



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:01 AM UTC

PDB ID : 6RDO / pdb_00006rdo
EMDB ID : EMD-4825
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 1C, composite map
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on : 2019-04-12
Resolution : 3.10 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

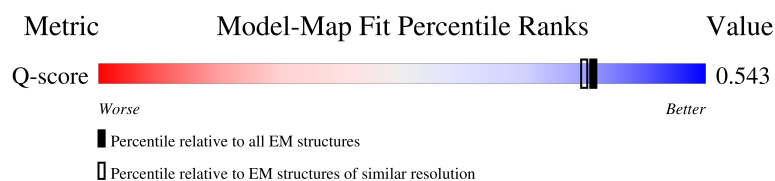
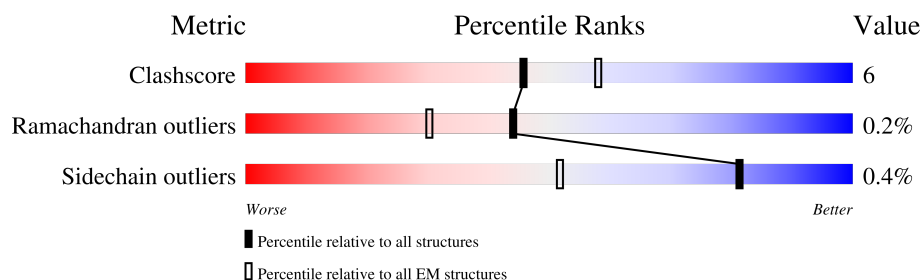
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



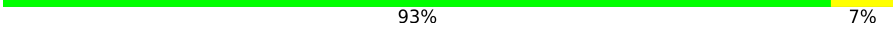
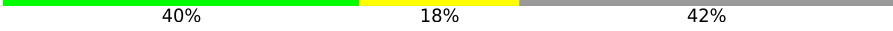
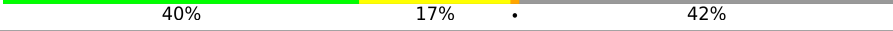
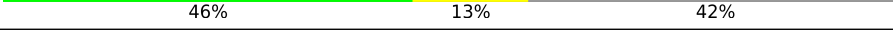
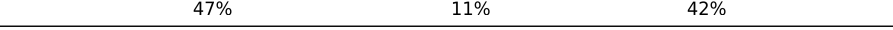
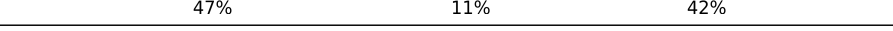
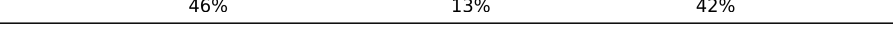
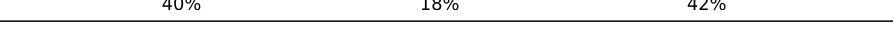
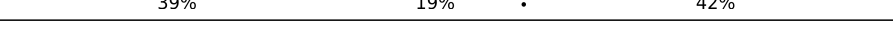
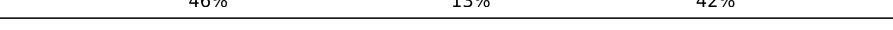
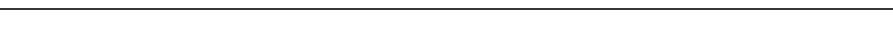
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	84% 12% .
3	2	441	87% 13%
4	3	325	64% 11% 25%

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Mol	Chain	Length	Quality of chain
5	4	294	 89% 10%
6	5	123	 82% 17%
7	6	151	 68% 14% 18%
8	7	190	 77% 16% 7%
9	8	89	 82% 17%
10	9	97	 93% 7%
11	A	127	 40% 18% 42%
11	B	127	 40% 17% 42%
11	C	127	 46% 13% 42%
11	D	127	 52% 6% 42%
11	E	127	 47% 11% 42%
11	F	127	 47% 11% 42%
11	G	127	 46% 13% 42%
11	H	127	 40% 18% 42%
11	I	127	 39% 19% 42%
11	J	127	 46% 13% 42%
12	M	327	 57% 9% 34%
13	P	229	 69% 16% 16%
14	Q	74	 82% 15%
15	R	199	 72% 17% 11%
16	S	317	 70% 18% 13%
17	T	562	 80% 12% 7%
17	U	562	 78% 14% 7%
17	V	562	 80% 12% 7%
18	X	574	 78% 16% 6%

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Mol	Chain	Length	Quality of chain
18	Y	574	 72% 18% 9%
18	Z	574	 82% 11% 6%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 53748 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		

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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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
17	V	520	Total	C	N	O	S	0	0
			3962	2527	700	724	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	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		
18	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
18	Z	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		

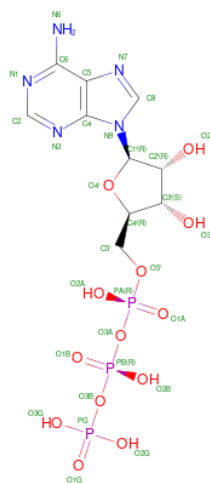
There are 6 discrepancies between the modelled and reference sequences:

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).

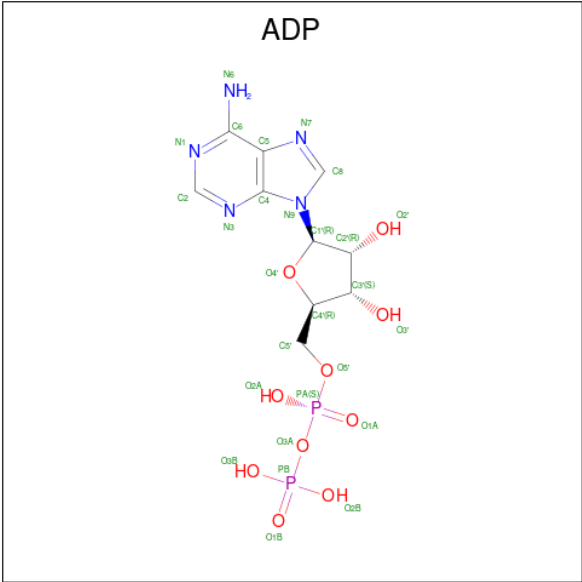


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total 31	C 10	N 5	O 13	P 3	0
20	U	1	Total 31	C 10	N 5	O 13	P 3	0
20	V	1	Total 31	C 10	N 5	O 13	P 3	0

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

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

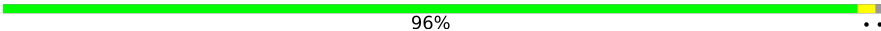
- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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.

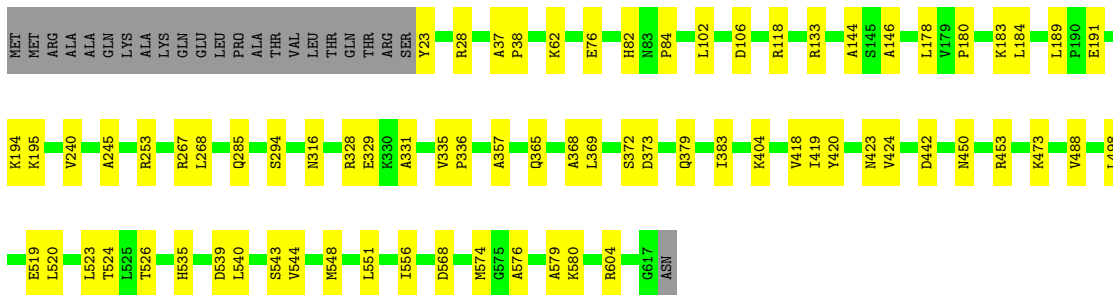
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

Chain 0:  96% ..



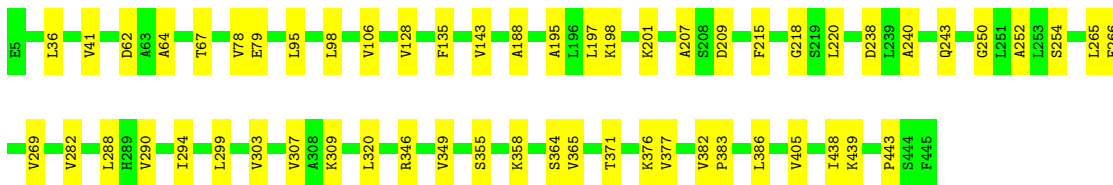
- Molecule 2: ATP synthase associated protein ASA1

Chain 1:  84% 12% .



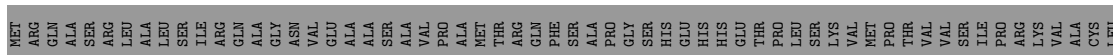
- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

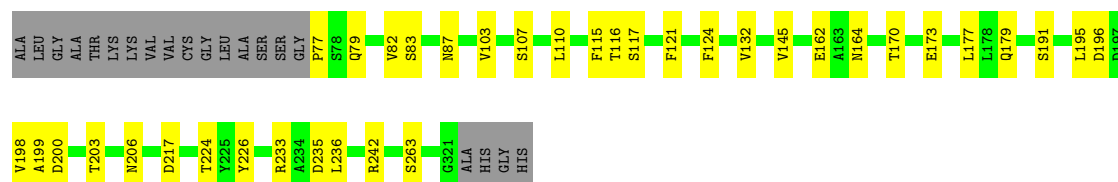
Chain 2:  87% 13%



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

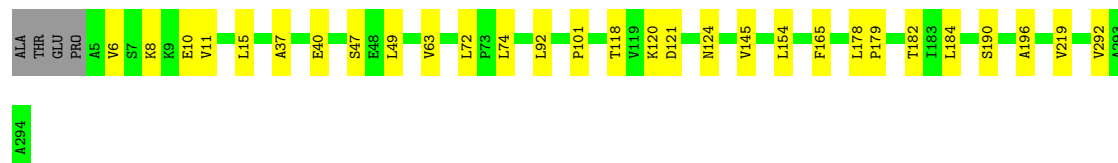
Chain 3:  64% 11% 25%





- Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4: 89% 10% .



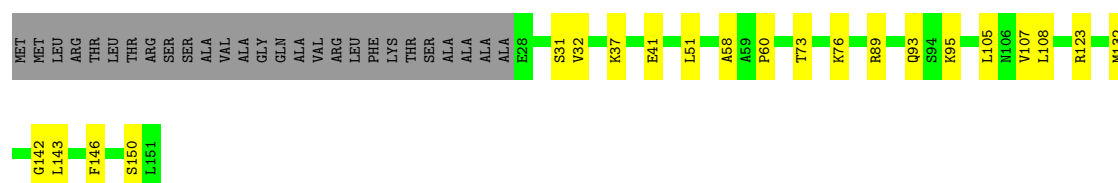
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5: 82% 17% .



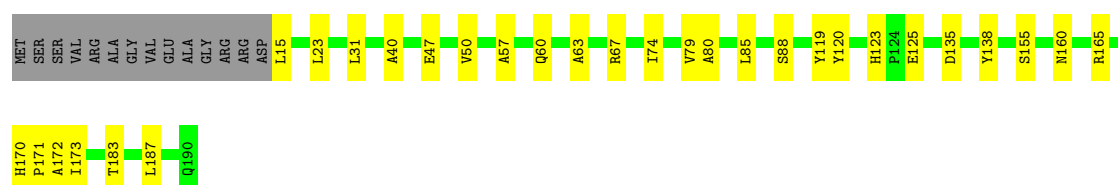
- Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6: 68% 14% 18%



- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7: 77% 16% 7%



- Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8: 82% 17% .

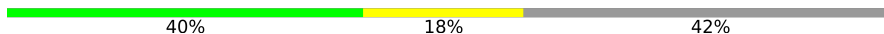


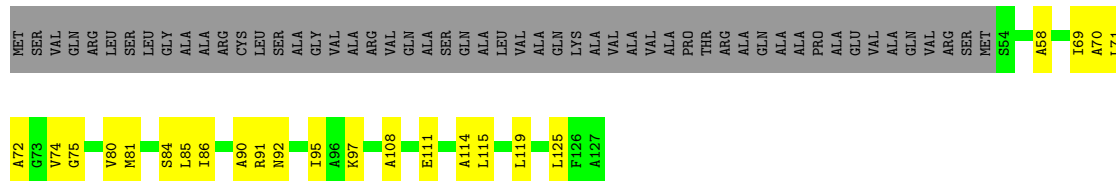
- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9:  93% 7%

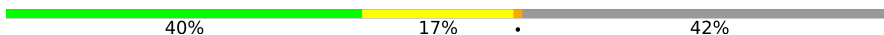


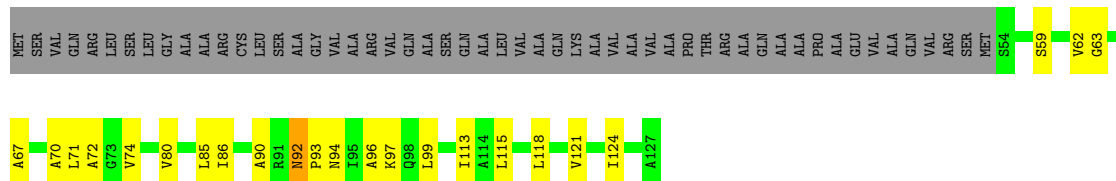
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain A:  40% 18% 42%

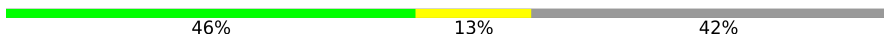


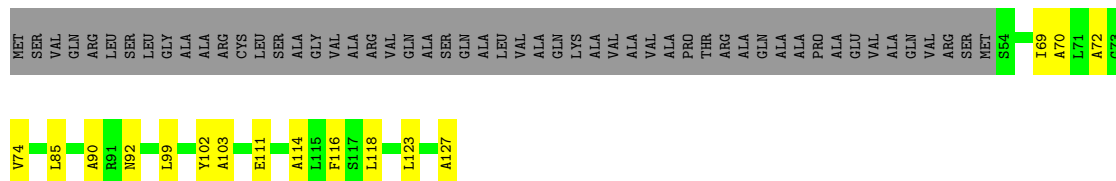
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain B:  40% 17% 42%



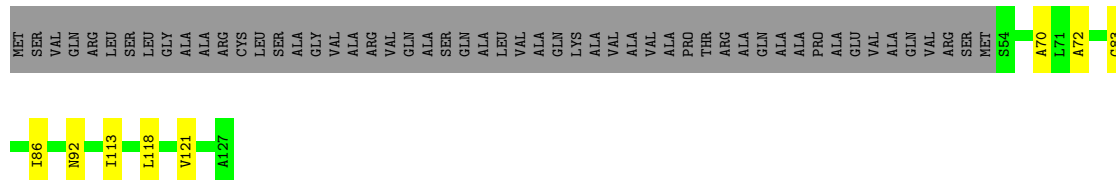
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain C:  46% 13% 42%



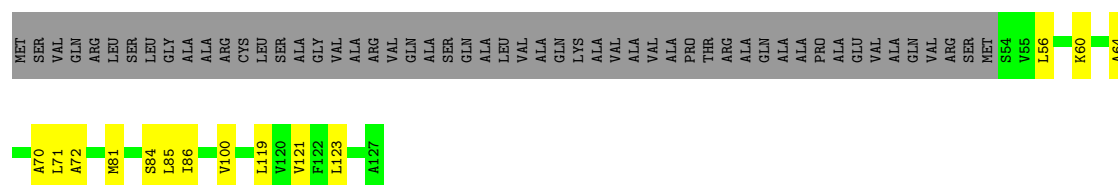
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain D:  52% 6% 42%

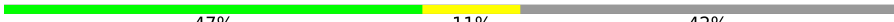


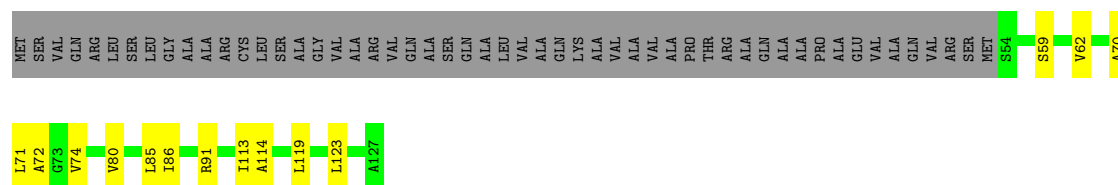
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain E:  47% 11% 42%

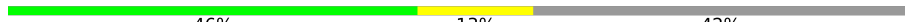


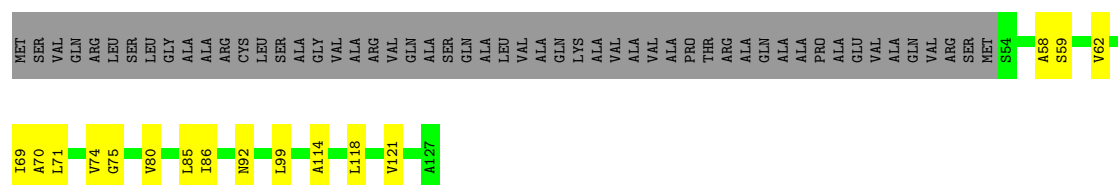
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain F:  47% 11% 42%

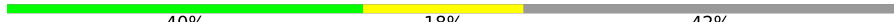


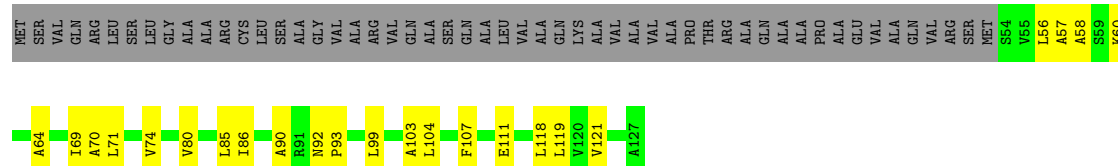
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain G:  46% 13% 42%

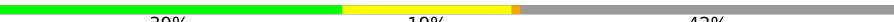


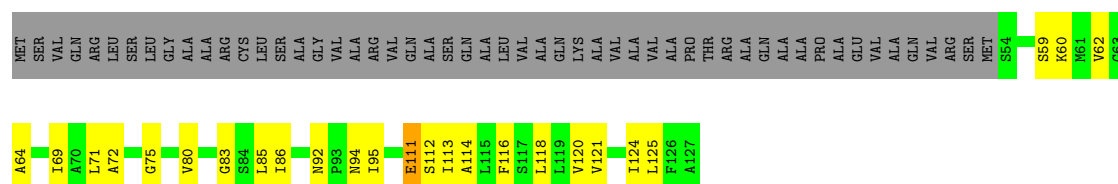
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain H:  40% 18% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

