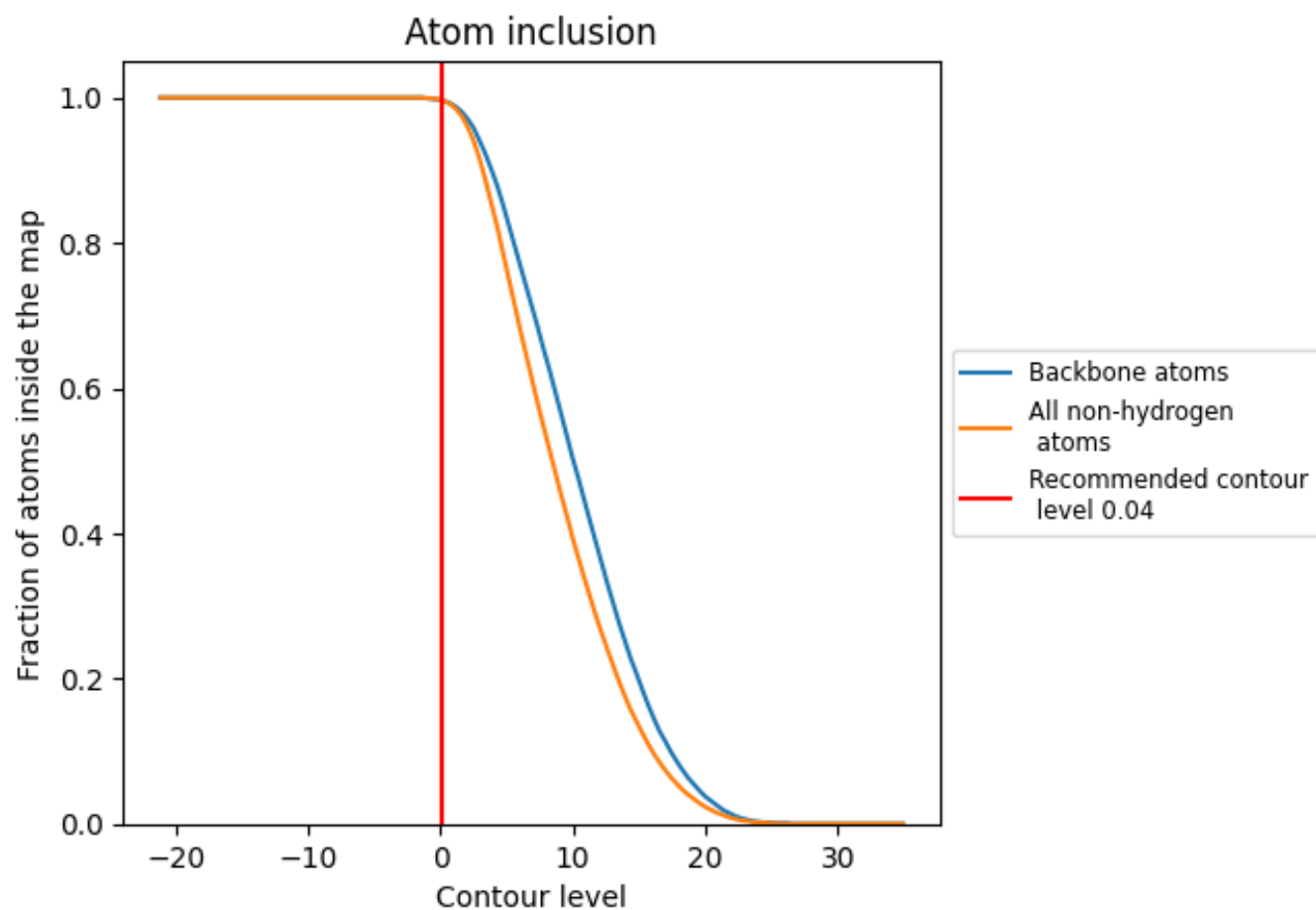
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.5300
0	 0.9920	 0.5140
1	 0.9970	 0.5320
2	 0.9980	 0.4920
3	 0.9970	 0.4850
4	 0.9990	 0.5090
5	 0.9940	 0.5520
6	 0.9970	 0.5440
7	 0.9960	 0.5320
8	 0.9970	 0.5410
9	 0.9960	 0.4780
A	 0.9940	 0.4890
B	 0.9900	 0.4690
C	 0.9960	 0.4660
D	 0.9980	 0.4760
E	 0.9940	 0.4720
F	 0.9900	 0.5020
G	 0.9920	 0.5380
H	 0.9960	 0.5350
I	 0.9980	 0.5140
J	 0.9980	 0.4880
M	 0.9940	 0.5350
P	 0.9990	 0.5030
Q	 1.0000	 0.5060
R	 0.9950	 0.4950
S	 0.9960	 0.5220
T	 0.9970	 0.5600
U	 0.9990	 0.5550
V	 0.9980	 0.5450
X	 0.9970	 0.5480
Y	 0.9960	 0.5590
Z	 0.9970	 0.5450

