Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:56 pm GMT

PDB ID	:	6ZPO
EMDB ID	:	EMD-11342
Title	:	bovine ATP synthase monomer state 1 (combined)
Authors	:	Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on	:	2020-07-09
Resolution	:	4.00 Å(reported)
Based on initial models	:	2CLY, 2V7Q

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:

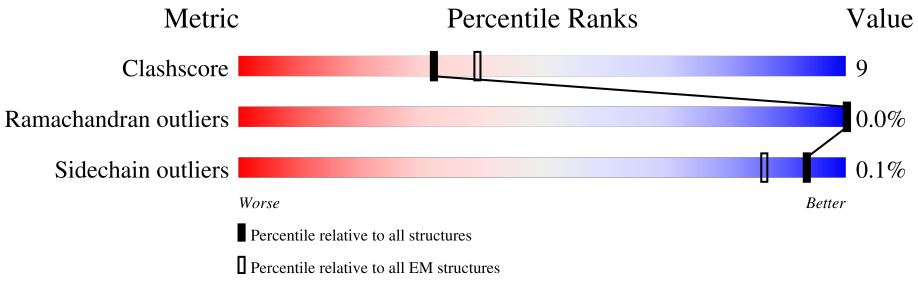
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	8	66	56% 6% 38%
2	A	510	5% 87% 13%
2	B	510	7% 83% 11% 6%
2	C	510	9% 80% 17%
3	D	482	79% 18%
3	E	482	6% 80% 16%
3	F	482	83% 13%
4	G	273	87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	146	67% 23% 10%
6	I	50	68% 26% 6%
7	J	66	20% 68% 29%
8	K	75	75% 24%
8	L	75	75% 23%
8	M	75	77% 23%
8	N	75	83% 17%
8	O	75	88% 12%
8	P	75	83% 16%
8	Q	75	85% 15%
8	R	75	73% 27%
9	S	190	22% 82% 17%
10	a	226	100%
11	b	214	5% 98%
12	d	160	19% 97%
13	e	70	59% 41%
14	f	87	95% 5%
15	g	102	77% 23%
16	h	76	49% 82% 18%
17	j	60	5% 80% 20%
18	k	57	11% 63% 37%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 81052 atoms, of which 41104 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 protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	8	41	696	231	352	52	58	3	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	508	7838	2434	3970	681	741	12	0	0
2	B	477	Total	C	H	N	O	S	0	0
			7392	2294	3751	645	690	12		
2	C	498	Total	C	H	N	O	S	0	0
			7698	2390	3904	669	723	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
C	1	GLU	GLN	variant	UNP P19483

- Molecule 3 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	469	7163	2254	3605	605	688	11	0	0
3	E	467	Total	C	H	N	O	S	0	0
			7132	2243	3593	601	684	11		
3	F	467	Total	C	H	N	O	S	0	0
			7131	2243	3592	601	684	11		

- Molecule 4 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	272	Total	C	H	N	O	S	0	0
			4300	1330	2185	368	409	8		

- Molecule 5 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	132	Total	C	H	N	O	S	0	0
			1957	614	978	165	198	2		

- Molecule 6 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	47	Total	C	H	N	O	S	0	0
			764	237	395	66	64	2		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	47	Total	C	H	N	O	0	0
			731	224	361	76	70		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
8	L	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
8	M	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
8	N	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
8	O	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
8	P	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
8	Q	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
8	R	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	S	188	Total	C	H	N	O	S	0	0
			3004	920	1557	249	269	9		

- Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	226	Total	C	H	N	O	S	0	0
			3611	1155	1870	276	298	12		

- Molecule 11 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	b	209	Total	C	H	N	O	S	0	0
			3454	1095	1753	292	308	6		

- Molecule 12 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	156	Total	C	H	N	O	S	0	0
			2567	827	1285	209	243	3		

- Molecule 13 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	e	41	Total	C	H	N	O	S	0	0
			687	218	352	61	55	1		

- Molecule 14 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	f	83	Total	C	H	N	O	S	0	0
			1410	456	717	120	114	3		

- Molecule 15 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	g	79	Total	C	H	N	O	S	0	0
			1291	420	662	100	108	1		

- Molecule 16 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	h	62	Total	C	H	N	O	S	0	0
			1009	326	495	87	99	2		

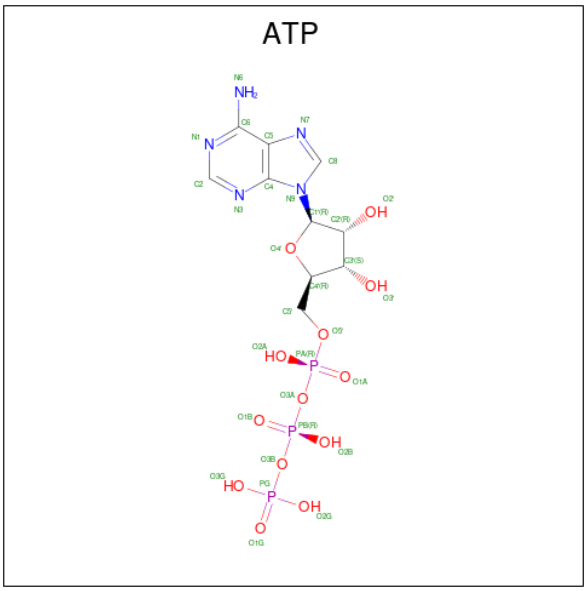
- Molecule 17 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	j	48	Total	C	H	N	O	S	0	0
			828	267	428	66	65	2		

- Molecule 18 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	k	36	Total	C	H	N	O	S	0	0
			596	192	307	47	48	2		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

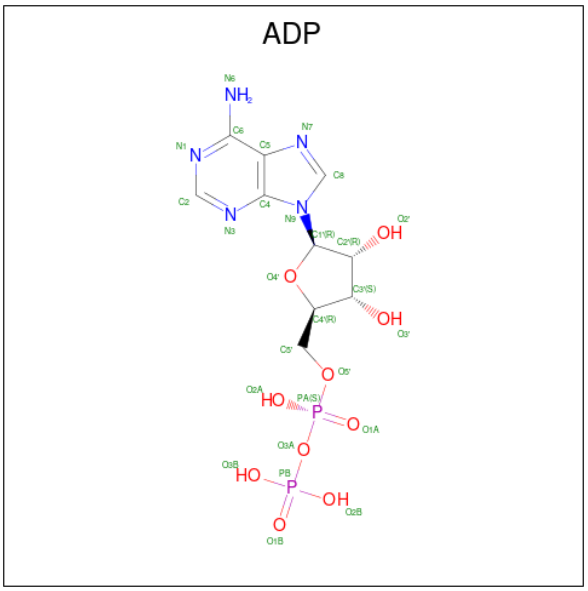


Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
19	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
19	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