Chain I:  39% 19% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

W80	W83	W86	W89	W92	W93	W94	W95	W99	A103	A113	A114	A124	A127	A130	A133	A136	A139	A142	A145	A148	A151	A154	A157	A160	A163	A166	A169	A172	A175	A178	A181	A184	A187	A190	A193	A196	A199	A202	A205	A208	A211	A214	A217	A220	A223	A226	A229	A232	A235	A238	A241	A244	A247	A250	A253	A256	A259	A262	A265	A268	A271	A274	A277	A280	A283	A286	A289	A292	A295	A298	A301	A304	A307	A310	A313	A316	A319	A322	A325	A328	A331	A334	A337	A340	A343	A346	A349	A352	A355	A358	A361	A364	A367	A370	A373	A376	A379	A382	A385	A388	A391	A394	A397	A400	A403	A406	A409	A412	A415	A418	A421	A424	A427	A430	A433	A436	A439	A442	A445	A448	A451	A454	A457	A460	A463	A466	A469	A472	A475	A478	A481	A484	A487	A490	A493	A496	A499	A502	A505	A508	A511	A514	A517	A520	A523	A526	A529	A532	A535	A538	A541	A544	A547	A550	A553	A556	A559	A562	A565	A568	A571	A574	A577	A580	A583	A586	A589	A592	A595	A598	A601	A604	A607	A610	A613	A616	A619	A622	A625	A628	A631	A634	A637	A640	A643	A646	A649	A652	A655	A658	A661	A664	A667	A670	A673	A676	A679	A682	A685	A688	A691	A694	A697	A700	A703	A706	A709	A712	A715	A718	A721	A724	A727	A730	A733	A736	A739	A742	A745	A748	A751	A754	A757	A760	A763	A766	A769	A772	A775	A778	A781	A784	A787	A790	A793	A796	A799	A802	A805	A808	A811	A814	A817	A820	A823	A826	A829	A832	A835	A838	A841	A844	A847	A850	A853	A856	A859	A862	A865	A868	A871	A874	A877	A880	A883	A886	A889	A892	A895	A898	A901	A904	A907	A910	A913	A916	A919	A922	A925	A928	A931	A934	A937	A940	A943	A946	A949	A952	A955	A958	A961	A964	A967	A970	A973	A976	A979	A982	A985	A988	A991	A994	A997	A1000	A1003	A1006	A1009	A1012	A1015	A1018	A1021	A1024	A1027	A1030	A1033	A1036	A1039	A1042	A1045	A1048	A1051	A1054	A1057	A1060	A1063	A1066	A1069	A1072	A1075	A1078	A1081	A1084	A1087	A1090	A1093	A1096	A1099	A1102	A1105	A1108	A1111	A1114	A1117	A1120	A1123	A1126	A1129	A1132	A1135	A1138	A1141	A1144	A1147	A1150	A1153	A1156	A1159	A1162	A1165	A1168	A1171	A1174	A1177	A1180	A1183	A1186	A1189	A1192	A1195	A1198	A1201	A1204	A1207	A1210	A1213	A1216	A1219	A1222	A1225	A1228	A1231	A1234	A1237	A1240	A1243	A1246	A1249	A1252	A1255	A1258	A1261	A1264	A1267	A1270	A1273	A1276	A1279	A1282	A1285	A1288	A1291	A1294	A1297	A1300	A1303	A1306	A1309	A1312	A1315	A1318	A1321	A1324	A1327	A1330	A1333	A1336	A1339	A1342	A1345	A1348	A1351	A1354	A1357	A1360	A1363	A1366	A1369	A1372	A1375	A1378	A1381	A1384	A1387	A1390	A1393	A1396	A1399	A1402	A1405	A1408	A1411	A1414	A1417	A1420	A1423	A1426	A1429	A1432	A1435	A1438	A1441	A1444	A1447	A1450	A1453	A1456	A1459	A1462	A1465	A1468	A1471	A1474	A1477	A1480	A1483	A1486	A1489	A1492	A1495	A1498	A1501	A1504	A1507	A1510	A1513	A1516	A1519	A1522	A1525	A1528	A1531	A1534	A1537	A1540	A1543	A1546	A1549
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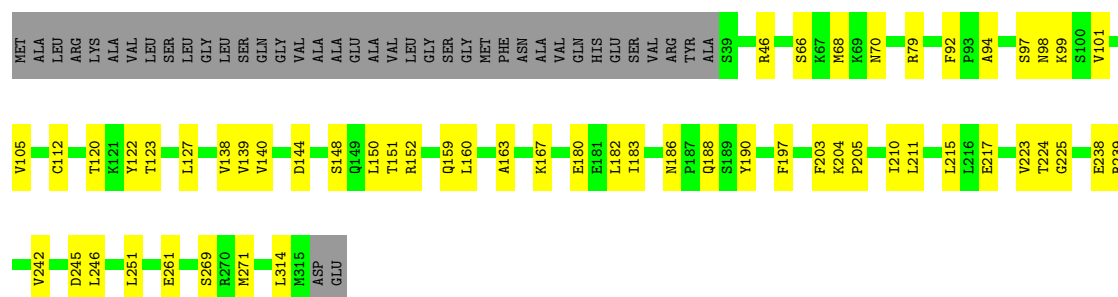
PRO	GLY	THR	TRP	PRO	MET	F219	V234	V238	V241	L250	L251	M257	P262	V271	F275	L281	L284	V285	I301	L302	T304	G308	N311	K324	LYS	ILE	HIS																			
SER	PRO	ASN	VAL	LEU	MET	SER	CYS	SER	ILE	LEU	PRO	THR	ARG	ILE	VAL	PHE	GLY	GLN	MET	ALA	MET	\$95	D99	T107	T111	G112	K125	P126	D132	T153	A181	T200	G201	P205	GLY	HIS	THR									
MET	SER	LEU	SER	VAL	LEU	GLY	ARG	SER	GLY	LEU	LEU	LYS	SER	ALA	VAL	PHE	GLY	GLN	THR	ARG	SER	ASN	LEU	ASN	GLY	SER	ILE	ASP	THR	SER	SER	VAL	PHE	GLN	ALA	LEU	SER	SER	ASP	ASN	GLU	ASN	LYS	PRO	ALA	ALA

[illegible]

MET
CYS
A3
P4
R10
L17
R18
K32
E33
P34
F35
K36
R48
Q49
Y52
K56
N74

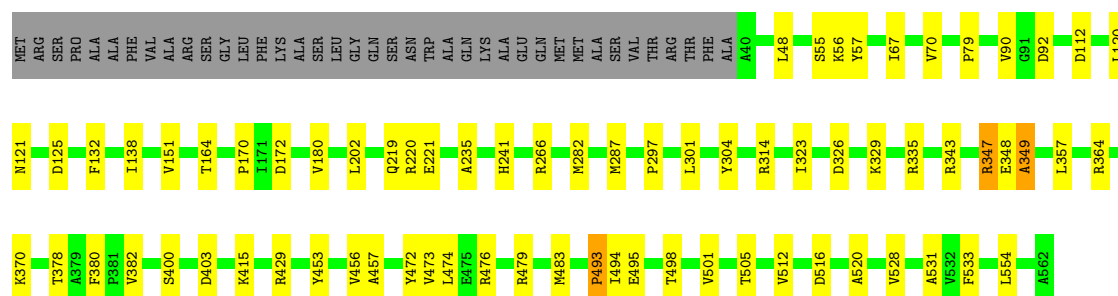
T142	T143	T144	T151	D152	D153	Q154	V155	E175	Q178	I185	S189	A190	L191	V195	K198	A199																														
Met	Phe	Gly	Leu	Lys	Arg	Ala	Val	Thr	Val	Gly	Arg	Arg	Phe	Ile	Ser	Thr	Ser	Ala	Ala	Arg	Met	E23	F33	W37	L45	T55	K58	P71	V72	N73	F74	Y75	T76	P77	H78	K86	V90	G99	V116	E117	L118	E125	V136	N139	G140	V141

Chain S:  70% 18% 13%



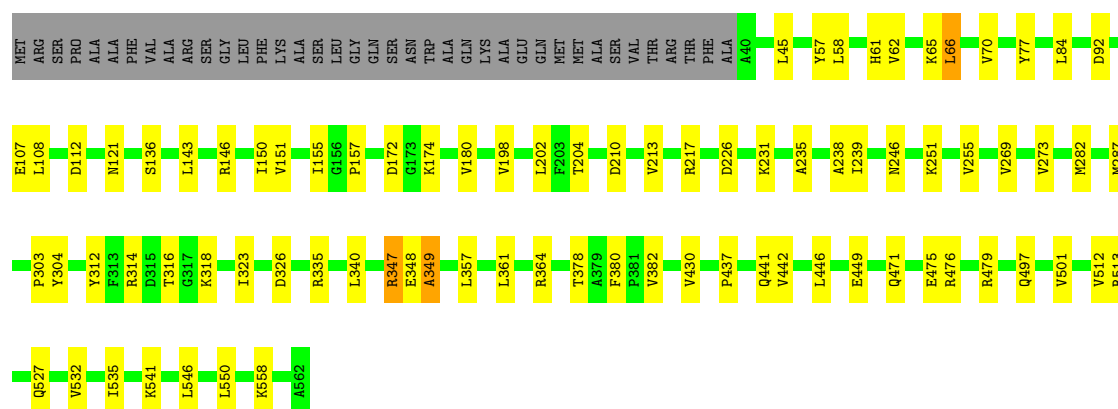
• Molecule 17: ATP synthase subunit alpha

Chain T:  80% 12% 7%



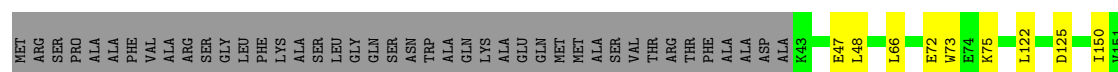
• Molecule 17: ATP synthase subunit alpha

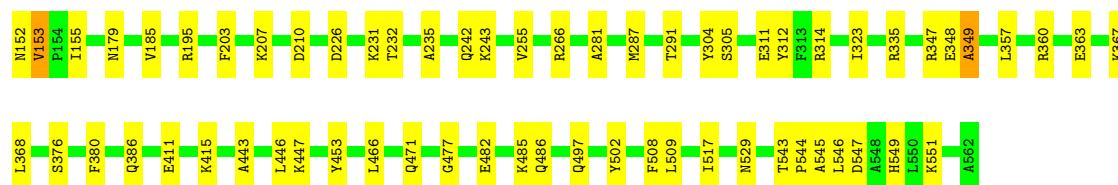
Chain U:  78% 14% 7%



• Molecule 17: ATP synthase subunit alpha

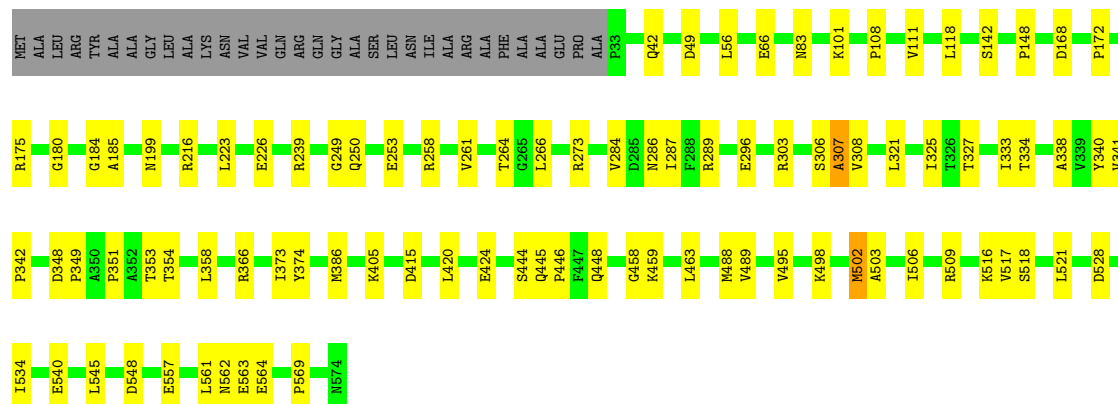
Chain V:  80% 12% 7%





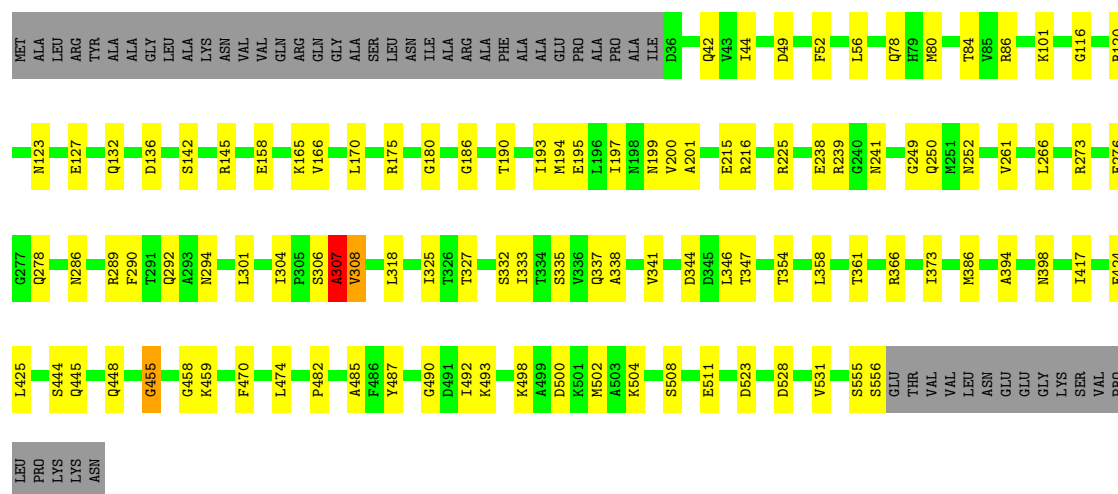
• Molecule 18: ATP synthase subunit beta

Chain X: 78% 16% 6%



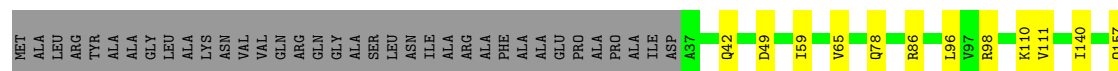
• Molecule 18: ATP synthase subunit beta

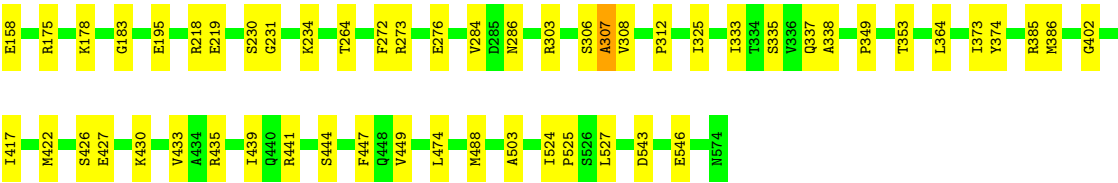
Chain Y: 72% 18% 9%



• Molecule 18: ATP synthase subunit beta

Chain Z: 82% 11% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112810	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	41.504	Depositor
Minimum map value	-23.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.038	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ADP, ATP, 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	0.38	0/628	0.43	0/856
2	1	0.43	0/4750	0.51	0/6434
3	2	0.31	0/3212	0.53	0/4371
4	3	0.36	0/1911	0.53	1/2601 (0.0%)
5	4	0.35	0/2216	0.51	0/3000
6	5	0.54	0/1011	0.61	0/1376
7	6	0.47	0/946	0.58	0/1287
8	7	0.44	0/1374	0.52	0/1865
9	8	0.46	0/715	0.58	0/974
10	9	0.29	0/802	0.54	0/1084
11	A	0.35	0/520	0.56	0/704
11	B	0.33	0/520	0.59	0/704
11	C	0.30	0/519	0.59	0/701
11	D	0.26	0/520	0.59	0/704
11	E	0.25	0/520	0.62	0/704
11	F	0.30	0/520	0.56	0/704
11	G	0.31	0/520	0.56	0/704
11	H	0.32	0/520	0.71	1/704 (0.1%)
11	I	0.30	0/520	0.64	1/704 (0.1%)
11	J	0.29	0/520	0.53	0/704
12	M	0.48	0/1683	0.61	0/2295
13	P	0.40	0/1553	0.65	2/2093 (0.1%)
14	Q	0.28	0/574	0.56	0/774
15	R	0.31	0/1336	0.53	0/1827
16	S	0.39	0/2153	0.60	0/2901
17	T	0.53	0/4048	0.63	2/5481 (0.0%)
17	U	0.54	0/4049	0.64	4/5481 (0.1%)
17	V	0.48	0/4031	0.58	2/5456 (0.0%)
18	X	0.52	0/4176	0.61	0/5659
18	Y	0.44	0/4015	0.60	0/5440
18	Z	0.48	0/4147	0.57	0/5619
All	All	0.44	0/54529	0.58	13/73911 (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
5	4	0	1
6	5	0	1
17	T	0	1
17	U	0	1
17	V	0	2
18	X	0	1
18	Y	0	4
18	Z	0	2
All	All	0	13

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	I	111	GLU	N-CA-C	-7.13	103.55	111.82
11	H	111	GLU	N-CA-C	-6.88	104.70	113.23
17	U	347	ARG	CA-C-N	6.75	134.43	121.54
17	U	347	ARG	C-N-CA	6.75	134.43	121.54
4	3	77	PRO	N-CA-CB	6.70	110.36	103.00
17	T	347	ARG	CA-C-N	6.26	133.50	121.54
17	T	347	ARG	C-N-CA	6.26	133.50	121.54
17	V	347	ARG	CA-C-N	6.13	133.25	121.54
17	V	347	ARG	C-N-CA	6.13	133.25	121.54
13	P	48	GLY	CA-C-N	5.61	132.26	121.54
13	P	48	GLY	C-N-CA	5.61	132.26	121.54
17	U	66	LEU	CA-C-N	5.19	123.51	120.24
17	U	66	LEU	C-N-CA	5.19	123.51	120.24

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4	47	SER	Peptide
6	5	119	LYS	Peptide
17	T	348	GLU	Peptide
17	U	348	GLU	Peptide
17	V	348	GLU	Peptide

