



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:10 AM UTC

PDB ID : 6TT7 / pdb_00006tt7
EMDB ID : EMD-10573
Title : Ovine ATP synthase 1a state
Authors : Pinke, G.; Zhou, L.; Sazanov, L.A.
Deposited on : 2019-12-23
Resolution : 3.50 Å(reported)
Based on initial model : 5ARA

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:

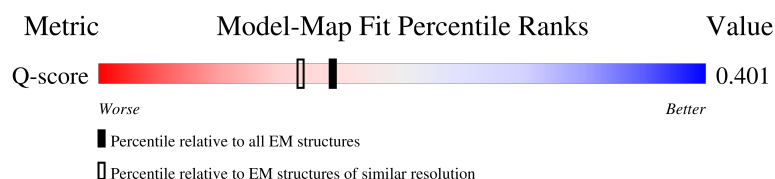
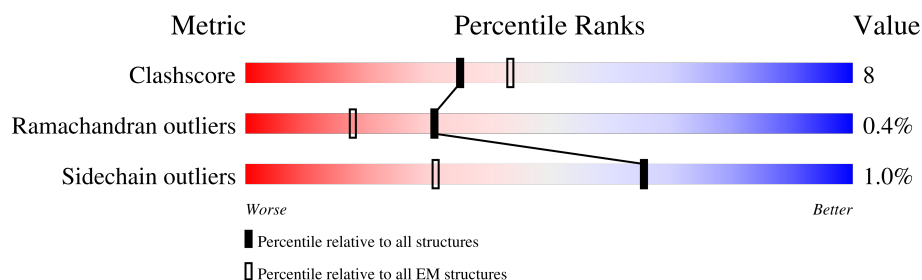
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.50 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.



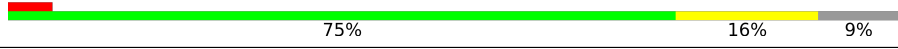
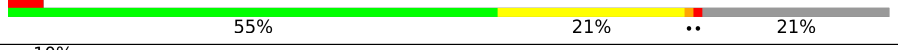
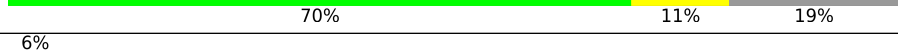
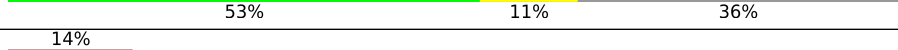
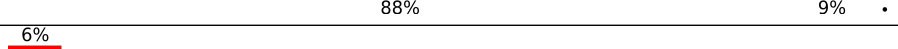
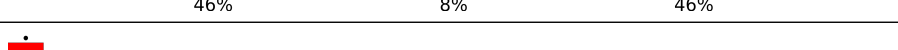
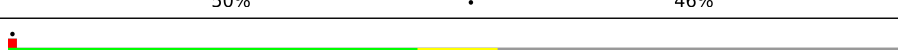
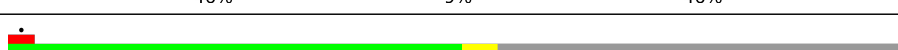
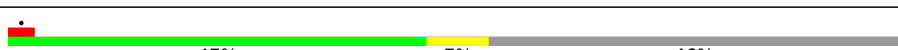
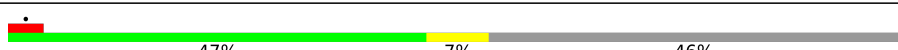
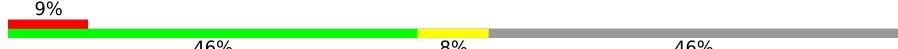
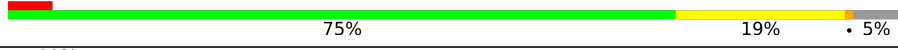
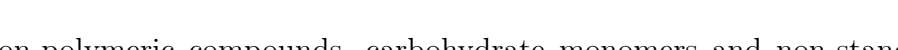
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	553	 71% 19% • 8%
1	B	553	 71% 17% • 12%
1	C	553	 6% 71% 19% • 9%
2	D	528	 66% 21% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	528	
2	F	528	
3	G	298	
4	H	168	
5	I	51	
6	J	213	
7	K	256	
8	L	108	
9	M	161	
10	1	136	
10	2	136	
10	3	136	
10	4	136	
10	5	136	
10	6	136	
10	7	136	
10	8	136	
11	N	226	
12	O	58	
13	P	60	
14	Q	66	
15	R	88	
16	S	103	
17	T	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CDL	R	301	X	-	-	-
22	CDL	R	302	X	-	-	-
22	CDL	R	303	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 40337 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	488	Total	C	N	O	S	0	0
			3724	2347	657	708	12		
1	C	503	Total	C	N	O	S	0	0
			3834	2414	675	733	12		
1	A	507	Total	C	N	O	S	0	0
			3860	2429	679	740	12		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	467	Total	C	N	O	S	0	0
			3536	2242	601	682	11		
2	D	469	Total	C	N	O	S	0	0
			3544	2246	603	684	11		
2	F	472	Total	C	N	O	S	0	0
			3570	2260	608	691	11		

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	272	Total	C	N	O	S	0	0
			2115	1330	368	409	8		

- Molecule 4 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	132	Total	C	N	O	S	0	0
			978	613	165	198	2		

- Molecule 5 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	47	Total	C	N	O	S	0	0
			368	236	66	64	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	10	LEU	VAL	conflict	UNP W5Q3H8

- Molecule 6 is a protein called ATP synthase peripheral stalk subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	188	Total	C	N	O	S	0	0
			1452	922	251	269	10		

- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	208	Total	C	N	O	S	0	0
			1689	1089	289	305	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	58	PHE	ALA	conflict	UNP W5QEA9

- Molecule 8 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	69	Total	C	N	O	S	0	0
			576	366	97	111	2		

- Molecule 9 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	156	Total	C	N	O	S	0	0
			1284	829	209	243	3		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	3	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	4	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	5	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	6	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	7	74	Total	C	N	O	S	0	0
			526	348	82	93	3		
10	8	74	Total	C	N	O	S	0	0
			526	348	82	93	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	225	Total	C	N	O	S	0	0
			1734	1150	277	295	12		

- Molecule 12 is a protein called Subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	40	Total	C	N	O	S	0	0
			327	219	53	53	2		

- Molecule 13 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	52	Total	C	N	O	S	0	0
			425	281	70	71	3		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	47	Total	C	N	O	S	0	0
			371	248	58	62	3		

- Molecule 15 is a protein called ATP synthase membrane subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	84	Total	C	N	O	S	0	0
			701	461	121	116	3		

- Molecule 16 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	85	Total	C	N	O	S	0	0
			673	448	106	118	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	96	ARG	HIS	conflict	UNP W5Q5U7
S	99	ILE	THR	conflict	UNP W5Q5U7

- Molecule 17 is a protein called Subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	70	Total	C	N	O	S	0	0
			577	364	106	106	1		

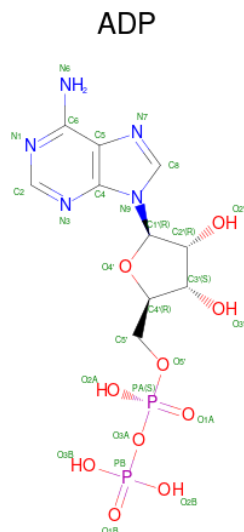
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	23	MET	VAL	conflict	UNP W5PF18
T	26	GLY	SER	conflict	UNP W5PF18
T	38	GLU	-	insertion	UNP W5PF18

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

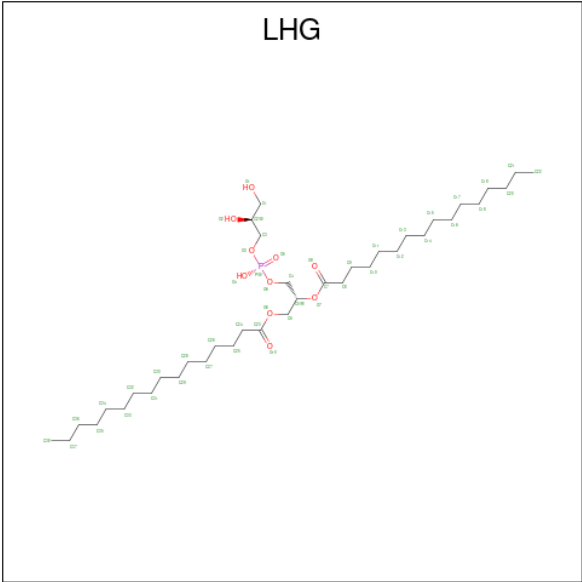
Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Mg	0
			1	1	
18	C	1	Total	Mg	0
			1	1	
18	A	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



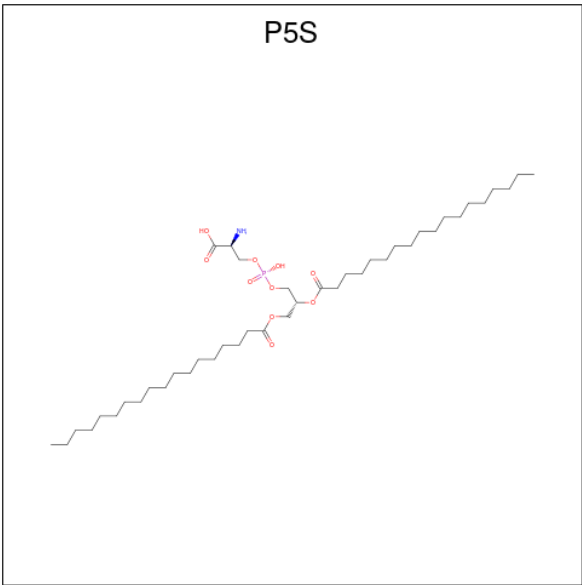
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 27	C 10	N 5	O 10	P 2	0
19	C	1	Total 27	C 10	N 5	O 10	P 2	0
19	A	1	Total 27	C 10	N 5	O 10	P 2	0
19	D	1	Total 27	C 10	N 5	O 10	P 2	0
19	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



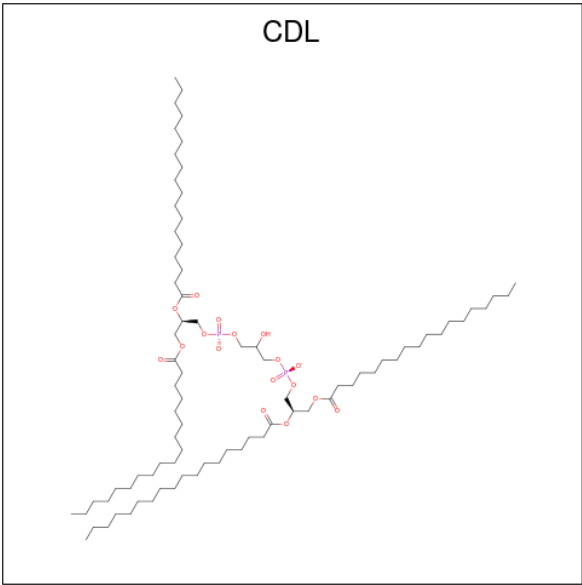
Mol	Chain	Residues	Atoms				AltConf
20	K	1	Total	C	O	P	0
			43	32	10	1	
20	K	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			45	34	10	1	
20	R	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			49	38	10	1	
20	S	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



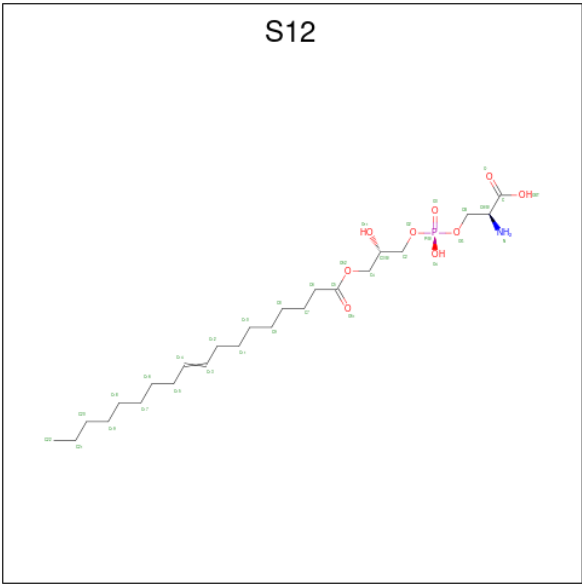
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
21	2	1	54	42	1	10	1	0

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	R	1	100	81	17	2	0
22	R	1	92	73	17	2	0
22	R	1	88	69	17	2	0

- Molecule 23 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).

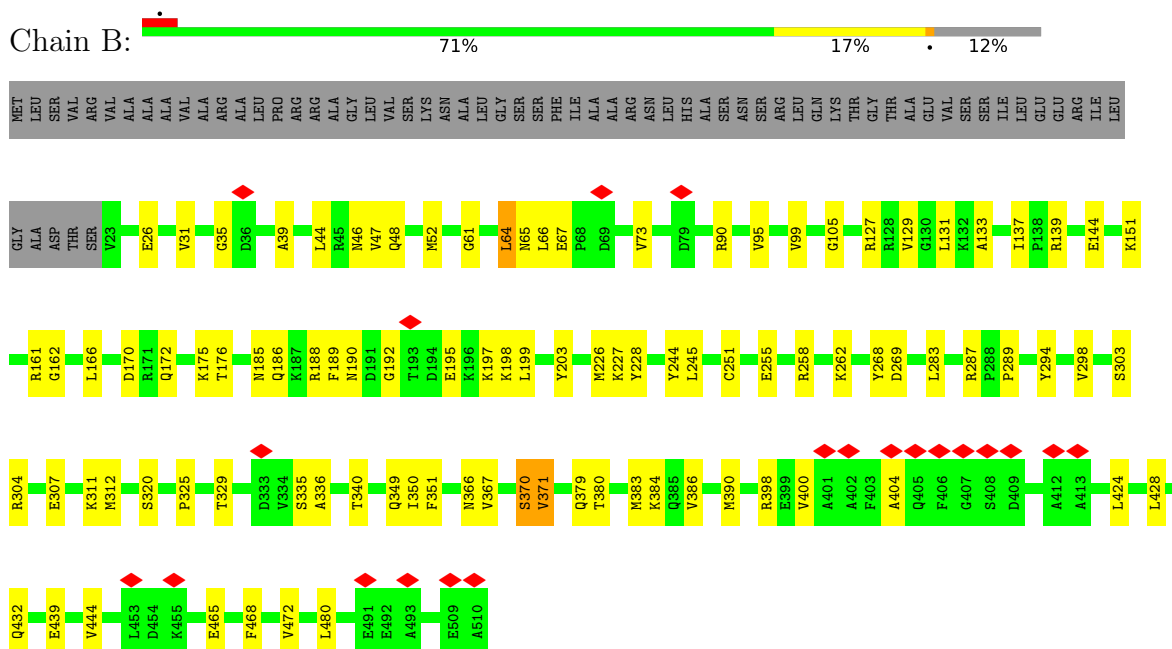


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	T	1	35	24	1	9	1	0

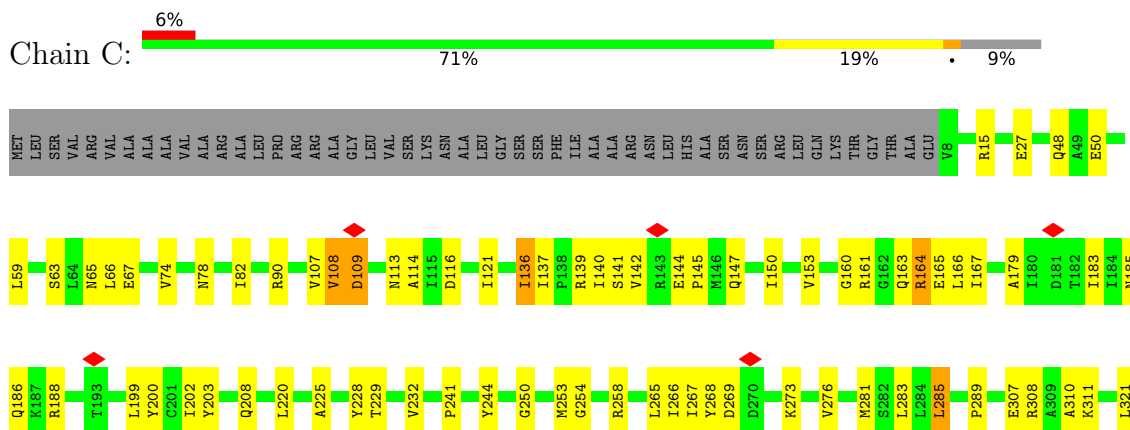
3 Residue-property plots

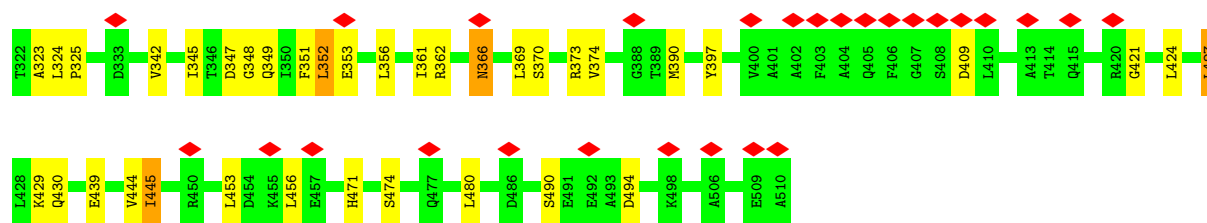
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP synthase subunit alpha



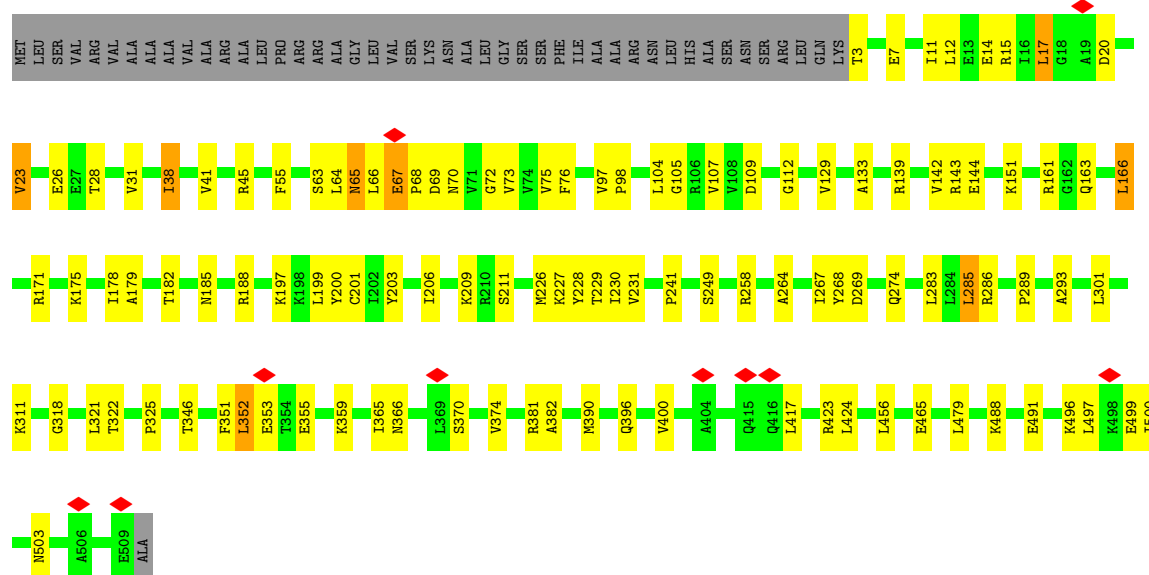
• Molecule 1: ATP synthase subunit alpha





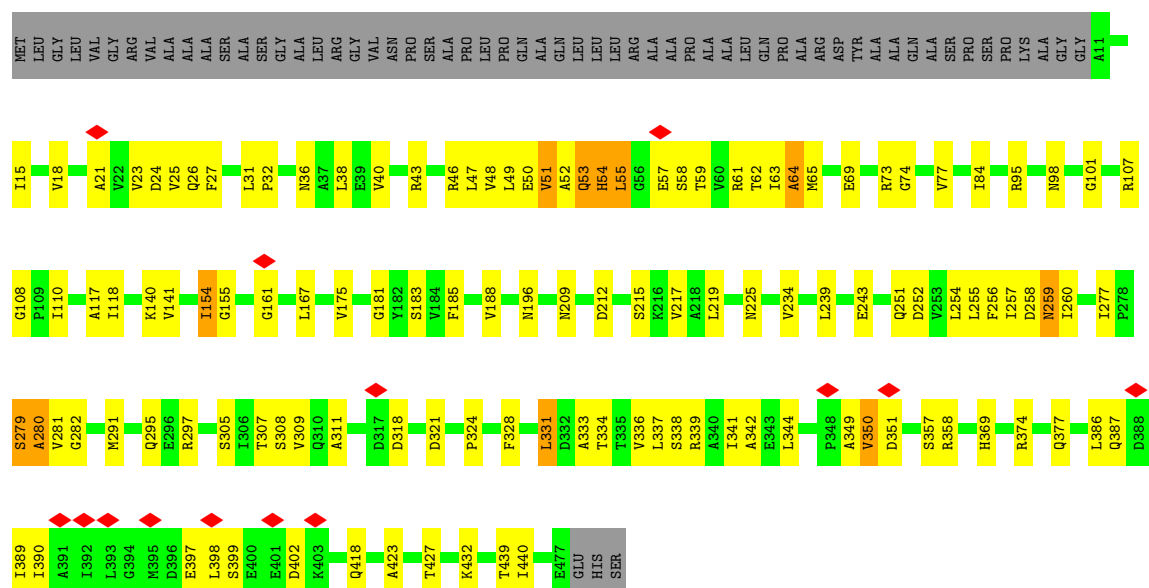
• Molecule 1: ATP synthase subunit alpha

Chain A: 71% 19% 8%

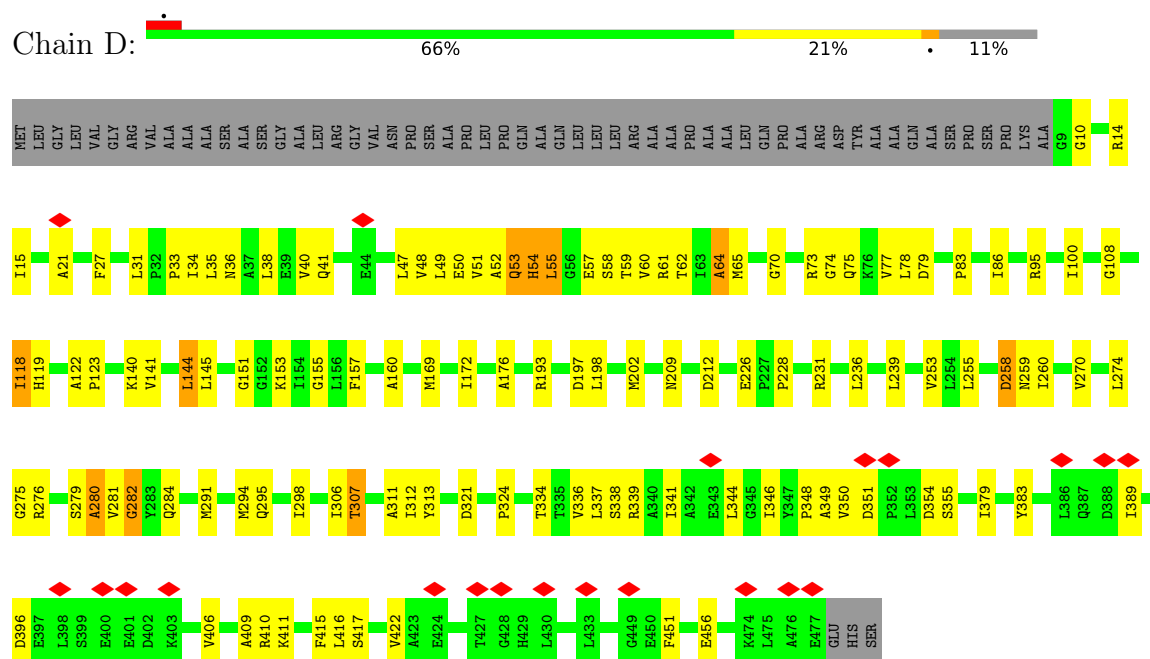


• Molecule 2: ATP synthase subunit beta

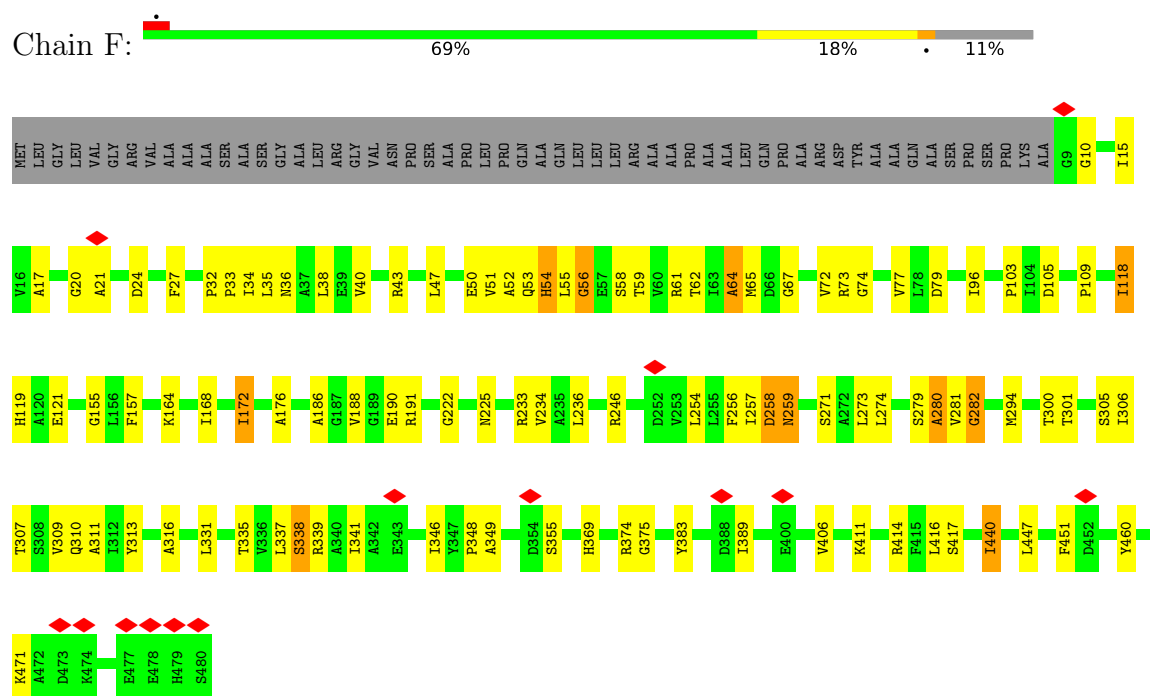
Chain E: 65% 21% 12%



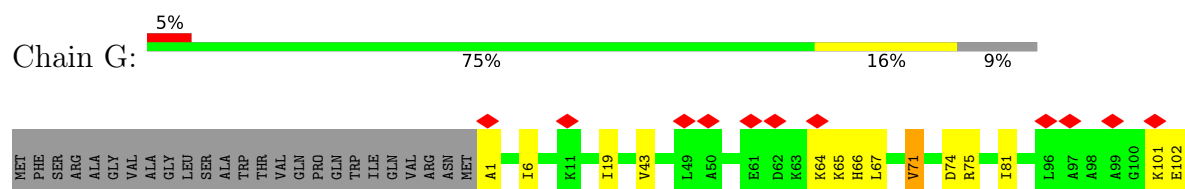
- Molecule 2: ATP synthase subunit beta

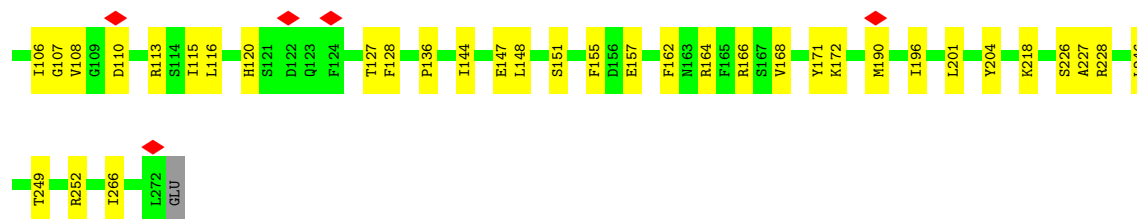


- Molecule 2: ATP synthase subunit beta

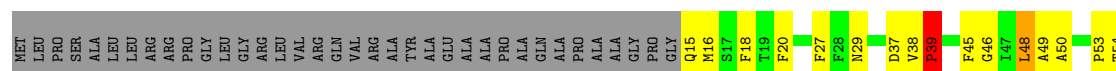


- Molecule 3: ATP synthase subunit gamma

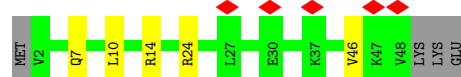
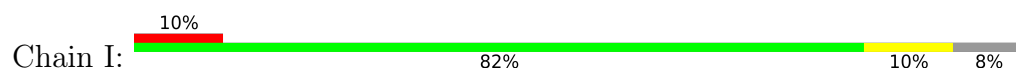