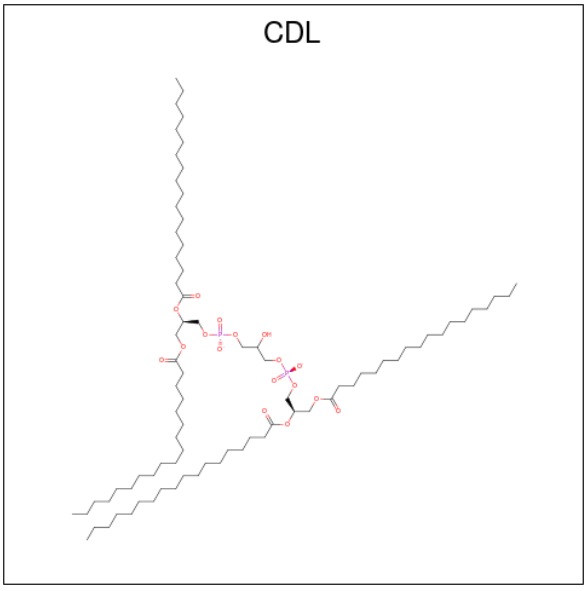
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	
20	B	1	Total	Mg	0
			1	1	
20	C	1	Total	Mg	0
			1	1	
20	D	1	Total	Mg	0
			1	1	
20	F	1	Total	Mg	0
			1	1	

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
21	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
21	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
21	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



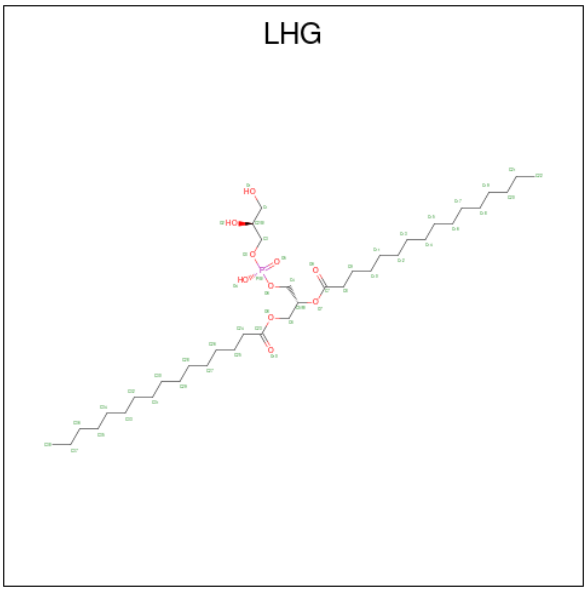
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	H	O	P	0
			202	64	119	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	f	1	Total	C	H	O	P	0
			392	124	230	34	4	
22	f	1	Total	C	H	O	P	0
			392	124	230	34	4	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
23	f	1	Total	C	H	O	P	0
			214	66	126	20	2	
23	f	1	Total	C	H	O	P	0
			214	66	126	20	2	

- Molecule 24 is water.

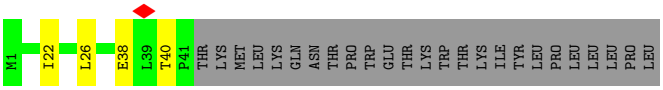
Mol	Chain	Residues	Atoms		AltConf
24	A	3	Total	O	0
			3	3	
24	B	3	Total	O	0
			3	3	
24	C	3	Total	O	0
			3	3	
24	D	4	Total	O	0
			4	4	
24	F	4	Total	O	0
			4	4	

3 Residue-property plots (i)

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

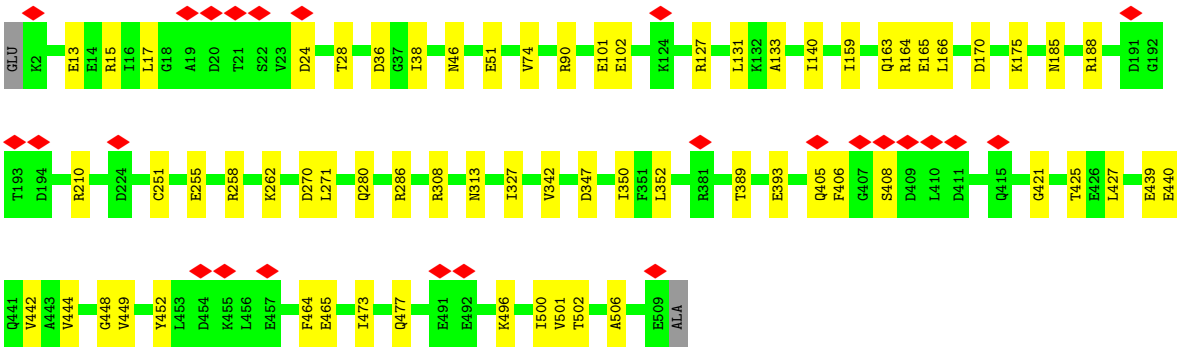
• Molecule 1: ATP synthase protein 8

Chain 8:



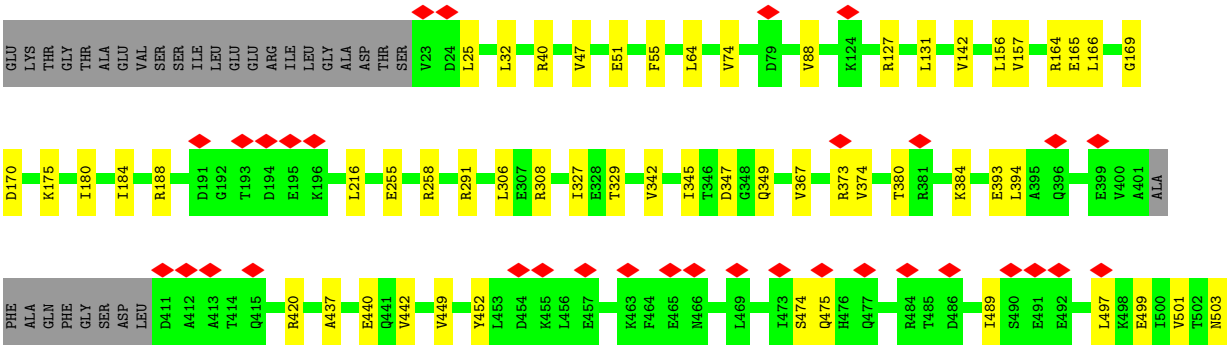
• Molecule 2: ATP synthase subunit alpha, mitochondrial

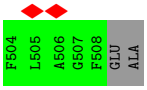
Chain A:



• Molecule 2: ATP synthase subunit alpha, mitochondrial

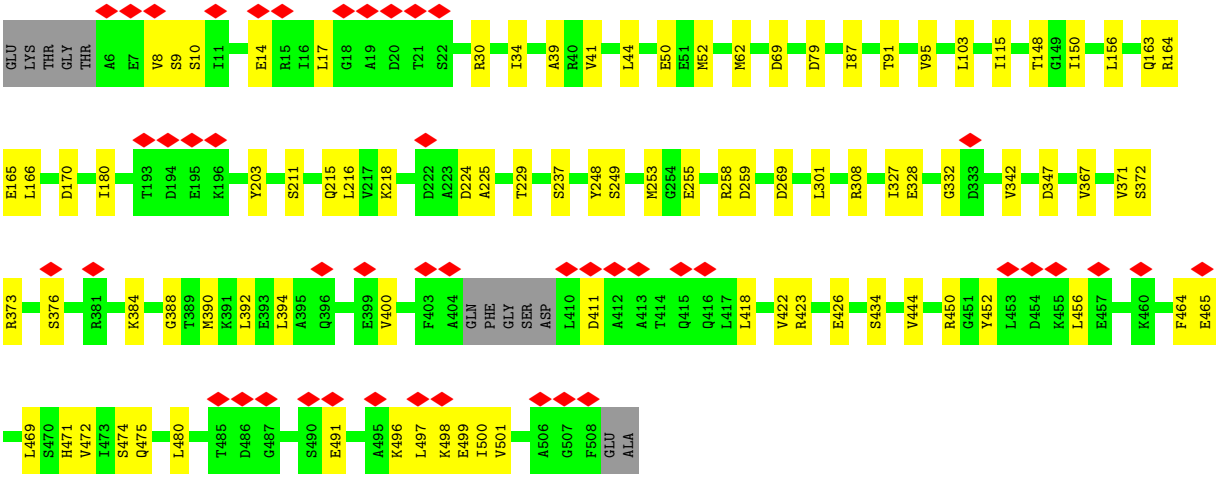
Chain B:





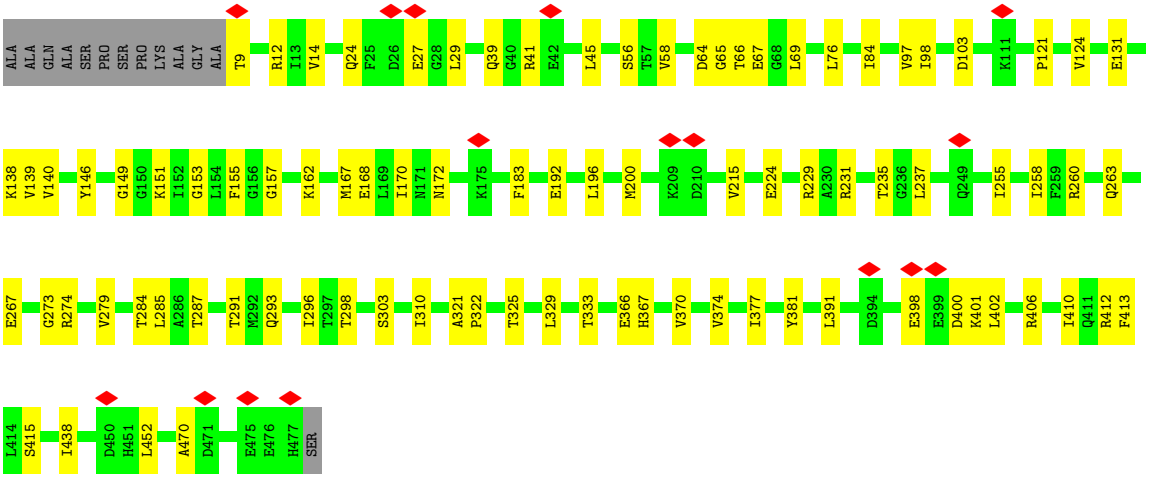
• Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain C:



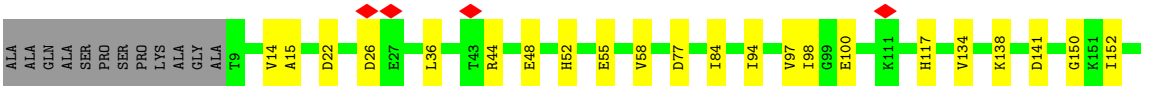
• Molecule 3: ATP synthase subunit beta, mitochondrial

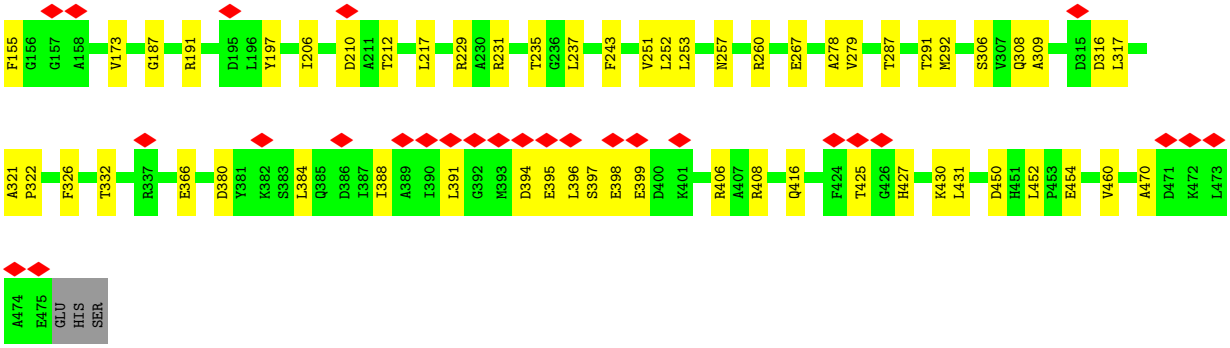
Chain D:



• Molecule 3: ATP synthase subunit beta, mitochondrial

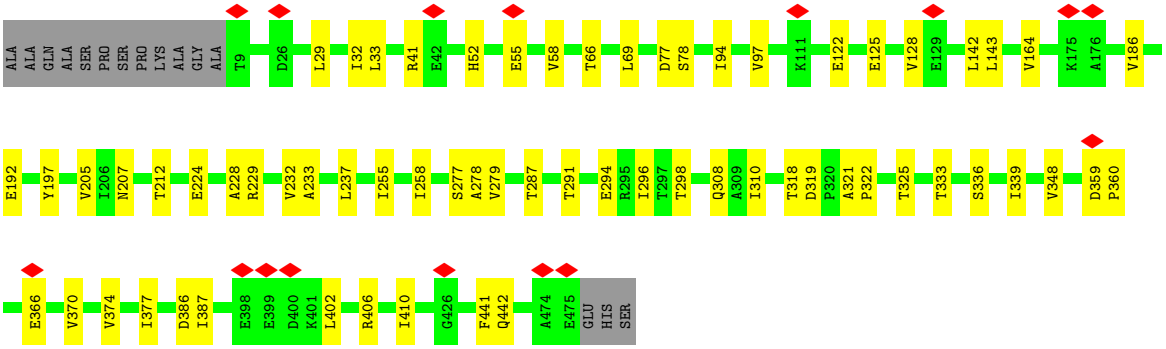
Chain E:





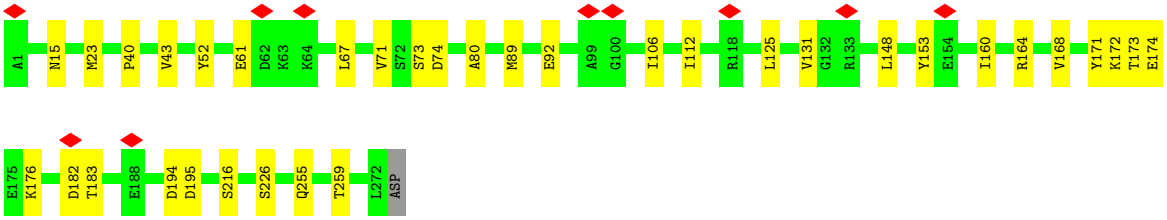
• Molecule 3: ATP synthase subunit beta, mitochondrial

Chain F:



• Molecule 4: ATP synthase subunit gamma, mitochondrial

Chain G:

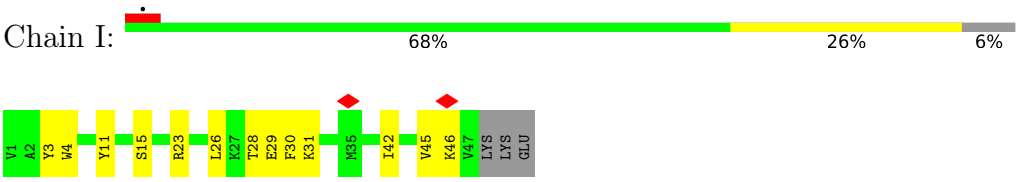


• Molecule 5: ATP synthase subunit delta, mitochondrial

Chain H:

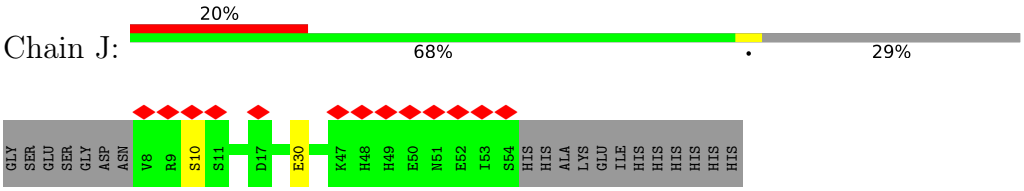
• Molecule 6: ATP synthase subunit epsilon, mitochondrial

Chain I:



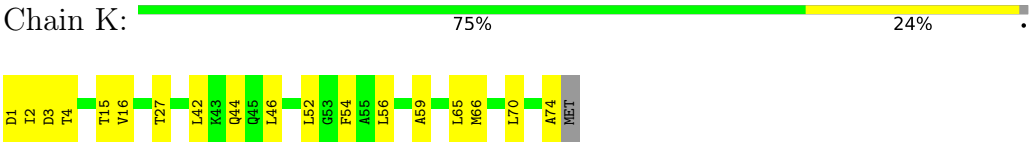
• Molecule 7: ATPase inhibitor, mitochondrial

Chain J:



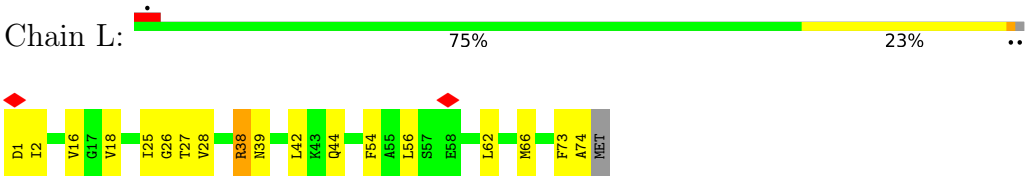
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain K:



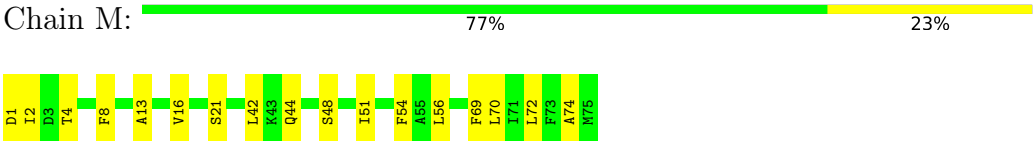
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain L:



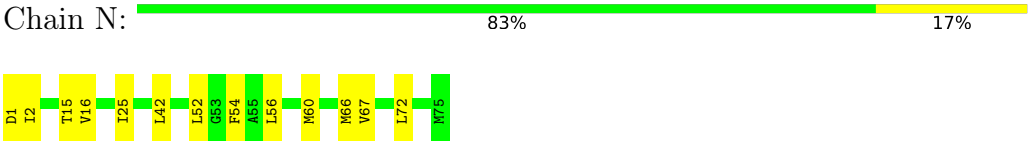
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain M:



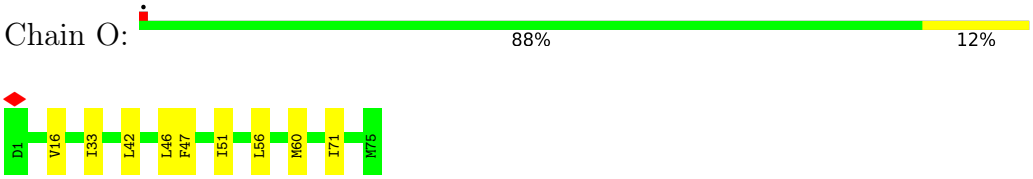
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain N:



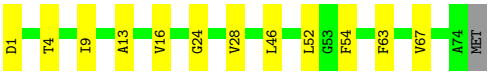
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain O:



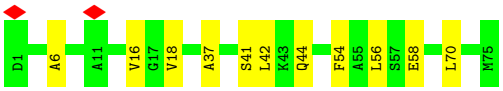
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain P:



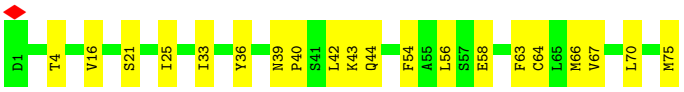
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain Q:



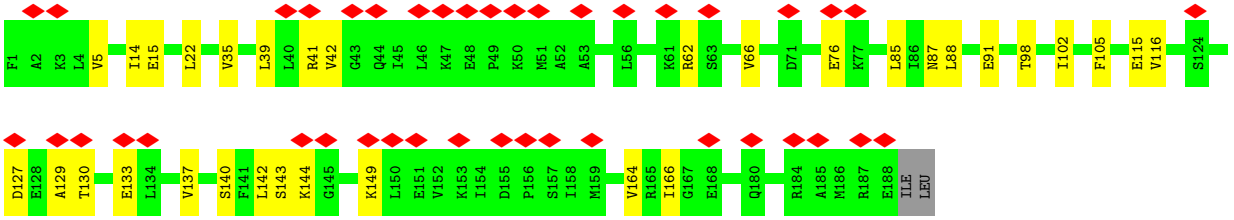
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain R:



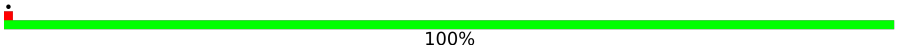
• Molecule 9: ATP synthase subunit O, mitochondrial

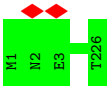
Chain S:



• Molecule 10: ATP synthase subunit a

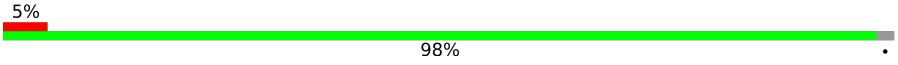
Chain a:

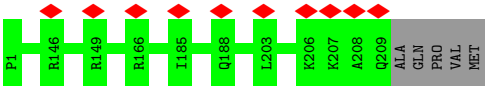




• Molecule 11: ATP synthase F(0) complex subunit B1, mitochondrial

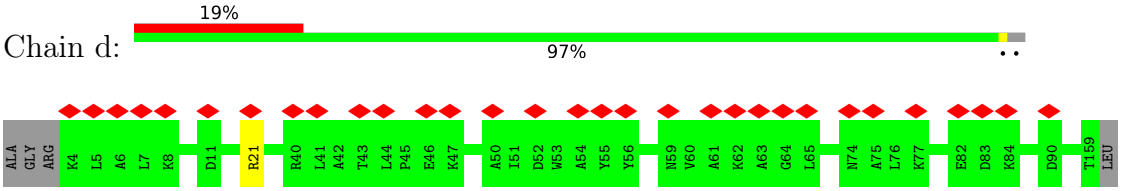
Chain b:





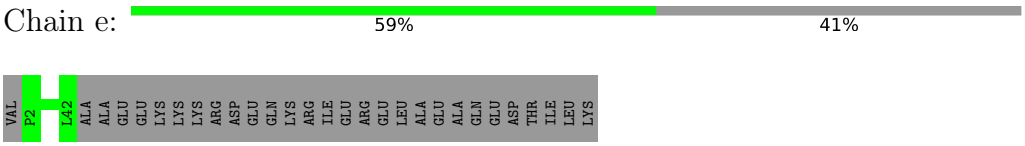
• Molecule 12: ATP synthase subunit d, mitochondrial

Chain d:



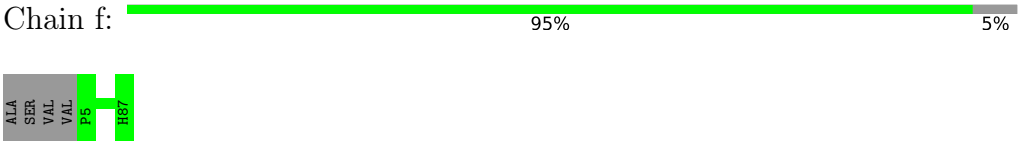
• Molecule 13: ATP synthase subunit e, mitochondrial

Chain e:



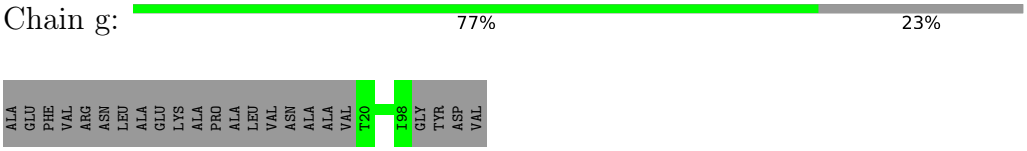
• Molecule 14: ATP synthase subunit f, mitochondrial

Chain f:



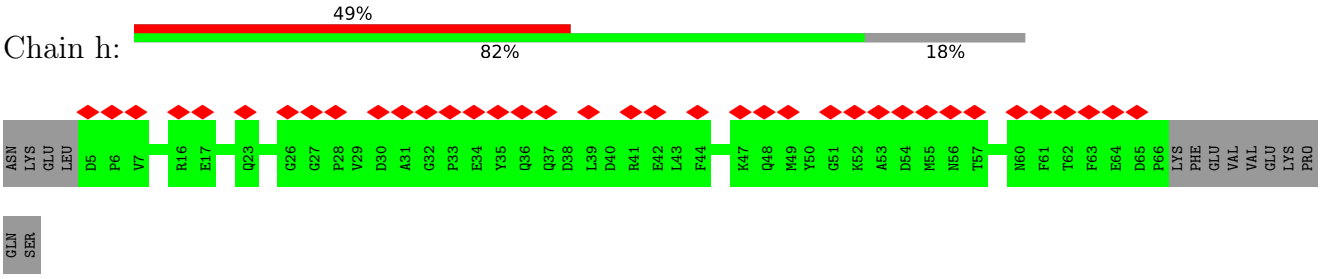
• Molecule 15: ATP synthase subunit g, mitochondrial

Chain g:



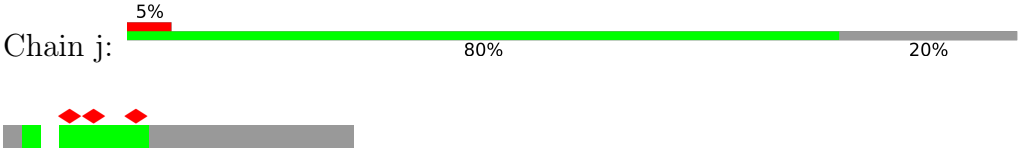
• Molecule 16: ATP synthase-coupling factor 6, mitochondrial

Chain h:



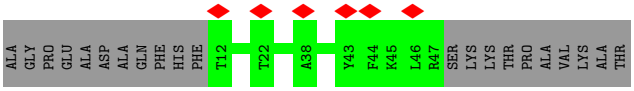
• Molecule 17: ATP synthase subunit ATP5MPL, mitochondrial

Chain j:



• Molecule 18: ATP synthase membrane subunit DAPIT, mitochondrial

Chain k:


ALA
GLY
PRO
GLU
ALA
ASP
ALA
GLN
PHE
HIS
PHE
T12
T22
A38
Y43
F44
K45
L46
R47
SER
LYS
LYS
THR
PRO
ALA
VAL
LYS
ALA
THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101165	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 ($e^-/Å^2$)	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	60.010	Depositor
Minimum map value	-26.621	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.116	Depositor
Recommended contour level	8.86	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, LHG, M3L, ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	8	0.41	0/355	0.54	0/483
2	A	0.34	0/3919	0.46	0/5287
2	B	0.34	0/3689	0.46	0/4975
2	C	0.34	0/3843	0.46	0/5184
3	D	0.34	0/3616	0.45	0/4906
3	E	0.33	0/3596	0.45	0/4879
3	F	0.34	0/3596	0.45	0/4879
4	G	0.36	0/2141	0.46	0/2876
5	H	0.39	0/991	0.50	0/1349
6	I	0.40	0/374	0.48	0/501
7	J	0.30	0/374	0.41	0/495
8	K	0.35	0/526	0.47	0/711
8	L	0.37	0/526	0.49	0/711
8	M	0.40	0/534	0.47	0/721
8	N	0.39	0/534	0.51	0/721
8	O	0.37	0/534	0.47	0/721
8	P	0.38	0/526	0.45	0/711
8	Q	0.38	0/534	0.49	0/721
8	R	0.35	0/534	0.49	0/721
9	S	0.29	0/1464	0.44	0/1969
10	a	0.33	0/1779	0.50	0/2433
11	b	0.33	0/1733	0.47	0/2334
12	d	0.30	0/1313	0.43	0/1779
13	e	0.35	0/343	0.52	0/460
14	f	0.38	0/711	0.46	0/952
15	g	0.33	0/646	0.49	0/879
16	h	0.31	0/526	0.47	0/707
17	j	0.32	0/410	0.44	0/552
18	k	0.27	0/294	0.43	0/395
All	All	0.34	0/39961	0.46	0/54012

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	344	352	352	3	0
2	A	3868	3970	3969	45	0
2	B	3641	3751	3750	44	0
2	C	3794	3904	3903	59	0
3	D	3558	3605	3605	66	0
3	E	3539	3593	3593	56	0
3	F	3539	3592	3592	45	0
4	G	2115	2185	2185	27	0
5	H	979	978	978	25	0
6	I	369	395	395	13	0
7	J	370	361	361	2	0
8	K	529	550	550	15	0
8	L	529	550	549	15	0
8	M	537	559	558	16	0
8	N	537	559	559	18	0
8	O	537	559	559	11	0
8	P	529	550	550	8	0
8	Q	537	559	559	12	0
8	R	537	559	558	18	0
9	S	1447	1557	1557	22	0
10	a	1741	1870	1870	0	0
11	b	1701	1753	1755	0	0
12	d	1282	1285	1288	0	0
13	e	335	352	352	0	0
14	f	693	717	718	0	0
15	g	629	662	662	0	0
16	h	514	495	495	0	0
17	j	400	428	428	0	0
18	k	289	307	307	0	0
19	A	31	12	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	31	12	12	0	0
19	C	31	12	12	0	0
20	A	1	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	1	0	0	0	0
21	D	27	12	12	1	0
21	E	27	12	12	0	0
21	F	27	12	12	3	0
22	b	83	119	113	0	0
22	f	162	230	218	0	0
23	f	88	126	122	0	0
24	A	3	0	0	0	0
24	B	3	0	0	0	0
24	C	3	0	0	0	0
24	D	4	0	0	2	0
24	F	4	0	0	2	0
All	All	39948	41104	41082	471	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 9.