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Mol	Chain	Res	Type	Group
17	V	75	LYS	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	424	GLU	Peptide
18	Y	425	LEU	Peptide
18	Y	455	GLY	Peptide
18	Z	307	ALA	Peptide
18	Z	503	ALA	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	2	0
2	1	4661	0	4695	49	0
3	2	3163	0	3262	33	0
4	3	1874	0	1826	21	0
5	4	2177	0	2169	19	0
6	5	986	0	1021	19	0
7	6	926	0	941	18	0
8	7	1347	0	1345	26	0
9	8	692	0	694	11	0
10	9	776	0	757	6	0
11	A	514	0	554	24	0
11	B	514	0	554	22	0
11	C	514	0	553	17	0
11	D	514	0	554	12	0
11	E	514	0	554	11	0
11	F	514	0	554	12	0
11	G	514	0	554	15	0
11	H	514	0	554	20	0
11	I	514	0	554	25	0
11	J	514	0	554	19	0
12	M	1640	0	1665	21	0
13	P	1532	0	1603	40	0
14	Q	561	0	565	13	0
15	R	1303	0	1266	21	0
16	S	2130	0	2180	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	T	3979	0	4119	56	0
17	U	3980	0	4119	55	0
17	V	3962	0	4105	44	0
18	X	4115	0	4137	56	0
18	Y	3957	0	3966	66	0
18	Z	4087	0	4110	39	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	1	0
20	V	31	0	12	1	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Y	1	0	0	0	0
22	X	27	0	12	0	0
22	Y	27	0	12	2	0
All	All	53748	0	54728	676	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 (676) 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)
13:P:180:ALA:HB3	13:P:182:PHE:CD2	1.59	1.35
17:T:453:TYR:CE1	17:T:474:LEU:HD12	1.63	1.32
13:P:180:ALA:CB	13:P:182:PHE:CE2	2.35	1.10
18:X:498:LYS:O	18:X:502:MET:HG3	1.52	1.09
13:P:180:ALA:HB3	13:P:182:PHE:CE2	1.88	1.09
13:P:154:CYS:HB2	13:P:184:LEU:HD11	1.35	1.05
13:P:171:THR:CA	13:P:186:MET:HE1	1.89	1.03
13:P:171:THR:HA	13:P:186:MET:CE	1.89	1.02
13:P:180:ALA:CB	13:P:182:PHE:CD2	2.44	0.99
17:T:453:TYR:CE1	17:T:474:LEU:CD1	2.50	0.93
13:P:180:ALA:HB2	13:P:182:PHE:CE2	2.03	0.90
7:6:89:ARG:O	7:6:93:GLN:HB2	1.71	0.90
13:P:154:CYS:HB2	13:P:184:LEU:CD1	2.02	0.89
17:T:453:TYR:HE1	17:T:474:LEU:HD12	1.29	0.88
13:P:154:CYS:CB	13:P:184:LEU:HD11	2.04	0.86
13:P:171:THR:HA	13:P:186:MET:HE1	0.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:180:ALA:HB2	13:P:182:PHE:HE2	1.44	0.80
18:X:498:LYS:O	18:X:502:MET:CG	2.29	0.80
11:C:111:GLU:OE1	11:D:113:ILE:HD11	1.87	0.75
18:X:327:THR:HG22	18:X:333:ILE:H	1.51	0.74
18:X:503:ALA:O	18:X:506:ILE:HG22	1.87	0.74
13:P:154:CYS:HB3	13:P:186:MET:HA	1.70	0.71
11:J:85:LEU:CD1	11:J:99:LEU:HB3	2.19	0.71
18:Y:498:LYS:O	18:Y:502:MET:HG3	1.89	0.71
17:V:335:ARG:HD2	17:V:349:ALA:HB3	1.74	0.70
2:1:316:ASN:HD21	2:1:331:ALA:H	1.36	0.70
17:T:400:SER:HB3	18:Y:289:ARG:HH22	1.57	0.68
11:G:86:ILE:HG21	11:H:85:LEU:HA	1.76	0.68
11:I:75:GLY:HA3	11:J:74:VAL:HG12	1.76	0.68
13:P:154:CYS:SG	13:P:184:LEU:HD11	2.34	0.67
17:U:335:ARG:HD2	17:U:349:ALA:HB3	1.78	0.66
11:F:86:ILE:HG21	11:G:85:LEU:HA	1.78	0.66
13:P:209:MET:HE2	17:T:79:PRO:HD2	1.78	0.65
18:Y:142:SER:O	18:Y:145:ARG:NH2	2.28	0.65
2:1:180:PRO:HG2	2:1:183:LYS:HB3	1.78	0.65
11:A:95:ILE:HD13	11:J:93:PRO:HG3	1.78	0.65
17:T:335:ARG:HD2	17:T:349:ALA:HB3	1.78	0.64
18:X:266:LEU:HD21	18:X:325:ILE:HG12	1.79	0.64
18:Y:197:ILE:O	18:Y:201:ALA:HB3	1.97	0.64
11:J:74:VAL:HG21	11:J:114:ALA:HB2	1.78	0.64
18:X:118:LEU:O	18:X:239:ARG:NH2	2.31	0.64
8:7:123:HIS:HD2	8:7:125:GLU:H	1.46	0.64
2:1:404:LYS:HZ1	6:5:78:GLU:HB3	1.62	0.63
17:U:479:ARG:NH2	17:U:512:VAL:O	2.31	0.63
17:U:479:ARG:NH2	17:U:513:ARG:O	2.32	0.62
11:C:111:GLU:CD	11:D:113:ILE:HD11	2.23	0.62
18:Y:80:MET:HE2	18:Y:86:ARG:HH11	1.64	0.62
17:T:202:LEU:HD22	17:T:378:THR:HG21	1.81	0.61
14:Q:32:LYS:HE3	15:R:154:GLN:HA	1.83	0.61
17:U:347:ARG:NH2	18:X:348:ASP:OD2	2.31	0.61
18:Z:417:ILE:HG23	18:Z:422:MET:HA	1.82	0.61
18:Y:238:GLU:OE1	18:Y:241:ASN:ND2	2.33	0.61
16:S:123:THR:O	16:S:127:LEU:HB2	2.01	0.61
18:Y:80:MET:HB2	18:Y:84:THR:HG23	1.83	0.61
17:V:153:VAL:HG21	17:V:305:SER:HB2	1.82	0.61
18:X:42:GLN:HG2	18:X:49:ASP:HB2	1.82	0.61
16:S:66:SER:O	16:S:70:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:323:ILE:HG12	17:T:380:PHE:HB2	1.83	0.60
18:Y:158:GLU:HG3	18:Y:175:ARG:HB3	1.83	0.60
17:U:155:ILE:HD12	17:U:312:TYR:HB2	1.84	0.60
17:T:479:ARG:NH1	17:T:512:VAL:O	2.35	0.59
17:V:207:LYS:HG3	17:V:486:GLN:HE21	1.67	0.59
17:U:449:GLU:OE1	17:U:476:ARG:NH1	2.35	0.59
2:1:267:ARG:NH1	2:1:519:GLU:OE1	2.35	0.59
11:A:70:ALA:HA	11:J:72:ALA:HB2	1.85	0.59
13:P:180:ALA:HB3	13:P:182:PHE:HD2	1.52	0.59
17:V:266:ARG:HG2	17:V:291:THR:HG21	1.84	0.59
17:U:246:ASN:HD21	17:U:255:VAL:H	1.51	0.59
17:V:155:ILE:HD12	17:V:312:TYR:HB2	1.85	0.59
18:X:373:ILE:HG23	18:X:444:SER:HB3	1.85	0.59
5:4:190:SER:HB3	5:4:196:ALA:HB2	1.85	0.59
11:G:59:SER:HA	11:G:62:VAL:HG12	1.84	0.59
11:I:71:LEU:HD11	11:I:118:LEU:HD21	1.84	0.59
10:9:64:PRO:HG2	12:M:257:MET:HE1	1.84	0.58
16:S:148:SER:O	16:S:152:ARG:NH2	2.36	0.58
11:I:111:GLU:O	11:I:114:ALA:N	2.36	0.58
13:P:185:VAL:HG12	13:P:185:VAL:O	2.02	0.58
17:U:226:ASP:O	17:U:231:LYS:NZ	2.33	0.58
17:T:326:ASP:H	17:T:382:VAL:HB	1.69	0.58
16:S:120:THR:HG23	16:S:150:LEU:HD23	1.85	0.58
17:V:210:ASP:HB2	17:V:497:GLN:HE22	1.68	0.58
11:F:72:ALA:HB2	11:G:70:ALA:HA	1.86	0.58
11:J:85:LEU:HD22	11:J:103:ALA:HB2	1.86	0.58
12:M:200:THR:OG1	12:M:201:GLY:N	2.36	0.58
2:1:450:ASN:OD1	2:1:453:ARG:NH2	2.37	0.57
18:Z:231:GLY:O	18:Z:234:LYS:NZ	2.36	0.57
11:A:80:VAL:HG21	11:J:80:VAL:HG12	1.85	0.57
13:P:174:ALA:HB3	13:P:186:MET:HE2	1.85	0.57
18:Y:266:LEU:HD21	18:Y:325:ILE:HG12	1.87	0.57
18:Z:218:ARG:NH2	18:Z:219:GLU:OE2	2.37	0.57
17:V:529:ASN:HD21	18:Z:527:LEU:HD23	1.68	0.57
3:2:128:VAL:HG21	3:2:143:VAL:HG11	1.86	0.57
13:P:157:ILE:HG23	13:P:199:VAL:HG13	1.85	0.57
17:T:235:ALA:HB1	17:T:323:ILE:HD13	1.86	0.57
11:A:71:LEU:HD12	11:B:113:ILE:HG23	1.87	0.57
11:G:74:VAL:HG11	11:G:114:ALA:HB2	1.86	0.57
18:Y:165:LYS:HE2	18:Y:445:GLN:HB2	1.86	0.57
11:A:75:GLY:HA3	11:B:74:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:314:ARG:NH1	17:T:364:ARG:O	2.38	0.57
11:I:72:ALA:HB2	11:J:70:ALA:HA	1.87	0.56
17:U:210:ASP:HB2	17:U:497:GLN:HE22	1.69	0.56
3:2:197:LEU:O	3:2:201:LYS:NZ	2.38	0.56
11:G:75:GLY:HA3	11:H:74:VAL:HG22	1.87	0.56
17:V:179:ASN:ND2	18:Z:546:GLU:OE2	2.38	0.56
2:1:368:ALA:O	2:1:379:GLN:NE2	2.36	0.56
5:4:118:THR:HG23	5:4:121:ASP:H	1.69	0.56
7:6:60:PRO:HB3	9:8:15:PRO:HB2	1.87	0.56
9:8:36:ALA:HA	9:8:40:LEU:HB3	1.88	0.56
11:A:80:VAL:HG12	11:B:80:VAL:HG21	1.87	0.56
15:R:151:THR:HG22	15:R:153:ASP:H	1.70	0.56
18:X:446:PRO:HB2	18:X:458:GLY:HA2	1.87	0.56
18:Y:306:SER:OG	18:Y:307:ALA:N	2.39	0.56
3:2:382:VAL:HG13	3:2:386:LEU:HB2	1.88	0.56
11:E:72:ALA:HB2	11:F:70:ALA:HA	1.88	0.56
16:S:46:ARG:NH1	18:X:415:ASP:OD1	2.39	0.56
18:X:216:ARG:O	18:X:250:GLN:NE2	2.39	0.56
14:Q:32:LYS:O	14:Q:36:LYS:N	2.39	0.56
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.87	0.56
8:7:165:ARG:NH2	8:7:171:PRO:O	2.38	0.56
17:U:269:VAL:HG13	17:U:287:MET:HE2	1.87	0.56
17:T:266:ARG:NH1	18:X:148:PRO:O	2.38	0.56
17:V:311:GLU:OE2	17:V:314:ARG:NH1	2.39	0.56
16:S:188:GLN:HG3	16:S:215:LEU:HB3	1.87	0.55
11:G:80:VAL:HG12	11:H:80:VAL:HG11	1.87	0.55
18:X:253:GLU:O	18:X:258:ARG:NH1	2.39	0.55
18:X:374:TYR:HB2	18:X:488:MET:HE1	1.88	0.55
2:1:76:GLU:OE2	2:1:133:ARG:NH2	2.39	0.55
4:3:83:SER:O	4:3:87:ASN:ND2	2.39	0.55
17:U:235:ALA:HB1	17:U:323:ILE:HG12	1.88	0.55
18:X:287:ILE:HD11	18:X:321:LEU:HD21	1.89	0.55
11:E:71:LEU:HD12	11:F:113:ILE:HG23	1.87	0.55
17:T:121:ASN:HB3	17:T:343:ARG:HH21	1.71	0.55
18:Y:216:ARG:O	18:Y:250:GLN:NE2	2.40	0.55
2:1:539:ASP:N	2:1:539:ASP:OD1	2.39	0.55
11:I:59:SER:HA	11:I:62:VAL:HG12	1.89	0.55
18:Z:157:GLN:HG2	18:Z:386:MET:HE1	1.88	0.55
11:B:90:ALA:O	11:C:92:ASN:ND2	2.39	0.54
5:4:8:LYS:HD2	5:4:40:GLU:HG2	1.88	0.54
12:M:308:GLY:HA2	12:M:311:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:371:THR:HG22	3:2:376:LYS:HG2	1.90	0.54
17:V:549:HIS:HE1	18:Z:524:ILE:HB	1.73	0.54
18:Y:485:ALA:HA	18:Y:498:LYS:HD3	1.90	0.54
18:Z:325:ILE:HG21	18:Z:335:SER:HB2	1.89	0.54
13:P:87:LEU:HB2	17:U:66:LEU:HD21	1.89	0.54
18:X:185:ALA:O	18:X:366:ARG:NH2	2.41	0.54
3:2:364:SER:OG	3:2:365:VAL:N	2.41	0.54
16:S:79:ARG:NH2	16:S:197:PHE:O	2.40	0.54
8:7:40:ALA:HB3	8:7:47:GLU:HB2	1.89	0.53
17:U:84:LEU:HD13	18:X:563:GLU:HG2	1.90	0.53
17:V:235:ALA:HB1	17:V:323:ILE:HD13	1.90	0.53
17:V:544:PRO:HA	17:V:547:ASP:HB3	1.89	0.53
4:3:242:ARG:NH2	12:M:132:ASP:OD2	2.41	0.53
7:6:132:MET:HE2	12:M:112:GLY:HA3	1.90	0.53
18:Y:52:PHE:HB2	18:Y:56:LEU:HD23	1.90	0.53
11:I:94:ASN:ND2	16:S:224:THR:O	2.41	0.53
18:Z:65:VAL:HG11	18:Z:96:LEU:HD11	1.89	0.53
11:H:57:ALA:HA	11:H:60:LYS:HG2	1.91	0.53
18:X:249:GLY:HA3	18:X:261:VAL:HG11	1.90	0.53
11:C:123:LEU:O	11:C:127:ALA:N	2.42	0.53
17:V:72:GLU:OE1	17:V:73:TRP:NE1	2.41	0.53
4:3:203:THR:HG21	4:3:235:ASP:HB2	1.90	0.53
11:E:56:LEU:O	11:E:60:LYS:NZ	2.42	0.53
18:Z:111:VAL:HG11	18:Z:264:THR:HG23	1.89	0.53
2:1:420:TYR:HB2	2:1:424:VAL:HG23	1.91	0.53
17:U:475:GLU:HB3	17:U:479:ARG:HH11	1.74	0.53
11:B:94:ASN:ND2	14:Q:4:PRO:O	2.42	0.53
15:R:33:PHE:O	15:R:37:TRP:HB2	2.09	0.53
18:Y:136:ASP:OD2	18:Y:239:ARG:NH2	2.42	0.53
4:3:79:GLN:HA	4:3:82:VAL:HB	1.90	0.52
5:4:178:LEU:HD11	8:7:183:THR:HG21	1.91	0.52
16:S:79:ARG:NE	16:S:261:GLU:OE2	2.41	0.52
2:1:245:ALA:HB1	2:1:498:LEU:HD13	1.92	0.52
2:1:329:GLU:HG3	7:6:123:ARG:HB2	1.90	0.52
4:3:116:THR:OG1	4:3:117:SER:N	2.43	0.52
11:E:85:LEU:HD11	11:E:100:VAL:HG22	1.90	0.52
17:T:531:ALA:HB1	18:Y:531:VAL:HG11	1.91	0.52
4:3:145:VAL:HG11	4:3:179:GLN:HE21	1.73	0.52
17:U:314:ARG:NH2	17:U:364:ARG:O	2.42	0.52
17:V:150:ILE:O	17:V:152:ASN:ND2	2.42	0.52
11:E:119:LEU:O	11:E:123:LEU:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:516:ASP:O	17:T:520:ALA:N	2.43	0.52
17:V:125:ASP:OD1	17:V:125:ASP:N	2.43	0.52
3:2:36:LEU:HD22	3:2:41:VAL:HG21	1.90	0.52
3:2:355:SER:O	3:2:358:LYS:NZ	2.42	0.52
4:3:235:ASP:OD1	4:3:235:ASP:N	2.41	0.52
11:C:111:GLU:OE2	11:D:113:ILE:HD11	2.08	0.52
17:U:303:PRO:HB2	17:U:361:LEU:HD11	1.90	0.52
11:H:86:ILE:HG21	11:I:85:LEU:HA	1.91	0.52
18:Y:123:ASN:HD22	18:Y:127:GLU:HB2	1.75	0.52
13:P:194:LEU:HD21	13:P:199:VAL:HG12	1.91	0.52
17:U:136:SER:HA	18:Z:59:ILE:HB	1.91	0.52
18:X:172:PRO:HG2	18:X:386:MET:HB2	1.92	0.52
11:I:86:ILE:HG21	11:J:85:LEU:HD13	1.91	0.52
17:T:304:TYR:OH	17:T:357:LEU:O	2.28	0.52
6:5:27:ASP:OD2	9:8:44:HIS:NE2	2.43	0.52
11:A:85:LEU:HA	11:J:86:ILE:HG21	1.93	0.52
11:A:69:ILE:HA	11:B:70:ALA:HB2	1.92	0.51
18:X:506:ILE:O	18:X:509:ARG:NH2	2.42	0.51
17:T:472:TYR:OH	17:T:476:ARG:NH1	2.44	0.51
11:C:69:ILE:HA	11:D:70:ALA:HB2	1.91	0.51
17:U:92:ASP:HB3	17:U:340:LEU:HD13	1.91	0.51
2:1:84:PRO:HG2	6:5:71:VAL:HG11	1.92	0.51
11:A:72:ALA:HB2	11:B:70:ALA:HA	1.91	0.51
13:P:155:THR:HA	13:P:187:GLN:HB3	1.92	0.51
17:T:121:ASN:HB2	18:Y:44:ILE:HG12	1.92	0.51
18:Y:78:GLN:NE2	18:Y:301:LEU:O	2.40	0.51
18:Y:286:ASN:H	18:Y:338:ALA:HB3	1.75	0.51
18:Y:394:ALA:O	18:Y:398:ASN:ND2	2.44	0.51
11:H:90:ALA:HA	11:I:95:ILE:HD11	1.91	0.51
11:I:86:ILE:HG21	11:J:85:LEU:CD1	2.40	0.51
15:R:55:THR:O	15:R:58:LYS:NZ	2.43	0.51
11:B:115:LEU:HD22	12:M:250:LEU:HD22	1.93	0.51
17:U:437:PRO:HB2	17:U:541:LYS:HB3	1.93	0.51
4:3:195:LEU:O	4:3:226:TYR:OH	2.26	0.51
15:R:86:LYS:HG3	15:R:118:LEU:HD12	1.91	0.51
18:Y:448:GLN:HG2	18:Y:458:GLY:HA3	1.93	0.51
2:1:28:ARG:NH2	8:7:160:ASN:OD1	2.43	0.51
11:E:86:ILE:HG21	11:F:85:LEU:HA	1.93	0.51
11:H:64:ALA:HB1	11:H:121:VAL:HG13	1.93	0.51
17:U:107:GLU:HA	17:U:150:ILE:HA	1.93	0.51
6:5:86:LYS:NZ	8:7:135:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:170:HIS:CD2	8:7:172:ALA:H	2.28	0.50
11:I:60:LYS:NZ	11:I:125:LEU:O	2.42	0.50
6:5:5:PRO:O	9:8:65:ARG:NH1	2.43	0.50
17:V:508:PHE:HZ	17:V:551:LYS:HG3	1.75	0.50
18:X:175:ARG:O	18:X:334:THR:OG1	2.23	0.50
3:2:266:PHE:HA	3:2:269:VAL:HG22	1.93	0.50
9:8:26:HIS:HD2	9:8:28:PHE:H	1.59	0.50
18:X:111:VAL:HG11	18:X:264:THR:HG23	1.94	0.50
18:X:557:GLU:HG2	18:X:569:PRO:HB3	1.94	0.50
18:X:284:VAL:HG11	18:X:287:ILE:HD13	1.94	0.50
17:V:243:LYS:HG3	17:V:281:ALA:HA	1.93	0.50
18:X:286:ASN:HB3	18:X:289:ARG:HG2	1.93	0.50
17:T:347:ARG:HD2	18:Y:308:VAL:HG12	1.93	0.50
18:Y:555:SER:OG	18:Y:556:SER:N	2.45	0.50
17:T:90:VAL:HG21	17:T:138:ILE:HB	1.93	0.49
18:Z:230:SER:HB3	18:Z:449:VAL:HB	1.93	0.49
3:2:377:VAL:HG11	3:2:438:ILE:HG23	1.94	0.49
11:C:111:GLU:OE1	11:D:113:ILE:CD1	2.60	0.49
5:4:63:VAL:HA	5:4:92:LEU:HD11	1.93	0.49
16:S:92:PHE:HB2	16:S:211:LEU:HD11	1.93	0.49
16:S:97:SER:OG	16:S:99:LYS:O	2.29	0.49
16:S:190:TYR:HB2	16:S:210:ILE:HB	1.94	0.49
17:T:151:VAL:HG11	17:T:301:LEU:HD21	1.94	0.49
5:4:6:VAL:HB	5:4:10:GLU:HB3	1.93	0.49
18:X:184:GLY:O	18:X:366:ARG:NH2	2.45	0.49
4:3:173:GLU:HA	4:3:206:ASN:HD21	1.77	0.49
13:P:69:LYS:NZ	17:U:57:TYR:OH	2.45	0.49
17:T:403:ASP:O	17:T:429:ARG:NH2	2.36	0.49
18:X:286:ASN:H	18:X:338:ALA:HB3	1.77	0.49
18:Z:426:SER:OG	18:Z:427:GLU:N	2.44	0.49
3:2:299:LEU:HD13	3:2:303:VAL:HG12	1.94	0.49
6:5:83:THR:O	8:7:119:TYR:OH	2.29	0.49
17:V:226:ASP:O	17:V:231:LYS:NZ	2.44	0.49
18:Z:195:GLU:HG3	18:Z:447:PHE:CG	2.48	0.49
17:V:47:GLU:HG2	17:V:48:LEU:HG	1.94	0.49
18:Y:42:GLN:HB3	18:Y:49:ASP:HB2	1.95	0.49
3:2:64:ALA:HB3	8:7:31:LEU:HD21	1.95	0.49
3:2:209:ASP:OD1	8:7:67:ARG:NH2	2.43	0.49
10:9:53:LEU:HD12	12:M:262:PRO:HB2	1.95	0.49
17:U:471:GLN:HE21	17:U:475:GLU:HG2	1.77	0.49
18:Y:318:LEU:HD21	18:Y:354:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:108:LEU:HD11	12:M:281:LEU:HD13	1.95	0.49
11:F:86:ILE:HG23	11:G:99:LEU:HD22	1.94	0.49
13:P:136:GLU:HG2	17:U:45:LEU:HD21	1.95	0.49
14:Q:48:ARG:HE	16:S:163:ALA:HB3	1.78	0.49
18:X:420:LEU:HD13	18:X:424:GLU:HG2	1.94	0.49
11:A:119:LEU:HD21	12:M:234:VAL:HG11	1.94	0.48
18:X:168:ASP:HB3	18:X:463:LEU:HD13	1.95	0.48
18:Z:178:LYS:HG3	18:Z:335:SER:HB3	1.95	0.48
18:Z:183:GLY:HA2	18:Z:364:LEU:HB2	1.95	0.48
18:Z:284:VAL:HB	18:Z:337:GLN:HG2	1.94	0.48
5:4:74:LEU:HD23	5:4:219:VAL:HG13	1.94	0.48
11:C:90:ALA:O	11:D:92:ASN:ND2	2.46	0.48
13:P:195:LEU:O	13:P:211:THR:OG1	2.31	0.48
17:T:241:HIS:CE1	17:T:493:PRO:HA	2.49	0.48
17:T:457:ALA:HB2	17:T:474:LEU:HD13	1.95	0.48
17:U:535:ILE:HD13	18:X:534:ILE:HD11	1.95	0.48
17:V:203:PHE:O	17:V:242:GLN:NE2	2.35	0.48
3:2:240:ALA:H	3:2:243:GLN:HE21	1.61	0.48
9:8:9:LYS:NZ	9:8:10:ASP:OD2	2.44	0.48
11:A:115:LEU:HD22	12:M:238:VAL:HG12	1.95	0.48
18:X:185:ALA:HB2	18:X:340:TYR:HE1	1.77	0.48
18:X:349:PRO:O	18:X:353:THR:OG1	2.27	0.48
11:G:86:ILE:HG23	11:H:99:LEU:HG	1.95	0.48
15:R:195:VAL:HA	15:R:198:LYS:HZ3	1.79	0.48
17:U:316:THR:OG1	17:U:318:LYS:NZ	2.45	0.48
17:V:314:ARG:HH21	17:V:368:LEU:HD21	1.78	0.48
18:Y:335:SER:OG	18:Y:337:GLN:NE2	2.45	0.48
2:1:253:ARG:HD3	2:1:369:LEU:HB3	1.95	0.48
2:1:365:GLN:HG2	2:1:383:ILE:HD12	1.95	0.48
3:2:282:VAL:HG21	5:4:15:LEU:HD22	1.95	0.48
4:3:199:ALA:HA	4:3:236:LEU:HD13	1.95	0.48
11:A:111:GLU:HG3	11:B:113:ILE:HD11	1.95	0.48
16:S:140:VAL:HG22	16:S:160:LEU:HB3	1.96	0.48
17:U:475:GLU:OE1	17:U:479:ARG:NH1	2.46	0.48
10:9:3:VAL:HG23	10:9:4:THR:HG23	1.95	0.48
11:C:74:VAL:HG21	11:C:114:ALA:HB2	1.96	0.48
11:I:92:ASN:OD1	11:I:92:ASN:N	2.46	0.48
17:U:204:THR:HG23	17:U:238:ALA:HB2	1.95	0.48
18:X:180:GLY:HA3	18:X:358:LEU:HD13	1.96	0.48
2:1:285:GLN:NE2	2:1:294:SER:OG	2.47	0.48
6:5:26:LEU:HD21	12:M:153:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:90:VAL:HB	15:R:117:GLU:HB2	1.96	0.48
18:X:258:ARG:NH2	18:X:296:GLU:OE1	2.47	0.48
18:Z:373:ILE:HG23	18:Z:444:SER:HB3	1.96	0.48
3:2:439:LYS:HD3	3:2:443:PRO:HA	1.94	0.48
6:5:91:HIS:ND1	8:7:138:TYR:OH	2.33	0.48
12:M:271:VAL:O	12:M:275:PHE:HB2	2.13	0.48
3:2:67:THR:HG22	3:2:106:VAL:HG23	1.96	0.48
4:3:200:ASP:OD1	4:3:233:ARG:NH1	2.42	0.48
13:P:201:GLU:OE2	13:P:206:ARG:NE	2.42	0.48
17:T:55:SER:O	17:T:57:TYR:N	2.45	0.48
9:8:26:HIS:CD2	9:8:28:PHE:H	2.32	0.47
11:F:91:ARG:O	15:R:99:GLY:N	2.46	0.47
16:S:211:LEU:HB2	16:S:217:GLU:HB2	1.95	0.47
17:V:367:LYS:HD2	17:V:376:SER:HB3	1.95	0.47
17:V:466:LEU:HG	17:V:471:GLN:HG3	1.96	0.47
17:V:509:LEU:HD23	17:V:517:ILE:HG23	1.95	0.47
18:Y:327:THR:HA	18:Y:332:SER:HA	1.95	0.47
11:H:93:PRO:HG3	11:I:95:ILE:HD13	1.95	0.47
17:T:164:THR:HA	17:T:170:PRO:HA	1.96	0.47
17:V:545:ALA:HA	18:Z:524:ILE:HG22	1.96	0.47
2:1:372:SER:OG	2:1:373:ASP:N	2.45	0.47
5:4:145:VAL:HG21	5:4:165:PHE:HA	1.96	0.47
17:T:456:VAL:HG21	17:T:473:VAL:HG23	1.96	0.47
17:V:323:ILE:HG12	17:V:380:PHE:HB2	1.95	0.47
3:2:215:PHE:HA	3:2:250:GLY:HA3	1.95	0.47
11:B:86:ILE:HG23	11:C:99:LEU:HB3	1.96	0.47
17:U:146:ARG:HG2	18:X:561:LEU:HD12	1.96	0.47
18:Y:166:VAL:HG23	18:Y:170:LEU:HD12	1.95	0.47
3:2:95:LEU:HD12	3:2:98:LEU:HD12	1.95	0.47
6:5:47:ALA:O	6:5:51:TYR:HB2	2.14	0.47
11:A:92:ASN:N	11:A:92:ASN:OD1	2.48	0.47
14:Q:32:LYS:HG2	14:Q:34:PRO:HD2	1.96	0.47
17:T:498:THR:HA	17:T:501:VAL:HG12	1.96	0.47
17:U:62:VAL:O	17:U:66:LEU:N	2.47	0.47
18:Y:249:GLY:HA3	18:Y:261:VAL:HG11	1.97	0.47
18:Z:195:GLU:HG2	18:Z:449:VAL:HG22	1.96	0.47
2:1:191:GLU:HA	2:1:194:LYS:HG2	1.95	0.47
2:1:568:ASP:HB2	2:1:580:LYS:HE3	1.97	0.47
3:2:290:VAL:HG22	3:2:405:VAL:HG21	1.97	0.47
8:7:50:VAL:HG23	8:7:57:ALA:HB3	1.97	0.47
17:U:121:ASN:OD1	17:U:121:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:199:ASN:HD21	18:X:448:GLN:HE22	1.62	0.47
18:Z:402:GLY:HA3	18:Z:474:LEU:HD21	1.95	0.47
11:C:116:PHE:HZ	12:M:284:LEU:HD21	1.80	0.47
11:E:81:MET:HE2	11:E:81:MET:HB3	1.82	0.47
17:U:198:VAL:HG22	17:U:430:VAL:HG12	1.96	0.47
11:H:58:ALA:HB1	11:I:59:SER:HB2	1.97	0.47
14:Q:49:GLN:HB2	16:S:160:LEU:HD11	1.97	0.47
18:Y:165:LYS:NZ	18:Y:490:GLY:O	2.39	0.47
4:3:132:VAL:O	4:3:164:ASN:ND2	2.47	0.47
13:P:40:PRO:O	13:P:59:GLN:NE2	2.47	0.47
13:P:77:PHE:HZ	13:P:109:LEU:HD11	1.80	0.47
2:1:418:VAL:HG23	2:1:419:ILE:HG13	1.96	0.46