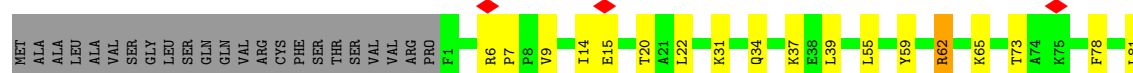
• Molecule 4: ATP synthase F1 subunit delta



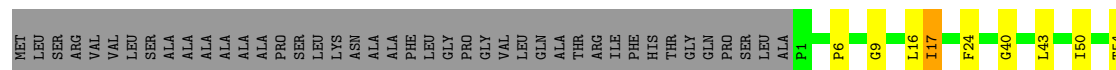
• Molecule 5: ATP synthase F1 subunit epsilon



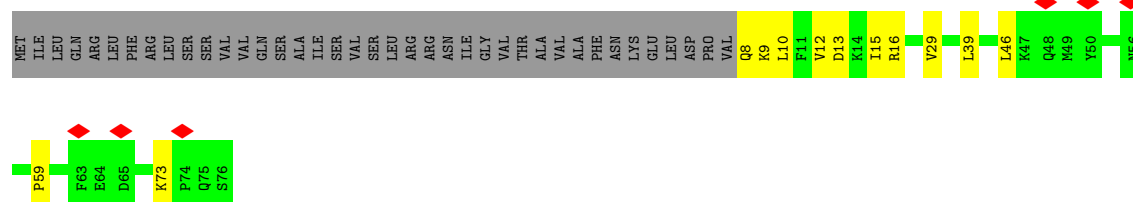
• Molecule 6: ATP synthase peripheral stalk subunit OSCP



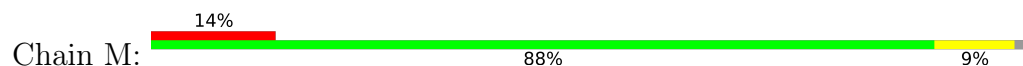
• Molecule 7: ATP synthase subunit b



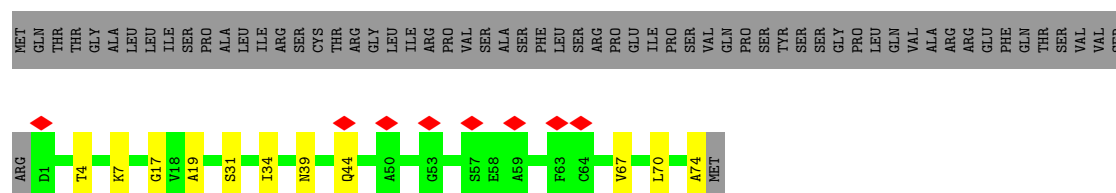
• Molecule 8: ATP synthase-coupling factor 6, mitochondrial



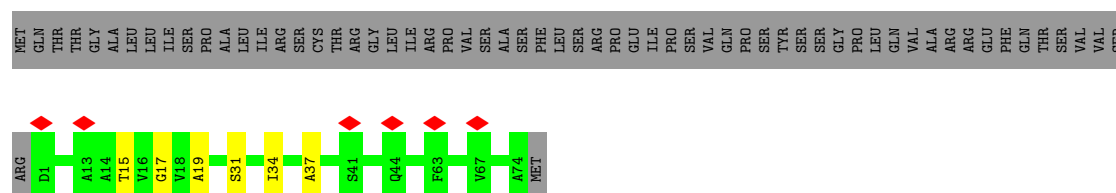
- Molecule 9: ATP synthase subunit d, mitochondrial



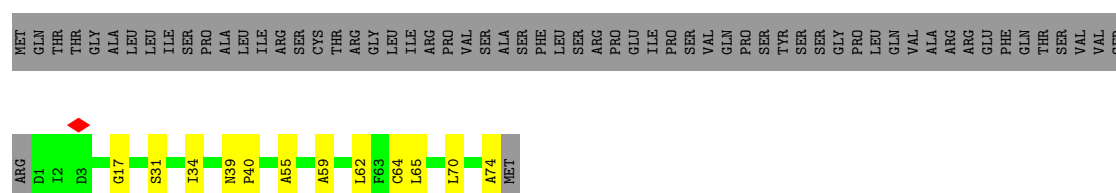
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 4:  51% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



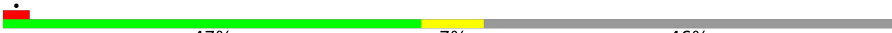
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 5:  7% 49% 5% 46%

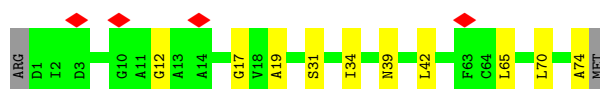
MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



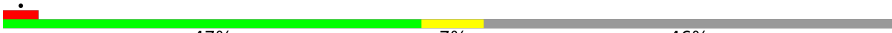
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 6:  47% 7% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 7:  47% 7% 46%

MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



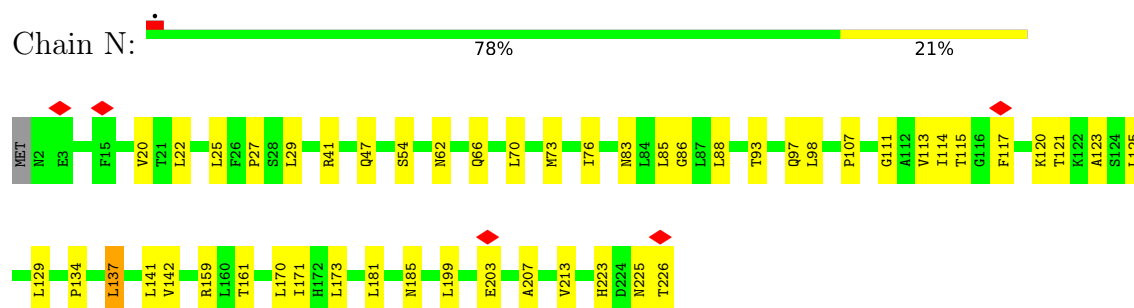
- Molecule 10: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 8:  9% 46% 8% 46%

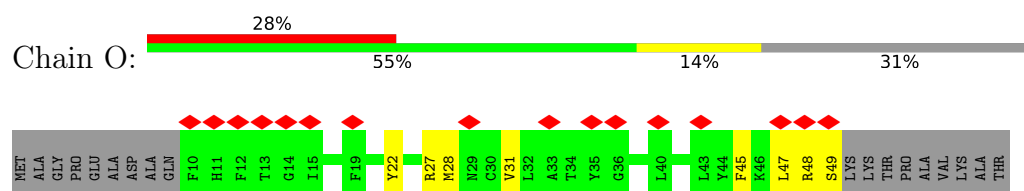
MET GLN THR THR GLY ALA LEU LEU ILE SER PRO PRO ARG ALA LEU LEU ILE ARG SER CYS THR THR ARG GLY LEU ILE ARG PRO VAL SER ALA SER PHE SER LEU SER ARG PRO PRO GLU ILE ILE PRO PRO VAL VAL GLN VAL ALA ARG ARG ARG PHE THR SER VAL VAL SER



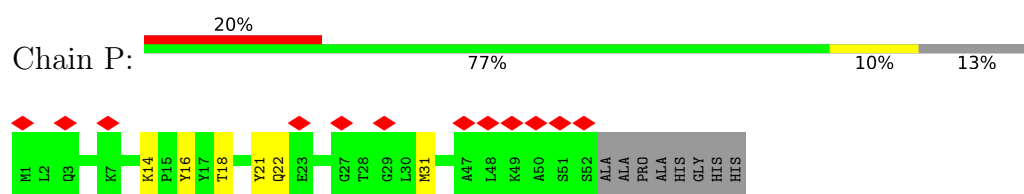
- Molecule 11: ATP synthase subunit a



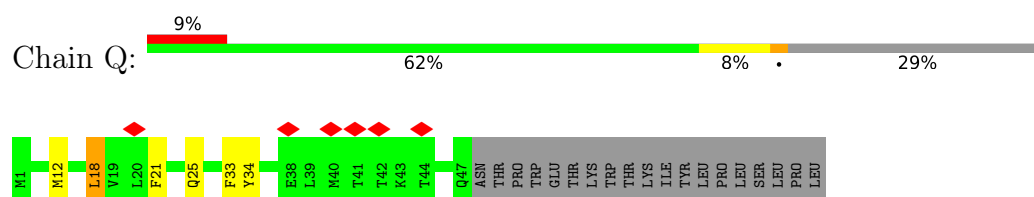
- Molecule 12: Subunit DAPIT



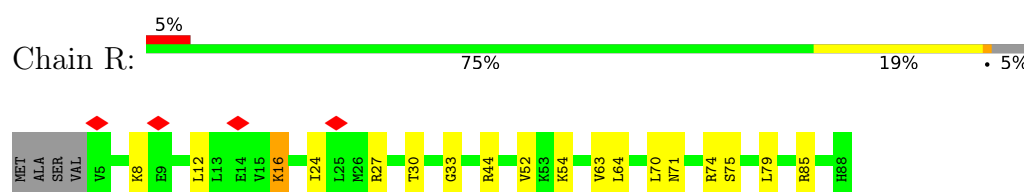
- Molecule 13: ATP synthase membrane subunit 6.8PL



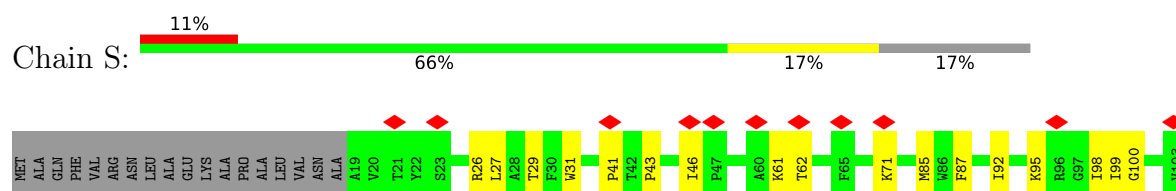
- Molecule 14: ATP synthase protein 8



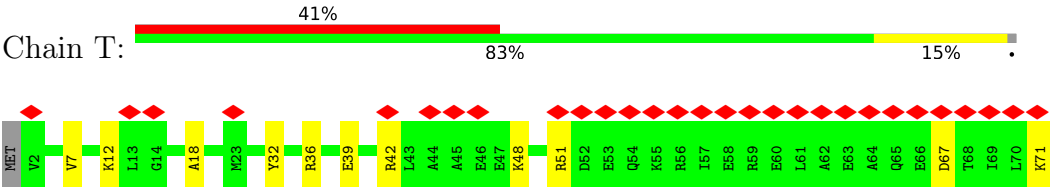
- Molecule 15: ATP synthase membrane subunit f



- Molecule 16: ATP synthase subunit



- Molecule 17: Subunit e



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35000	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 ($e^-/\text{\AA}^2$)	106	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	131951	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	146.418, 147.479, 244.03	wwPDB
Map dimensions	230, 139, 138	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, S12, CDL, ADP, P5S, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3911	0.77	6/5278 (0.1%)
1	B	0.38	0/3775	0.72	4/5092 (0.1%)
1	C	0.37	0/3885	0.75	2/5241 (0.0%)
2	D	0.35	0/3601	0.75	6/4884 (0.1%)
2	E	0.37	0/3593	0.74	2/4874 (0.0%)
2	F	0.37	0/3628	0.77	9/4919 (0.2%)
3	G	0.28	0/2141	0.68	1/2876 (0.0%)
4	H	0.31	0/990	0.75	1/1346 (0.1%)
5	I	0.23	0/373	0.54	0/499
6	J	0.29	0/1470	0.65	0/1977
7	K	0.26	0/1722	0.61	0/2321
8	L	0.27	0/589	0.72	1/788 (0.1%)
9	M	0.23	0/1315	0.53	0/1781
10	1	0.28	0/535	0.59	0/722
10	2	0.29	0/535	0.60	0/722
10	3	0.31	0/535	0.63	0/722
10	4	0.28	0/535	0.60	0/722
10	5	0.27	0/535	0.55	0/722
10	6	0.29	0/535	0.59	0/722
10	7	0.27	0/535	0.57	0/722
10	8	0.29	0/535	0.59	0/722
11	N	0.30	0/1772	0.62	2/2421 (0.1%)
12	O	0.19	0/335	0.50	0/450
13	P	0.23	0/435	0.51	0/585
14	Q	0.25	0/381	0.61	0/518
15	R	0.29	0/719	0.58	0/963
16	S	0.27	0/691	0.61	0/940
17	T	0.25	0/585	0.60	0/780
All	All	0.33	0/40191	0.70	34/54309 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	3
2	D	0	7
2	E	0	6
2	F	0	6
4	H	0	1
All	All	0	32

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	ALA	CA-C-N	8.40	134.95	120.58
2	D	64	ALA	C-N-CA	8.40	134.95	120.58
2	F	258	ASP	CA-C-N	8.20	136.45	121.70
2	F	258	ASP	C-N-CA	8.20	136.45	121.70
2	D	258	ASP	CA-C-N	7.48	135.17	121.70
2	D	258	ASP	C-N-CA	7.48	135.17	121.70
1	A	352	LEU	CA-C-N	-6.73	111.79	121.42
1	A	352	LEU	C-N-CA	-6.73	111.79	121.42
1	C	352	LEU	CA-C-N	-6.13	109.75	122.07
1	C	352	LEU	C-N-CA	-6.13	109.75	122.07
2	F	348	PRO	CA-C-N	-5.96	111.24	122.27
2	F	348	PRO	C-N-CA	-5.96	111.24	122.27
11	N	137	LEU	CA-C-N	5.93	125.07	120.33
11	N	137	LEU	C-N-CA	5.93	125.07	120.33
2	F	259	ASN	N-CA-C	-5.89	94.50	111.00
1	B	380	THR	CA-C-N	5.75	132.52	121.54
1	B	380	THR	C-N-CA	5.75	132.52	121.54
4	H	62	LEU	N-CA-C	5.58	118.92	107.37
3	G	115	ILE	N-CA-C	-5.49	107.40	112.83
2	F	64	ALA	CA-C-N	5.34	132.00	122.06
2	F	64	ALA	C-N-CA	5.34	132.00	122.06
2	F	338	SER	CA-C-N	5.26	132.15	122.79
2	F	338	SER	C-N-CA	5.26	132.15	122.79
8	L	9	LYS	N-CA-C	5.18	117.34	111.02
1	A	143	ARG	CA-C-N	-5.17	107.40	122.38
1	A	143	ARG	C-N-CA	-5.17	107.40	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	CA-C-N	5.11	131.30	121.54
1	A	23	VAL	C-N-CA	5.11	131.30	121.54
1	B	370	SER	CA-C-N	-5.04	116.88	122.27
1	B	370	SER	C-N-CA	-5.04	116.88	122.27
2	E	46	ARG	CA-C-N	-5.03	115.54	123.13
2	E	46	ARG	C-N-CA	-5.03	115.54	123.13
2	D	53	GLN	CA-C-N	5.00	130.51	122.86
2	D	53	GLN	C-N-CA	5.00	130.51	122.86

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	LYS	Peptide
1	A	64	LEU	Mainchain,Peptide
1	A	65	ASN	Peptide
1	A	67	GLU	Peptide
1	B	162	GLY	Peptide
1	B	227	LYS	Peptide
1	B	371	VAL	Peptide
1	B	64	LEU	Peptide
1	C	109	ASP	Peptide
1	C	352	LEU	Peptide
1	C	366	ASN	Peptide
2	D	118	ILE	Peptide
2	D	122	ALA	Peptide
2	D	258	ASP	Peptide
2	D	280	ALA	Peptide
2	D	54	HIS	Peptide
2	D	57	GLU	Peptide
2	D	83	PRO	Peptide
2	E	258	ASP	Peptide
2	E	397	GLU	Peptide
2	E	51	VAL	Peptide
2	E	52	ALA	Peptide
2	E	54	HIS	Peptide
2	E	64	ALA	Peptide
2	F	118	ILE	Peptide
2	F	20	GLY	Peptide
2	F	258	ASP	Peptide
2	F	280	ALA	Peptide
2	F	54	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	56	GLY	Peptide
4	H	39	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3860	0	3961	69	0
1	B	3724	0	3825	58	0
1	C	3834	0	3937	76	0
2	D	3544	0	3597	80	0
2	E	3536	0	3591	84	0
2	F	3570	0	3615	75	0
3	G	2115	0	2185	33	0
4	H	978	0	976	28	0
5	I	368	0	390	4	0
6	J	1452	0	1557	28	0
7	K	1689	0	1739	23	0
8	L	576	0	560	10	0
9	M	1284	0	1292	13	0
10	1	526	0	544	8	0
10	2	526	0	544	5	0
10	3	526	0	544	10	0
10	4	526	0	544	6	0
10	5	526	0	544	6	0
10	6	526	0	544	9	0
10	7	526	0	544	8	0
10	8	526	0	544	9	0
11	N	1734	0	1856	36	0
12	O	327	0	337	6	0
13	P	425	0	455	6	0
14	Q	371	0	357	8	0
15	R	701	0	726	15	0
16	S	673	0	701	13	0
17	T	577	0	601	7	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	27	0	12	0	0
19	B	27	0	12	2	0
19	C	27	0	12	1	0
19	D	27	0	12	0	0
19	F	27	0	12	1	0
20	2	45	0	63	0	0
20	K	92	0	133	3	0
20	R	49	0	74	2	0
20	S	98	0	148	5	0
21	2	54	0	80	2	0
22	R	280	0	422	13	0
23	T	35	0	44	1	0
All	All	40337	0	41634	650	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 8.