All (471) 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:A:405:GLN:NE2	3:D:400:ASP:OD2	1.91	1.02
5:H:95:GLU:OE2	6:I:15:SER:OG	1.86	0.94
5:H:59:ARG:NH2	5:H:136:GLU:OE2	2.04	0.91
2:B:127:ARG:NH2	2:B:255:GLU:OE1	2.05	0.89
3:D:192:GLU:OE1	24:D:701:HOH:O	1.91	0.89
3:D:381:TYR:OH	7:J:30:GLU:OE2	1.90	0.88
3:E:306:SER:OG	3:E:308:GLN:OE1	1.91	0.88
2:B:291:ARG:NH2	3:F:319:ASP:OD1	2.07	0.86
3:E:206:ILE:HD11	3:E:217:LEU:HD11	1.59	0.84
2:B:420:ARG:NH1	2:B:449:VAL:O	2.13	0.82
8:M:42:LEU:O	8:M:44:GLN:N	2.13	0.81
2:B:258:ARG:NH1	2:B:308:ARG:O	2.14	0.81
2:A:101:GLU:OE1	2:A:262:LYS:NZ	2.15	0.80
2:A:102:GLU:OE1	2:A:102:GLU:N	2.15	0.79
8:L:16:VAL:HG21	8:M:16:VAL:HG13	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:42:LEU:O	8:R:44:GLN:N	2.17	0.78
3:E:48:GLU:OE1	3:E:231:ARG:NE	2.18	0.77
8:N:54:PHE:CE1	8:O:56:LEU:HD21	2.19	0.77
4:G:67:LEU:HD11	4:G:106:ILE:HD11	1.67	0.77
3:E:138:LYS:NZ	3:E:460:VAL:O	2.18	0.77
2:C:163:GLN:NE2	2:C:165:GLU:OE2	2.18	0.77
4:G:61:GLU:OE1	4:G:61:GLU:N	2.18	0.76
2:C:452:TYR:OH	2:C:498:LYS:NZ	2.18	0.76
2:B:499:GLU:OE2	2:B:503:ASN:ND2	2.18	0.76
3:F:192:GLU:OE2	24:F:701:HOH:O	2.03	0.75
8:M:13:ALA:O	8:M:16:VAL:HG12	1.85	0.75
3:D:138:LYS:NZ	3:D:413:PHE:O	2.18	0.75
3:D:310:ILE:HD13	3:D:325:THR:HG21	1.68	0.75
3:D:398:GLU:OE1	3:D:401:LYS:NZ	2.20	0.74
8:N:1:ASP:OD1	8:N:2:ILE:N	2.21	0.74
3:F:287:THR:O	3:F:291:THR:HG23	1.89	0.73
2:B:64:LEU:HD13	2:B:74:VAL:HG13	1.70	0.73
3:F:192:GLU:OE1	24:F:702:HOH:O	2.05	0.73
2:A:185:ASN:OD1	2:A:188:ARG:NH1	2.21	0.73
8:Q:54:PHE:CE2	8:R:56:LEU:HD21	2.25	0.72
5:H:55:LEU:HD12	5:H:55:LEU:O	1.90	0.71
2:B:437:ALA:HB3	2:B:440:GLU:OE1	1.88	0.71
2:A:163:GLN:NE2	2:A:165:GLU:OE1	2.21	0.71
3:E:52:HIS:HD2	3:E:58:VAL:HG12	1.55	0.71
2:B:157:VAL:O	2:B:157:VAL:HG23	1.91	0.71
2:C:255:GLU:OE1	2:C:308:ARG:NE	2.22	0.71
5:H:58:LEU:HD11	5:H:92:LEU:HD11	1.72	0.71
4:G:15:ASN:OD1	7:J:10:SER:OG	2.07	0.70
5:H:124:ASP:OD2	5:H:125:GLU:N	2.25	0.70
8:O:42:LEU:HD12	8:O:42:LEU:O	1.91	0.70
2:A:210:ARG:NH1	3:D:121:PRO:O	2.25	0.70
3:D:12:ARG:NH2	3:D:24:GLN:OE1	2.25	0.69
3:D:151:LYS:NZ	3:D:293:GLN:O	2.25	0.69
6:I:26:LEU:O	6:I:31:LYS:NZ	2.26	0.69
2:B:442:VAL:CG1	2:B:489:ILE:HD11	2.23	0.69
3:D:192:GLU:OE2	24:D:702:HOH:O	2.11	0.69
3:E:399:GLU:OE2	3:E:399:GLU:N	2.26	0.69
3:E:388:ILE:HD11	3:E:396:LEU:HD11	1.75	0.69
2:A:473:ILE:O	2:A:477:GLN:NE2	2.27	0.68
3:E:278:ALA:O	4:G:259:THR:OG1	2.04	0.68
3:D:412:ARG:O	3:D:415:SER:OG	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:287:THR:O	3:D:291:THR:HG23	1.92	0.68
2:B:164:ARG:NH2	2:B:347:ASP:OD1	2.26	0.68
8:K:3:ASP:OD1	8:K:4:THR:N	2.27	0.67
3:D:229:ARG:NH2	3:D:267:GLU:OE1	2.28	0.67
3:D:298:THR:HG23	3:D:303:SER:HA	1.77	0.67
2:A:38:ILE:CD1	2:A:74:VAL:HG12	2.26	0.66
9:S:41:ARG:NH2	9:S:76:GLU:OE1	2.29	0.66
3:E:287:THR:O	3:E:291:THR:HG23	1.96	0.66
8:Q:42:LEU:O	8:Q:44:GLN:N	2.27	0.65
8:R:25:ILE:HD12	8:R:54:PHE:HD1	1.61	0.65
3:D:167:MET:SD	3:D:196:LEU:HD13	2.35	0.65
2:A:258:ARG:NH1	2:A:308:ARG:O	2.29	0.65
2:C:52:MET:O	2:C:91:THR:OG1	2.12	0.65
5:H:64:VAL:HG22	5:H:74:LYS:HG3	1.78	0.65
2:C:496:LYS:O	2:C:500:ILE:HD12	1.97	0.64
2:C:491:GLU:OE1	2:C:491:GLU:N	2.31	0.64
9:S:22:LEU:HD22	9:S:85:LEU:HD22	1.81	0.63
2:B:255:GLU:OE2	2:B:308:ARG:NE	2.31	0.63
2:A:36:ASP:OD2	3:D:274:ARG:NE	2.32	0.63
4:G:67:LEU:HD11	4:G:106:ILE:CD1	2.28	0.63
3:F:336:SER:HB3	3:F:339:ILE:HD13	1.81	0.62
9:S:98:THR:O	9:S:102:ILE:HD12	1.98	0.62
9:S:116:VAL:HG21	9:S:142:LEU:HD22	1.80	0.62
2:A:421:GLY:O	2:A:425:THR:HG23	1.99	0.62
6:I:46:LYS:HE3	6:I:46:LYS:HA	1.79	0.62
3:D:168:GLU:OE2	3:D:172:ASN:ND2	2.32	0.62
2:B:393:GLU:OE1	2:B:420:ARG:NH1	2.32	0.61
2:C:376:SER:O	2:C:384:LYS:NZ	2.33	0.61
2:A:38:ILE:HD13	2:A:74:VAL:HG12	1.82	0.61
2:C:180:ILE:HD11	2:C:216:LEU:CD1	2.31	0.61
9:S:137:VAL:O	9:S:140:SER:OG	2.05	0.61
3:F:122:GLU:N	3:F:125:GLU:OE2	2.32	0.61
2:C:471:HIS:O	2:C:475:GLN:NE2	2.34	0.61
8:O:56:LEU:HD23	8:O:56:LEU:O	2.01	0.61
2:B:170:ASP:O	2:B:175:LYS:NZ	2.34	0.60
3:D:366:GLU:O	3:D:370:VAL:HG23	2.01	0.60
3:E:84:ILE:HD13	3:E:235:THR:HG23	1.82	0.60
8:K:1:ASP:OD1	8:K:2:ILE:N	2.34	0.60
5:H:114:LYS:O	5:H:118:GLU:OE1	2.20	0.60
3:E:237:LEU:HD11	3:E:292:MET:HG2	1.83	0.60
5:H:37:ASP:OD2	8:Q:41:SER:OG	2.06	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:MET:HE3	2:C:95:VAL:HG21	1.84	0.60
3:E:44:ARG:NH1	3:E:100:GLU:OE2	2.35	0.60