11:B:71:LEU:HD11	11:B:118:LEU:HD21	1.97	0.46
11:C:72:ALA:HB2	11:D:70:ALA:HA	1.96	0.46
11:I:80:VAL:HG12	11:J:80:VAL:HG21	1.96	0.46
13:P:209:MET:CE	17:T:79:PRO:HD2	2.45	0.46
17:U:527:GLN:OE1	17:U:558:LYS:N	2.45	0.46
18:X:528:ASP:OD2	18:X:528:ASP:N	2.49	0.46
18:Y:344:ASP:OD1	18:Y:366:ARG:NH1	2.45	0.46
5:4:101:PRO:HG3	8:7:170:HIS:CD2	2.50	0.46
18:Z:286:ASN:H	18:Z:338:ALA:HB3	1.80	0.46
18:Z:441:ARG:O	18:Z:444:SER:OG	2.33	0.46
11:G:58:ALA:HB2	11:H:56:LEU:HD23	1.97	0.46
18:Y:290:PHE:O	18:Y:294:ASN:ND2	2.49	0.46
2:1:520:LEU:O	2:1:524:THR:OG1	2.33	0.46
12:M:251:LEU:HD21	12:M:285:VAL:HG22	1.96	0.46
13:P:109:LEU:HD23	13:P:119:LYS:HA	1.97	0.46
13:P:121:LEU:HD13	17:V:66:LEU:HD11	1.98	0.46
2:1:556:ILE:HG21	6:5:36:ARG:HA	1.97	0.46
5:4:120:LYS:HE2	5:4:124:ASN:HD21	1.80	0.46
7:6:143:LEU:HD12	7:6:143:LEU:HA	1.77	0.46
11:I:83:GLY:O	11:J:84:SER:OG	2.34	0.46
16:S:242:VAL:O	16:S:246:LEU:HB2	2.15	0.46
17:T:415:LYS:O	18:X:405:LYS:NZ	2.45	0.46
17:T:516:ASP:OD1	17:T:516:ASP:N	2.48	0.46
17:V:549:HIS:NE2	18:Z:525:PRO:O	2.48	0.46
11:A:90:ALA:O	11:B:92:ASN:ND2	2.39	0.46
15:R:33:PHE:HD2	16:S:94:ALA:HB2	1.80	0.46
17:T:67:ILE:HA	17:T:70:VAL:HG12	1.96	0.46
17:T:453:TYR:CZ	17:T:474:LEU:HD12	2.39	0.46
17:U:441:GLN:HE22	17:U:541:LYS:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:487:TYR:O	18:Y:498:LYS:NZ	2.48	0.46
2:1:604:ARG:NH2	4:3:196:ASP:OD2	2.49	0.46
15:R:58:LYS:O	15:R:139:ASN:ND2	2.48	0.46
17:U:446:LEU:HD22	17:U:501:VAL:HG21	1.98	0.46
18:Y:289:ARG:NH1	18:Y:292:GLN:OE1	2.43	0.46
3:2:128:VAL:HG22	3:2:135:PHE:HE2	1.81	0.46
11:B:92:ASN:OD1	11:B:92:ASN:N	2.46	0.46
11:I:118:LEU:HA	11:I:121:VAL:HG22	1.97	0.46
18:Y:180:GLY:HA3	18:Y:358:LEU:HD13	1.97	0.46
18:Z:158:GLU:OE2	18:Z:175:ARG:NH1	2.49	0.46
3:2:195:ALA:HA	3:2:198:LYS:HE3	1.97	0.46
4:3:177:LEU:HD22	4:3:198:VAL:HG22	1.98	0.46
2:1:568:ASP:OD2	6:5:38:HIS:NE2	2.47	0.46
8:7:23:LEU:HD12	8:7:63:ALA:HA	1.98	0.46
11:C:85:LEU:HD13	11:C:103:ALA:HB2	1.98	0.46
13:P:184:LEU:HG	13:P:186:MET:HG3	1.98	0.46
16:S:101:VAL:HG11	16:S:182:LEU:HD22	1.98	0.46
17:T:429:ARG:NH1	22:Y:601:ADP:O2B	2.37	0.46
18:Y:445:GLN:NE2	18:Y:459:LYS:O	2.48	0.46
3:2:218:GLY:HA2	3:2:254:SER:HB2	1.98	0.45
4:3:103:VAL:O	4:3:107:SER:OG	2.31	0.45
11:A:84:SER:OG	11:J:83:GLY:O	2.29	0.45
15:R:71:PRO:HG2	15:R:141:VAL:HG12	1.98	0.45
17:U:202:LEU:HD22	17:U:378:THR:HG21	1.98	0.45
4:3:121:PHE:HA	4:3:124:PHE:HB2	1.99	0.45
17:T:241:HIS:HE1	17:T:493:PRO:HA	1.80	0.45
17:U:532:VAL:HG21	17:U:550:LEU:HD13	1.98	0.45
18:Y:195:GLU:O	18:Y:199:ASN:HB2	2.16	0.45
11:D:83:GLY:O	11:E:84:SER:OG	2.34	0.45
11:J:85:LEU:HD22	11:J:103:ALA:CB	2.47	0.45
16:S:210:ILE:HD13	16:S:251:LEU:HA	1.98	0.45
16:S:314:LEU:HD12	18:Y:304:ILE:HG22	1.97	0.45
18:Y:528:ASP:HA	18:Y:531:VAL:HG22	1.97	0.45
2:1:118:ARG:HH21	6:5:70:ALA:HB2	1.81	0.45
18:Y:273:ARG:HD3	18:Y:333:ILE:HG13	1.98	0.45
18:Y:358:LEU:HB2	18:Y:361:THR:HG22	1.99	0.45
5:4:8:LYS:HA	5:4:11:VAL:HG12	1.98	0.45
11:H:85:LEU:HD13	11:H:103:ALA:HB2	1.98	0.45
17:V:122:LEU:HB3	18:Z:98:ARG:HD3	1.98	0.45
18:Y:186:GLY:HA2	22:Y:601:ADP:H5'1	1.98	0.45
17:T:287:MET:HE2	17:T:287:MET:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:267:ARG:NE	7:6:150:SER:O	2.43	0.45
3:2:309:LYS:NZ	5:4:37:ALA:O	2.42	0.45
10:9:56:ASN:OD1	10:9:56:ASN:N	2.50	0.45
11:B:72:ALA:HB2	11:C:70:ALA:HA	1.99	0.45
11:F:80:VAL:HG12	11:G:80:VAL:HG21	1.98	0.45
17:T:112:ASP:OD1	17:T:112:ASP:N	2.49	0.45
17:U:84:LEU:HD23	17:U:143:LEU:HD12	1.99	0.45
17:V:232:THR:OG1	20:V:1001:ATP:O2B	2.34	0.45
18:X:341:VAL:HA	18:X:342:PRO:HD3	1.78	0.45
18:Y:508:SER:OG	18:Y:511:GLU:OE1	2.34	0.45
2:1:189:LEU:HD12	2:1:189:LEU:HA	1.88	0.45
2:1:576:ALA:HB1	2:1:579:ALA:HB3	1.99	0.45
13:P:46:LEU:HD13	13:P:140:ASN:HB3	1.99	0.45
1:0:62:PRO:HG2	7:6:95:LYS:HD3	1.98	0.45
11:B:93:PRO:HA	11:B:96:ALA:HB2	1.99	0.45
11:G:71:LEU:HB2	11:H:70:ALA:HB1	1.98	0.45
17:U:323:ILE:HG13	17:U:380:PHE:HB2	1.98	0.45
5:4:49:LEU:HD21	13:P:215:VAL:HG22	1.99	0.44
5:4:184:LEU:HD21	8:7:187:LEU:HB2	1.99	0.44
11:D:118:LEU:HA	11:D:121:VAL:HB	1.99	0.44
11:F:119:LEU:HG	11:F:123:LEU:HD12	1.98	0.44
18:Y:523:ASP:OD1	18:Y:523:ASP:N	2.51	0.44
2:1:184:LEU:HG	2:1:488:VAL:HG21	1.99	0.44
14:Q:52:TYR:N	16:S:159:GLN:O	2.43	0.44
16:S:167:LYS:HE2	16:S:167:LYS:HB3	1.85	0.44
17:T:92:ASP:OD1	18:X:303:ARG:NH2	2.50	0.44
17:U:108:LEU:HG	17:U:151:VAL:HA	1.99	0.44
2:1:62:LYS:HD2	2:1:144:ALA:HB3	1.99	0.44
2:1:102:LEU:HD12	2:1:106:ASP:HB3	1.99	0.44
2:1:523:LEU:HA	2:1:526:THR:HG22	1.99	0.44
18:Z:273:ARG:HD3	18:Z:333:ILE:HG13	1.98	0.44
8:7:47:GLU:OE1	8:7:60:GLN:NE2	2.46	0.44
11:D:72:ALA:HB2	11:E:70:ALA:HA	2.00	0.44
11:J:92:ASN:OD1	11:J:92:ASN:N	2.50	0.44
17:V:357:LEU:HA	17:V:360:ARG:HH11	1.82	0.44
18:X:562:ASN:ND2	18:X:564:GLU:OE1	2.50	0.44
18:Z:42:GLN:HB2	18:Z:49:ASP:HB2	1.98	0.44
3:2:78:VAL:HA	8:7:74:ILE:HB	1.99	0.44
5:4:292:VAL:HG22	17:T:48:LEU:HD12	2.00	0.44
8:7:79:VAL:HG13	17:T:48:LEU:HB3	2.00	0.44
11:G:92:ASN:OD1	11:G:92:ASN:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:111:GLU:O	11:I:112:SER:C	2.60	0.44
14:Q:17:LEU:HD23	14:Q:17:LEU:HA	1.89	0.44
3:2:188:ALA:HB2	3:2:220:LEU:HD22	2.00	0.44
17:V:386:GLN:HB3	18:Y:347:THR:HB	1.99	0.44
3:2:62:ASP:OD1	3:2:62:ASP:N	2.46	0.44
16:S:112:CYS:O	16:S:269:SER:OG	2.26	0.44
17:T:476:ARG:NH2	17:T:505:THR:O	2.50	0.44
18:Y:116:GLY:HA3	18:Y:136:ASP:HB2	2.00	0.44
2:1:328:ARG:NH1	10:9:12:GLU:OE1	2.51	0.44
11:A:81:MET:HE2	11:A:81:MET:HB3	1.88	0.44
17:V:304:TYR:OH	17:V:357:LEU:O	2.34	0.44
17:U:172:ASP:OD1	17:U:172:ASP:N	2.51	0.44
18:X:273:ARG:HD3	18:X:333:ILE:HG13	2.00	0.44
18:X:516:LYS:HE2	18:X:518:SER:HB2	2.00	0.44
18:Y:286:ASN:HB3	18:Y:289:ARG:HG2	1.98	0.44
18:Y:482:PRO:HB2	18:Y:502:MET:HE1	1.99	0.44
7:6:37:LYS:O	7:6:41:GLU:HG2	2.18	0.43
17:T:453:TYR:CZ	17:T:474:LEU:CD1	2.99	0.43
16:S:68:MET:HE2	16:S:68:MET:HB3	1.80	0.43
17:T:132:PHE:HE1	17:T:297:PRO:HB2	1.83	0.43
18:Y:215:GLU:OE1	18:Y:286:ASN:ND2	2.47	0.43
18:Y:470:PHE:O	18:Y:474:LEU:HB2	2.18	0.43
18:Z:78:GLN:HG3	18:Z:86:ARG:HB3	2.00	0.43
4:3:110:LEU:HB3	4:3:115:PHE:HD2	1.82	0.43
8:7:173:ILE:HD12	8:7:173:ILE:HA	1.88	0.43
11:A:91:ARG:NH1	16:S:238:GLU:OE1	2.46	0.43
18:Y:120:ARG:NH1	18:Y:132:GLN:O	2.51	0.43
18:Y:386:MET:HE3	18:Y:386:MET:HB3	1.91	0.43
11:H:104:LEU:HA	11:H:107:PHE:HB3	1.99	0.43
13:P:174:ALA:HB3	13:P:186:MET:CE	2.47	0.43
2:1:23:TYR:O	8:7:155:SER:OG	2.36	0.43
2:1:543:SER:OG	12:M:99:ASP:OD2	2.33	0.43
17:T:172:ASP:OD2	17:T:172:ASP:N	2.46	0.43
17:V:195:ARG:NH2	17:V:363:GLU:O	2.51	0.43
18:Y:276:GLU:OE1	18:Y:278:GLN:NE2	2.52	0.43
18:Y:361:THR:O	18:Y:361:THR:OG1	2.36	0.43
2:1:420:TYR:OH	2:1:442:ASP:OD2	2.28	0.43
17:T:282:MET:HE1	17:T:287:MET:HG3	1.99	0.43
17:U:239:ILE:HD11	17:U:323:ILE:HD13	2.00	0.43
17:U:273:VAL:HG13	17:U:282:MET:HE3	2.01	0.43
18:Y:252:ASN:OD1	18:Y:252:ASN:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:195:LYS:HD2	2:1:195:LYS:HA	1.73	0.43
4:3:217:ASP:N	4:3:217:ASP:OD1	2.51	0.43
7:6:105:LEU:HA	7:6:105:LEU:HD23	1.75	0.43
9:8:11:ILE:HG22	9:8:12:LEU:HG	2.01	0.43
11:B:63:GLY:O	11:B:67:ALA:N	2.52	0.43
11:B:97:LYS:NZ	11:C:102:TYR:OH	2.35	0.43
11:E:64:ALA:HB1	11:E:121:VAL:HG13	2.01	0.43
11:F:71:LEU:HA	11:F:74:VAL:HG22	2.01	0.43
15:R:136:VAL:HG22	15:R:142:THR:HG22	2.01	0.43
2:1:268:LEU:HD22	2:1:357:ALA:HB1	2.00	0.43
3:2:207:ALA:HB3	3:2:238:ASP:HB3	2.00	0.43
9:8:26:HIS:HB3	9:8:29:GLN:HG3	2.01	0.43
11:H:92:ASN:N	11:H:92:ASN:OD1	2.51	0.43
17:T:120:LEU:HD23	17:T:120:LEU:HA	1.79	0.43
17:T:125:ASP:OD1	17:T:125:ASP:N	2.40	0.43
17:T:220:ARG:H	17:T:220:ARG:HG2	1.65	0.43
18:Y:500:ASP:O	18:Y:504:LYS:HG3	2.19	0.43
3:2:79:GLU:OE1	8:7:15:LEU:N	2.51	0.42
12:M:301:ILE:O	12:M:304:THR:OG1	2.36	0.42
17:U:92:ASP:OD1	18:Z:303:ARG:NH2	2.43	0.42
17:V:287:MET:HE2	17:V:287:MET:HB3	1.90	0.42
18:X:66:GLU:HG3	18:X:101:LYS:HD3	2.01	0.42
11:A:86:ILE:HG21	11:B:85:LEU:HA	2.00	0.42
13:P:157:ILE:HB	13:P:189:LYS:HB2	2.01	0.42
14:Q:32:LYS:N	15:R:154:GLN:O	2.49	0.42
17:T:528:VAL:HG21	17:T:554:LEU:HD23	2.01	0.42
18:X:445:GLN:NE2	18:X:459:LYS:O	2.49	0.42
11:F:59:SER:HA	11:F:62:VAL:HG12	2.00	0.42
16:S:186:ASN:OD1	16:S:186:ASN:N	2.52	0.42
17:V:447:LYS:HE2	17:V:447:LYS:HB3	1.91	0.42
18:Z:272:PHE:HD1	18:Z:276:GLU:HG3	1.85	0.42
14:Q:48:ARG:NH1	16:S:144:ASP:OD1	2.52	0.42
17:U:304:TYR:OH	17:U:357:LEU:O	2.34	0.42
11:H:118:LEU:HD22	11:I:120:VAL:HG21	2.00	0.42
14:Q:10:ARG:NH2	16:S:245:ASP:OD1	2.50	0.42
15:R:76:THR:HG22	15:R:78:HIS:H	1.85	0.42
16:S:271:MET:HE2	16:S:271:MET:HB3	1.82	0.42
17:U:217:ARG:O	17:U:378:THR:OG1	2.36	0.42
17:V:543:THR:HG23	17:V:546:LEU:H	1.84	0.42
3:2:252:ALA:HB1	3:2:294:ILE:HB	2.00	0.42
5:4:179:PRO:HB2	5:4:182:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:51:TYR:HE2	7:6:143:LEU:HD13	1.85	0.42
6:5:62:TYR:OH	7:6:146:PHE:O	2.27	0.42
18:Y:225:ARG:HA	18:Y:225:ARG:HD3	1.82	0.42
2:1:535:HIS:HB3	2:1:540:LEU:HB2	2.01	0.42
11:A:108:ALA:HB1	12:M:302:LEU:HD11	2.01	0.42
16:S:98:ASN:HB3	16:S:188:GLN:HE21	1.85	0.42
17:V:411:GLU:HG2	17:V:415:LYS:HE3	2.00	0.42
2:1:178:LEU:HD23	2:1:178:LEU:HA	1.88	0.42
4:3:224:THR:HG21	4:3:263:SER:HB2	2.01	0.42
8:7:170:HIS:HD2	8:7:172:ALA:H	1.65	0.42
17:U:251:LYS:HB2	18:X:540:GLU:HB2	2.00	0.42
18:Z:306:SER:HB3	18:Z:312:PRO:HA	2.01	0.42
5:4:118:THR:HA	5:4:154:LEU:HA	2.01	0.42
17:V:453:TYR:CG	17:V:477:GLY:HA3	2.54	0.42
18:Z:349:PRO:O	18:Z:353:THR:OG1	2.31	0.42
4:3:162:GLU:OE2	4:3:191:SER:OG	2.31	0.42
11:A:74:VAL:HG11	11:A:114:ALA:HB2	2.02	0.42
15:R:175:GLU:HA	15:R:178:GLN:HB3	2.02	0.42
17:U:58:LEU:HA	17:U:61:HIS:HB3	2.02	0.42
18:Y:341:VAL:HG11	18:Y:346:LEU:HD23	2.02	0.42
5:4:72:LEU:HB3	5:4:74:LEU:HG	2.02	0.41
9:8:82:THR:HA	9:8:83:PRO:HD3	1.91	0.41
11:A:86:ILE:HG23	11:B:99:LEU:HB3	2.01	0.41
14:Q:18:ARG:NE	16:S:180:GLU:OE1	2.53	0.41
17:T:219:GLN:NE2	17:T:221:GLU:OE1	2.53	0.41
17:U:326:ASP:H	17:U:382:VAL:HB	1.83	0.41
18:Z:374:TYR:HB2	18:Z:488:MET:HE1	2.01	0.41
3:2:346:ARG:HA	3:2:349:VAL:HG22	2.01	0.41
6:5:35:MET:O	6:5:39:LYS:HB2	2.21	0.41
11:G:69:ILE:HA	11:H:70:ALA:HB2	2.02	0.41
15:R:116:VAL:HG11	15:R:144:ILE:HD13	2.02	0.41
17:V:311:GLU:HG2	17:V:314:ARG:HE	1.84	0.41
18:Z:430:LYS:HA	18:Z:433:VAL:HB	2.03	0.41
3:2:288:LEU:HD23	3:2:307:VAL:HG11	2.02	0.41
11:G:118:LEU:HA	11:G:121:VAL:HG12	2.02	0.41
15:R:118:LEU:HB2	15:R:125:GLU:HG2	2.01	0.41
16:S:204:LYS:HA	16:S:205:PRO:HD3	1.83	0.41
17:U:112:ASP:OD2	17:U:112:ASP:N	2.51	0.41
18:Z:110:LYS:HB3	18:Z:140:ILE:HG22	2.01	0.41
18:Z:435:ARG:NH2	18:Z:474:LEU:O	2.53	0.41
1:0:71:MET:HE2	1:0:71:MET:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:111:GLU:O	11:C:114:ALA:N	2.54	0.41
11:H:71:LEU:HD13	11:I:113:ILE:HG23	2.02	0.41
11:J:85:LEU:HD11	11:J:99:LEU:HB3	1.97	0.41
11:J:113:ILE:HD13	11:J:113:ILE:HA	1.95	0.41
13:P:193:LYS:HE3	13:P:193:LYS:HB3	1.92	0.41
18:Y:493:LYS:HE2	18:Y:493:LYS:HB2	1.89	0.41
6:5:44:TRP:CE3	7:6:142:GLY:HA3	2.55	0.41
11:C:118:LEU:HD23	11:C:118:LEU:HA	1.95	0.41
12:M:181:ALA:HB3	12:M:241:TRP:HB2	2.02	0.41
16:S:101:VAL:HG22	16:S:138:VAL:HB	2.02	0.41
18:X:489:VAL:HG21	18:X:495:VAL:HG22	2.02	0.41
11:D:92:ASN:OD1	11:D:92:ASN:N	2.53	0.41
12:M:324:LYS:HB3	12:M:324:LYS:HE2	1.76	0.41
13:P:162:LEU:HD21	13:P:170:LEU:HD21	2.03	0.41
6:5:58:LEU:HD23	6:5:58:LEU:HA	1.93	0.41
7:6:32:VAL:HG23	9:8:14:THR:HG21	2.02	0.41
7:6:51:LEU:HD23	7:6:51:LEU:HA	1.92	0.41
7:6:107:VAL:HG11	10:9:48:GLY:HA3	2.03	0.41
11:I:125:LEU:HD21	11:J:124:ILE:HG12	2.02	0.41
15:R:185:ILE:O	15:R:189:SER:OG	2.37	0.41
17:U:174:LYS:HE2	17:U:174:LYS:HB3	1.89	0.41
17:U:546:LEU:O	17:U:550:LEU:HB2	2.20	0.41
17:V:502:TYR:OH	17:V:547:ASP:OD2	2.23	0.41
18:X:548:ASP:OD2	18:X:548:ASP:N	2.52	0.41
18:Z:543:ASP:OD1	18:Z:543:ASP:N	2.52	0.41
2:1:335:VAL:HA	2:1:336:PRO:HD3	1.91	0.41
7:6:31:SER:HB2	7:6:58:ALA:HB1	2.03	0.41
8:7:85:LEU:O	8:7:88:SER:OG	2.37	0.41
11:B:59:SER:HA	11:B:62:VAL:HG22	2.03	0.41
11:D:86:ILE:HG21	11:E:85:LEU:HA	2.02	0.41
18:X:223:LEU:HA	18:X:226:GLU:HG2	2.02	0.41
2:1:551:LEU:HD21	4:3:170:THR:HB	2.03	0.41
3:2:320:LEU:HD23	3:2:320:LEU:HA	1.92	0.41
11:A:125:LEU:HD21	11:B:124:ILE:HG22	2.03	0.41
11:F:74:VAL:HG21	11:F:114:ALA:HB2	2.02	0.41
13:P:108:VAL:HG23	13:P:109:LEU:HD12	2.03	0.41
13:P:184:LEU:HD12	13:P:185:VAL:H	1.85	0.41
17:V:360:ARG:HE	17:V:360:ARG:HB3	1.67	0.41
18:X:56:LEU:HD11	18:X:83:ASN:HA	2.02	0.41
18:X:108:PRO:HB2	18:X:142:SER:HB2	2.03	0.41
18:X:306:SER:OG	18:X:307:ALA:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:351:PRO:HA	18:X:354:THR:HG22	2.02	0.41
18:X:516:LYS:HB3	18:X:518:SER:H	1.86	0.41
18:Y:194:MET:HE2	18:Y:194:MET:HB2	1.93	0.41
11:I:64:ALA:HB2	11:I:124:ILE:HB	2.03	0.41
17:U:70:VAL:HG13	17:U:77:TYR:HE2	1.86	0.41
20:U:1001:ATP:PG	18:Z:385:ARG:HH12	2.44	0.41
18:Y:190:THR:HA	18:Y:193:ILE:HG22	2.03	0.41
2:1:37:ALA:HA	2:1:38:PRO:HD3	1.91	0.40
2:1:423:ASN:HD22	2:1:423:ASN:HA	1.67	0.40
11:H:118:LEU:HD11	11:I:116:PHE:HB3	2.03	0.40
15:R:45:LEU:HB3	16:S:122:TYR:HE1	1.86	0.40
17:T:326:ASP:HB3	17:T:329:LYS:HB2	2.03	0.40
17:V:482:GLU:HA	17:V:485:LYS:HD3	2.03	0.40
18:Y:492:ILE:HD12	18:Y:492:ILE:HA	1.92	0.40
3:2:265:LEU:HD23	3:2:265:LEU:HA	1.96	0.40
6:5:120:PRO:HB3	8:7:80:ALA:HA	2.03	0.40
14:Q:56:LYS:HE3	16:S:151:THR:HG21	2.04	0.40
15:R:73:ASN:HB3	15:R:75:TYR:CZ	2.56	0.40
16:S:239:ARG:HA	16:S:242:VAL:HG12	2.03	0.40
17:U:157:PRO:HB3	18:X:545:LEU:HB3	2.02	0.40
17:U:442:VAL:HG11	17:U:501:VAL:HG13	2.04	0.40
18:Y:101:LYS:HD3	18:Y:101:LYS:HA	1.93	0.40
18:Y:165:LYS:H	18:Y:165:LYS:HG2	1.71	0.40
8:7:170:HIS:HB3	8:7:173:ILE:HB	2.04	0.40
16:S:197:PHE:N	16:S:261:GLU:OE1	2.48	0.40
17:U:65:LYS:HE2	17:U:65:LYS:HB3	1.89	0.40
11:A:58:ALA:O	11:B:59:SER:OG	2.27	0.40
11:A:97:LYS:HD2	11:A:97:LYS:HA	1.94	0.40
11:I:94:ASN:HD21	16:S:225:GLY:HA3	1.85	0.40
16:S:127:LEU:HD12	16:S:127:LEU:HA	1.93	0.40
17:T:132:PHE:CE1	17:T:297:PRO:HB2	2.56	0.40
17:T:483:MET:HE3	17:T:483:MET:HB3	1.93	0.40
18:Y:373:ILE:HG23	18:Y:444:SER:HB2	2.03	0.40
2:1:82:HIS:NE2	8:7:120:TYR:O	2.52	0.40
2:1:473:LYS:HD3	6:5:92:LEU:HD22	2.04	0.40
2:1:544:VAL:HG12	2:1:548:MET:HE2	2.03	0.40
2:1:574:MET:HE2	2:1:574:MET:HB3	1.88	0.40
7:6:73:THR:HA	7:6:76:LYS:HE2	2.04	0.40
11:H:69:ILE:HD12	11:I:69:ILE:HD11	2.02	0.40
12:M:107:THR:O	12:M:111:THR:OG1	2.34	0.40
12:M:125:LYS:HA	12:M:126:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:155:VAL:HG21	15:R:191:LEU:HD21	2.03	0.40
17:T:370:LYS:HE2	17:T:370:LYS:HB2	1.95	0.40
17:T:495:GLU:HG3	17:T:533:PHE:HB3	2.04	0.40
17:V:443:ALA:HA	17:V:446:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
2	1	593/618 (96%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	420 (96%)	18 (4%)	1 (0%)	43	73
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	281 (98%)	7 (2%)	0	100	100
6	5	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	16	47
7	6	122/151 (81%)	109 (89%)	13 (11%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	B	72/127 (57%)	69 (96%)	3 (4%)	0	100	100
11	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
11	D	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	E	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	F	72/127 (57%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	H	72/127 (57%)	72 (100%)	0	0	100	100
11	I	72/127 (57%)	66 (92%)	6 (8%)	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%)	174 (91%)	17 (9%)	0	100	100
14	Q	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
15	R	175/199 (88%)	160 (91%)	15 (9%)	0	100	100
16	S	275/317 (87%)	262 (95%)	13 (5%)	0	100	100
17	T	521/562 (93%)	490 (94%)	27 (5%)	4 (1%)	16	47
17	U	521/562 (93%)	489 (94%)	31 (6%)	1 (0%)	43	73
17	V	518/562 (92%)	496 (96%)	21 (4%)	1 (0%)	43	73
18	X	540/574 (94%)	504 (93%)	35 (6%)	1 (0%)	43	73
18	Y	519/574 (90%)	478 (92%)	38 (7%)	3 (1%)	21	52
18	Z	536/574 (93%)	503 (94%)	31 (6%)	2 (0%)	30	61
All	All	7038/8234 (86%)	6659 (95%)	365 (5%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	308	VAL
18	Z	308	VAL
3	2	383	PRO
17	T	493	PRO
17	U	349	ALA
17	V	349	ALA
18	Y	308	VAL
17	T	56	LYS
17	T	349	ALA
18	Z	307	ALA
18	Y	307	ALA
18	Y	455	GLY
17	T	494	ILE
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%)	492 (100%)	1 (0%)	87	89
3	2	312/312 (100%)	312 (100%)	0	100	100
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%)	106 (99%)	1 (1%)	70	80
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%)	48 (96%)	2 (4%)	28	60
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%)	50 (100%)	0	100	100
11	F	50/86 (58%)	50 (100%)	0	100	100
11	G	50/86 (58%)	50 (100%)	0	100	100
11	H	50/86 (58%)	49 (98%)	1 (2%)	48	72
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%)	134 (100%)	0	100	100
16	S	235/265 (89%)	230 (98%)	5 (2%)	47	71
17	T	419/448 (94%)	418 (100%)	1 (0%)	87	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	U	419/448 (94%)	417 (100%)	2 (0%)	81	85
17	V	418/448 (93%)	415 (99%)	3 (1%)	76	82
18	X	449/469 (96%)	446 (99%)	3 (1%)	76	82
18	Y	430/469 (92%)	428 (100%)	2 (0%)	81	85
18	Z	446/469 (95%)	445 (100%)	1 (0%)	87	89
All	All	5631/6445 (87%)	5608 (100%)	23 (0%)	81	86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	240	VAL
6	5	113	VAL
11	B	92	ASN
11	B	121	VAL
11	H	119	LEU
11	J	95	ILE
16	S	105	VAL
16	S	139	VAL
16	S	183	ILE
16	S	203	PHE
16	S	223	VAL
17	T	180	VAL
17	U	180	VAL
17	U	213	VAL
17	V	153	VAL
17	V	185	VAL
17	V	255	VAL
18	X	502	MET
18	X	517	VAL
18	X	521	LEU
18	Y	200	VAL
18	Y	417	ILE
18	Z	439	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	48	ASN
1	0	60	GLN