All (650) 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)
2:D:259:ASN:HA	2:D:311:ALA:O	1.38	1.22
2:F:259:ASN:HA	2:F:311:ALA:O	1.52	1.07
2:D:338:SER:O	2:D:349:ALA:HB3	1.54	1.05
2:F:338:SER:O	2:F:349:ALA:HB3	1.54	1.04
1:B:199:LEU:O	1:B:228:TYR:HB3	1.59	1.02
2:D:10:GLY:HA2	2:D:79:ASP:O	1.64	0.97
2:E:27:PHE:O	2:E:58:SER:HB2	1.65	0.97
2:E:338:SER:O	2:E:349:ALA:HB3	1.66	0.95
4:H:16:MET:HA	4:H:88:SER:O	1.70	0.91
1:A:199:LEU:O	1:A:228:TYR:HB3	1.75	0.85
6:J:115:GLU:HA	6:J:147:VAL:O	1.74	0.85
1:C:199:LEU:O	1:C:228:TYR:HB3	1.76	0.85
2:F:21:ALA:HA	2:F:64:ALA:H	1.42	0.83
2:F:27:PHE:O	2:F:58:SER:HA	1.81	0.81
2:E:21:ALA:O	2:E:63:ILE:HA	1.82	0.78
2:D:54:HIS:HA	2:D:59:THR:O	1.83	0.78
4:H:15:GLN:O	4:H:88:SER:HB2	1.85	0.76
2:E:259:ASN:HA	2:E:311:ALA:O	1.86	0.76
3:G:66:HIS:HA	3:G:157:GLU:O	1.87	0.74
2:D:27:PHE:O	2:D:58:SER:HB2	1.87	0.74
2:E:336:VAL:O	2:E:350:VAL:HA	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:70:LEU:O	10:5:74:ALA:HB3	1.88	0.73
2:F:54:HIS:HA	2:F:59:THR:O	1.88	0.72
10:3:70:LEU:O	10:3:74:ALA:HB3	1.88	0.72
1:C:362:ARG:HH22	2:F:374:ARG:HD2	1.57	0.70
2:D:21:ALA:HA	2:D:64:ALA:H	1.56	0.69
2:E:21:ALA:HA	2:E:64:ALA:O	1.93	0.69
1:C:164:ARG:HA	1:C:323:ALA:O	1.93	0.68
2:D:259:ASN:CA	2:D:311:ALA:O	2.30	0.68
2:E:36:ASN:O	2:E:50:GLU:HA	1.92	0.68
2:E:50:GLU:O	2:E:62:THR:HA	1.93	0.68
2:F:259:ASN:CA	2:F:311:ALA:O	2.36	0.67
2:E:40:VAL:HB	2:E:47:LEU:HB3	1.75	0.67
2:F:54:HIS:C	2:F:59:THR:O	2.37	0.67
2:D:40:VAL:HB	2:D:47:LEU:HB3	1.77	0.67
2:F:346:ILE:HG23	2:F:417:SER:HB3	1.77	0.67
1:C:347:ASP:OD2	2:D:193:ARG:NH1	2.29	0.66
1:B:268:TYR:HB2	1:B:325:PRO:HA	1.77	0.66
2:F:40:VAL:HB	2:F:47:LEU:HB3	1.77	0.66
10:6:19:ALA:HB2	10:7:17:GLY:HA2	1.77	0.66
1:B:144:GLU:HB2	1:B:161:ARG:HB2	1.76	0.66
2:D:141:VAL:HG11	2:D:350:VAL:HG11	1.78	0.66
2:D:54:HIS:CA	2:D:59:THR:O	2.44	0.65
2:D:54:HIS:C	2:D:59:THR:O	2.40	0.65
2:F:27:PHE:O	2:F:58:SER:CA	2.45	0.64
2:E:31:LEU:HD13	2:E:58:SER:HB3	1.78	0.64
2:F:300:THR:HG23	2:F:305:SER:HA	1.78	0.64
7:K:6:PRO:HG2	15:R:52:VAL:HG12	1.78	0.64
2:F:15:ILE:O	2:F:74:GLY:N	2.30	0.64
1:B:251:CYS:SG	1:B:268:TYR:OH	2.56	0.64
2:F:369:HIS:HD2	2:F:440:ILE:HD11	1.63	0.64
2:F:54:HIS:CA	2:F:59:THR:O	2.45	0.64
2:D:50:GLU:HB2	2:D:65:MET:HE1	1.80	0.63
1:B:137:ILE:HG13	2:F:105:ASP:HA	1.80	0.63
1:A:144:GLU:HB2	1:A:161:ARG:HB2	1.80	0.63
2:F:21:ALA:CA	2:F:64:ALA:H	2.11	0.63
2:F:96:ILE:HD12	2:F:105:ASP:HB3	1.81	0.63
1:A:423:ARG:NH2	1:A:456:LEU:O	2.32	0.63
1:C:59:LEU:HD11	1:C:82:ILE:HD11	1.81	0.62
1:C:351:PHE:H	1:C:370:SER:HB3	1.63	0.62
4:H:136:GLU:HA	4:H:139:GLU:HG2	1.81	0.62
2:F:10:GLY:HA2	2:F:79:ASP:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:ASN:O	2:F:50:GLU:HA	2.00	0.62
4:H:39:PRO:HB2	4:H:62:LEU:H	1.63	0.62
1:C:144:GLU:HB2	1:C:161:ARG:HB2	1.82	0.62
1:B:133:ALA:HB3	2:F:225:ASN:HD22	1.65	0.62
1:B:170:ASP:O	1:B:175:LYS:NZ	2.32	0.62
1:C:66:LEU:HD23	2:D:73:ARG:HG3	1.83	0.61
2:D:14:ARG:HA	2:D:75:GLN:O	2.00	0.61
11:N:97:GLN:HG3	14:Q:12:MET:HE3	1.83	0.61
1:C:349:GLN:NE2	1:C:369:LEU:O	2.33	0.61
2:E:54:HIS:HA	2:E:59:THR:O	2.00	0.61
7:K:172:HIS:NE2	8:L:29:VAL:O	2.31	0.61
4:H:48:LEU:HD23	4:H:49:ALA:H	1.64	0.61
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.34	0.60
7:K:79:GLY:O	11:N:41:ARG:NH2	2.34	0.60
1:A:161:ARG:HH12	1:A:197:LYS:HA	1.67	0.60
10:4:66:MET:HG2	11:N:170:LEU:HD13	1.84	0.60
2:E:15:ILE:O	2:E:74:GLY:N	2.34	0.60
20:S:201:LHG:H172	20:S:201:LHG:H371	1.84	0.60
2:D:34:ILE:HG23	2:D:52:ALA:HA	1.84	0.60
1:B:349:GLN:HG3	1:B:371:VAL:HG12	1.83	0.60
7:K:54:THR:HG22	7:K:56:GLU:H	1.67	0.60
22:R:301:CDL:H851	22:R:301:CDL:H381	1.84	0.60
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.84	0.60
10:7:19:ALA:HB2	10:8:17:GLY:HA2	1.84	0.60
2:E:95:ARG:NH2	2:E:108:GLY:O	2.35	0.60
10:6:31:SER:HA	10:6:34:ILE:HG22	1.84	0.59
1:B:390:MET:HE3	1:B:424:LEU:HD12	1.84	0.59
11:N:29:LEU:HD21	22:R:302:CDL:H162	1.84	0.59
1:B:251:CYS:O	1:B:255:GLU:HB2	2.02	0.59
1:B:350:ILE:HA	1:B:371:VAL:O	2.02	0.59
1:C:185:ASN:OD1	1:C:188:ARG:NH2	2.36	0.59
22:R:303:CDL:H351	22:R:303:CDL:H211	1.83	0.59
2:D:226:GLU:O	2:D:231:ARG:NH1	2.36	0.59
1:A:390:MET:HE2	1:A:424:LEU:HB3	1.85	0.59
2:D:31:LEU:HD13	2:D:58:SER:HB3	1.84	0.59
9:M:15:ALA:O	9:M:19:ILE:HB	2.02	0.59
1:A:63:SER:HA	1:A:73:VAL:HA	1.85	0.59
2:F:27:PHE:O	2:F:58:SER:CB	2.51	0.59
3:G:166:ARG:HE	3:G:172:LYS:HB2	1.68	0.59
16:S:41:PRO:HG3	17:T:12:LYS:HE2	1.84	0.59
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:ILE:HG12	2:D:409:ALA:HB2	1.84	0.59
1:A:65:ASN:O	1:A:72:GLY:N	2.36	0.58
2:D:172:ILE:O	2:D:176:ALA:HB3	2.04	0.58
2:E:54:HIS:C	2:E:59:THR:O	2.47	0.58
16:S:87:PHE:HB2	17:T:18:ALA:HB1	1.85	0.58
2:E:31:LEU:HD12	2:E:32:PRO:HD2	1.83	0.58
2:E:336:VAL:HB	2:E:351:ASP:HB2	1.85	0.58
4:H:66:HIS:ND1	4:H:71:THR:O	2.37	0.58
11:N:25:LEU:HB3	22:R:302:CDL:H341	1.86	0.58
1:A:151:LYS:NZ	1:A:465:GLU:OE2	2.34	0.58
10:7:31:SER:HA	10:7:34:ILE:HG22	1.86	0.58
2:F:43:ARG:NH2	2:F:67:GLY:O	2.37	0.58
23:T:201:S12:H27	23:T:201:S12:H7	1.86	0.58
2:E:140:LYS:HG2	2:E:439:THR:HG22	1.85	0.57
2:F:280:ALA:O	2:F:282:GLY:N	2.34	0.57
2:E:84:ILE:O	2:E:117:ALA:HA	2.04	0.57
2:D:155:GLY:O	2:D:334:THR:HA	2.04	0.57
10:7:70:LEU:O	10:7:74:ALA:HB3	2.04	0.57
1:C:140:ILE:O	1:C:311:LYS:HB3	2.04	0.57
2:D:253:VAL:O	2:D:306:ILE:HA	2.04	0.57
10:8:7:LYS:NZ	10:8:72:LEU:O	2.38	0.57
2:F:341:ILE:HG22	2:F:346:ILE:HB	1.87	0.57
1:B:64:LEU:HD23	1:B:65:ASN:H	1.70	0.57
1:C:145:PRO:HB2	1:C:147:GLN:HE21	1.69	0.57
1:A:107:VAL:HG22	1:A:231:VAL:HB	1.87	0.57
3:G:75:ARG:O	3:G:228:ARG:NH2	2.38	0.57
10:1:44:GLN:NE2	12:O:22:TYR:OH	2.37	0.57
1:C:67:GLU:O	2:D:73:ARG:NH1	2.37	0.57
1:C:307:GLU:HG3	1:C:345:ILE:HD11	1.85	0.57
4:H:53:PRO:HA	4:H:84:VAL:HG23	1.86	0.57
1:B:383:MET:HA	1:B:386:VAL:HG12	1.87	0.57
1:A:286:ARG:NH2	2:D:275:GLY:O	2.38	0.57
2:D:15:ILE:O	2:D:74:GLY:N	2.31	0.57
11:N:25:LEU:HD21	14:Q:18:LEU:HD12	1.87	0.57
1:C:74:VAL:HG11	1:C:281:MET:HE3	1.86	0.56
1:A:3:THR:HG23	6:J:14:ILE:HD11	1.87	0.56
1:A:67:GLU:O	1:A:69:ASP:N	2.38	0.56
1:A:479:LEU:HD13	1:A:496:LYS:HD3	1.87	0.56
2:F:38:LEU:HD22	2:F:51:VAL:HG23	1.87	0.56
4:H:96:GLU:OE2	5:I:24:ARG:NH2	2.38	0.56
15:R:75:SER:O	15:R:79:LEU:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:30:THR:HG23	15:R:33:GLY:H	1.68	0.56
1:C:50:GLU:HA	1:C:63:SER:O	2.05	0.56
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.87	0.56
2:E:399:SER:H	2:E:402:ASP:HB3	1.71	0.56
1:C:183:ILE:HG23	1:C:228:TYR:HE2	1.70	0.56
1:A:355:GLU:O	1:A:359:LYS:HB2	2.05	0.56
2:F:34:ILE:HG23	2:F:52:ALA:HA	1.87	0.56
10:3:31:SER:HA	10:3:34:ILE:HG22	1.87	0.56
14:Q:21:PHE:O	14:Q:25:GLN:CB	2.54	0.56
20:S:201:LHG:H111	20:S:201:LHG:H282	1.87	0.56
2:D:209:ASN:ND2	2:D:212:ASP:OD1	2.39	0.56
6:J:31:LYS:HD2	6:J:81:LEU:HD23	1.86	0.56
10:8:31:SER:HA	10:8:34:ILE:HG22	1.88	0.56
1:A:133:ALA:HB3	2:E:225:ASN:HD22	1.71	0.56
7:K:16:LEU:HD12	7:K:17:ILE:HG23	1.88	0.56
1:C:147:GLN:O	1:C:186:GLN:NE2	2.39	0.56
10:2:31:SER:HA	10:2:34:ILE:HG22	1.86	0.56
16:S:61:LYS:HG3	16:S:62:THR:HG23	1.87	0.56
2:D:396:ASP:HB3	3:G:75:ARG:HD2	1.87	0.55
1:B:294:TYR:HB3	1:B:298:VAL:HG21	1.88	0.55
21:2:201:P5S:H33A	21:2:201:P5S:H52A	1.88	0.55
2:E:53:GLN:OE1	2:E:61:ARG:NH1	2.39	0.55
2:F:335:THR:HA	2:F:355:SER:HB2	1.88	0.55
17:T:48:LYS:HD2	17:T:51:ARG:HD2	1.88	0.55
1:C:390:MET:HG3	1:C:424:LEU:HD13	1.89	0.55
2:D:36:ASN:O	2:D:50:GLU:HA	2.05	0.55
2:D:95:ARG:NH2	2:D:108:GLY:O	2.39	0.55
3:G:164:ARG:HH21	3:G:166:ARG:HD3	1.71	0.55
10:6:70:LEU:O	10:6:74:ALA:HB3	2.06	0.55
1:B:379:GLN:HB2	1:B:384:LYS:HE3	1.89	0.55
11:N:86:GLY:HA3	11:N:93:THR:HG22	1.89	0.55
16:S:27:LEU:O	16:S:31:TRP:N	2.37	0.55
1:C:220:LEU:HD13	1:C:229:THR:HG21	1.89	0.55
15:R:85:ARG:NH2	16:S:99:ILE:O	2.39	0.55
2:E:95:ARG:HE	2:E:110:ILE:HG12	1.72	0.55
1:B:31:VAL:O	6:J:59:TYR:OH	2.25	0.55
2:E:418:GLN:NE2	2:E:432:LYS:O	2.40	0.55
16:S:92:ILE:HD12	16:S:95:LYS:HD3	1.88	0.55
2:D:280:ALA:O	2:D:282:GLY:N	2.39	0.55
6:J:98:THR:HA	6:J:101:VAL:HG12	1.88	0.55
2:E:155:GLY:O	2:E:334:THR:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1:31:SER:HA	10:1:34:ILE:HG22	1.88	0.55
11:N:41:ARG:NE	15:R:54:LYS:O	2.38	0.55
1:B:67:GLU:O	2:F:73:ARG:NH1	2.40	0.54
2:E:38:LEU:HB2	2:E:49:LEU:HB2	1.89	0.54
2:E:53:GLN:O	2:E:59:THR:O	2.24	0.54
2:F:341:ILE:HB	2:F:349:ALA:HB1	1.88	0.54
7:K:204:LEU:HA	7:K:207:LYS:HG2	1.89	0.54
9:M:145:LEU:HB3	9:M:155:HIS:HB2	1.89	0.54
1:A:258:ARG:HD3	1:A:321:LEU:HB2	1.90	0.54
2:D:38:LEU:HB2	2:D:49:LEU:HB2	1.89	0.54
2:E:374:ARG:NH2	2:E:377:GLN:OE1	2.40	0.54
2:D:270:VAL:O	2:D:274:LEU:N	2.40	0.54
1:A:499:GLU:OE2	1:A:503:ASN:ND2	2.40	0.54
9:M:84:ASP:OD2	9:M:87:THR:OG1	2.23	0.54
1:A:201:CYS:HB2	1:A:229:THR:HG22	1.90	0.54
8:L:73:LYS:NZ	9:M:93:GLU:OE2	2.41	0.54
2:F:17:ALA:HB3	2:F:24:ASP:HB2	1.89	0.54
10:6:65:LEU:HD11	10:7:67:VAL:HG21	1.89	0.54
17:T:32:TYR:OH	17:T:36:ARG:NH2	2.41	0.54
2:E:54:HIS:CA	2:E:59:THR:O	2.56	0.54
2:D:21:ALA:CA	2:D:64:ALA:H	2.19	0.54
15:R:63:VAL:HG22	22:R:303:CDL:H591	1.89	0.54
1:B:439:GLU:HG3	1:B:480:LEU:HB3	1.90	0.54
1:A:163:GLN:O	1:A:322:THR:HA	2.08	0.54
1:C:136:ILE:HD12	1:C:137:ILE:HG12	1.90	0.54
1:A:14:GLU:HA	1:A:17:LEU:HD22	1.89	0.54
4:H:59:ARG:HH11	4:H:60:PRO:HD2	1.72	0.53
1:C:166:LEU:HD23	1:C:325:PRO:HG2	1.90	0.53
14:Q:21:PHE:O	14:Q:25:GLN:HB2	2.07	0.53
1:C:139:ARG:NH2	1:C:307:GLU:O	2.36	0.53
1:A:15:ARG:NH1	6:J:91:GLU:OE1	2.39	0.53
2:D:169:MET:HB3	2:D:422:VAL:HG21	1.90	0.53
4:H:50:ALA:HB3	10:7:41:SER:HB2	1.89	0.53
1:C:166:LEU:HD21	1:C:342:VAL:HG12	1.90	0.53
1:C:203:TYR:OH	1:C:269:ASP:OD2	2.26	0.53
1:A:66:LEU:C	1:A:70:ASN:O	2.51	0.53
6:J:22:LEU:HG	6:J:85:LEU:HD22	1.89	0.53
6:J:55:LEU:O	6:J:65:LYS:NZ	2.42	0.53
2:E:84:ILE:HB	2:E:118:ILE:HG12	1.91	0.53
2:F:257:ILE:O	2:F:310:GLN:HA	2.09	0.53
21:2:201:P5S:H24	21:2:201:P5S:H43A	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:ALA:O	2:E:282:GLY:N	2.42	0.53
2:F:21:ALA:HA	2:F:64:ALA:N	2.17	0.53
2:F:32:PRO:HG2	2:F:51:VAL:HG21	1.91	0.53
10:1:19:ALA:HB2	10:2:17:GLY:HA2	1.90	0.53
2:D:51:VAL:HA	2:D:62:THR:HG22	1.90	0.53
2:D:346:ILE:HG23	2:D:417:SER:HB2	1.91	0.53
2:F:460:TYR:O	2:F:471:LYS:NZ	2.41	0.53
15:R:85:ARG:HD2	16:S:100:GLY:HA3	1.90	0.53
1:C:199:LEU:O	1:C:228:TYR:CB	2.51	0.53
2:E:95:ARG:HH12	2:E:107:ARG:HB2	1.73	0.53
2:F:279:SER:OG	2:F:280:ALA:N	2.41	0.53
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.90	0.53
1:C:65:ASN:HD22	1:C:285:LEU:HG	1.74	0.53
1:A:12:LEU:HG	6:J:88:LEU:HD21	1.91	0.53
2:D:341:ILE:HG22	2:D:346:ILE:HB	1.90	0.53
6:J:183:SER:HA	6:J:186:MET:HG2	1.91	0.53
11:N:181:LEU:O	11:N:185:ASN:N	2.40	0.53
1:C:139:ARG:HD3	1:C:310:ALA:HB3	1.91	0.52
2:D:239:LEU:HD22	2:D:298:ILE:HB	1.91	0.52
2:D:294:MET:SD	2:D:295:GLN:NE2	2.77	0.52
10:4:31:SER:HA	10:4:34:ILE:HG22	1.90	0.52
9:M:153:TRP:HB3	11:N:70:LEU:HB2	1.91	0.52
2:F:50:GLU:O	2:F:62:THR:HA	2.09	0.52
2:D:41:GLN:HE22	2:D:78:LEU:HB2	1.74	0.52
3:G:65:LYS:HB2	3:G:155:PHE:HA	1.90	0.52
2:E:38:LEU:O	2:E:48:VAL:HA	2.10	0.52
2:D:260:ILE:HG13	2:D:312:ILE:HG12	1.92	0.52
4:H:46:GLY:H	10:6:39:ASN:HA	1.75	0.52
20:K:302:LHG:H321	20:K:302:LHG:H122	1.91	0.52
10:1:70:LEU:O	10:1:74:ALA:HB3	2.09	0.52
2:F:33:PRO:O	2:F:36:ASN:ND2	2.42	0.52
2:E:256:PHE:HA	2:E:309:VAL:O	2.10	0.52
11:N:98:LEU:HA	11:N:161:THR:HG21	1.91	0.52
1:B:303:SER:O	1:B:307:GLU:HB2	2.09	0.52
2:F:164:LYS:NZ	19:F:600:ADP:O1B	2.38	0.52
11:N:20:VAL:HG21	14:Q:12:MET:HE1	1.92	0.52
2:D:351:ASP:O	2:D:355:SER:OG	2.26	0.52
22:R:302:CDL:H181	22:R:303:CDL:H601	1.90	0.52
2:F:10:GLY:CA	2:F:79:ASP:O	2.57	0.52
7:K:9:GLY:HA3	15:R:52:VAL:HG11	1.91	0.52
17:T:7:VAL:HG23	17:T:12:LYS:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:PRO:HA	1:C:244:TYR:HB3	1.92	0.51
1:A:353:GLU:HG2	1:A:366:ASN:HB3	1.92	0.51
1:A:497:LEU:HA	1:A:500:ILE:HG22	1.92	0.51
3:G:64:LYS:O	3:G:66:HIS:ND1	2.40	0.51
1:C:27:GLU:OE1	1:C:90:ARG:NH2	2.42	0.51
2:D:151:GLY:H	2:D:307:THR:HB	1.74	0.51
11:N:107:PRO:HD3	13:P:31:MET:HG3	1.92	0.51
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.92	0.51
2:F:40:VAL:HG22	2:F:77:VAL:HG22	1.92	0.51
2:F:65:MET:HE1	2:F:233:ARG:HG3	1.93	0.51
1:B:340:THR:HG21	2:F:316:ALA:HA	1.91	0.51
1:C:220:LEU:HB3	1:C:225:ALA:HB3	1.92	0.51
1:C:453:LEU:HA	1:C:456:LEU:HD13	1.92	0.51
2:E:40:VAL:HG22	2:E:77:VAL:HG22	1.92	0.51
2:D:153:LYS:HZ3	2:D:298:ILE:HG23	1.76	0.51
10:8:70:LEU:O	10:8:74:ALA:HB3	2.11	0.51
11:N:54:SER:HA	11:N:73:MET:HE3	1.93	0.51
2:E:48:VAL:HG13	2:E:65:MET:HG3	1.93	0.51
6:J:62:ARG:HA	6:J:65:LYS:HD3	1.92	0.51
1:B:176:THR:N	19:B:602:ADP:O2A	2.41	0.51
1:A:109:ASP:O	1:A:112:GLY:N	2.40	0.51
1:B:366:ASN:O	1:B:370:SER:N	2.34	0.50
10:2:19:ALA:HB2	10:3:17:GLY:HA2	1.92	0.50
16:S:98:ILE:HG21	20:S:201:LHG:H132	1.93	0.50
17:T:39:GLU:OE1	17:T:42:ARG:NH2	2.44	0.50
1:C:108:VAL:HA	1:C:114:ALA:HA	1.93	0.50
6:J:135:LYS:HE2	6:J:148:LEU:HD21	1.92	0.50
1:B:186:GLN:O	1:B:190:ASN:ND2	2.39	0.50
1:B:170:ASP:OD1	1:B:329:THR:OG1	2.27	0.50
1:C:167:ILE:HD11	1:C:324:LEU:HD12	1.94	0.50
1:C:186:GLN:HG3	1:C:199:LEU:HD22	1.94	0.50
1:A:382:ALA:HB2	1:A:488:LYS:HA	1.93	0.50
2:F:103:PRO:HG3	2:F:109:PRO:HA	1.93	0.50
1:A:178:ILE:O	1:A:182:THR:OG1	2.28	0.50
3:G:64:LYS:HG2	3:G:101:LYS:HE2	1.92	0.50
3:G:166:ARG:NH2	3:G:171:TYR:O	2.38	0.50
6:J:34:GLN:HA	6:J:37:LYS:HE2	1.93	0.50
7:K:43:LEU:HD21	20:S:201:LHG:H212	1.93	0.50
1:A:199:LEU:O	1:A:228:TYR:CB	2.54	0.50
2:E:209:ASN:ND2	2:E:212:ASP:OD1	2.45	0.50
2:E:181:GLY:HA2	2:E:251:GLN:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:GLY:H	2:F:59:THR:HB	1.77	0.49
4:H:20:PHE:HB3	4:H:27:PHE:HB2	1.94	0.49
9:M:54:TRP:O	9:M:58:LYS:HB2	2.11	0.49
2:D:336:VAL:HB	2:D:351:ASP:HB3	1.93	0.49
2:F:259:ASN:OD1	2:F:313:TYR:N	2.45	0.49
11:N:137:LEU:O	11:N:141:LEU:HB2	2.11	0.49
1:B:44:LEU:HG	1:B:47:VAL:HB	1.94	0.49
2:D:33:PRO:O	2:D:36:ASN:ND2	2.46	0.49
6:J:7:PRO:HG3	6:J:20:THR:HG22	1.93	0.49
2:E:243:GLU:OE1	2:E:297:ARG:NH2	2.39	0.49
2:E:341:ILE:HG13	2:E:344:LEU:HD12	1.93	0.49
2:D:276:ARG:HH12	2:D:284:GLN:HB2	1.76	0.49
3:G:246:LEU:HA	3:G:249:THR:HG22	1.93	0.49
1:C:254:GLY:HA3	1:C:266:ILE:HD11	1.94	0.49
1:C:361:ILE:HA	1:C:429:LYS:HG2	1.93	0.49
7:K:118:VAL:HG11	9:M:105:LEU:HD13	1.94	0.49
7:K:152:LYS:NZ	7:K:156:ASP:OD2	2.35	0.49
1:C:78:ASN:ND2	2:F:121:GLU:OE2	2.46	0.49
2:D:157:PHE:O	2:D:337:LEU:HB2	2.13	0.49
1:A:396:GLN:HB3	1:A:417:LEU:HD21	1.94	0.49
2:F:38:LEU:HB2	2:F:79:ASP:HA	1.95	0.49
5:I:10:LEU:HD11	5:I:14:ARG:HG2	1.95	0.49
13:P:18:THR:O	13:P:22:GLN:NE2	2.43	0.49
15:R:70:LEU:HB3	22:R:302:CDL:H442	1.95	0.49
1:C:273:LYS:HA	1:C:276:VAL:HG12	1.95	0.49
2:F:118:ILE:O	2:F:119:HIS:ND1	2.46	0.49
4:H:45:PHE:HA	10:6:39:ASN:HB3	1.95	0.49
10:3:55:ALA:HB3	11:N:213:VAL:HG21	1.95	0.49
10:5:19:ALA:HB2	10:6:17:GLY:HA2	1.95	0.49
1:C:165:GLU:HA	1:C:348:GLY:O	2.12	0.49
2:D:410:ARG:NE	2:D:456:GLU:OE1	2.42	0.49
2:F:338:SER:O	2:F:349:ALA:CB	2.45	0.48
2:D:279:SER:OG	2:D:280:ALA:N	2.46	0.48
2:D:411:LYS:NZ	2:D:451:PHE:O	2.34	0.48
2:F:172:ILE:O	2:F:176:ALA:HB3	2.12	0.48
2:D:118:ILE:O	2:D:119:HIS:ND1	2.45	0.48
2:F:346:ILE:HD11	2:F:414:ARG:HD3	1.95	0.48
1:A:66:LEU:HD13	2:E:18:VAL:HB	1.94	0.48
2:D:198:LEU:HD11	2:D:202:MET:HE3	1.95	0.48
1:B:311:LYS:HD2	1:B:320:SER:HB3	1.95	0.48
8:L:12:VAL:HA	8:L:15:ILE:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:HH22	1:B:131:LEU:HD12	1.78	0.48
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.95	0.48
2:E:255:LEU:O	2:E:308:SER:HA	2.14	0.48
2:E:279:SER:OG	2:E:280:ALA:N	2.40	0.48
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.96	0.48
2:E:185:PHE:HB3	2:E:219:LEU:HD23	1.95	0.48
2:F:254:LEU:HD23	2:F:307:THR:HB	1.96	0.48
10:1:17:GLY:HA2	10:8:19:ALA:HB2	1.96	0.48
3:G:74:ASP:OD1	3:G:110:ASP:N	2.46	0.48
22:R:301:CDL:H552	22:R:301:CDL:H422	1.96	0.48
10:8:70:LEU:O	10:8:74:ALA:CB	2.62	0.47
11:N:134:PRO:HG2	11:N:137:LEU:HD13	1.96	0.47
13:P:14:LYS:O	13:P:18:THR:OG1	2.33	0.47
15:R:44:ARG:NH1	20:R:304:LHG:O5	2.46	0.47
1:C:353:GLU:H	1:C:366:ASN:HB2	1.79	0.47
3:G:136:PRO:HG2	3:G:218:LYS:HG2	1.95	0.47
4:H:16:MET:HE3	4:H:90:VAL:HG21	1.95	0.47
1:B:367:VAL:HB	1:B:398:ARG:HH21	1.79	0.47
1:C:258:ARG:HD3	1:C:321:LEU:HB2	1.95	0.47
3:G:81:ILE:HD11	3:G:227:ALA:HB3	1.97	0.47
4:H:133:ILE:HA	4:H:136:GLU:HG2	1.96	0.47
7:K:154:ARG:HH21	8:L:59:PRO:HD2	1.79	0.47
1:A:203:TYR:OH	1:A:269:ASP:OD2	2.27	0.47
2:E:175:VAL:HG21	2:E:254:LEU:HD11	1.96	0.47
10:4:19:ALA:HB2	10:5:17:GLY:HA2	1.95	0.47
1:B:203:TYR:OH	1:B:269:ASP:OD2	2.29	0.47
2:D:389:ILE:HA	3:G:19:ILE:HD13	1.95	0.47
22:R:303:CDL:H531	22:R:303:CDL:H322	1.97	0.47
2:E:51:VAL:HA	2:E:62:THR:HG22	1.97	0.47
11:N:83:ASN:HB3	11:N:207:ALA:HB1	1.96	0.47
2:E:209:ASN:H	2:E:215:SER:HB3	1.80	0.47
2:F:55:LEU:HD13	2:F:61:ARG:HH21	1.80	0.47
4:H:87:ASP:OD1	4:H:87:ASP:N	2.47	0.47
11:N:113:VAL:HA	11:N:225:ASN:HD21	1.80	0.47
1:B:283:LEU:HD21	1:B:289:PRO:HB3	1.97	0.47
1:C:141:SER:OG	2:D:197:ASP:OD1	2.26	0.47
1:A:7:GLU:OE2	6:J:94:ARG:NH1	2.47	0.47
1:A:206:ILE:HG21	1:A:274:GLN:HB2	1.96	0.47
2:F:168:ILE:HD11	2:F:311:ALA:HB2	1.96	0.47
2:F:246:ARG:HD3	2:F:306:ILE:HG13	1.98	0.47
4:H:54:THR:HG22	4:H:84:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:186:MET:HG3	7:K:174:ILE:HD11	1.97	0.47
1:C:136:ILE:H	1:C:136:ILE:HG13	1.60	0.46
1:C:424:LEU:HD23	1:C:427:LEU:HD13	1.96	0.46
2:E:24:ASP:OD1	2:E:24:ASP:N	2.47	0.46
2:F:222:GLY:HA3	2:F:234:VAL:HG21	1.98	0.46
3:G:71:VAL:HA	3:G:108:VAL:HG22	1.97	0.46
16:S:26:ARG:NH2	16:S:29:THR:OG1	2.49	0.46
2:D:169:MET:HE1	2:D:198:LEU:HB2	1.96	0.46
1:B:26:GLU:HG3	1:B:46:ASN:HB2	1.98	0.46
4:H:115:ALA:HA	4:H:131:ILE:HD11	1.97	0.46
6:J:121:THR:HB	6:J:163:ILE:HG13	1.98	0.46
1:C:48:GLN:HB2	2:D:70:GLY:HA2	1.97	0.46
1:A:20:ASP:OD1	1:A:20:ASP:N	2.48	0.46
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.96	0.46
1:A:209:LYS:HE2	1:A:211:SER:HB3	1.97	0.46
3:G:113:ARG:HG2	3:G:127:THR:HG21	1.97	0.46
7:K:130:ASN:HB2	9:M:8:LEU:HD13	1.97	0.46
1:B:139:ARG:NH2	1:B:307:GLU:O	2.33	0.46
3:G:147:GLU:O	3:G:151:SER:OG	2.27	0.46
2:D:21:ALA:HA	2:D:64:ALA:N	2.29	0.46
2:D:55:LEU:HD11	2:D:61:ARG:HE	1.80	0.46
1:B:195:GLU:OE2	1:B:262:LYS:NZ	2.43	0.46
1:C:347:ASP:HB2	1:C:373:ARG:HD3	1.98	0.46
3:G:64:LYS:HE2	3:G:102:GLU:HG2	1.97	0.46
1:A:23:VAL:O	1:A:28:THR:OG1	2.34	0.46
1:A:26:GLU:HG2	1:A:45:ARG:HB2	1.97	0.46
2:D:49:LEU:HB3	2:D:62:THR:HB	1.97	0.46
15:R:8:LYS:O	15:R:27:ARG:NH2	2.49	0.46
1:B:105:GLY:HA2	1:B:226:MET:HG3	1.98	0.46
1:B:351:PHE:HB3	1:B:370:SER:HA	1.98	0.46
1:C:362:ARG:O	1:C:430:GLN:N	2.44	0.46
1:A:55:PHE:HE2	1:A:75:VAL:HG22	1.81	0.46
11:N:47:GLN:HG3	14:Q:33:PHE:HE1	1.81	0.46
2:D:291:MET:HA	2:D:294:MET:HG3	1.98	0.45
10:1:39:ASN:ND2	10:8:37:ALA:O	2.49	0.45
11:N:27:PRO:HG3	11:N:85:LEU:HD22	1.97	0.45
1:C:199:LEU:HD11	1:C:265:LEU:HD23	1.99	0.45
2:E:341:ILE:HB	2:E:349:ALA:HB1	1.98	0.45
2:E:21:ALA:CA	2:E:64:ALA:O	2.64	0.45
2:D:35:LEU:N	2:D:51:VAL:O	2.48	0.45
2:D:160:ALA:O	2:D:339:ARG:NH2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:127:THR:HB	5:I:46:VAL:HB	1.98	0.45
9:M:54:TRP:O	9:M:58:LYS:CB	2.64	0.45
10:7:65:LEU:HD11	10:8:67:VAL:HG21	1.98	0.45
1:C:444:VAL:HG13	1:C:445:ILE:HD12	1.99	0.45
1:A:274:GLN:HE22	1:A:301:LEU:HD21	1.81	0.45
1:A:65:ASN:HA	1:A:66:LEU:HD12	1.99	0.45
3:G:204:TYR:HH	4:H:83:THR:HG1	1.63	0.45
6:J:165:ARG:HB2	6:J:170:TYR:HD1	1.82	0.45
11:N:22:LEU:HD12	22:R:302:CDL:H372	1.98	0.45
11:N:73:MET:HA	11:N:76:ILE:HG22	1.99	0.45
11:N:111:GLY:O	11:N:115:THR:OG1	2.32	0.45
1:A:166:LEU:HB2	1:A:346:THR:HG21	1.99	0.45
2:D:40:VAL:HG22	2:D:77:VAL:HG12	1.98	0.45
6:J:155:ASP:N	6:J:155:ASP:OD1	2.50	0.45
2:D:321:ASP:HB3	2:D:324:PRO:HD2	1.99	0.45
3:G:168:VAL:O	3:G:226:SER:OG	2.35	0.45
11:N:120:LYS:HB3	11:N:123:ALA:HB3	1.99	0.45
13:P:14:LYS:O	13:P:18:THR:CB	2.64	0.45
1:B:39:ALA:HB3	1:B:73:VAL:HG13	1.99	0.45
1:C:258:ARG:NH2	1:C:308:ARG:O	2.50	0.45
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.99	0.45
1:C:471:HIS:O	1:C:474:SER:OG	2.34	0.45
1:A:31:VAL:HA	1:A:41:VAL:HG12	1.99	0.45
1:A:381:ARG:HB2	1:A:488:LYS:HB3	1.99	0.45
2:E:43:ARG:NH1	2:E:69:GLU:O	2.42	0.45
2:D:140:LYS:NZ	2:D:415:PHE:O	2.46	0.45
2:F:186:ALA:HB3	2:F:257:ILE:HG12	1.99	0.45
7:K:50:ILE:HD13	20:K:302:LHG:HC91	1.99	0.45
2:F:155:GLY:HA3	2:F:331:LEU:HD21	1.99	0.44
7:K:121:ARG:HH11	9:M:19:ILE:HG13	1.81	0.44
12:O:45:PHE:O	12:O:49:SER:OG	2.29	0.44
2:E:333:ALA:HA	2:E:357:SER:HA	1.98	0.44
3:G:106:ILE:HD13	3:G:148:LEU:HD13	1.99	0.44
11:N:129:LEU:HD11	12:O:27:ARG:HG2	1.99	0.44
2:E:154:ILE:HB	2:E:333:ALA:HB3	1.99	0.44
7:K:154:ARG:O	7:K:158:HIS:ND1	2.38	0.44
2:D:348:PRO:O	2:D:350:VAL:N	2.51	0.44
1:A:139:ARG:O	2:E:196:ASN:ND2	2.51	0.44
2:E:49:LEU:HB3	2:E:62:THR:HB	1.99	0.44
6:J:179:ILE:O	6:J:183:SER:OG	2.27	0.44
7:K:168:LYS:HD3	8:L:39:LEU:HD22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HD2	1:A:112:GLY:HA3	2.00	0.44
2:F:188:VAL:HG22	2:F:234:VAL:HB	1.99	0.44
2:F:411:LYS:NZ	2:F:451:PHE:O	2.43	0.44
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.79	0.44
1:C:142:VAL:HG21	1:C:374:VAL:HB	2.00	0.44
2:E:18:VAL:HA	2:E:23:VAL:HG12	2.00	0.44
6:J:175:ALA:HB1	8:L:10:LEU:HD21	2.00	0.44
8:L:13:ASP:OD1	8:L:16:ARG:NH2	2.47	0.44
1:C:15:ARG:HG2	6:J:186:MET:HA	1.99	0.43
1:C:199:LEU:O	1:C:228:TYR:HA	2.18	0.43
2:D:236:LEU:HD13	2:D:239:LEU:HD12	1.99	0.43
2:F:375:GLY:HA3	2:F:447:LEU:HD11	2.00	0.43
1:B:35:GLY:HA2	2:E:53:GLN:HG2	1.99	0.43
2:E:239:LEU:HD21	2:E:297:ARG:HB2	1.99	0.43
2:D:259:ASN:OD1	2:D:313:TYR:N	2.51	0.43
12:O:47:LEU:HG	12:O:48:ARG:HE	1.81	0.43
3:G:107:GLY:O	3:G:127:THR:HA	2.17	0.43
5:I:7:GLN:HE22	10:3:40:PRO:HB2	1.82	0.43
6:J:15:GLU:HG2	6:J:100:ALA:HB3	2.01	0.43
2:E:369:HIS:CD2	2:E:440:ILE:HD11	2.53	0.43
10:2:37:ALA:O	10:3:39:ASN:ND2	2.51	0.43
1:B:351:PHE:H	1:B:370:SER:HB2	1.83	0.43
2:E:38:LEU:HD13	2:E:77:VAL:HG11	2.01	0.43
2:F:118:ILE:HG23	2:F:236:LEU:HB3	1.99	0.43
2:F:338:SER:OG	2:F:339:ARG:N	2.51	0.43
3:G:71:VAL:HG13	3:G:162:PHE:HA	1.99	0.43
1:B:189:PHE:HB3	1:B:197:LYS:HG3	2.01	0.43
2:E:341:ILE:HA	2:E:344:LEU:HB2	2.01	0.43
1:C:200:TYR:HA	1:C:228:TYR:HA	2.01	0.43
1:C:342:VAL:HA	1:C:345:ILE:HG22	2.01	0.43
2:E:387:GLN:HA	2:E:390:ILE:HG22	2.00	0.43
2:F:157:PHE:O	2:F:337:LEU:HB2	2.18	0.43
6:J:73:THR:HG23	6:J:78:PHE:HB2	2.01	0.43
1:C:108:VAL:HG13	1:C:232:VAL:HG22	2.00	0.43
3:G:1:ALA:HB3	3:G:6:ILE:HD11	2.01	0.43
10:3:62:LEU:HD13	10:3:65:LEU:HB3	1.99	0.43
3:G:190:MET:HG2	3:G:201:LEU:HD11	2.00	0.43
6:J:178:LYS:HB2	8:L:10:LEU:HD22	2.01	0.43
7:K:157:TYR:HE1	8:L:46:LEU:HB3	1.84	0.43
11:N:88:LEU:HD11	15:R:64:LEU:HD22	2.00	0.43
15:R:71:ASN:HA	15:R:74:ARG:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:43:PRO:HA	16:S:46:ILE:HG12	2.00	0.43
1:A:11:ILE:HA	1:A:14:GLU:HG3	2.01	0.43
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.01	0.43
2:F:190:GLU:HG3	2:F:191:ARG:H	1.84	0.43
3:G:164:ARG:HB3	3:G:172:LYS:HB3	2.01	0.43
1:B:251:CYS:O	1:B:255:GLU:CB	2.65	0.42
1:C:362:ARG:HB3	19:C:602:ADP:C6	2.53	0.42
2:F:27:PHE:O	2:F:58:SER:OG	2.37	0.42
4:H:37:ASP:HA	4:H:46:GLY:HA2	2.01	0.42
10:4:70:LEU:HD12	11:N:173:LEU:HD11	2.01	0.42
11:N:142:VAL:HG21	12:O:31:VAL:HG22	2.01	0.42
11:N:171:ILE:HD11	11:N:203:GLU:HG3	2.01	0.42
2:D:341:ILE:HB	2:D:349:ALA:HB1	2.00	0.42
2:F:383:TYR:HE1	2:F:406:VAL:HG13	1.83	0.42
4:H:128:ARG:HA	4:H:131:ILE:HG22	2.01	0.42
10:4:34:ILE:HD12	10:5:34:ILE:HG23	2.00	0.42
1:C:356:LEU:HB3	1:C:361:ILE:HG22	2.01	0.42
1:C:397:TYR:CG	1:C:421:GLY:HA3	2.54	0.42
1:A:66:LEU:HB3	2:E:73:ARG:HD2	2.01	0.42
1:A:352:LEU:HD23	1:A:365:ILE:HA	2.01	0.42
2:E:26:GLN:NE2	2:E:57:GLU:OE1	2.51	0.42
11:N:125:LEU:HD23	12:O:28:MET:HG3	2.00	0.42
15:R:12:LEU:H	20:R:304:LHG:HC11	1.84	0.42
1:B:151:LYS:NZ	1:B:465:GLU:OE2	2.49	0.42
1:C:250:GLY:HA2	1:C:253:MET:HE3	2.01	0.42
1:A:105:GLY:HA2	1:A:226:MET:HE3	2.01	0.42
2:E:98:ASN:O	2:E:101:GLY:N	2.41	0.42
2:D:341:ILE:HG23	2:D:344:LEU:HD12	2.01	0.42
7:K:196:LYS:HZ2	8:L:8:GLN:N	2.18	0.42
10:5:40:PRO:HG3	10:6:42:LEU:HD21	2.02	0.42
17:T:67:ASP:HA	17:T:71:LYS:HE2	2.00	0.42
1:B:52:MET:HA	1:B:61:GLY:O	2.18	0.42
1:B:432:GLN:HG3	19:B:602:ADP:C6	2.54	0.42
1:C:160:GLY:N	1:C:163:GLN:OE1	2.45	0.42
1:C:490:SER:O	1:C:494:ASP:N	2.50	0.42
2:D:21:ALA:HA	2:D:64:ALA:O	2.20	0.42
4:H:84:VAL:HG12	4:H:90:VAL:HA	2.00	0.42
10:1:4:THR:HA	10:1:7:LYS:HG2	2.01	0.42
1:B:258:ARG:HE	1:B:312:MET:HE2	1.84	0.42
1:A:104:LEU:HD13	1:A:230:ILE:HG13	2.01	0.42
2:E:15:ILE:HD13	2:E:25:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:ALA:O	2:E:427:THR:OG1	2.32	0.42
2:D:228:PRO:HB2	2:D:270:VAL:HG13	2.00	0.42
10:1:67:VAL:HG21	10:8:65:LEU:HD11	2.00	0.42
1:A:166:LEU:HD23	1:A:325:PRO:HG2	2.00	0.42
2:E:252:ASP:OD1	2:E:305:SER:OG	2.33	0.42
2:D:144:LEU:HG	2:D:145:LEU:HG	2.00	0.42
13:P:21:TYR:HE2	14:Q:25:GLN:HE22	1.66	0.42
1:B:472:VAL:HG12	1:B:480:LEU:HD11	2.01	0.42
2:E:257:ILE:HG22	2:E:259:ASN:H	1.84	0.42
2:E:260:ILE:HD12	2:E:260:ILE:HA	1.90	0.42
9:M:153:TRP:N	13:P:16:TYR:OH	2.53	0.42
1:A:264:ALA:O	1:A:321:LEU:HA	2.20	0.42
3:G:249:THR:HA	3:G:252:ARG:HG2	2.00	0.42
4:H:18:PHE:HA	4:H:90:VAL:HB	2.02	0.42
15:R:16:LYS:HD2	15:R:16:LYS:HA	1.75	0.42
1:A:311:LYS:NZ	1:A:318:GLY:O	2.53	0.42
2:E:188:VAL:HG22	2:E:234:VAL:HB	2.01	0.42
10:4:19:ALA:HB1	10:5:20:GLY:HA3	2.02	0.42
1:A:66:LEU:CA	1:A:70:ASN:O	2.68	0.41
2:E:328:PHE:HA	2:E:331:LEU:HB2	2.01	0.41
2:D:86:ILE:HD13	2:D:118:ILE:HD11	2.01	0.41
1:C:202:ILE:HB	1:C:266:ILE:HG13	2.02	0.41
1:A:38:ILE:HG12	1:A:285:LEU:HD22	2.01	0.41
1:A:76:PHE:HE1	1:A:241:PRO:HB2	1.85	0.41
1:A:200:TYR:HA	1:A:228:TYR:HA	2.02	0.41
2:D:383:TYR:HE1	2:D:406:VAL:HG13	1.85	0.41
6:J:6:ARG:HD3	6:J:7:PRO:HD2	2.02	0.41
7:K:40:GLY:HA3	16:S:85:MET:HB3	2.01	0.41
7:K:108:ILE:HG23	9:M:112:ILE:HD11	2.02	0.41
20:K:302:LHG:H222	22:R:303:CDL:H392	2.02	0.41
2:E:321:ASP:HB3	2:E:324:PRO:HD2	2.01	0.41
10:3:59:ALA:HB1	11:N:159:ARG:HB2	2.01	0.41
1:B:335:SER:HA	1:B:340:THR:HG23	2.02	0.41
2:E:23:VAL:HG22	2:E:64:ALA:HB2	2.02	0.41
22:R:302:CDL:H181	22:R:303:CDL:H741	2.01	0.41
1:A:97:VAL:HG21	1:A:249:SER:HA	2.03	0.41
2:F:35:LEU:N	2:F:51:VAL:O	2.51	0.41
4:H:137:ALA:O	4:H:141:LEU:HB2	2.20	0.41
1:C:321:LEU:HA	1:C:321:LEU:HD12	1.83	0.41
1:A:479:LEU:HD21	1:A:497:LEU:HG	2.02	0.41
2:E:55:LEU:H	2:E:55:LEU:HG	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:342:ALA:N	2:E:349:ALA:HB2	2.34	0.41
11:N:22:LEU:HB3	22:R:302:CDL:H402	2.02	0.41
11:N:62:ASN:O	11:N:66:GLN:N	2.54	0.41
11:N:117:PHE:O	11:N:121:THR:OG1	2.30	0.41
1:B:44:LEU:HD11	1:B:90:ARG:HG3	2.03	0.41
1:B:172:GLN:OE1	2:E:358:ARG:NH2	2.54	0.41
1:A:171:ARG:NH2	2:D:354:ASP:OD1	2.53	0.41
7:K:24:PHE:HE1	16:S:71:LYS:HG3	1.86	0.41
1:B:244:TYR:OH	1:B:304:ARG:NH2	2.54	0.41
1:C:150:ILE:HG22	1:C:153:VAL:H	1.85	0.41
1:C:268:TYR:HE2	1:C:323:ALA:HB1	1.85	0.41
2:E:161:GLY:H	2:E:339:ARG:HH11	1.68	0.41
2:E:291:MET:O	2:E:295:GLN:HB2	2.21	0.41
3:G:43:VAL:HG11	4:H:29:ASN:HD22	1.86	0.41
3:G:116:LEU:HD12	3:G:120:HIS:HB2	2.03	0.41
6:J:9:VAL:HG23	6:J:111:VAL:HG11	2.02	0.41
6:J:39:LEU:HD12	6:J:102:ILE:HG12	2.03	0.41
10:2:15:THR:HG22	10:3:64:CYS:HB2	2.03	0.41
10:6:12:GLY:HA2	10:7:14:ALA:HB2	2.03	0.41
16:S:92:ILE:HD11	16:S:98:ILE:HA	2.02	0.41
1:C:107:VAL:HB	1:C:116:ASP:HB3	2.03	0.41
1:C:208:GLN:NE2	1:C:269:ASP:OD2	2.54	0.41
1:A:142:VAL:HG21	1:A:374:VAL:HG11	2.02	0.41
2:E:386:LEU:HD23	2:E:389:ILE:HD12	2.03	0.41
2:D:54:HIS:CD2	2:D:60:VAL:HG12	2.56	0.41
11:N:223:HIS:HA	11:N:226:THR:HB	2.02	0.41
1:B:287:ARG:HH12	2:F:273:LEU:HD21	1.86	0.40
1:B:400:VAL:O	1:B:404:ALA:N	2.54	0.40
1:C:109:ASP:HB3	1:C:113:ASN:O	2.21	0.40
1:C:409:ASP:OD1	1:C:409:ASP:N	2.54	0.40
1:A:66:LEU:HA	1:A:70:ASN:O	2.20	0.40
2:E:183:SER:O	2:E:217:VAL:HA	2.21	0.40
2:D:259:ASN:HD21	2:D:313:TYR:HB2	1.85	0.40
2:F:256:PHE:HA	2:F:309:VAL:O	2.21	0.40
2:F:294:MET:HE3	2:F:294:MET:HB3	1.86	0.40
3:G:67:LEU:HD11	3:G:106:ILE:HG23	2.03	0.40
9:M:156:ARG:NH1	14:Q:34:TYR:O	2.54	0.40
10:3:70:LEU:O	10:3:74:ALA:CB	2.64	0.40
20:S:202:LHG:H142	20:S:202:LHG:H112	1.91	0.40
1:B:99:VAL:HG11	1:B:127:ARG:HB2	2.04	0.40
2:F:271:SER:HA	2:F:274:LEU:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:108:VAL:HA	3:G:128:PHE:HB2	2.03	0.40
1:B:444:VAL:HA	1:B:468:PHE:HZ	1.86	0.40
1:A:351:PHE:H	1:A:370:SER:HB2	1.85	0.40
4:H:132:GLN:HA	4:H:135:ILE:HG22	2.04	0.40
2:E:167:LEU:HD13	2:E:337:LEU:HD21	2.03	0.40
2:E:277:ILE:HG23	3:G:266:ILE:HG21	2.03	0.40
2:D:48:VAL:HG11	2:D:100:ILE:HG12	2.02	0.40
7:K:182:VAL:O	7:K:186:SER:OG	2.35	0.40
1:B:48:GLN:HB3	2:F:72:VAL:HG22	2.03	0.40
1:B:66:LEU:HB3	2:F:73:ARG:HD3	2.02	0.40
1:B:192:GLY:O	1:B:198:LYS:NZ	2.53	0.40
1:C:356:LEU:HD13	1:C:361:ILE:HG21	2.03	0.40
2:E:254:LEU:HA	2:E:307:THR:O	2.21	0.40
2:E:318:ASP:OD2	2:E:321:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	505/553 (91%)	457 (90%)	46 (9%)	2 (0%)	30	62
1	B	486/553 (88%)	448 (92%)	37 (8%)	1 (0%)	43	74
1	C	501/553 (91%)	456 (91%)	45 (9%)	0	100	100
2	D	467/528 (88%)	420 (90%)	42 (9%)	5 (1%)	11	43
2	E	465/528 (88%)	425 (91%)	33 (7%)	7 (2%)	8	37
2	F	470/528 (89%)	433 (92%)	34 (7%)	3 (1%)	21	54
3	G	270/298 (91%)	256 (95%)	14 (5%)	0	100	100
4	H	130/168 (77%)	119 (92%)	10 (8%)	1 (1%)	16	49
5	I	45/51 (88%)	43 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	24	57
7	K	206/256 (80%)	193 (94%)	13 (6%)	0	100	100
8	L	67/108 (62%)	60 (90%)	7 (10%)	0	100	100
9	M	154/161 (96%)	150 (97%)	4 (3%)	0	100	100
10	1	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	2	72/136 (53%)	72 (100%)	0	0	100	100
10	3	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	4	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	5	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
10	6	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	7	72/136 (53%)	71 (99%)	1 (1%)	0	100	100
10	8	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
11	N	223/226 (99%)	212 (95%)	11 (5%)	0	100	100
12	O	38/58 (66%)	37 (97%)	1 (3%)	0	100	100
13	P	50/60 (83%)	49 (98%)	1 (2%)	0	100	100
14	Q	45/66 (68%)	42 (93%)	3 (7%)	0	100	100
15	R	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	S	83/103 (81%)	78 (94%)	5 (6%)	0	100	100
17	T	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5117/6258 (82%)	4767 (93%)	330 (6%)	20 (0%)	31	62