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Mol	Chain	Res	Type
1	0	80	HIS
2	1	257	HIS
2	1	285	GLN
2	1	298	GLN
2	1	313	GLN
2	1	316	ASN
2	1	346	GLN
2	1	365	GLN
2	1	394	GLN
2	1	423	ASN
2	1	477	GLN
2	1	482	ASN
2	1	547	HIS
2	1	562	ASN
2	1	587	ASN
2	1	590	HIS
2	1	606	ASN
3	2	40	GLN
3	2	59	GLN
3	2	68	ASN
3	2	122	ASN
3	2	243	GLN
3	2	289	HIS
3	2	427	GLN
4	3	97	ASN
4	3	179	GLN
4	3	189	HIS
4	3	206	ASN
5	4	38	GLN
5	4	61	GLN
5	4	124	ASN
5	4	240	GLN
6	5	25	HIS
6	5	107	ASN
7	6	40	ASN
7	6	74	GLN
8	7	24	GLN
8	7	86	HIS
8	7	98	ASN
8	7	123	HIS
8	7	170	HIS
8	7	184	ASN

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Mol	Chain	Res	Type
8	7	190	GLN
9	8	26	HIS
10	9	27	ASN
10	9	80	GLN
11	A	87	ASN
11	D	98	GLN
11	H	94	ASN
11	I	94	ASN
11	J	98	GLN
12	M	121	ASN
12	M	163	ASN
12	M	295	GLN
13	P	65	ASN
13	P	220	ASN
13	P	223	ASN
14	Q	21	ASN
14	Q	40	GLN
15	R	38	ASN
15	R	85	GLN
15	R	171	GLN
15	R	181	ASN
16	S	70	ASN
16	S	116	ASN
16	S	188	GLN
16	S	257	ASN
16	S	262	ASN
16	S	293	ASN
16	S	297	GLN
17	T	64	GLN
17	T	126	HIS
17	T	134	ASN
17	T	241	HIS
17	T	461	GLN
17	T	497	GLN
17	T	549	HIS
17	U	179	ASN
17	U	246	ASN
17	U	248	GLN
17	U	264	GLN
17	U	319	HIS
17	U	358	HIS
17	U	405	GLN

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Mol	Chain	Res	Type
17	U	441	GLN
17	U	471	GLN
17	U	497	GLN
17	U	529	ASN
17	V	60	GLN
17	V	104	GLN
17	V	121	ASN
17	V	126	HIS
17	V	139	HIS
17	V	149	GLN
17	V	152	ASN
17	V	244	ASN
17	V	271	GLN
17	V	278	GLN
17	V	405	GLN
17	V	486	GLN
17	V	497	GLN
17	V	529	ASN
18	X	199	ASN
18	X	448	GLN
18	Y	68	HIS
18	Y	123	ASN
18	Y	221	ASN
18	Y	398	ASN
18	Z	132	GLN
18	Z	199	ASN
18	Z	221	ASN
18	Z	250	GLN
18	Z	278	GLN
18	Z	294	ASN
18	Z	414	GLN
18	Z	574	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	X	601	21	28,29,29	1.40	5 (17%)	43,45,45	1.86	10 (23%)
20	ATP	U	1001	21	32,33,33	1.30	5 (15%)	48,52,52	1.78	8 (16%)
20	ATP	T	1001	21	32,33,33	1.31	5 (15%)	48,52,52	1.77	10 (20%)
22	ADP	Y	601	21	28,29,29	1.38	5 (17%)	43,45,45	1.84	10 (23%)
20	ATP	V	1001	21	32,33,33	1.34	5 (15%)	48,52,52	1.73	7 (14%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	601	ADP	C5-C4	4.38	1.46	1.39
20	V	1001	ATP	C5-C4	4.04	1.46	1.39
20	U	1001	ATP	C5-C4	3.96	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	601	ADP	C5-C4	3.84	1.45	1.39
20	T	1001	ATP	C5-C4	3.67	1.45	1.39
20	V	1001	ATP	C5-N7	-3.04	1.33	1.39
20	T	1001	ATP	C5-N7	-2.90	1.33	1.39
22	X	601	ADP	C5-N7	-2.85	1.33	1.39
20	U	1001	ATP	C5-N7	-2.81	1.34	1.39
22	Y	601	ADP	C5-N7	-2.57	1.34	1.39
22	X	601	ADP	C8-N9	-2.52	1.33	1.37
22	Y	601	ADP	C5-C6	2.47	1.47	1.41
22	X	601	ADP	C4-N9	-2.45	1.32	1.37
20	T	1001	ATP	C8-N9	-2.42	1.33	1.37
20	T	1001	ATP	C4-N9	-2.42	1.32	1.37
20	V	1001	ATP	C4-N9	-2.37	1.32	1.37
20	V	1001	ATP	C8-N9	-2.31	1.33	1.37
20	V	1001	ATP	C5-C6	2.24	1.47	1.41
20	U	1001	ATP	C5-C6	2.24	1.47	1.41
22	Y	601	ADP	C4-N9	-2.20	1.33	1.37
20	U	1001	ATP	C4-N9	-2.18	1.33	1.37
20	U	1001	ATP	C8-N9	-2.16	1.33	1.37
20	T	1001	ATP	C5-C6	2.06	1.46	1.41
22	X	601	ADP	C5-C6	2.03	1.46	1.41
22	Y	601	ADP	C8-N9	-2.03	1.34	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	1001	ATP	C5-C4-N3	-5.99	118.47	126.72
22	Y	601	ADP	C5-C4-N3	-5.74	118.82	126.72
20	V	1001	ATP	C5-C4-N3	-5.72	118.84	126.72
22	X	601	ADP	C5-C4-N3	-5.44	119.22	126.72
20	T	1001	ATP	C5-C4-N3	-5.38	119.31	126.72
20	U	1001	ATP	N3-C4-N9	5.02	135.71	127.17
20	V	1001	ATP	N3-C4-N9	4.68	135.13	127.17
22	Y	601	ADP	N3-C4-N9	4.64	135.06	127.17
22	X	601	ADP	N3-C4-N9	4.62	135.03	127.17
20	T	1001	ATP	N3-C4-N9	4.45	134.74	127.17
20	U	1001	ATP	C2-N3-C4	3.66	120.77	111.83
22	Y	601	ADP	C2-N3-C4	3.64	120.71	111.83
22	X	601	ADP	C2-N3-C4	3.55	120.50	111.83
20	T	1001	ATP	C2-N3-C4	3.53	120.46	111.83
20	V	1001	ATP	C2-N3-C4	3.52	120.44	111.83
20	T	1001	ATP	N3-C2-N1	-3.52	123.25	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	601	ADP	N3-C2-N1	-3.38	123.47	128.58
22	X	601	ADP	C4-N9-C8	3.28	109.19	105.74
22	Y	601	ADP	C4-C5-N7	-3.28	106.83	110.58
20	V	1001	ATP	C4-C5-N7	-3.19	106.94	110.58
22	X	601	ADP	C4-C5-N7	-3.18	106.95	110.58
20	V	1001	ATP	N3-C2-N1	-3.16	123.79	128.58
20	U	1001	ATP	N3-C2-N1	-3.16	123.80	128.58
20	T	1001	ATP	C4-C5-N7	-3.14	107.00	110.58
22	Y	601	ADP	N3-C2-N1	-3.12	123.86	128.58
20	U	1001	ATP	C4-C5-N7	-2.99	107.17	110.58
20	T	1001	ATP	C4-N9-C8	2.96	108.85	105.74
22	Y	601	ADP	C2'-C1'-N9	-2.94	106.00	113.30
22	X	601	ADP	C2'-C1'-N9	-2.94	106.01	113.30
20	U	1001	ATP	C4-N9-C8	2.69	108.56	105.74
22	Y	601	ADP	C4-N9-C8	2.62	108.49	105.74
20	V	1001	ATP	C4-N9-C8	2.53	108.39	105.74
22	X	601	ADP	C5-N7-C8	2.40	107.22	103.45
20	T	1001	ATP	C3'-C2'-C1'	2.39	105.98	101.46
20	T	1001	ATP	C5-N7-C8	2.36	107.16	103.45
20	U	1001	ATP	C3'-C2'-C1'	2.34	105.90	101.46
20	V	1001	ATP	C5-N7-C8	2.31	107.08	103.45
22	Y	601	ADP	C5-N7-C8	2.27	107.02	103.45
20	U	1001	ATP	C5-N7-C8	2.26	107.00	103.45
22	X	601	ADP	C3'-C2'-C1'	2.18	105.59	101.46
20	T	1001	ATP	C2-N1-C6	2.17	122.30	118.73
22	X	601	ADP	N9-C8-N7	-2.14	110.90	113.94
22	Y	601	ADP	C3'-C2'-C1'	2.11	105.45	101.46
22	Y	601	ADP	C6-C5-N7	2.06	136.07	132.09
20	T	1001	ATP	N9-C8-N7	-2.02	111.06	113.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	Y	601	ADP	C5'-O5'-PA-O1A
22	Y	601	ADP	C5'-O5'-PA-O2A
22	Y	601	ADP	C5'-O5'-PA-O3A
20	U	1001	ATP	PA-O3A-PB-O1B
20	T	1001	ATP	C5'-O5'-PA-O3A
20	U	1001	ATP	PA-O3A-PB-O2B
20	T	1001	ATP	PG-O3B-PB-O1B
20	T	1001	ATP	PG-O3B-PB-O2B

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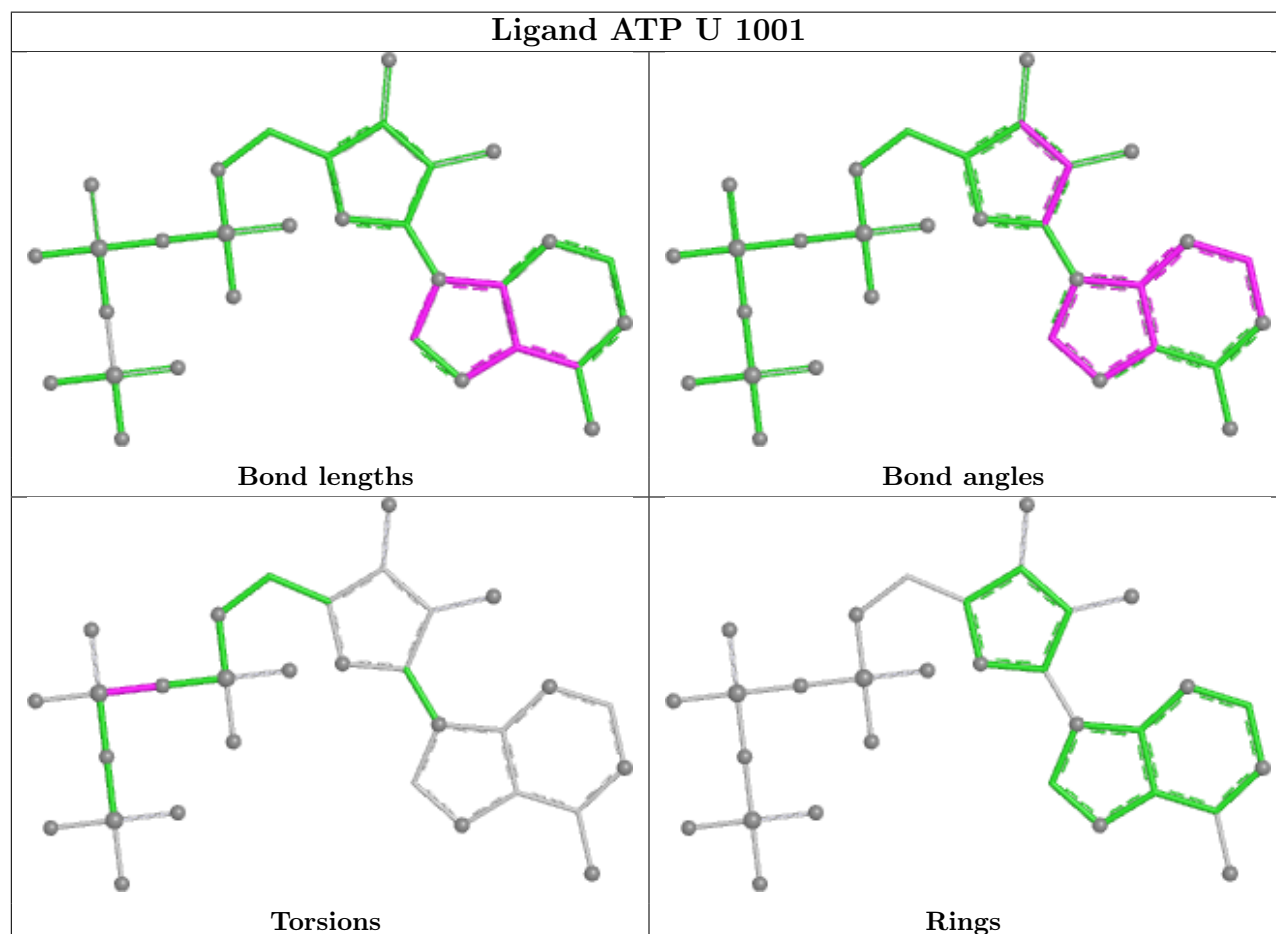
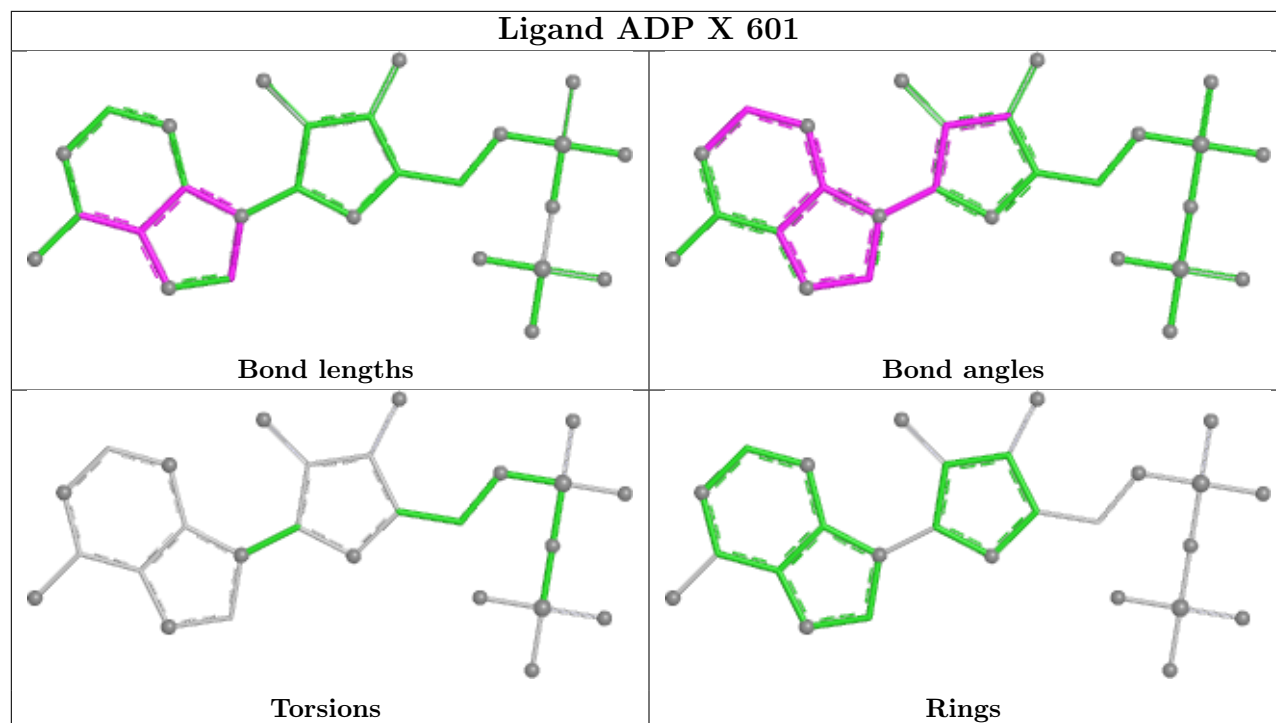
Mol	Chain	Res	Type	Atoms
20	V	1001	ATP	PB-O3A-PA-O1A
20	V	1001	ATP	PB-O3A-PA-O2A
22	Y	601	ADP	PB-O3A-PA-O1A
22	Y	601	ADP	PB-O3A-PA-O2A