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	53	GLN
2	E	259	ASN
2	E	280	ALA
2	E	281	VAL
2	D	281	VAL
2	F	281	VAL
2	D	55	LEU
4	H	39	PRO
2	E	279	SER
2	D	53	GLN
6	J	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	491	GLU
2	E	398	LEU
2	F	53	GLN
1	B	336	ALA
1	A	68	PRO
2	E	55	LEU
2	F	282	GLY
2	D	123	PRO
2	D	282	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/443 (93%)	403 (98%)	7 (2%)	53	70
1	B	394/443 (89%)	390 (99%)	4 (1%)	68	75
1	C	407/443 (92%)	400 (98%)	7 (2%)	53	70
2	D	376/415 (91%)	372 (99%)	4 (1%)	65	74
2	E	376/415 (91%)	372 (99%)	4 (1%)	65	74
2	F	379/415 (91%)	374 (99%)	5 (1%)	61	72
3	G	230/251 (92%)	227 (99%)	3 (1%)	61	72
4	H	104/127 (82%)	102 (98%)	2 (2%)	50	68
5	I	38/42 (90%)	38 (100%)	0	100	100
6	J	164/185 (89%)	164 (100%)	0	100	100
7	K	184/218 (84%)	182 (99%)	2 (1%)	65	74
8	L	63/98 (64%)	63 (100%)	0	100	100
9	M	141/144 (98%)	141 (100%)	0	100	100
10	1	50/105 (48%)	50 (100%)	0	100	100
10	2	50/105 (48%)	50 (100%)	0	100	100
10	3	50/105 (48%)	50 (100%)	0	100	100
10	4	50/105 (48%)	50 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	5	50/105 (48%)	50 (100%)	0	100	100
10	6	50/105 (48%)	50 (100%)	0	100	100
10	7	50/105 (48%)	50 (100%)	0	100	100
10	8	50/105 (48%)	50 (100%)	0	100	100
11	N	197/198 (100%)	195 (99%)	2 (1%)	68	75
12	O	35/47 (74%)	35 (100%)	0	100	100
13	P	45/49 (92%)	45 (100%)	0	100	100
14	Q	39/66 (59%)	38 (97%)	1 (3%)	40	62
15	R	73/76 (96%)	71 (97%)	2 (3%)	39	62
16	S	71/84 (84%)	71 (100%)	0	100	100
17	T	59/60 (98%)	59 (100%)	0	100	100
All	All	4185/5059 (83%)	4142 (99%)	43 (1%)	65	75

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	VAL
1	B	129	VAL
1	B	166	LEU
1	B	245	LEU
1	C	108	VAL
1	C	121	ILE
1	C	136	ILE
1	C	164	ARG
1	C	285	LEU
1	C	427	LEU
1	C	445	ILE
1	A	17	LEU
1	A	38	ILE
1	A	129	VAL
1	A	166	LEU
1	A	175	LYS
1	A	285	LEU
1	A	400	VAL
2	E	141	VAL
2	E	154	ILE
2	E	331	LEU
2	E	350	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	144	LEU
2	D	255	LEU
2	D	307	THR
2	D	416	LEU
2	F	172	ILE
2	F	301	THR
2	F	389	ILE
2	F	416	LEU
2	F	440	ILE
3	G	71	VAL
3	G	144	ILE
3	G	196	ILE
4	H	48	LEU
4	H	103	LEU
7	K	17	ILE
7	K	86	ASN
11	N	114	ILE
11	N	199	LEU
14	Q	18	LEU
15	R	16	LYS
15	R	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	260	ASN
1	B	341	ASN
1	B	366	ASN
1	C	147	GLN
1	C	405	GLN
1	C	476	HIS
1	A	341	ASN
1	A	405	GLN
1	A	466	ASN
2	E	54	HIS
2	E	132	GLN
2	E	179	HIS
2	E	196	ASN
2	E	200	HIS
2	E	248	GLN
2	E	259	ASN
2	D	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	41	GLN
2	D	265	GLN
2	D	310	GLN
2	F	75	GLN
2	F	132	GLN
2	F	173	ASN
2	F	200	HIS
2	F	429	HIS
3	G	205	GLN
3	G	225	GLN
3	G	234	ASN
4	H	15	GLN
4	H	32	ASN
5	I	7	GLN
5	I	34	ASN
6	J	10	GLN
7	K	86	ASN
7	K	98	GLN
7	K	145	HIS
9	M	89	GLN
10	1	44	GLN
14	Q	31	HIS
17	T	6	GLN