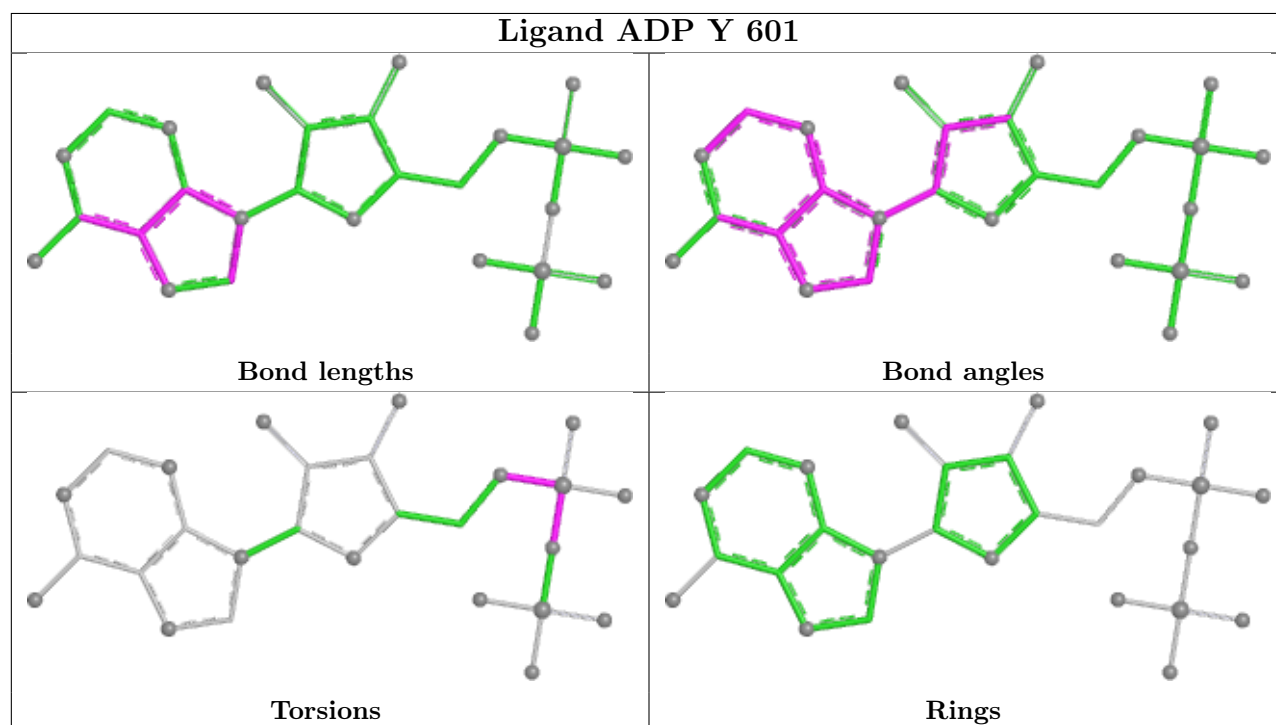
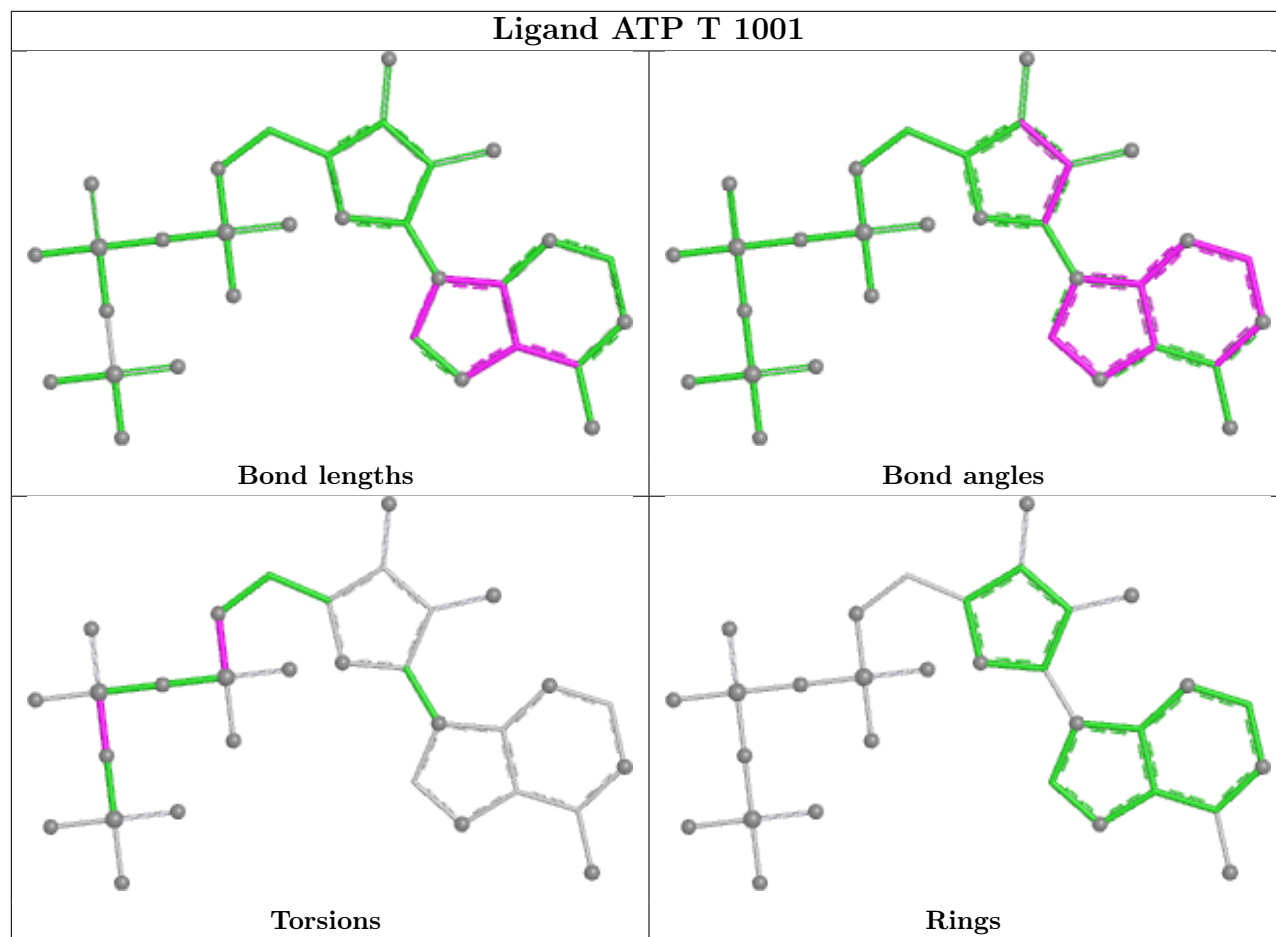
There are no ring outliers.

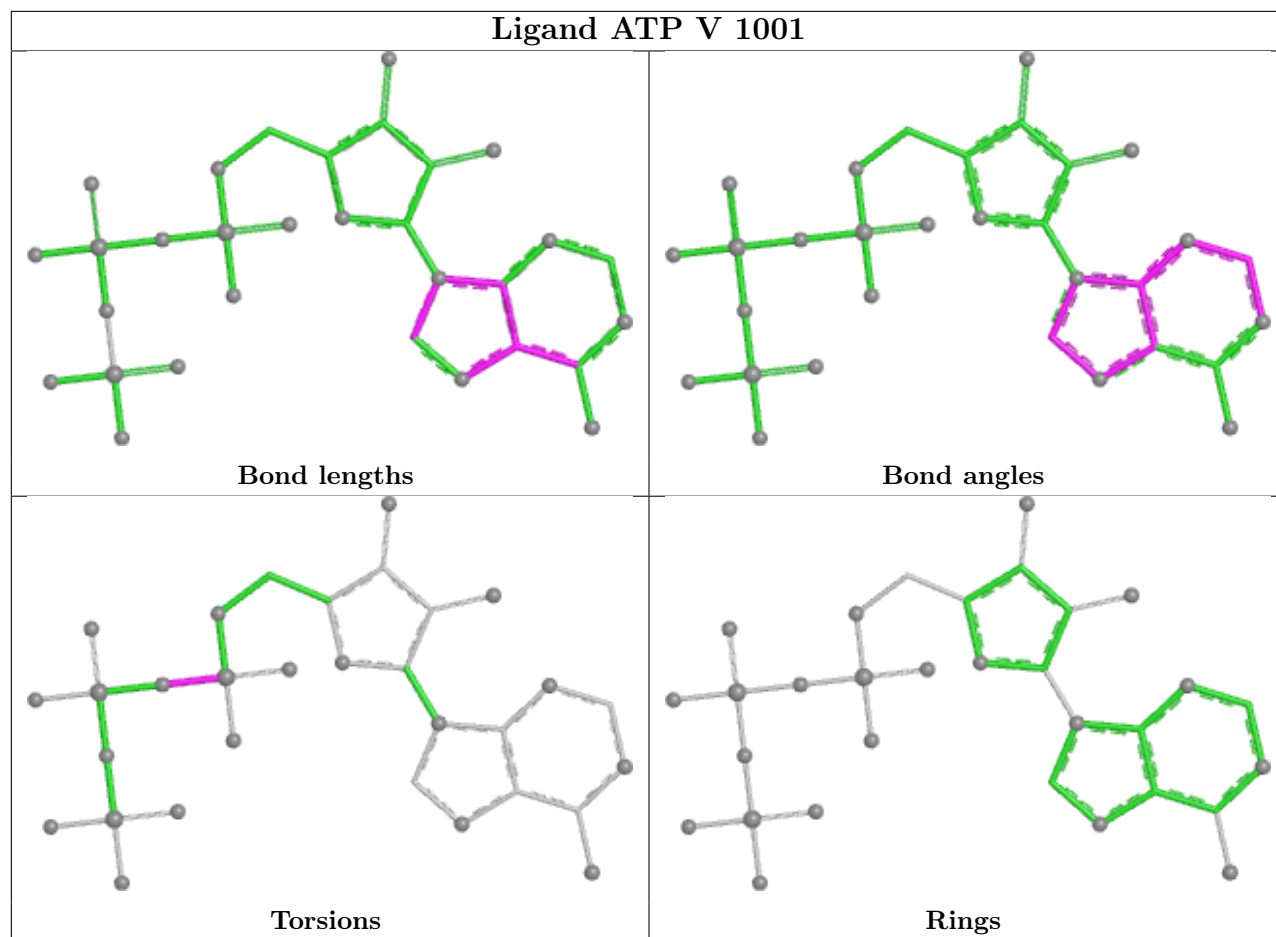
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	U	1001	ATP	1	0
22	Y	601	ADP	2	0
20	V	1001	ATP	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	3.51

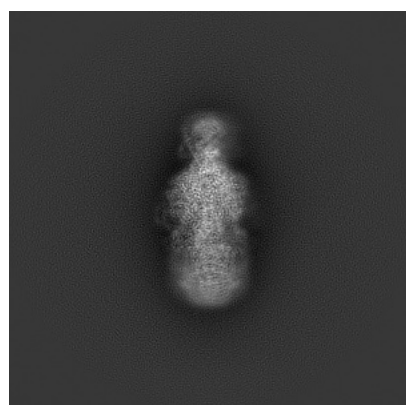
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4825. These allow visual inspection of the internal detail of the map and identification of artifacts.

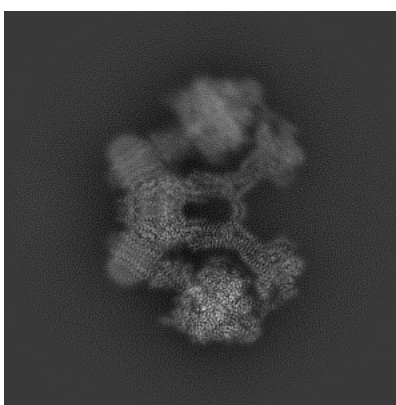
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

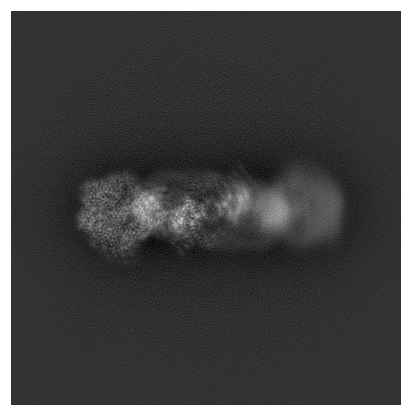
6.1.1 Primary map



X



Y

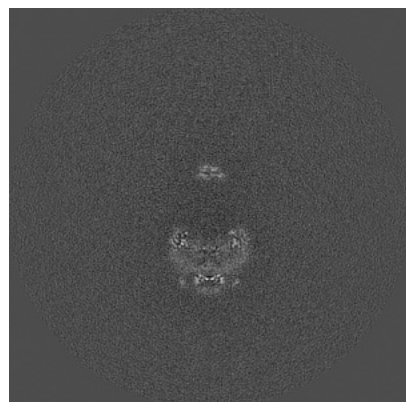


Z

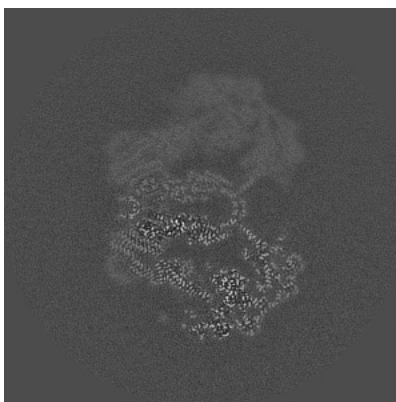
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

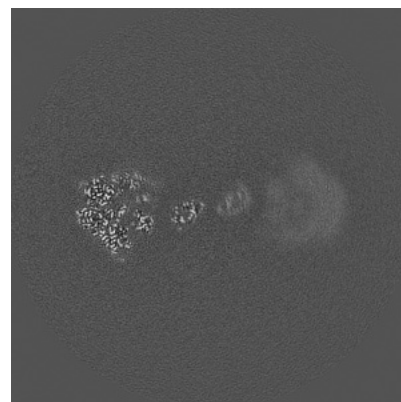
6.2.1 Primary map



X Index: 240



Y Index: 240

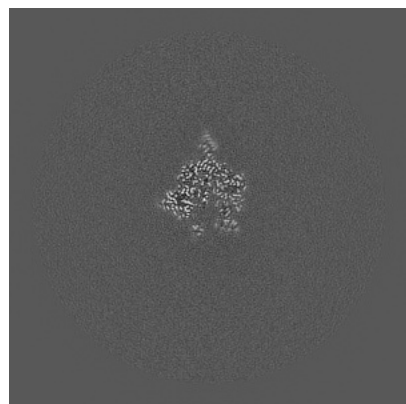


Z Index: 240

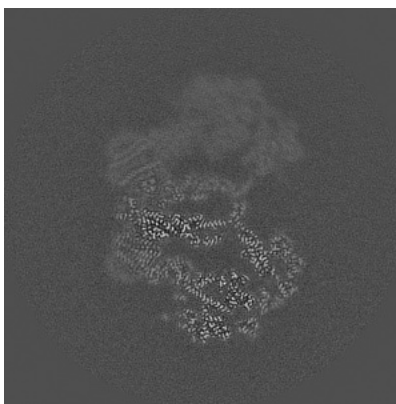
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 124



Y Index: 235

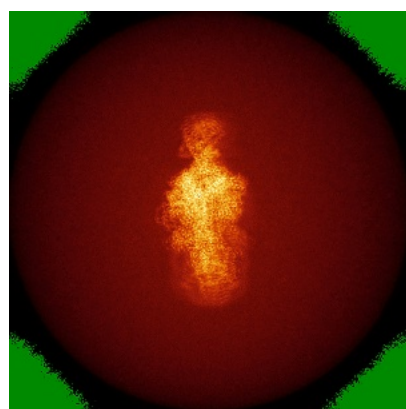


Z Index: 257

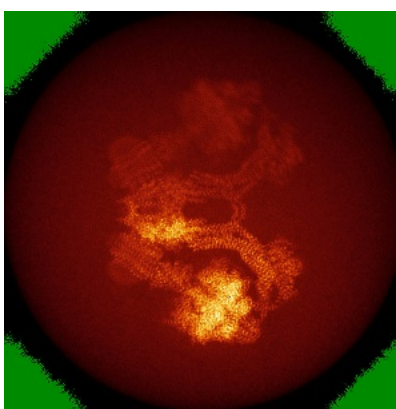
The images above show the largest variance slices of the map in three orthogonal directions.

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

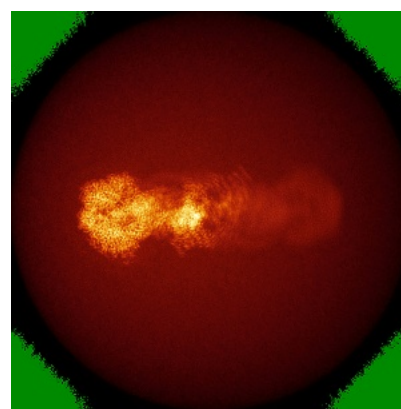
6.4.1 Primary map



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

This section was not generated.