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 [i](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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$
19	ADP	B	602	18	28,29,29	1.38	4 (14%)	43,45,45	1.88	12 (27%)
20	LHG	K	301	-	42,42,48	0.65	0	45,48,54	1.24	4 (8%)
22	CDL	R	303	-	87,87,99	1.06	6 (6%)	93,99,111	1.03	14 (15%)
22	CDL	R	302	-	91,91,99	1.08	7 (7%)	97,103,111	0.98	12 (12%)
19	ADP	F	600	-	28,29,29	1.37	5 (17%)	43,45,45	1.79	7 (16%)
20	LHG	S	202	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
19	ADP	A	602	18	28,29,29	1.38	4 (14%)	43,45,45	1.98	8 (18%)
22	CDL	R	301	-	99,99,99	1.15	8 (8%)	105,111,111	1.00	16 (15%)
23	S12	T	201	-	33,34,34	0.68	1 (3%)	34,40,40	0.45	0
21	P5S	2	201	-	52,53,53	0.33	0	54,60,60	0.55	1 (1%)
20	LHG	R	304	-	48,48,48	0.66	1 (2%)	51,54,54	1.26	6 (11%)
20	LHG	2	202	-	44,44,48	0.69	1 (2%)	47,50,54	1.35	6 (12%)
20	LHG	S	201	-	48,48,48	0.67	1 (2%)	51,54,54	1.27	6 (11%)
20	LHG	K	302	-	48,48,48	0.70	1 (2%)	51,54,54	1.33	7 (13%)
19	ADP	C	602	18	28,29,29	1.37	4 (14%)	43,45,45	1.84	8 (18%)
19	ADP	D	600	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	7 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	B	602	18	-	10/16/32/32	0/3/3/3
20	LHG	K	301	-	-	27/47/47/53	-
22	CDL	R	303	-	2/2/9/9	29/98/98/110	-
22	CDL	R	302	-	1/1/9/9	39/102/102/110	-
19	ADP	F	600	-	-	2/16/32/32	0/3/3/3
22	CDL	R	301	-	1/1/9/9	39/110/110/110	-
19	ADP	A	602	18	-	10/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	S	202	-	-	30/53/53/53	-
23	S12	T	201	-	-	14/38/38/38	-
21	P5S	2	201	-	-	14/59/59/59	-
20	LHG	R	304	-	-	32/53/53/53	-
20	LHG	2	202	-	-	26/49/49/53	-
20	LHG	S	201	-	-	27/53/53/53	-
20	LHG	K	302	-	-	26/53/53/53	-
19	ADP	C	602	18	-	3/16/32/32	0/3/3/3
19	ADP	D	600	-	-	3/16/32/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	600	ADP	C5-C4	4.47	1.47	1.39
19	C	602	ADP	C5-C4	4.44	1.47	1.39
19	A	602	ADP	C5-C4	4.43	1.47	1.39
19	B	602	ADP	C5-C4	4.38	1.46	1.39
19	F	600	ADP	C5-C4	4.27	1.46	1.39
22	R	302	CDL	C42-C41	-3.98	1.32	1.51
22	R	301	CDL	C42-C41	-3.98	1.32	1.51
22	R	302	CDL	C39-C38	-3.97	1.32	1.51
22	R	301	CDL	C19-C18	-3.96	1.32	1.51
22	R	301	CDL	C22-C21	-3.96	1.32	1.51
22	R	302	CDL	C22-C21	-3.95	1.32	1.51
22	R	303	CDL	C19-C18	-3.95	1.32	1.51
22	R	302	CDL	C19-C18	-3.94	1.32	1.51
22	R	303	CDL	C62-C61	-3.93	1.32	1.51
22	R	303	CDL	C59-C58	-3.92	1.32	1.51
22	R	301	CDL	C39-C38	-3.92	1.32	1.51
22	R	301	CDL	C79-C78	-3.92	1.32	1.51
22	R	301	CDL	C62-C61	-3.92	1.32	1.51
22	R	301	CDL	C59-C58	-3.92	1.32	1.51
22	R	303	CDL	C22-C21	-3.92	1.32	1.51
22	R	301	CDL	C82-C81	-3.91	1.32	1.51
22	R	302	CDL	C59-C58	-3.91	1.32	1.51
22	R	302	CDL	C62-C61	-3.89	1.32	1.51
22	R	303	CDL	C42-C41	-3.88	1.32	1.51
22	R	303	CDL	C39-C38	-3.83	1.32	1.51
23	T	201	S12	C14-C13	3.58	1.52	1.31
19	F	600	ADP	C5-N7	-2.88	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	602	ADP	C5-C6	2.67	1.48	1.41
20	R	304	LHG	O7-C5	-2.64	1.40	1.46
20	2	202	LHG	O7-C5	-2.64	1.40	1.46
20	K	302	LHG	O7-C5	-2.61	1.40	1.46
19	D	600	ADP	C5-N7	-2.61	1.34	1.39
19	B	602	ADP	C5-C6	2.58	1.48	1.41
19	C	602	ADP	C5-N7	-2.55	1.34	1.39
22	R	302	CDL	C79-C78	-2.55	1.32	1.50
19	A	602	ADP	C5-N7	-2.54	1.34	1.39
19	D	600	ADP	C5-C6	2.51	1.48	1.41
19	C	602	ADP	C5-C6	2.50	1.47	1.41
20	S	202	LHG	O7-C5	-2.43	1.40	1.46
19	B	602	ADP	C5-N7	-2.33	1.34	1.39
19	F	600	ADP	C4-N9	-2.30	1.32	1.37
19	B	602	ADP	C8-N7	2.25	1.36	1.31
20	S	201	LHG	P-O6	2.20	1.68	1.59
19	A	602	ADP	C8-N7	2.18	1.35	1.31
19	F	600	ADP	C5-C6	2.17	1.47	1.41
19	D	600	ADP	C8-N7	2.15	1.35	1.31
19	C	602	ADP	C8-N7	2.09	1.35	1.31
19	F	600	ADP	C8-N7	2.07	1.35	1.31

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	602	ADP	C5-C4-N3	-6.46	117.82	126.72
19	D	600	ADP	C5-C4-N3	-6.04	118.40	126.72
19	C	602	ADP	C5-C4-N3	-5.96	118.51	126.72
19	B	602	ADP	C5-C4-N3	-5.89	118.60	126.72
19	F	600	ADP	C5-C4-N3	-5.77	118.77	126.72
19	D	600	ADP	N3-C4-N9	4.93	135.55	127.17
19	C	602	ADP	N3-C4-N9	4.83	135.38	127.17
19	A	602	ADP	N3-C4-N9	4.79	135.31	127.17
19	B	602	ADP	N3-C4-N9	4.57	134.94	127.17
19	F	600	ADP	N3-C4-N9	4.52	134.85	127.17
20	2	202	LHG	O4-P-O5	4.48	133.29	112.44
20	K	302	LHG	O4-P-O5	4.42	133.02	112.44
20	K	301	LHG	O4-P-O5	4.40	132.92	112.44
20	S	202	LHG	O4-P-O5	4.38	132.82	112.44
20	S	201	LHG	O4-P-O5	4.38	132.80	112.44
20	R	304	LHG	O4-P-O5	4.33	132.57	112.44
19	A	602	ADP	O4'-C1'-N9	4.13	116.01	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	602	ADP	C2-N3-C4	3.91	121.39	111.83
19	A	602	ADP	C4-C5-N7	-3.87	106.15	110.58
19	C	602	ADP	C2-N3-C4	3.78	121.07	111.83
19	D	600	ADP	C2-N3-C4	3.75	121.00	111.83
19	F	600	ADP	C2-N3-C4	3.72	120.91	111.83
19	B	602	ADP	C2-N3-C4	3.67	120.80	111.83
19	B	602	ADP	C4-C5-N7	-3.62	106.44	110.58
19	C	602	ADP	N3-C2-N1	-3.41	123.42	128.58
19	F	600	ADP	N3-C2-N1	-3.37	123.48	128.58
20	K	302	LHG	O8-C23-C24	3.34	122.03	111.83
19	D	600	ADP	N3-C2-N1	-3.22	123.70	128.58
19	D	600	ADP	C4-C5-N7	-3.20	106.92	110.58
19	C	602	ADP	C4-C5-N7	-3.19	106.94	110.58
19	A	602	ADP	N3-C2-N1	-3.14	123.83	128.58
19	B	602	ADP	N3-C2-N1	-3.09	123.90	128.58
19	B	602	ADP	O4'-C1'-N9	2.96	113.78	108.09
19	F	600	ADP	C4-C5-N7	-2.90	107.26	110.58
20	2	202	LHG	O8-C23-C24	2.86	120.56	111.83
19	A	602	ADP	C5-N7-C8	2.77	107.80	103.45
19	F	600	ADP	C3'-C2'-C1'	2.74	106.64	101.46
19	B	602	ADP	C4-N9-C8	2.73	108.61	105.74
22	R	303	CDL	C40-C39-C38	2.63	127.67	114.37
19	B	602	ADP	C5-N7-C8	2.63	107.58	103.45
20	K	301	LHG	O8-C23-C24	2.62	119.83	111.83
20	S	202	LHG	O8-C23-C24	2.61	119.80	111.83
20	R	304	LHG	C11-C10-C9	-2.58	101.32	114.37
20	K	302	LHG	C11-C10-C9	-2.58	101.32	114.37
22	R	301	CDL	C62-C61-C60	2.58	127.42	114.37
22	R	303	CDL	C62-C61-C60	2.57	127.38	114.37
22	R	303	CDL	C22-C21-C20	2.55	127.24	114.37
19	C	602	ADP	C4-N9-C8	2.55	108.41	105.74
22	R	301	CDL	C40-C39-C38	2.54	127.23	114.37
19	D	600	ADP	C4-N9-C8	2.54	108.41	105.74
22	R	302	CDL	C60-C59-C58	2.53	127.14	114.37
22	R	302	CDL	C40-C39-C38	2.52	127.11	114.37
22	R	301	CDL	C80-C79-C78	2.52	127.09	114.37
22	R	302	CDL	C19-C18-C17	2.52	127.08	114.37
22	R	302	CDL	C62-C61-C60	2.51	127.07	114.37
22	R	301	CDL	C22-C21-C20	2.51	127.05	114.37
20	S	202	LHG	C11-C10-C9	-2.51	101.69	114.37
20	S	201	LHG	C11-C10-C9	-2.51	101.69	114.37
22	R	303	CDL	C60-C59-C58	2.51	127.03	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	301	CDL	C20-C19-C18	2.50	127.02	114.37
22	R	302	CDL	C42-C41-C40	2.49	126.96	114.37
20	S	201	LHG	O8-C23-C24	2.49	119.43	111.83
22	R	302	CDL	C22-C21-C20	2.48	126.91	114.37
20	R	304	LHG	O8-C23-C24	2.47	119.37	111.83
22	R	303	CDL	C19-C18-C17	2.46	126.81	114.37
22	R	303	CDL	C42-C41-C40	2.46	126.80	114.37
22	R	301	CDL	C60-C59-C58	2.45	126.74	114.37
20	K	302	LHG	C20-C19-C18	-2.44	102.02	114.37
22	R	301	CDL	C42-C41-C40	2.44	126.71	114.37
19	D	600	ADP	C5-N7-C8	2.44	107.29	103.45
22	R	303	CDL	C20-C19-C18	2.43	126.66	114.37
20	2	202	LHG	C5-O7-C7	-2.42	112.00	117.80
22	R	302	CDL	C20-C19-C18	2.42	126.58	114.37
22	R	301	CDL	C82-C81-C80	2.41	126.57	114.37
22	R	301	CDL	C59-C58-C57	2.41	126.57	114.37
20	2	202	LHG	C11-C10-C9	-2.41	102.20	114.37
22	R	303	CDL	C63-C62-C61	2.40	126.49	114.37
22	R	303	CDL	C43-C42-C41	2.40	126.49	114.37
22	R	302	CDL	C23-C22-C21	2.39	126.45	114.37
22	R	302	CDL	C59-C58-C57	2.39	126.45	114.37
22	R	302	CDL	C39-C38-C37	2.38	126.40	114.37
22	R	301	CDL	C23-C22-C21	2.38	126.38	114.37
22	R	302	CDL	C63-C62-C61	2.37	126.37	114.37
20	K	301	LHG	C11-C10-C9	-2.37	102.41	114.37
20	2	202	LHG	C20-C19-C18	-2.36	102.44	114.37
22	R	302	CDL	C43-C42-C41	2.36	126.30	114.37
22	R	301	CDL	C79-C78-C77	2.36	126.29	114.37
19	C	602	ADP	C5-N7-C8	2.36	107.15	103.45
22	R	301	CDL	C19-C18-C17	2.34	126.20	114.37
20	S	202	LHG	C20-C19-C18	-2.32	102.67	114.37
22	R	301	CDL	C39-C38-C37	2.31	126.03	114.37
20	S	201	LHG	C20-C19-C18	-2.31	102.71	114.37
20	R	304	LHG	C20-C19-C18	-2.30	102.72	114.37
20	2	202	LHG	C18-C17-C16	-2.29	102.80	114.37
22	R	303	CDL	C23-C22-C21	2.28	125.89	114.37
22	R	303	CDL	C59-C58-C57	2.28	125.89	114.37
22	R	301	CDL	C43-C42-C41	2.28	125.88	114.37
20	K	302	LHG	C18-C17-C16	-2.27	102.91	114.37
20	S	202	LHG	C18-C17-C16	-2.26	102.96	114.37
20	R	304	LHG	C18-C17-C16	-2.24	103.02	114.37
22	R	301	CDL	C63-C62-C61	2.22	125.57	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	303	CDL	C39-C38-C37	2.20	125.48	114.37
20	S	201	LHG	C18-C17-C16	-2.19	103.31	114.37
20	S	202	LHG	C27-C26-C25	-2.16	103.47	114.37
19	B	602	ADP	N9-C8-N7	-2.14	110.90	113.94
19	B	602	ADP	C6-C5-N7	2.14	136.21	132.09
19	A	602	ADP	C6-C5-N7	2.13	136.21	132.09
22	R	301	CDL	C83-C82-C81	2.13	125.11	114.37
19	B	602	ADP	C4'-O4'-C1'	-2.13	104.77	109.47
22	R	303	CDL	CB4-OB6-CB5	2.12	122.87	117.80
20	K	301	LHG	C27-C26-C25	-2.11	103.68	114.37
20	S	201	LHG	C27-C26-C25	-2.10	103.75	114.37
20	R	304	LHG	C27-C26-C25	-2.10	103.75	114.37
22	R	303	CDL	CA4-OA6-CA5	2.09	122.79	117.80
20	K	302	LHG	C5-O7-C7	-2.08	112.82	117.80
19	B	602	ADP	O3B-PB-O2B	2.07	115.55	107.80
19	C	602	ADP	C3'-C2'-C1'	2.05	105.34	101.46
19	F	600	ADP	C4-N9-C8	2.04	107.88	105.74
20	K	302	LHG	C27-C26-C25	-2.02	104.16	114.37
21	2	201	P5S	C2-O37-C38	2.00	122.59	117.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	R	301	CDL	CB4
22	R	302	CDL	CB4
22	R	303	CDL	CA4
22	R	303	CDL	CB4

All (331) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	602	ADP	C5'-O5'-PA-O3A
19	B	602	ADP	C2'-C1'-N9-C8
19	C	602	ADP	C5'-O5'-PA-O1A
19	A	602	ADP	PA-O3A-PB-O2B
19	A	602	ADP	PA-O3A-PB-O3B
19	A	602	ADP	C5'-O5'-PA-O2A
19	A	602	ADP	C5'-O5'-PA-O3A
19	D	600	ADP	C5'-O5'-PA-O1A
19	F	600	ADP	C5'-O5'-PA-O3A
20	K	301	LHG	C1-C2-C3-O3
20	K	301	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	K	301	LHG	C3-O3-P-O6
20	K	301	LHG	C4-O6-P-O3
20	K	301	LHG	C4-O6-P-O5
20	K	302	LHG	C3-O3-P-O5
20	K	302	LHG	C8-C7-O7-C5
20	K	302	LHG	O10-C23-O8-C6
20	K	302	LHG	C24-C23-O8-C6
20	2	202	LHG	O1-C1-C2-C3
20	2	202	LHG	C1-C2-C3-O3
20	2	202	LHG	C3-O3-P-O6
20	2	202	LHG	C4-O6-P-O5
20	2	202	LHG	C8-C7-O7-C5
20	R	304	LHG	O1-C1-C2-C3
20	R	304	LHG	C3-O3-P-O4
20	R	304	LHG	C3-O3-P-O5
20	R	304	LHG	C3-O3-P-O6
20	R	304	LHG	C4-O6-P-O4
20	R	304	LHG	C4-O6-P-O5
20	S	201	LHG	O1-C1-C2-C3
20	S	201	LHG	C3-O3-P-O6
20	S	201	LHG	C4-O6-P-O5
20	S	201	LHG	O6-C4-C5-O7
20	S	201	LHG	O9-C7-O7-C5
20	S	201	LHG	C8-C7-O7-C5
20	S	202	LHG	O1-C1-C2-C3
20	S	202	LHG	C1-C2-C3-O3
20	S	202	LHG	C4-O6-P-O3
20	S	202	LHG	C4-O6-P-O5
21	2	201	P5S	CA-CB-OG-P12
21	2	201	P5S	CB-OG-P12-O15
21	2	201	P5S	C3-O16-P12-O13
22	R	301	CDL	CB2-C1-CA2-OA2
22	R	301	CDL	CA2-OA2-PA1-OA3
22	R	301	CDL	CA3-OA5-PA1-OA2
22	R	301	CDL	CA3-OA5-PA1-OA4
22	R	301	CDL	CB3-OB5-PB2-OB2
22	R	301	CDL	CB3-OB5-PB2-OB3
22	R	302	CDL	CA3-OA5-PA1-OA2
22	R	302	CDL	CA3-OA5-PA1-OA3
22	R	302	CDL	CA3-OA5-PA1-OA4
22	R	303	CDL	O1-C1-CA2-OA2
22	R	303	CDL	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	R	303	CDL	CA3-OA5-PA1-OA3
22	R	303	CDL	CA3-OA5-PA1-OA4
22	R	303	CDL	CB2-OB2-PB2-OB4
22	R	303	CDL	CB2-OB2-PB2-OB5
23	T	201	S12	CB-OG-P-O4
23	T	201	S12	C2-O2-P-OG
23	T	201	S12	C2-O2-P-O3
23	T	201	S12	C2-O2-P-O4
20	S	202	LHG	C24-C23-O8-C6
20	2	202	LHG	O10-C23-O8-C6
20	S	201	LHG	O10-C23-O8-C6
20	K	301	LHG	O9-C7-O7-C5
20	2	202	LHG	O9-C7-O7-C5
20	S	201	LHG	C24-C23-O8-C6
22	R	302	CDL	C37-C38-C39-C40
22	R	301	CDL	C20-C21-C22-C23
22	R	302	CDL	C57-C58-C59-C60
20	S	202	LHG	O10-C23-O8-C6
20	K	302	LHG	O9-C7-O7-C5
22	R	301	CDL	C37-C38-C39-C40
22	R	301	CDL	C40-C41-C42-C43
22	R	301	CDL	C80-C81-C82-C83
22	R	302	CDL	C20-C21-C22-C23
22	R	302	CDL	C40-C41-C42-C43
22	R	303	CDL	C57-C58-C59-C60
20	K	301	LHG	O2-C2-C3-O3
20	2	202	LHG	O2-C2-C3-O3
20	S	202	LHG	O2-C2-C3-O3
22	R	301	CDL	O1-C1-CA2-OA2
22	R	302	CDL	O1-C1-CB2-OB2
20	2	202	LHG	C24-C23-O8-C6
22	R	303	CDL	C61-C62-C63-C64
20	K	301	LHG	C24-C23-O8-C6
20	R	304	LHG	C1-C2-C3-O3
22	R	302	CDL	CA2-C1-CB2-OB2
22	R	303	CDL	CB2-C1-CA2-OA2
20	R	304	LHG	O2-C2-C3-O3
22	R	301	CDL	O1-C1-CB2-OB2
22	R	302	CDL	O1-C1-CA2-OA2
22	R	301	CDL	CA7-C31-C32-C33
22	R	301	CDL	C61-C62-C63-C64
19	B	602	ADP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	201	P5S	C38-C39-C40-C41
22	R	302	CDL	CA5-C11-C12-C13
20	K	301	LHG	O10-C23-O8-C6
20	R	304	LHG	C7-C8-C9-C10
20	S	201	LHG	C7-C8-C9-C10
20	K	302	LHG	O2-C2-C3-O3
20	S	202	LHG	C23-C24-C25-C26
19	B	602	ADP	C4'-C5'-O5'-PA
20	K	302	LHG	O1-C1-C2-C3
22	R	302	CDL	C18-C19-C20-C21
20	S	201	LHG	C24-C25-C26-C27
22	R	302	CDL	C39-C40-C41-C42
22	R	301	CDL	C19-C20-C21-C22
20	K	302	LHG	C32-C33-C34-C35
22	R	301	CDL	C36-C37-C38-C39
20	S	201	LHG	O1-C1-C2-O2
20	S	202	LHG	O1-C1-C2-O2
23	T	201	S12	C11-C10-C9-C8
20	K	301	LHG	C8-C7-O7-C5
20	K	301	LHG	C7-C8-C9-C10
21	2	201	P5S	OXT-C-CA-N
20	K	301	LHG	C28-C29-C30-C31
20	S	202	LHG	C30-C31-C32-C33
22	R	301	CDL	C39-C40-C41-C42
22	R	302	CDL	C36-C37-C38-C39
20	R	304	LHG	C24-C25-C26-C27
22	R	303	CDL	C38-C39-C40-C41
20	S	202	LHG	C4-C5-C6-O8
20	2	202	LHG	C27-C28-C29-C30
22	R	301	CDL	C21-C22-C23-C24
20	K	302	LHG	C30-C31-C32-C33
20	S	201	LHG	C27-C28-C29-C30
20	K	301	LHG	C31-C32-C33-C34
22	R	302	CDL	C16-C17-C18-C19
20	K	302	LHG	C28-C29-C30-C31
22	R	303	CDL	CB7-C71-C72-C73
22	R	303	CDL	C18-C19-C20-C21
22	R	303	CDL	C52-C53-C54-C55
20	S	202	LHG	C28-C29-C30-C31
20	R	304	LHG	C29-C30-C31-C32
21	2	201	P5S	C22-C23-C24-C25
22	R	303	CDL	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	R	302	CDL	C61-C62-C63-C64
22	R	302	CDL	C51-CB5-OB6-CB4
20	2	202	LHG	C23-C24-C25-C26
20	S	202	LHG	C24-C25-C26-C27
20	K	301	LHG	C23-C24-C25-C26
20	K	302	LHG	C7-C8-C9-C10
20	S	202	LHG	C29-C30-C31-C32
20	2	202	LHG	C11-C12-C13-C14
22	R	302	CDL	C62-C63-C64-C65
20	S	202	LHG	C27-C28-C29-C30
20	K	302	LHG	C9-C10-C11-C12
20	S	202	LHG	C32-C33-C34-C35
22	R	301	CDL	OA6-CA4-CA6-OA8
22	R	302	CDL	OA6-CA4-CA6-OA8
22	R	302	CDL	C19-C20-C21-C22
22	R	301	CDL	C78-C79-C80-C81
22	R	303	CDL	C1-CB2-OB2-PB2
22	R	301	CDL	CA2-C1-CB2-OB2
22	R	301	CDL	C41-C42-C43-C44
22	R	302	CDL	C59-C60-C61-C62
20	S	202	LHG	C12-C13-C14-C15
20	2	202	LHG	O1-C1-C2-O2
20	R	304	LHG	O1-C1-C2-O2
20	K	301	LHG	O6-C4-C5-C6
22	R	302	CDL	OB7-CB5-OB6-CB4
19	B	602	ADP	O4'-C4'-C5'-O5'
20	S	201	LHG	C12-C13-C14-C15
22	R	301	CDL	CA3-CA4-CA6-OA8
20	R	304	LHG	C27-C28-C29-C30
22	R	302	CDL	CA4-CA3-OA5-PA1
20	K	301	LHG	C24-C25-C26-C27
20	K	301	LHG	C4-C5-O7-C7
20	R	304	LHG	C12-C13-C14-C15
20	K	301	LHG	C9-C10-C11-C12
20	K	302	LHG	C19-C20-C21-C22
20	K	301	LHG	C30-C31-C32-C33
20	K	302	LHG	C34-C35-C36-C37
20	R	304	LHG	C19-C20-C21-C22
22	R	302	CDL	CB5-C51-C52-C53
20	K	302	LHG	C18-C19-C20-C21
20	S	202	LHG	C7-C8-C9-C10
20	K	302	LHG	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	S	201	LHG	C32-C33-C34-C35
22	R	302	CDL	C56-C57-C58-C59
20	2	202	LHG	C2-C3-O3-P
20	R	304	LHG	C15-C16-C17-C18
20	S	202	LHG	C15-C16-C17-C18
20	K	302	LHG	O6-C4-C5-C6
22	R	301	CDL	C58-C59-C60-C61
20	2	202	LHG	C19-C20-C21-C22
20	K	302	LHG	C33-C34-C35-C36
23	T	201	S12	C7-C8-C9-C10
21	2	201	P5S	O-C-CA-N
20	R	304	LHG	C30-C31-C32-C33
20	R	304	LHG	C9-C10-C11-C12
20	S	202	LHG	O9-C7-O7-C5
20	K	302	LHG	O6-C4-C5-O7
20	R	304	LHG	O6-C4-C5-O7
19	A	602	ADP	C4'-C5'-O5'-PA
20	K	301	LHG	C2-C3-O3-P
20	2	202	LHG	C7-C8-C9-C10
20	K	302	LHG	O7-C5-C6-O8
20	2	202	LHG	C29-C30-C31-C32
22	R	303	CDL	C58-C59-C60-C61
20	2	202	LHG	C13-C14-C15-C16
20	S	202	LHG	C9-C10-C11-C12
22	R	301	CDL	C81-C82-C83-C84
20	S	202	LHG	C8-C7-O7-C5
20	R	304	LHG	C28-C29-C30-C31
22	R	302	CDL	CB2-C1-CA2-OA2
20	R	304	LHG	C33-C34-C35-C36
22	R	302	CDL	C76-C77-C78-C79
20	R	304	LHG	O6-C4-C5-C6
20	S	201	LHG	O6-C4-C5-C6
22	R	302	CDL	OB5-CB3-CB4-CB6
20	K	301	LHG	C26-C27-C28-C29
20	R	304	LHG	C11-C10-C9-C8
20	S	201	LHG	C9-C10-C11-C12
20	K	301	LHG	C35-C36-C37-C38
20	S	202	LHG	C11-C10-C9-C8
20	K	301	LHG	O6-C4-C5-O7
22	R	302	CDL	OB5-CB3-CB4-OB6
22	R	302	CDL	CA3-CA4-CA6-OA8
20	K	301	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	R	302	CDL	OB6-CB4-CB6-OB8
22	R	303	CDL	C16-C17-C18-C19
20	K	302	LHG	C31-C32-C33-C34
19	A	602	ADP	C2'-C1'-N9-C8
23	T	201	S12	C9-C10-C11-C12
21	2	201	P5S	N-CA-CB-OG
23	T	201	S12	C13-C14-C15-C16
20	2	202	LHG	O6-C4-C5-C6
22	R	301	CDL	C62-C63-C64-C65
22	R	301	CDL	C1-CB2-OB2-PB2
22	R	301	CDL	C84-C85-C86-C87
20	S	201	LHG	C15-C16-C17-C18
20	S	202	LHG	C16-C17-C18-C19
20	R	304	LHG	O7-C5-C6-O8
20	S	202	LHG	O7-C5-C6-O8
20	S	201	LHG	C26-C27-C28-C29
19	B	602	ADP	C5'-O5'-PA-O1A
19	C	602	ADP	C5'-O5'-PA-O3A
19	F	600	ADP	C5'-O5'-PA-O1A
20	K	301	LHG	C3-O3-P-O4
20	2	202	LHG	C3-O3-P-O5
20	R	304	LHG	C4-O6-P-O3
20	S	201	LHG	C3-O3-P-O5
20	S	201	LHG	C4-O6-P-O3
21	2	201	P5S	CB-OG-P12-O16
22	R	301	CDL	CA3-OA5-PA1-OA3
22	R	301	CDL	CB2-OB2-PB2-OB3
22	R	303	CDL	CA2-OA2-PA1-OA3
22	R	303	CDL	CA2-OA2-PA1-OA4
22	R	303	CDL	CA2-OA2-PA1-OA5
23	T	201	S12	CB-OG-P-O3
22	R	303	CDL	CB5-C51-C52-C53
20	S	201	LHG	C30-C31-C32-C33
20	R	304	LHG	C2-C3-O3-P
22	R	301	CDL	C1-CA2-OA2-PA1
22	R	301	CDL	CB4-CB3-OB5-PB2
22	R	301	CDL	C52-C51-CB5-OB6
20	R	304	LHG	C25-C26-C27-C28
20	K	302	LHG	O1-C1-C2-O2
23	T	201	S12	C11-C12-C13-C14
22	R	303	CDL	C59-C60-C61-C62
21	2	201	P5S	C1-C2-O37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	R	302	CDL	C12-C11-CA5-OA6
20	S	201	LHG	C31-C32-C33-C34
22	R	303	CDL	C12-C13-C14-C15
20	2	202	LHG	O6-C4-C5-O7
20	2	202	LHG	C12-C13-C14-C15
19	B	602	ADP	C3'-C4'-C5'-O5'
20	K	302	LHG	C16-C17-C18-C19
22	R	301	CDL	C79-C80-C81-C82
21	2	201	P5S	C45-C46-C48-C49
20	R	304	LHG	C13-C14-C15-C16
19	A	602	ADP	C2'-C1'-N9-C4
19	D	600	ADP	C3'-C4'-C5'-O5'
20	R	304	LHG	C10-C11-C12-C13
22	R	302	CDL	C58-C59-C60-C61
20	K	302	LHG	C27-C28-C29-C30
20	2	202	LHG	C18-C19-C20-C21
22	R	303	CDL	C51-C52-C53-C54
20	S	202	LHG	C25-C26-C27-C28
20	S	202	LHG	C14-C15-C16-C17
20	S	201	LHG	C10-C11-C12-C13
22	R	303	CDL	C1-CA2-OA2-PA1
19	B	602	ADP	PA-O3A-PB-O1B
20	S	201	LHG	C28-C29-C30-C31
22	R	302	CDL	C1-CB2-OB2-PB2
20	R	304	LHG	C14-C15-C16-C17
22	R	301	CDL	C11-C12-C13-C14
19	A	602	ADP	O4'-C1'-N9-C8
22	R	302	CDL	C74-C75-C76-C77
21	2	201	P5S	C23-C24-C25-C26
20	2	202	LHG	C9-C10-C11-C12
20	K	301	LHG	C27-C28-C29-C30
21	2	201	P5S	C46-C48-C49-C50
22	R	301	CDL	C14-C15-C16-C17
22	R	302	CDL	C71-CB7-OB8-CB6
19	A	602	ADP	O4'-C1'-N9-C4
19	B	602	ADP	PA-O3A-PB-O2B
19	B	602	ADP	PA-O3A-PB-O3B
20	R	304	LHG	C31-C32-C33-C34
20	S	201	LHG	C34-C35-C36-C37
20	K	302	LHG	C4-C5-C6-O8
22	R	302	CDL	CB3-CB4-CB6-OB8
22	R	303	CDL	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	T	201	S12	OXT-C-CA-N
22	R	303	CDL	C14-C15-C16-C17
20	2	202	LHG	C24-C25-C26-C27
20	K	302	LHG	C24-C25-C26-C27
22	R	302	CDL	C32-C33-C34-C35
20	S	202	LHG	O8-C23-C24-C25
23	T	201	S12	O52-C5-C6-C7
20	S	201	LHG	C29-C30-C31-C32
20	S	202	LHG	O7-C7-C8-C9
23	T	201	S12	CA-CB-OG-P
22	R	302	CDL	C52-C53-C54-C55
22	R	303	CDL	CA6-CA4-OA6-CA5
22	R	303	CDL	CB6-CB4-OB6-CB5
22	R	301	CDL	C82-C83-C84-C85
23	T	201	S12	O51-C5-C6-C7
20	S	202	LHG	O9-C7-C8-C9
20	2	202	LHG	C28-C29-C30-C31
20	R	304	LHG	O9-C7-C8-C9
20	K	301	LHG	O9-C7-C8-C9
20	S	201	LHG	C33-C34-C35-C36
22	R	301	CDL	C35-C36-C37-C38
19	C	602	ADP	PB-O3A-PA-O1A
19	D	600	ADP	PB-O3A-PA-O2A
19	A	602	ADP	O4'-C4'-C5'-O5'
21	2	201	P5S	O19-C17-C20-C21
22	R	301	CDL	C52-C51-CB5-OB7