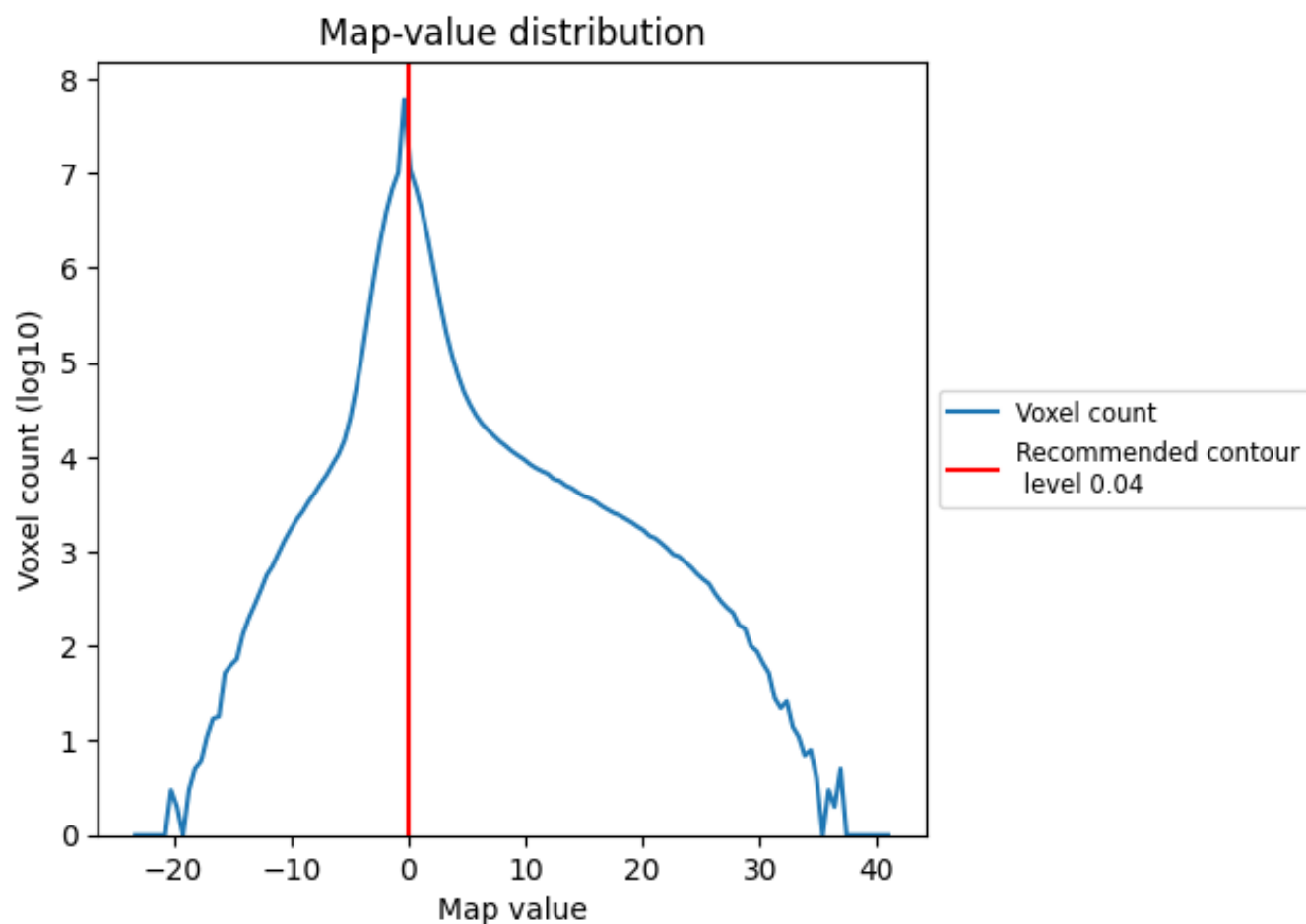
6.6 Mask visualisation

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

7 Map analysis [i](#)

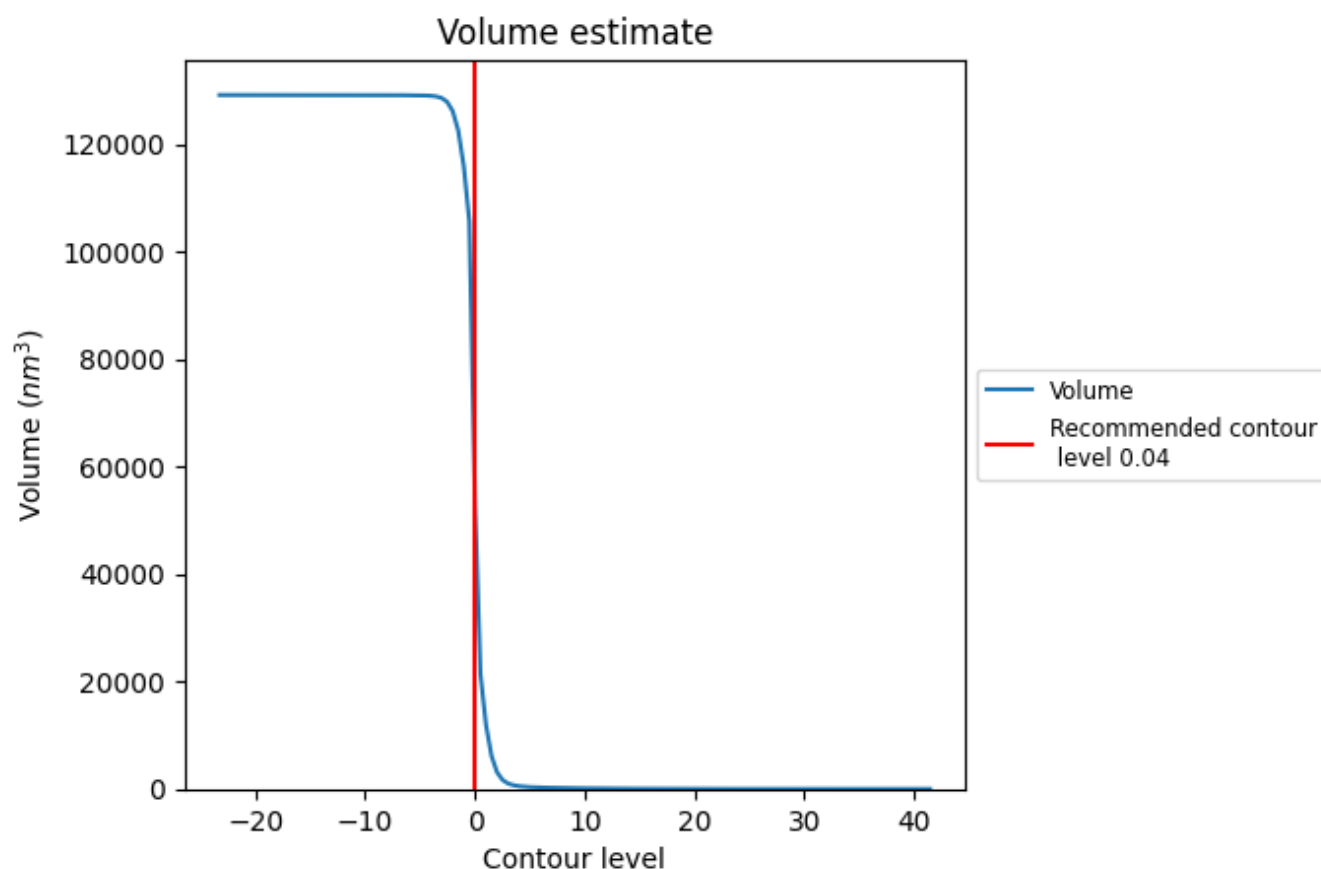
This section contains the results of statistical analysis of the map.

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.

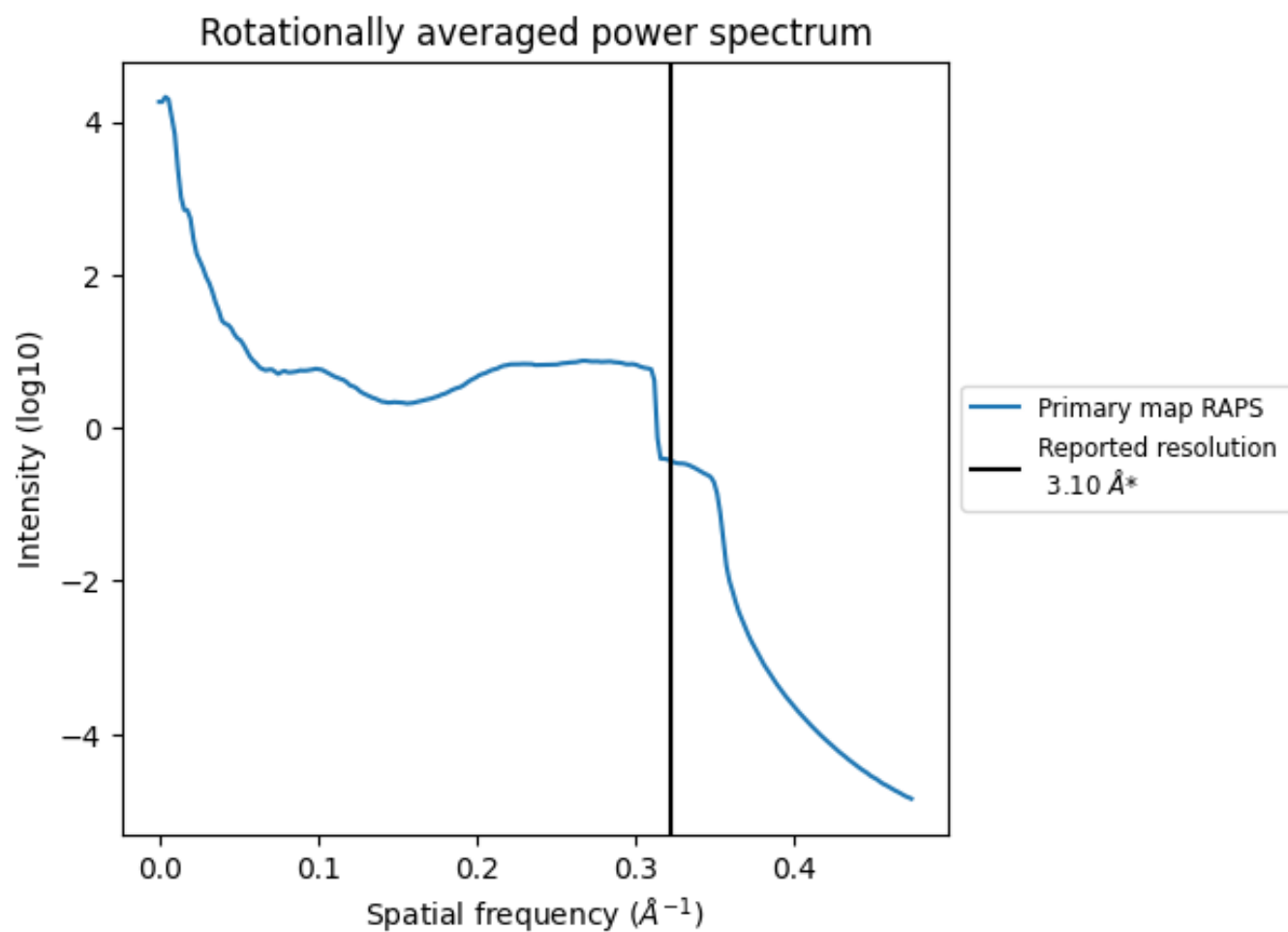
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52187 nm^3 ; this corresponds to an approximate mass of 47142 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 0.323 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

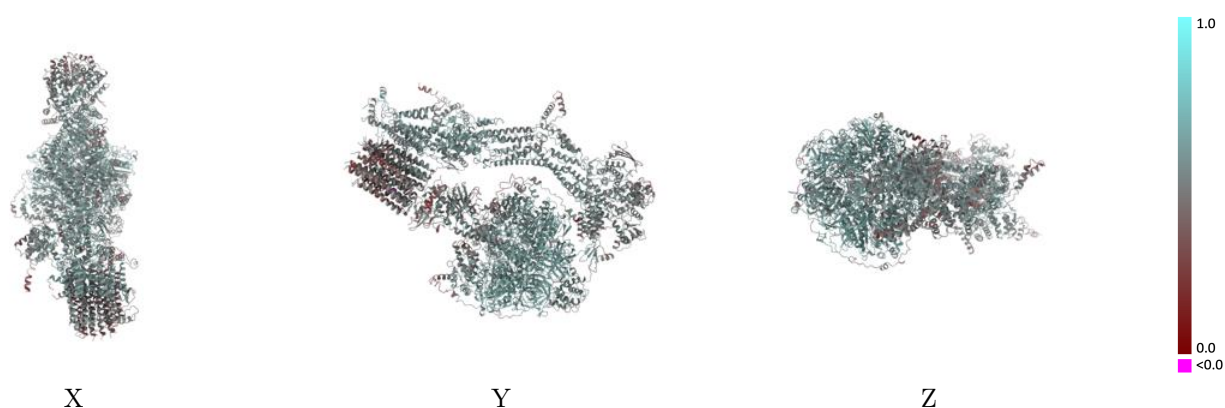
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4825 and PDB model 6RDO. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

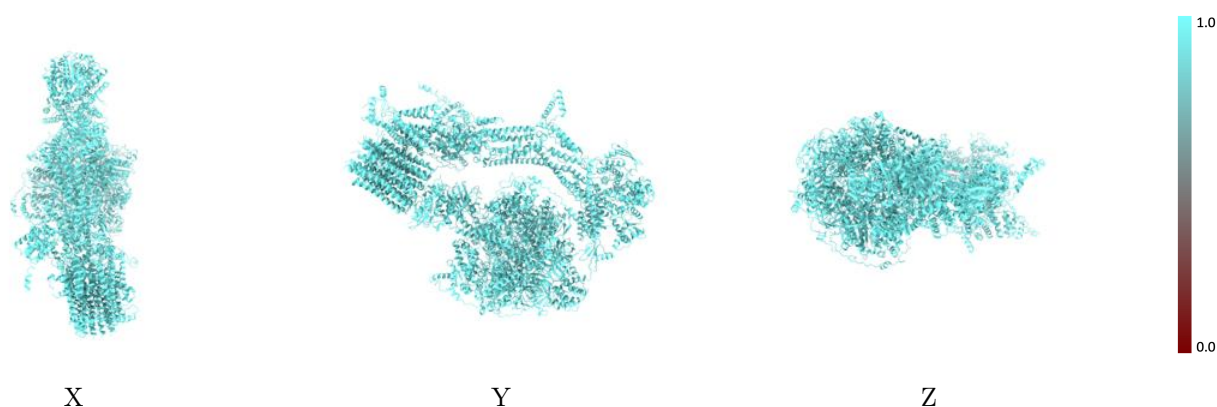
This section was not generated.

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



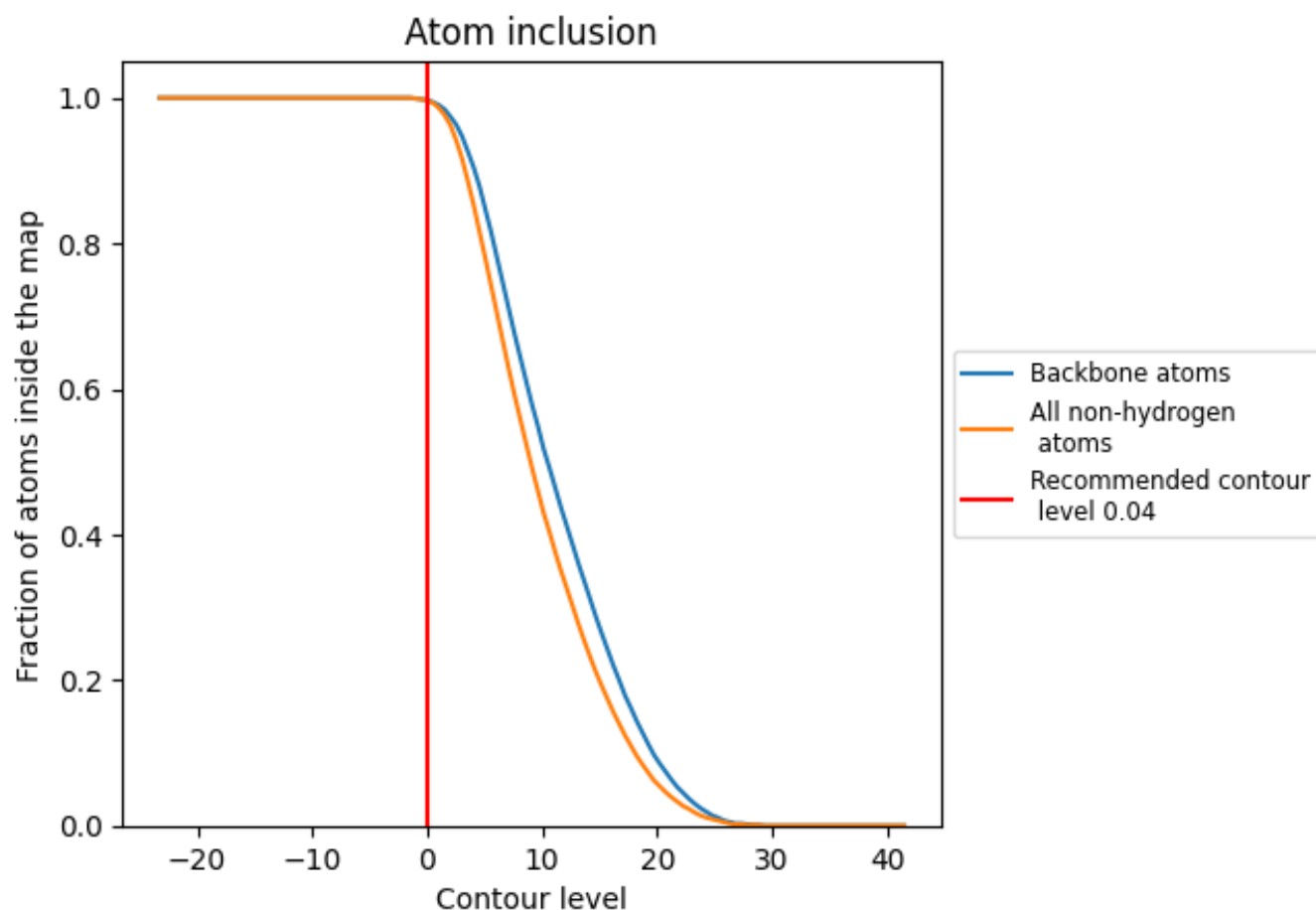
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.9960	 0.5430
0	 0.9930	 0.5530
1	 0.9970	 0.5480
2	 0.9990	 0.5010
3	 0.9990	 0.5080
4	 0.9990	 0.5180
5	 0.9980	 0.5750
6	 0.9950	 0.5590
7	 0.9980	 0.5360
8	 0.9990	 0.5750
9	 0.9970	 0.4970
A	 0.9820	 0.4770
B	 0.9800	 0.4690
C	 0.9860	 0.4530
D	 0.9820	 0.4200
E	 0.9940	 0.4310
F	 0.9940	 0.4480
G	 0.9900	 0.4170
H	 0.9860	 0.3650
I	 0.9880	 0.3960
J	 0.9730	 0.4440
M	 0.9960	 0.5570
P	 0.9940	 0.5290
Q	 0.9960	 0.4640
R	 0.9950	 0.4490
S	 0.9950	 0.5230
T	 0.9970	 0.5840
U	 0.9980	 0.5920
V	 0.9980	 0.5830
X	 0.9970	 0.5940
Y	 0.9960	 0.5690
Z	 0.9960	 0.5730