There are no ring outliers.

12 monomers are involved in 29 short contacts:

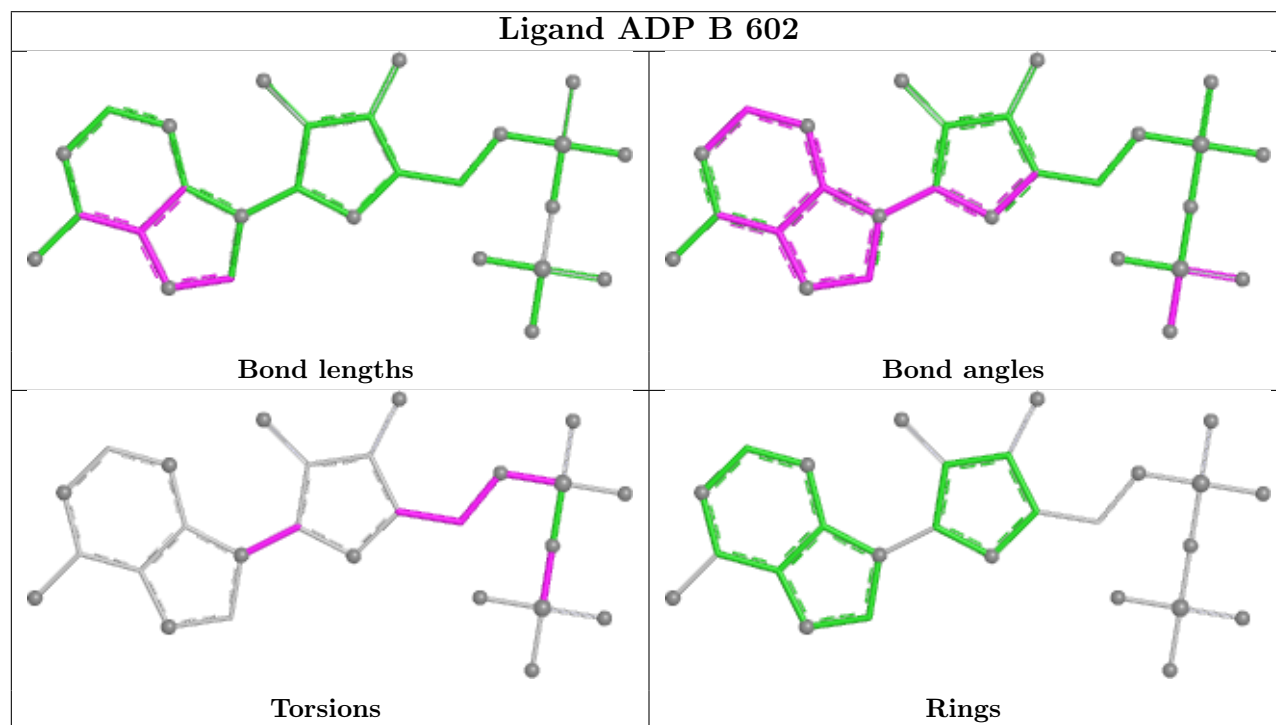
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	602	ADP	2	0
22	R	303	CDL	6	0
22	R	302	CDL	7	0
19	F	600	ADP	1	0
20	S	202	LHG	1	0
22	R	301	CDL	2	0
23	T	201	S12	1	0
21	2	201	P5S	2	0
20	R	304	LHG	2	0
20	S	201	LHG	4	0
20	K	302	LHG	3	0

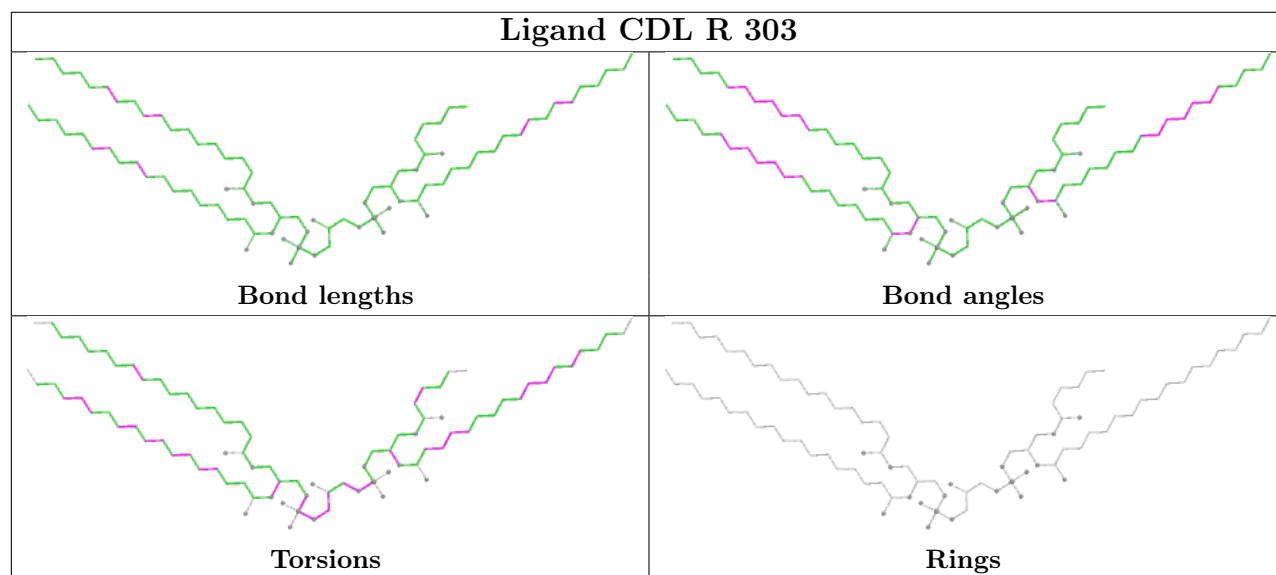
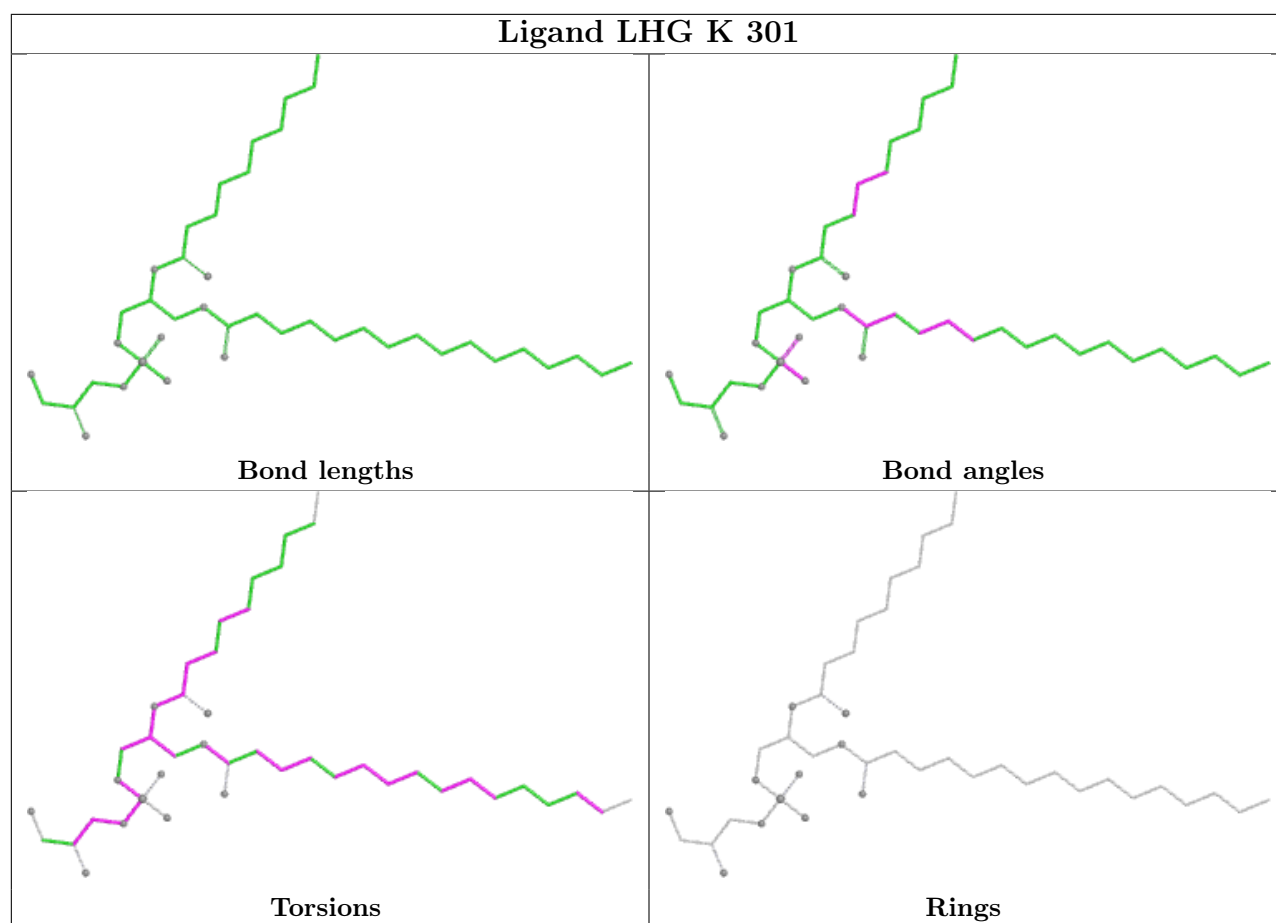
Continued on next page...

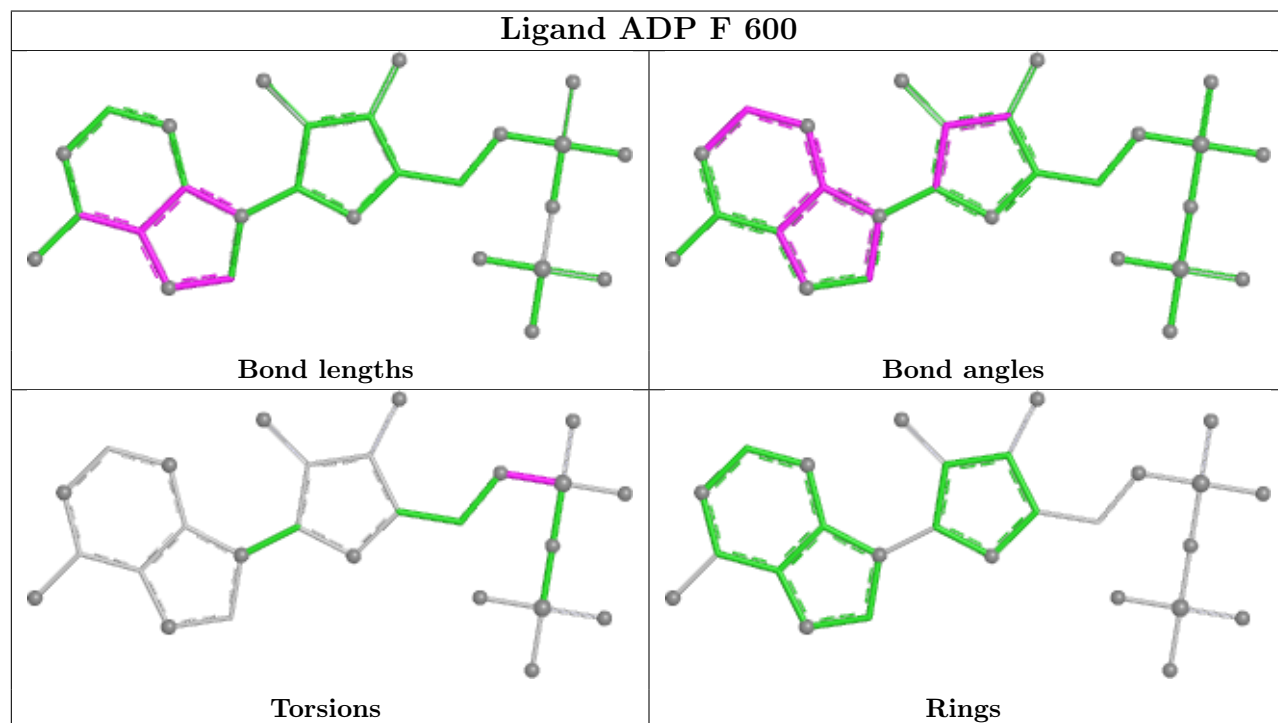
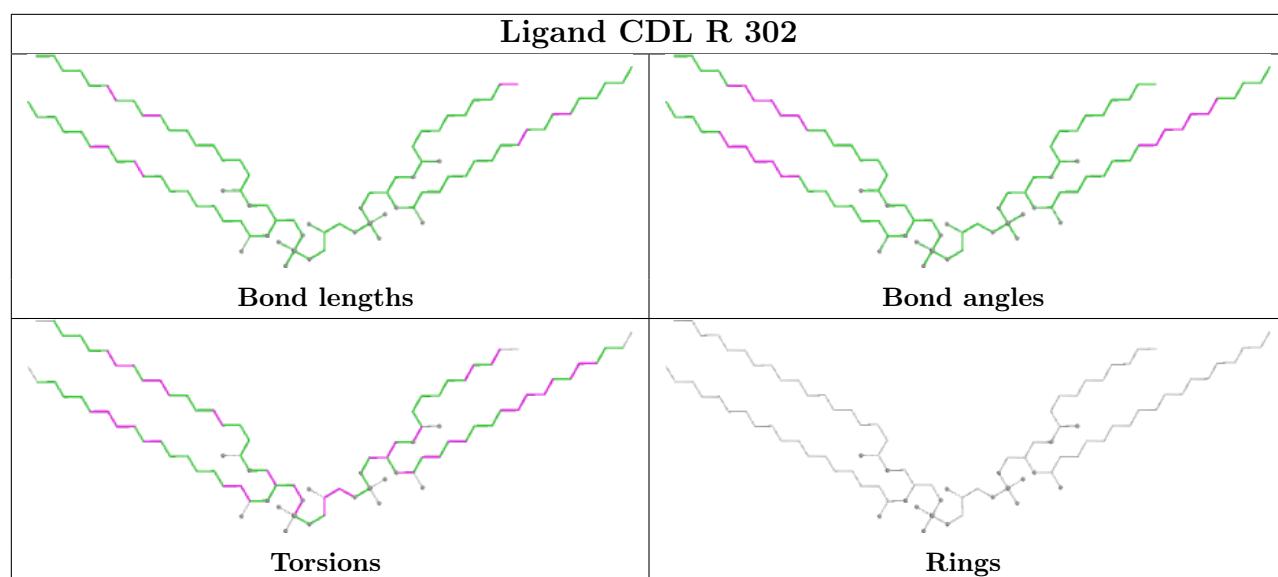
Continued from previous page...

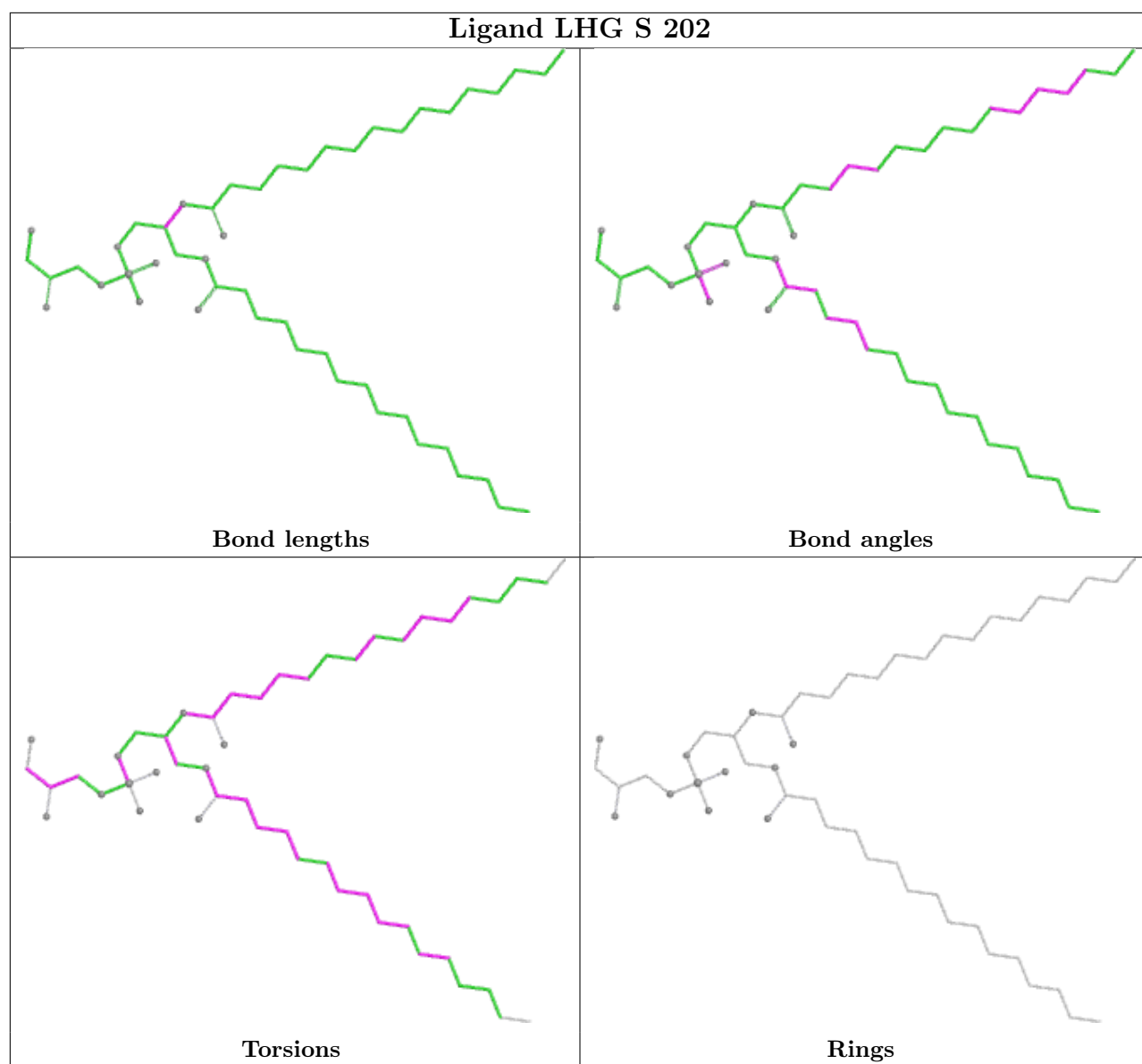
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	602	ADP	1	0

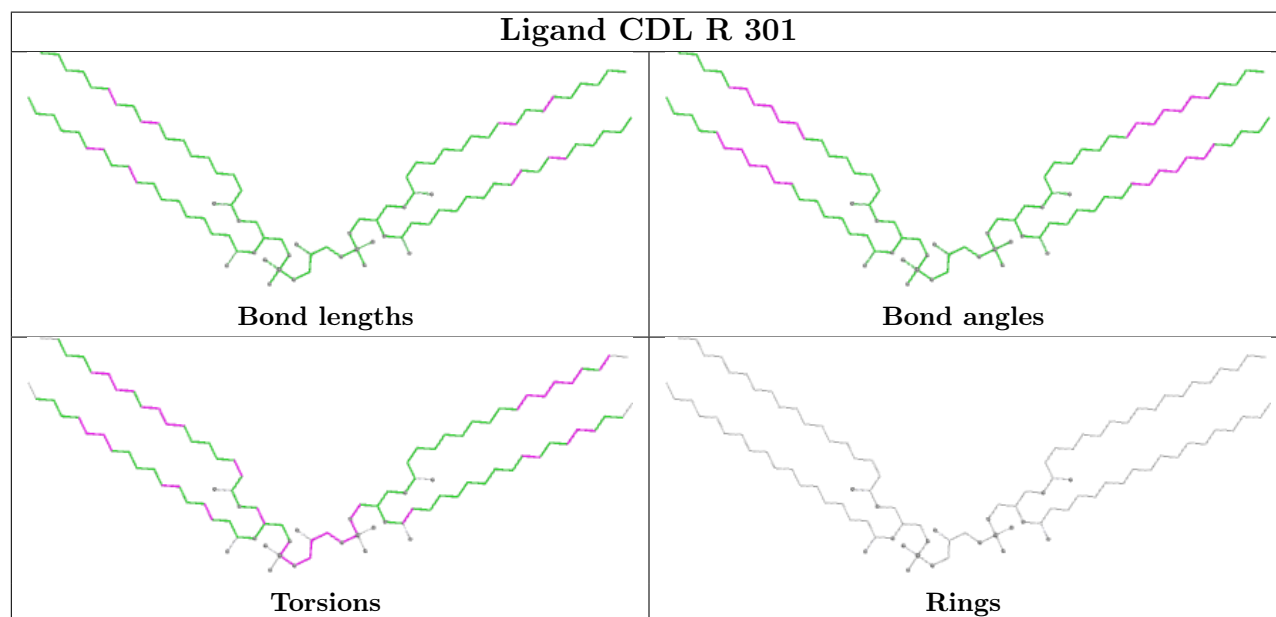
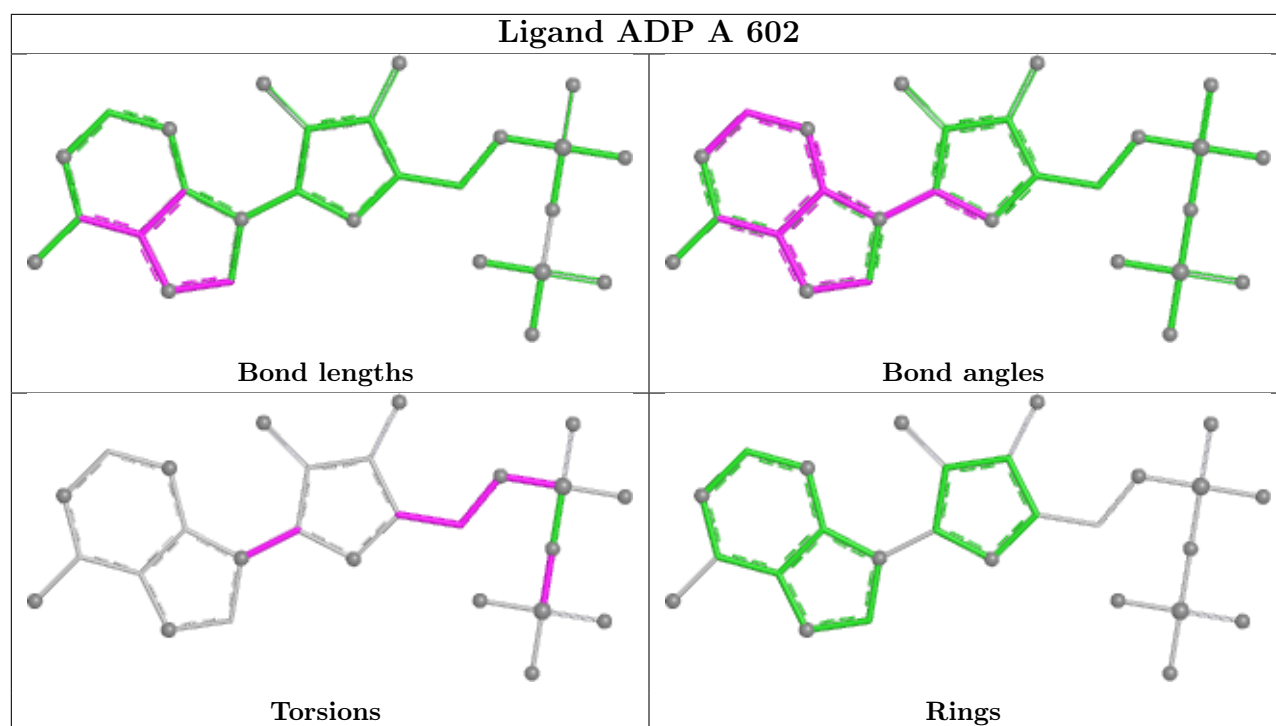
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

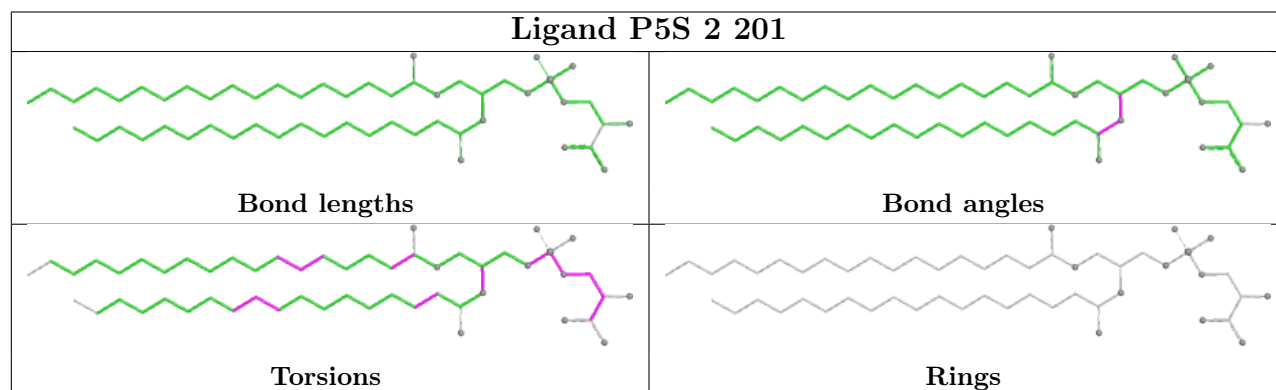
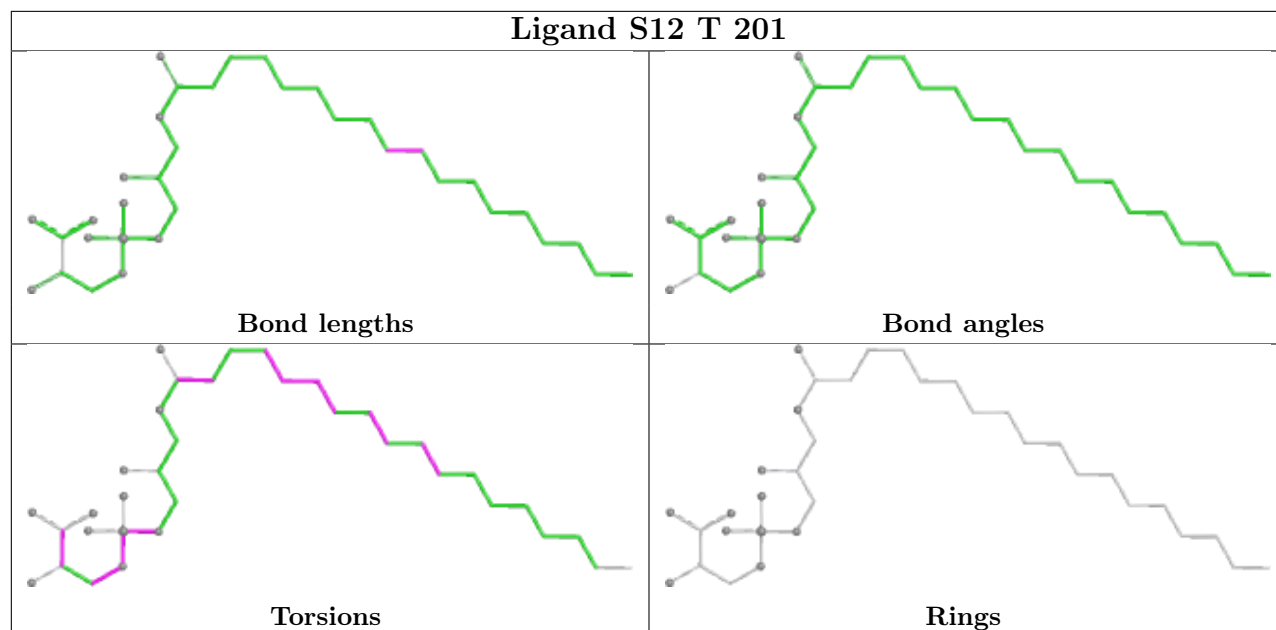


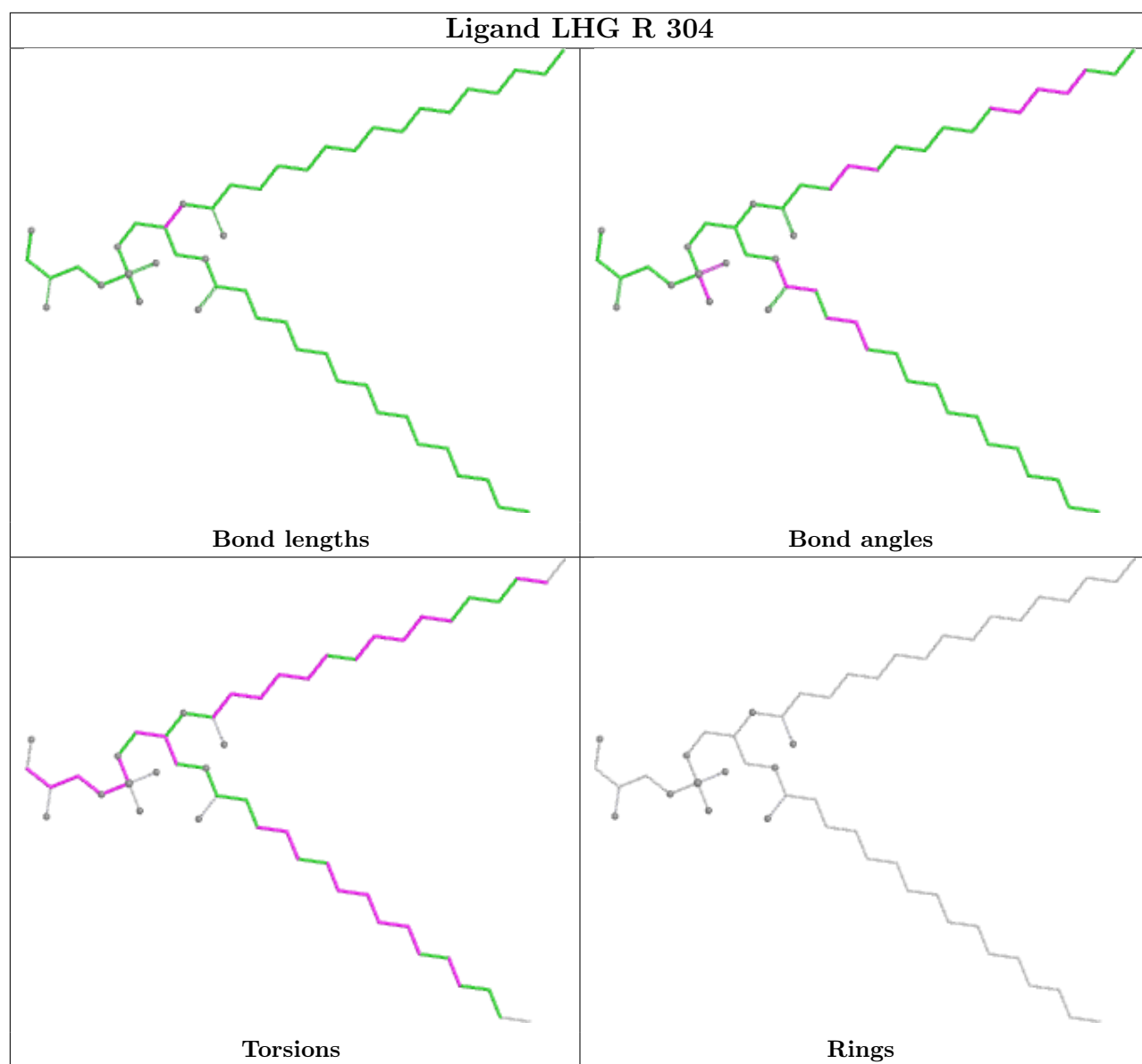


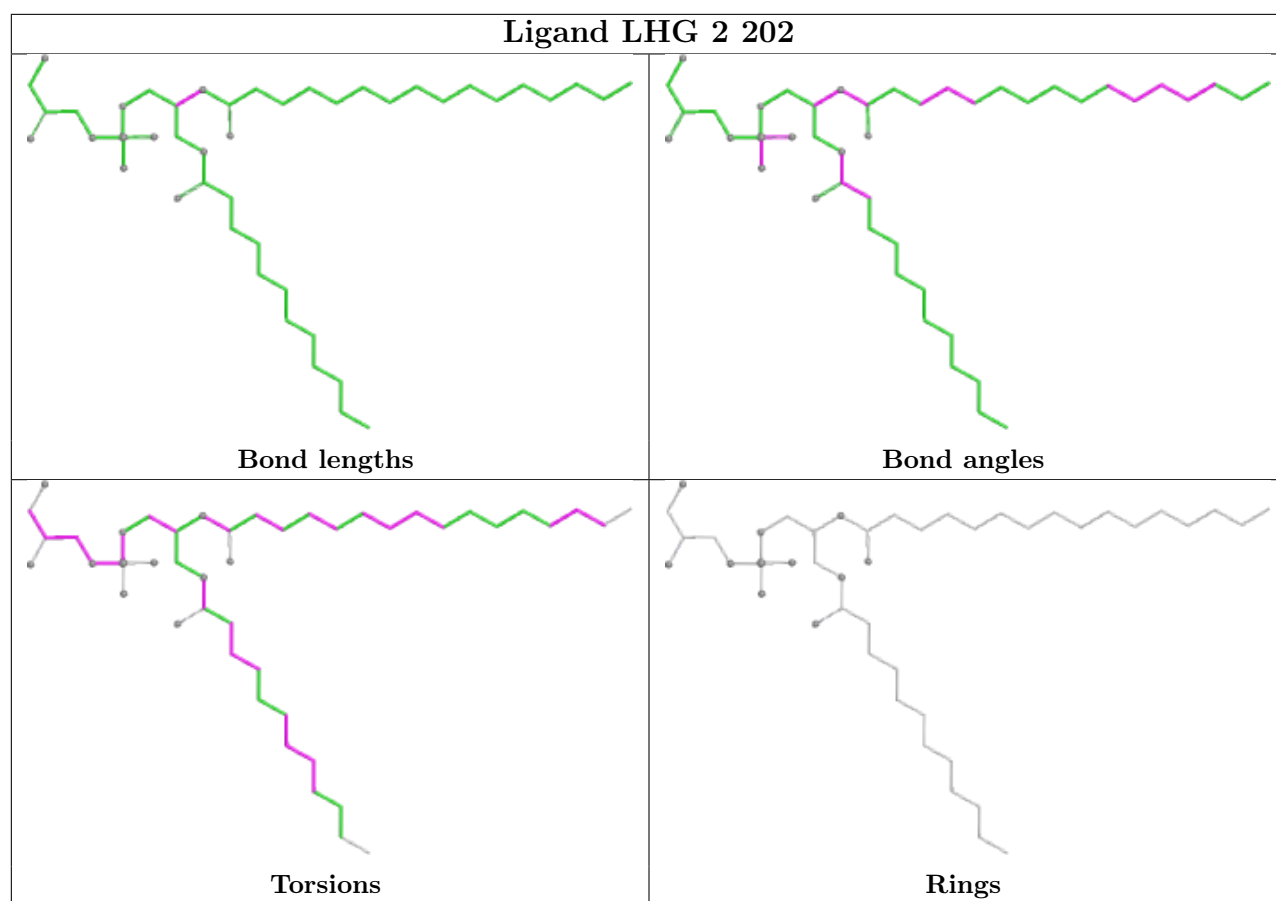


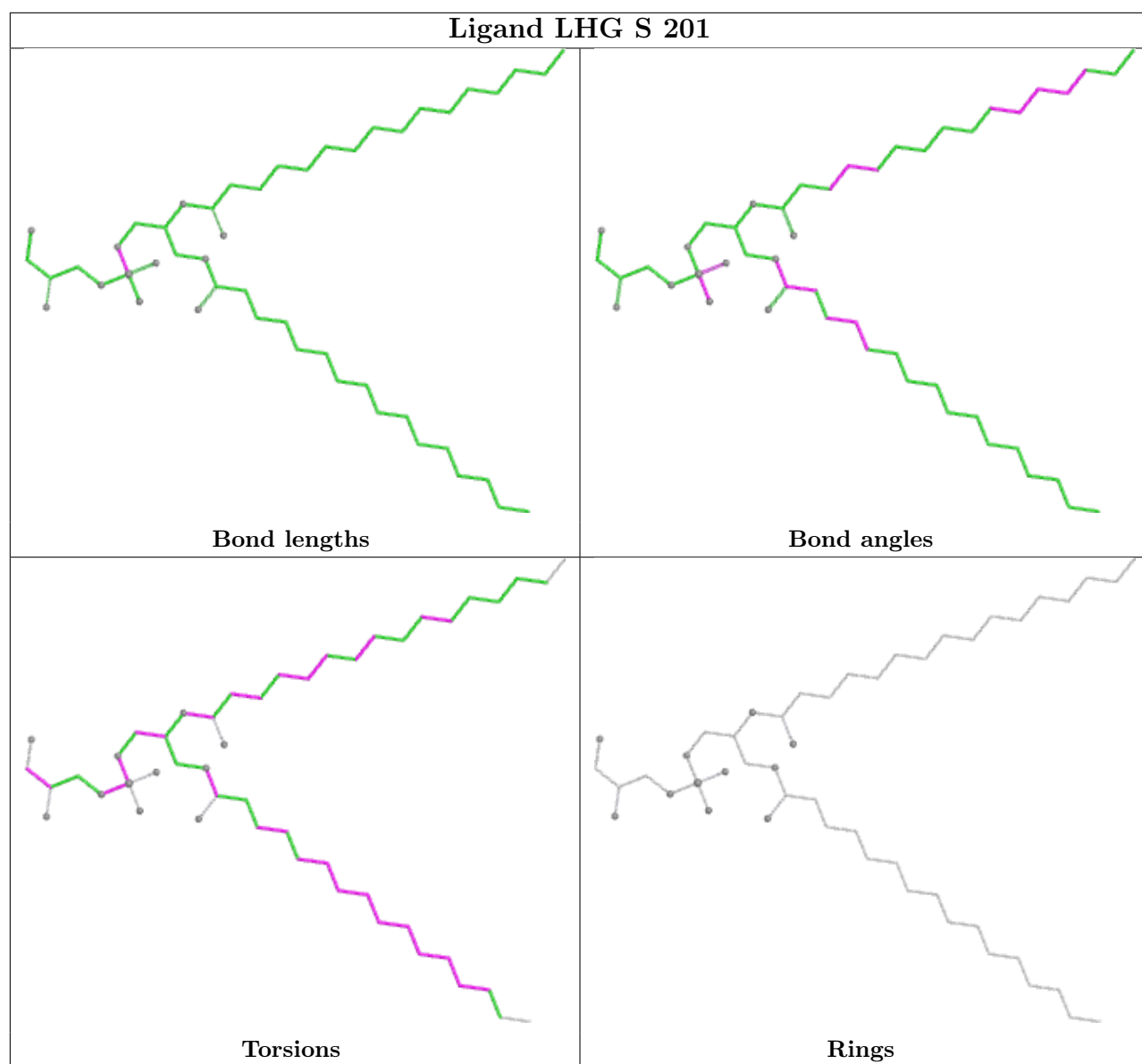


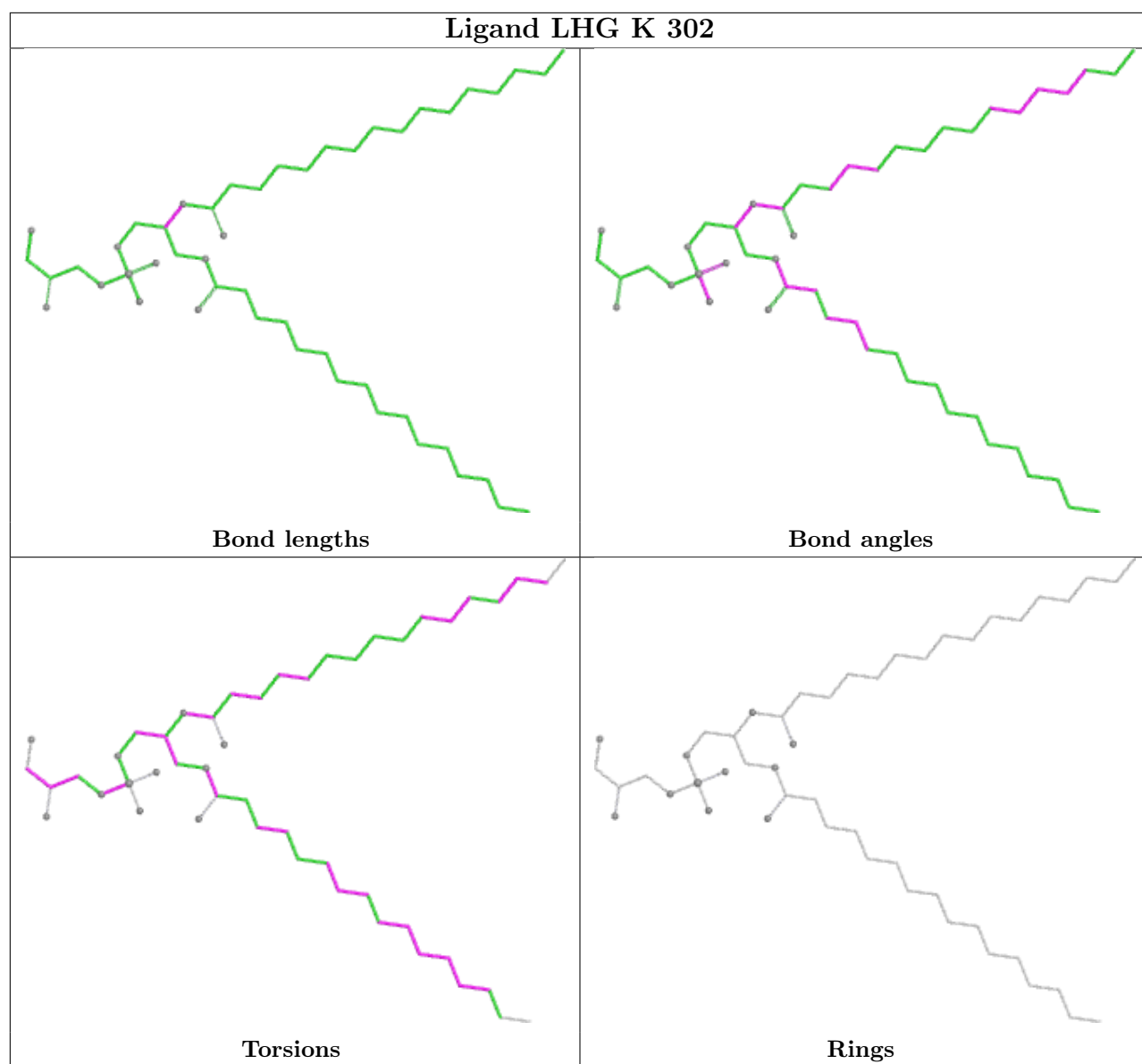


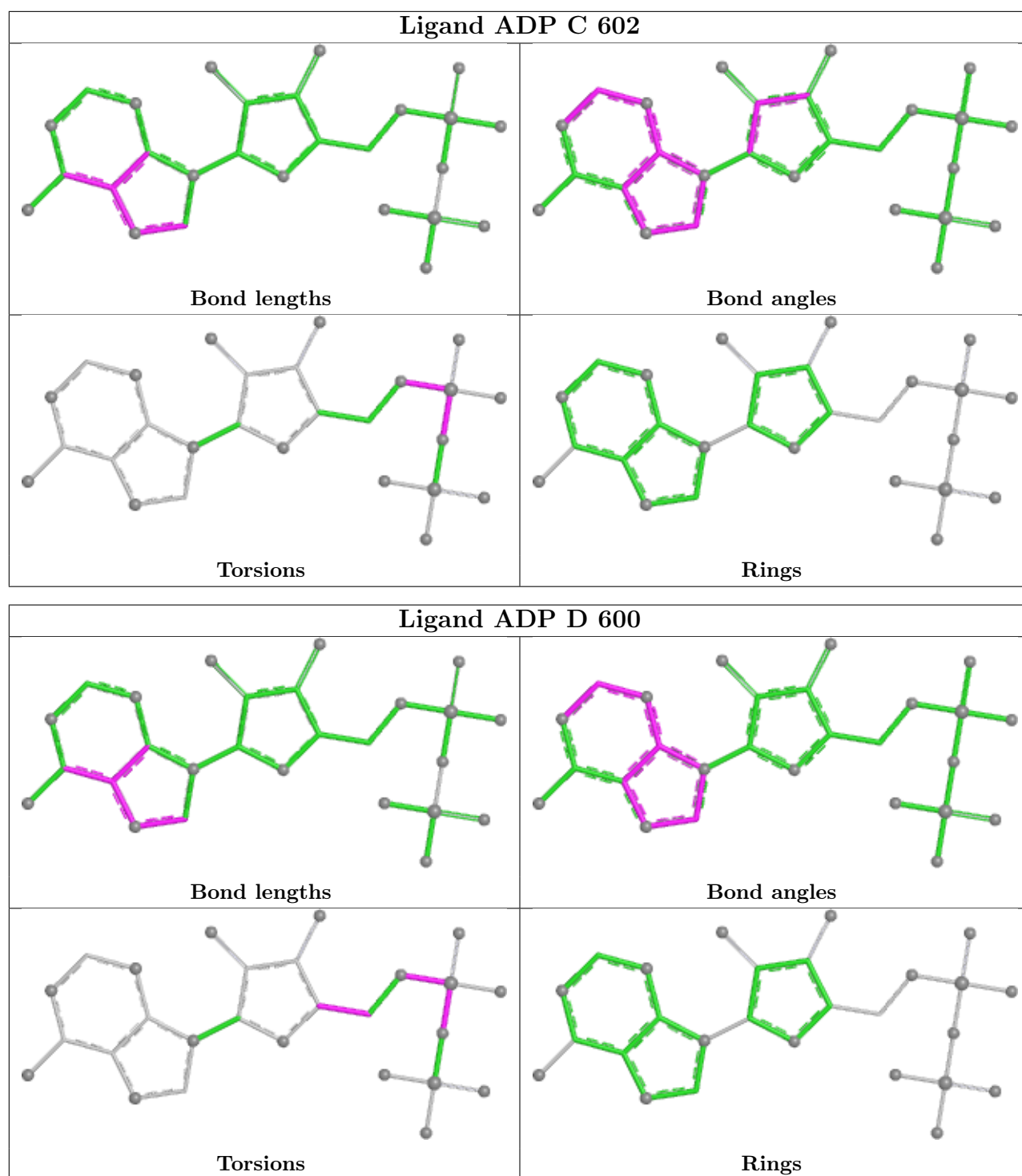












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	143:ARG	C	144:GLU	N	1.61

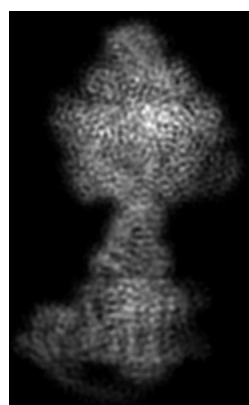
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10573. These allow visual inspection of the internal detail of the map and identification of artifacts.

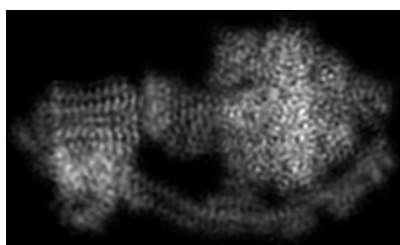
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

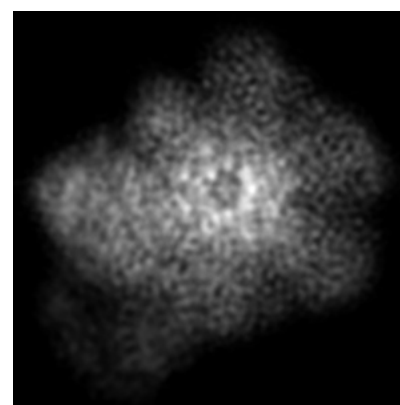
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

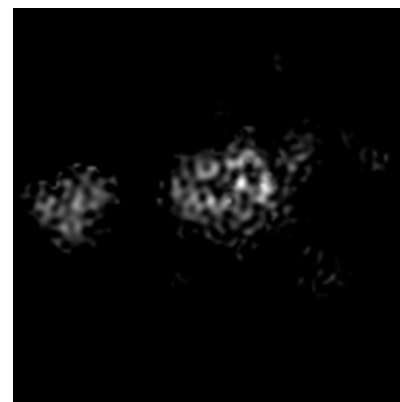
6.2.1 Primary map



X Index: 69



Y Index: 69



Z Index: 115

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

6.3 Largest variance slices [i](#)

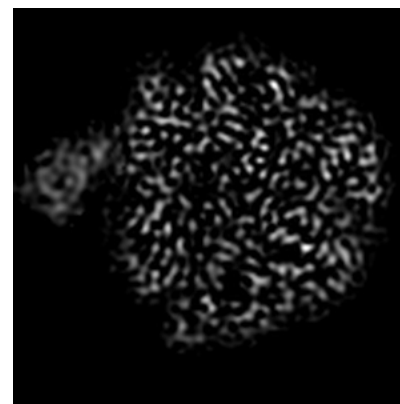
6.3.1 Primary map



X Index: 81



Y Index: 69



Z Index: 167

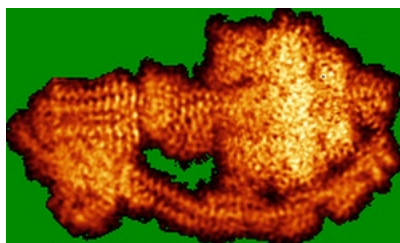
The images above show the largest variance slices of the map in three orthogonal directions.

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

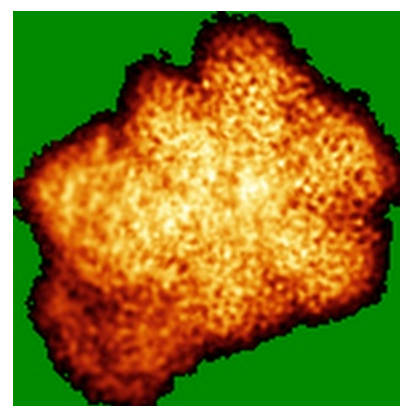
6.4.1 Primary map



X



Y

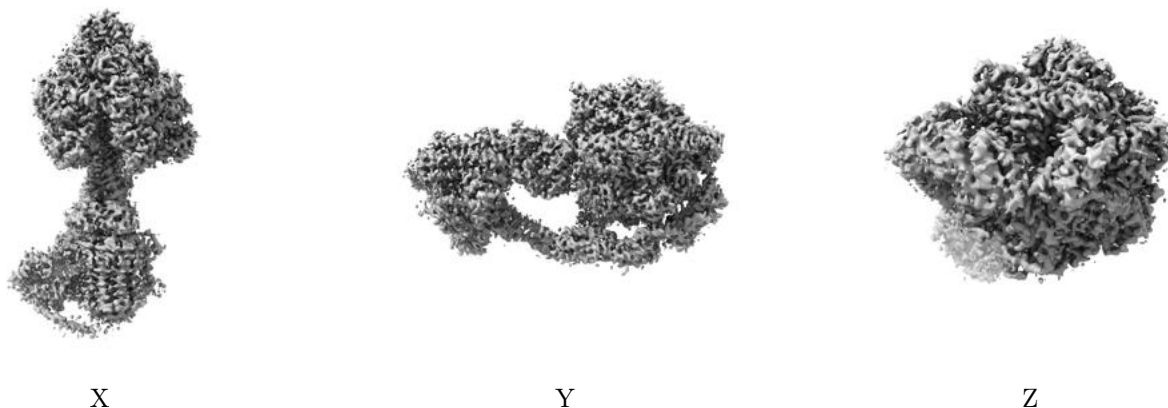


Z

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

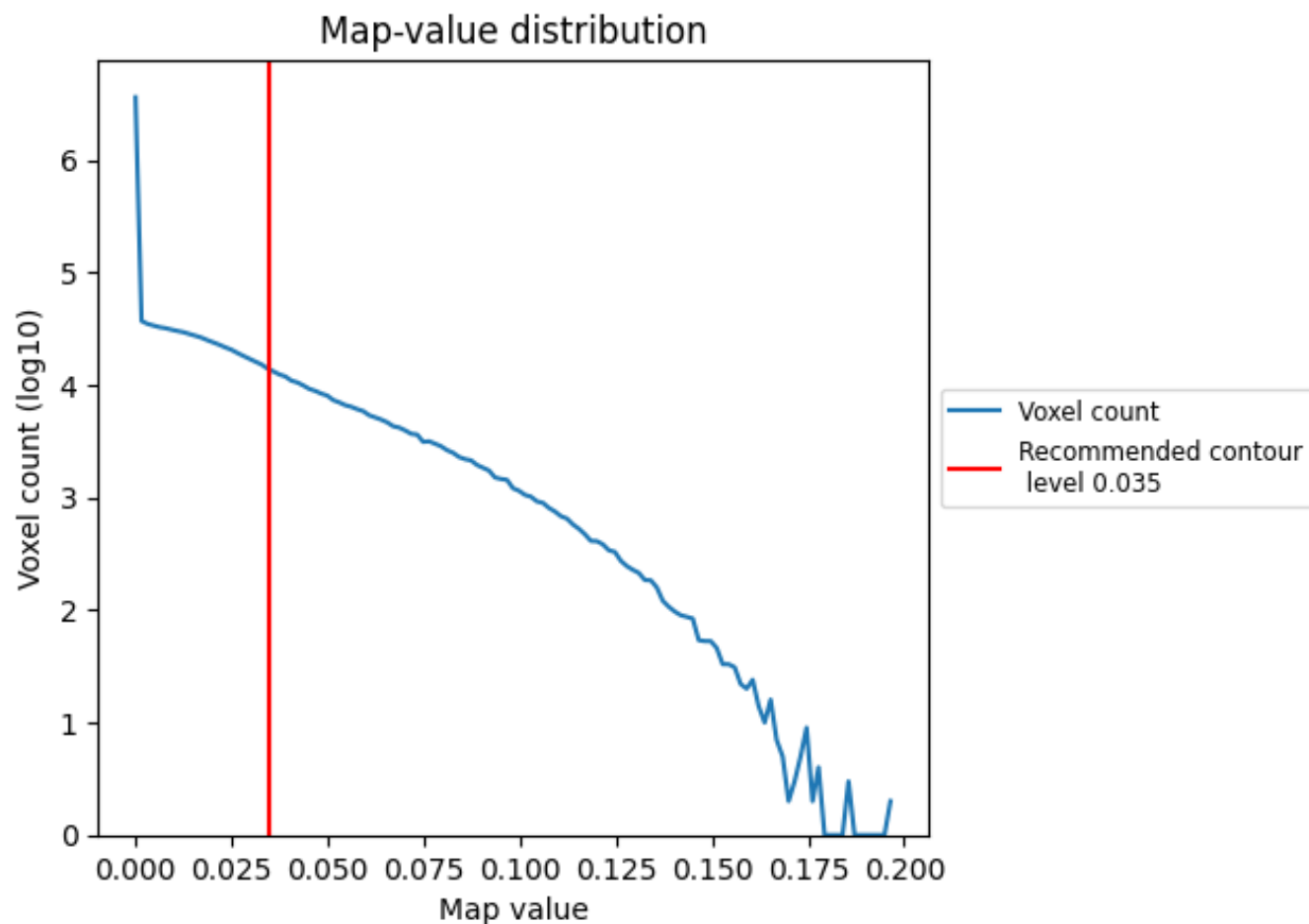
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

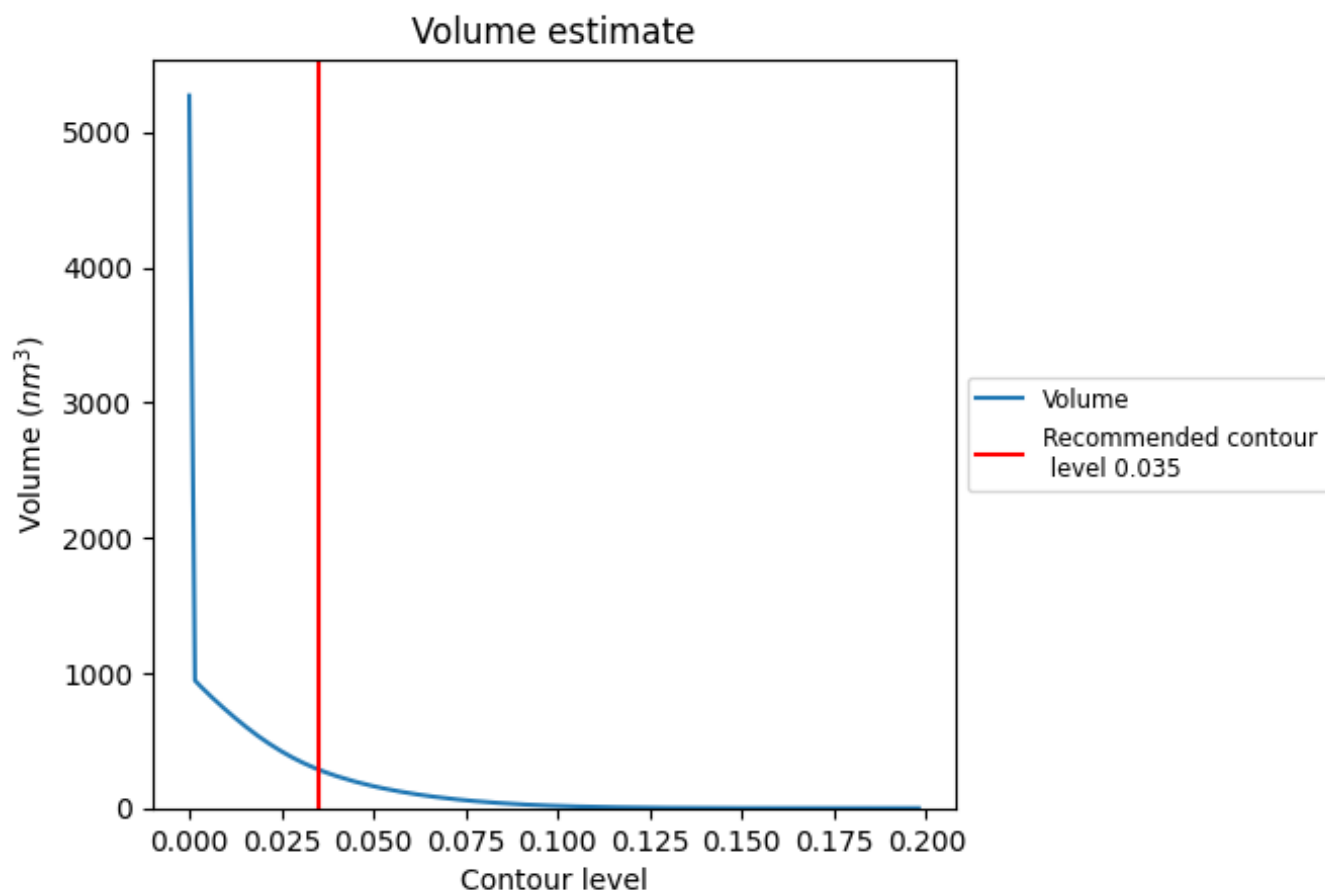
This section contains the results of statistical analysis of the map.

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 286 nm^3 ; this corresponds to an approximate mass of 259 kDa.

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

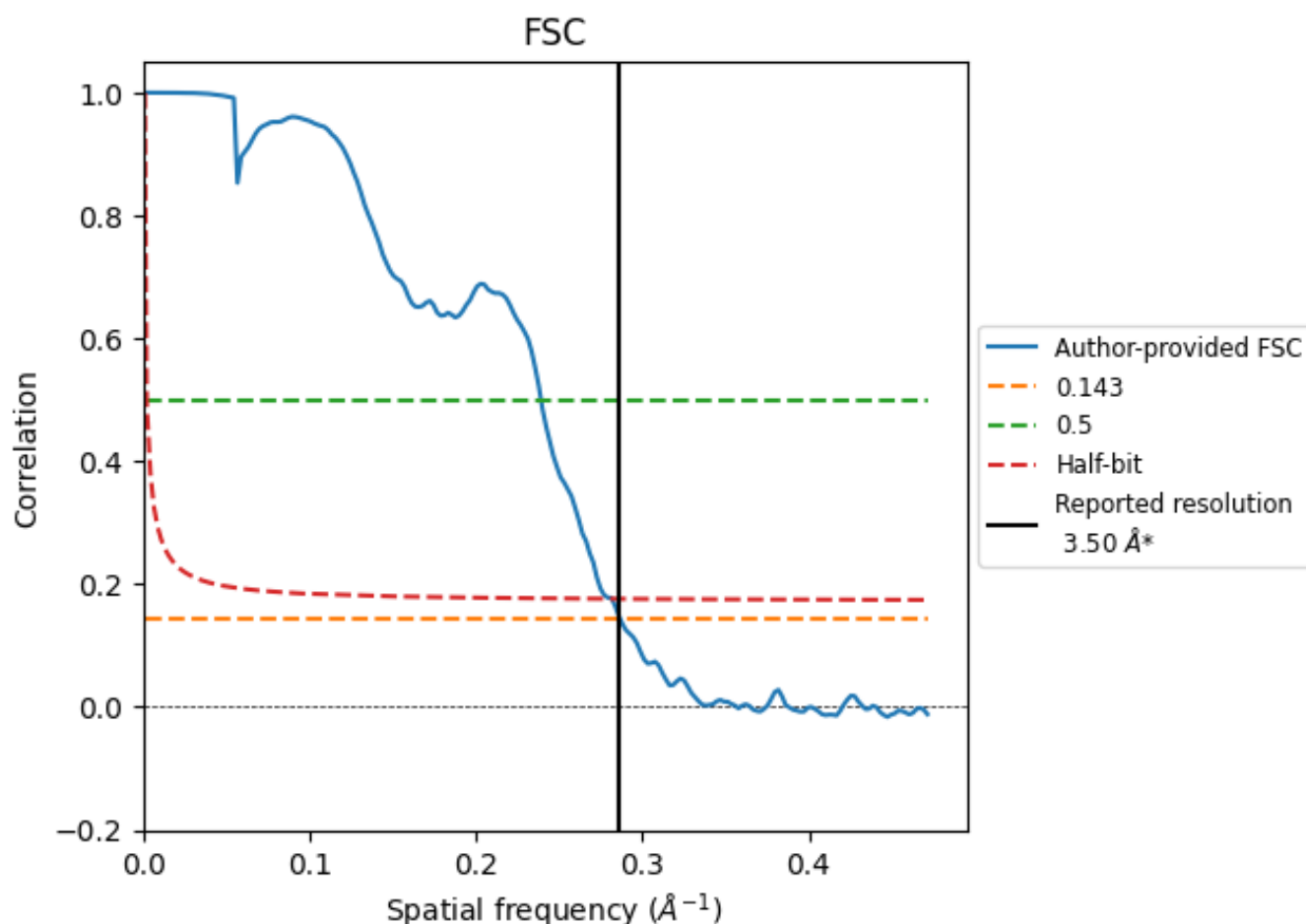
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

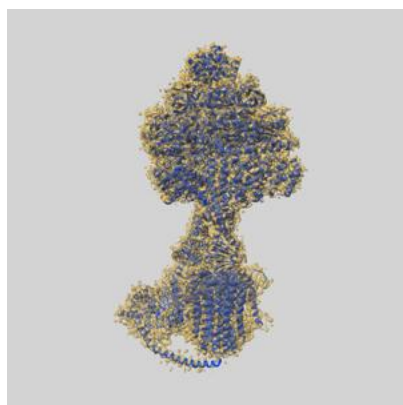
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.18	3.55
Unmasked-calculated*	-	-	-

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

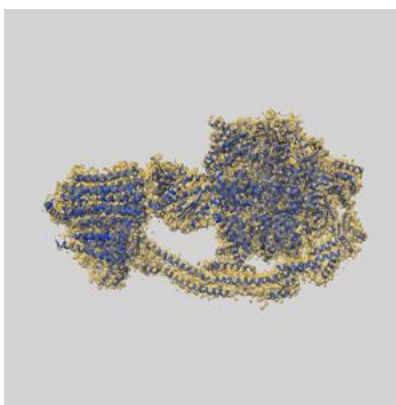
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10573 and PDB model 6TT7. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

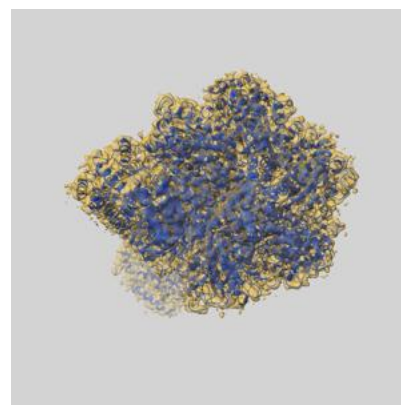
9.1 Map-model overlay [i](#)



X



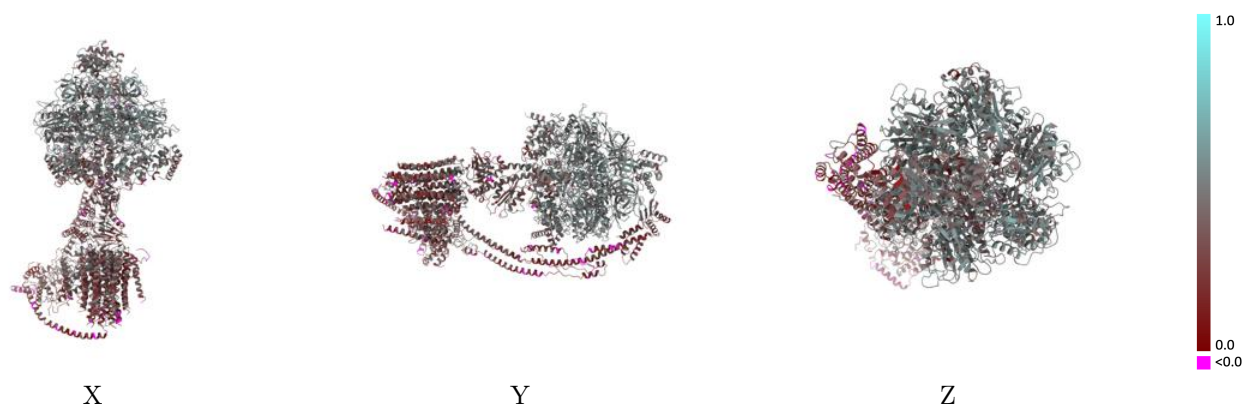
Y



Z

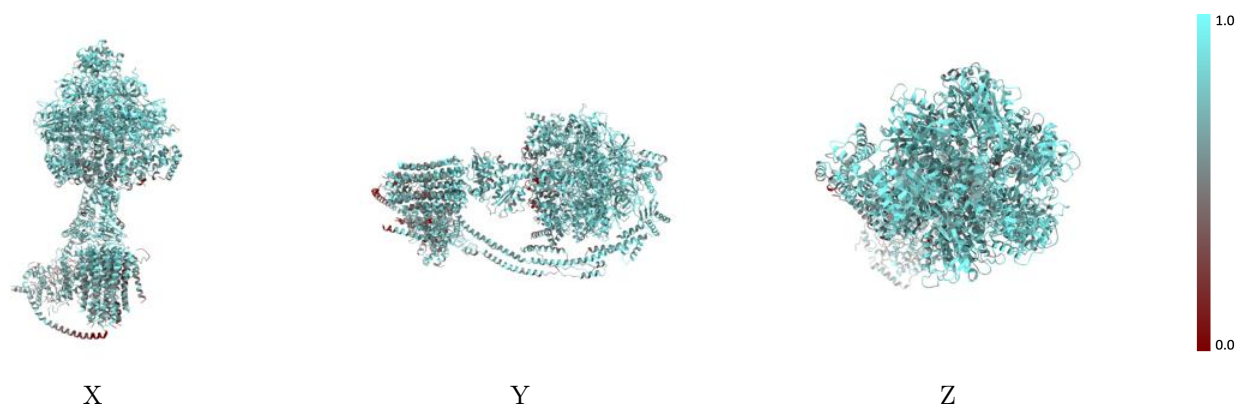
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



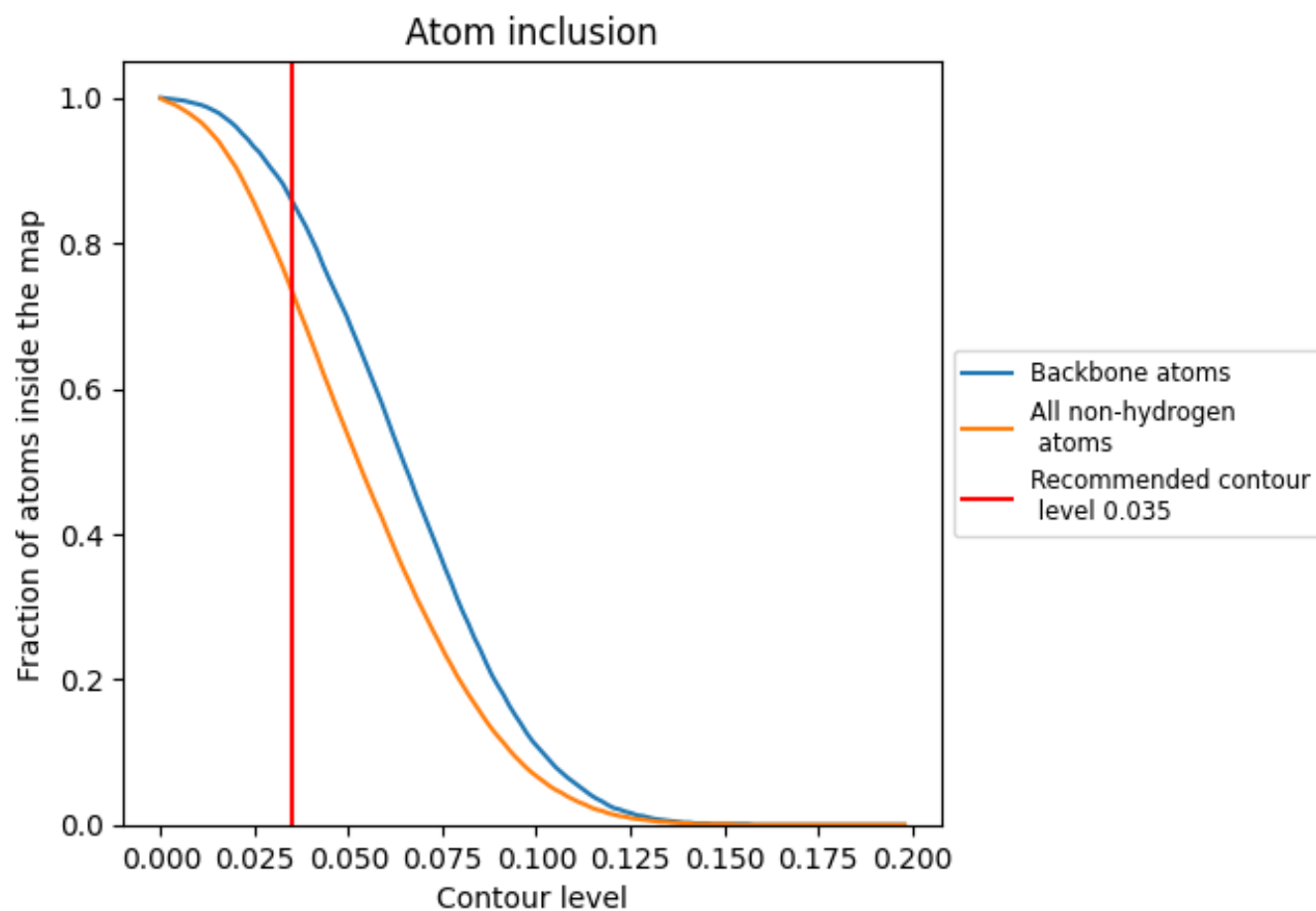
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.4010
1	 0.6700	 0.3020
2	 0.6220	 0.3180
3	 0.7180	 0.3370
4	 0.6800	 0.3380
5	 0.6670	 0.3030
6	 0.7110	 0.3270
7	 0.7110	 0.3430
8	 0.6740	 0.3060
A	 0.7750	 0.4720
B	 0.7800	 0.4810
C	 0.7480	 0.4500
D	 0.7480	 0.4660
E	 0.7750	 0.4770
F	 0.7920	 0.4940
G	 0.7530	 0.3780
H	 0.7180	 0.3100
I	 0.7430	 0.3210
J	 0.7740	 0.4110
K	 0.7440	 0.2870
L	 0.7310	 0.2230
M	 0.6640	 0.2340
N	 0.7300	 0.3570
O	 0.4550	 0.1830
P	 0.6420	 0.2780
Q	 0.7180	 0.3620
R	 0.5790	 0.2890
S	 0.5800	 0.2090
T	 0.5070	 0.2110