3:E:366:GLU:OE2	3:E:366:GLU:N	2.30	0.60
8:O:33:ILE:HG23	8:P:46:LEU:HD22	1.84	0.59
3:D:452:LEU:HD22	3:D:470:ALA:CB	2.33	0.59
8:L:25:ILE:HD12	8:L:54:PHE:HD1	1.66	0.59
3:E:279:VAL:HG12	3:E:279:VAL:O	2.01	0.59
8:K:42:LEU:HD23	8:R:36:TYR:CE2	2.37	0.59
8:N:15:THR:HG22	8:N:15:THR:O	2.03	0.59
8:P:24:GLY:O	8:P:28:VAL:HG23	2.02	0.59
3:F:255:ILE:HG21	3:F:258:ILE:HD13	1.85	0.59
5:H:69:ASP:OD1	5:H:71:THR:OG1	2.11	0.59
2:B:156:LEU:HD22	2:B:367:VAL:HG11	1.85	0.59
3:E:210:ASP:OD2	3:E:212:THR:HG22	2.03	0.58
8:K:16:VAL:HG23	8:R:16:VAL:HG23	1.84	0.58
2:B:166:LEU:HD11	2:B:327:ILE:HG12	1.85	0.58
3:E:416:GLN:NE2	3:E:430:LYS:O	2.37	0.58
3:D:279:VAL:HG23	3:D:279:VAL:O	2.04	0.58
3:E:229:ARG:NH2	3:E:267:GLU:OE1	2.37	0.58
2:A:140:ILE:HG23	2:A:313:ASN:HB3	1.86	0.58
1:8:38:GLU:OE1	1:8:40:THR:N	2.37	0.57
9:S:22:LEU:HD22	9:S:85:LEU:CD2	2.33	0.57
3:E:317:LEU:HD22	3:E:326:PHE:CE2	2.39	0.57
8:L:16:VAL:CG2	8:M:16:VAL:HG13	2.33	0.57
9:S:115:GLU:OE1	9:S:149:LYS:NZ	2.28	0.57
5:H:131:ILE:O	5:H:135:ILE:HD12	2.04	0.57
2:C:164:ARG:NH2	2:C:347:ASP:OD1	2.38	0.57
2:A:255:GLU:OE2	2:A:258:ARG:NH2	2.38	0.57
2:C:225:ALA:O	2:C:229:THR:OG1	2.15	0.57
3:F:296:ILE:HG22	3:F:296:ILE:O	2.03	0.57
2:C:62:MET:CE	2:C:95:VAL:HG21	2.34	0.56
2:C:400:VAL:O	2:C:418:LEU:HD11	2.05	0.56
2:B:188:ARG:HE	2:B:437:ALA:HB2	1.71	0.56
8:M:21:SER:HB2	8:N:60:MET:SD	2.46	0.56
2:B:47:VAL:HG23	2:B:51:GLU:OE1	2.05	0.56
2:C:258:ARG:NH1	2:C:259:ASP:OD2	2.39	0.56
3:D:255:ILE:HG21	3:D:258:ILE:HD13	1.88	0.56
3:E:317:LEU:HD22	3:E:326:PHE:HE2	1.69	0.55
3:E:452:LEU:HD22	3:E:470:ALA:CB	2.35	0.55
8:P:1:ASP:OD2	8:P:4:THR:N	2.39	0.55
2:B:180:ILE:HD11	2:B:216:LEU:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:164:ARG:N	4:G:172:LYS:O	2.40	0.55
8:R:4:THR:HG22	8:R:4:THR:O	2.05	0.55
2:A:170:ASP:O	2:A:175:LYS:NZ	2.38	0.55
8:M:54:PHE:CE1	8:N:56:LEU:HD22	2.41	0.55
3:E:397:SER:OG	3:E:398:GLU:N	2.40	0.55
3:F:55:GLU:O	3:F:55:GLU:HG2	2.07	0.55
3:D:162:LYS:N	21:D:600:ADP:O1B	2.40	0.55
2:A:15:ARG:HE	9:S:88:LEU:HD13	1.72	0.54
2:A:51:GLU:OE2	2:A:90:ARG:NH2	2.40	0.54
2:A:101:GLU:OE2	2:A:101:GLU:N	2.40	0.54
4:G:89:MET:CE	4:G:112:ILE:HD12	2.37	0.54
5:H:107:ALA:O	5:H:111:ASN:OD1	2.25	0.54
3:D:41:ARG:NH1	3:D:67:GLU:O	2.36	0.54
3:F:142:LEU:HD22	3:F:441:PHE:CD1	2.42	0.54
8:P:13:ALA:O	8:P:16:VAL:HG12	2.07	0.54
8:R:25:ILE:HD12	8:R:54:PHE:CD1	2.42	0.54
1:8:22:ILE:O	1:8:26:LEU:HD13	2.07	0.54
3:D:97:VAL:HG13	3:D:98:ILE:HG23	1.89	0.54
4:G:131:VAL:HG22	6:I:42:ILE:CD1	2.38	0.54
3:D:153:GLY:HA3	3:D:329:LEU:HD13	1.90	0.54
2:B:452:TYR:CE1	2:B:501:VAL:HG13	2.42	0.54
2:C:34:ILE:HD11	2:C:79:ASP:OD1	2.08	0.54
8:K:3:ASP:OD1	8:K:4:THR:HG23	2.07	0.53
9:S:116:VAL:HG23	9:S:116:VAL:O	2.08	0.53
4:G:164:ARG:NH1	4:G:174:GLU:OE1	2.41	0.53
2:A:46:ASN:O	2:A:90:ARG:NH1	2.41	0.53
3:E:48:GLU:OE2	3:E:117:HIS:NE2	2.41	0.53
8:L:54:PHE:CE1	8:M:56:LEU:HD23	2.44	0.53
8:K:52:LEU:O	8:K:56:LEU:HD23	2.09	0.53
3:E:380:ASP:O	3:E:384:LEU:HD13	2.09	0.53
2:C:422:VAL:O	2:C:426:GLU:OE1	2.27	0.53
3:D:29:LEU:HD21	3:D:56:SER:O	2.08	0.53
8:M:54:PHE:CE1	8:N:56:LEU:HD13	2.43	0.53
2:C:203:TYR:OH	2:C:269:ASP:OD2	2.18	0.52
3:D:29:LEU:HD22	3:D:58:VAL:CG1	2.39	0.52
3:D:97:VAL:HG21	3:D:231:ARG:HB2	1.91	0.52
8:M:48:SER:O	8:M:51:ILE:HG22	2.09	0.52
2:B:166:LEU:HD13	2:B:342:VAL:CG1	2.40	0.52
5:H:24:THR:HG22	5:H:24:THR:O	4.70	0.52
3:D:155:PHE:CZ	3:D:310:ILE:HD12	2.45	0.52
3:E:425:THR:O	3:E:427:HIS:ND1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:472:VAL:HG12	2:C:480:LEU:HD11	1.90	0.52
3:F:255:ILE:HD12	3:F:308:GLN:HG2	1.92	0.52
3:F:386:ASP:OD2	3:F:387:ILE:N	2.42	0.52
5:H:133:ILE:HD11	6:I:4:TRP:HB3	1.92	0.52
8:N:72:LEU:HD11	8:O:71:ILE:HD11	1.92	0.52
2:B:32:LEU:N	2:B:40:ARG:O	2.43	0.51
2:C:444:VAL:CG2	2:C:469:LEU:HD21	2.40	0.51
9:S:129:ALA:O	9:S:133:GLU:OE1	2.27	0.51
2:C:218:LYS:HD3	3:F:128:VAL:HG11	1.93	0.51
3:E:173:VAL:HG21	3:E:252:LEU:HD11	1.92	0.51
8:M:70:LEU:HD12	8:M:74:ALA:HB3	1.93	0.51
2:C:444:VAL:HG23	2:C:469:LEU:HD21	1.92	0.51
3:E:316:ASP:OD1	4:G:255:GLN:NE2	2.43	0.51
8:O:42:LEU:HD12	8:O:46:LEU:HG	1.90	0.51
2:C:411:ASP:OD1	2:C:411:ASP:N	2.44	0.51
2:C:497:LEU:O	2:C:501:VAL:HG23	2.11	0.51
3:E:52:HIS:CD2	3:E:58:VAL:HG12	2.42	0.51
2:C:69:ASP:OD2	2:C:69:ASP:N	2.43	0.51
3:F:377:ILE:HD11	3:F:406:ARG:HB2	1.93	0.51
3:D:157:GLY:O	3:D:162:LYS:NZ	2.42	0.50
2:B:170:ASP:OD1	2:B:329:THR:OG1	2.29	0.50
3:E:173:VAL:HG21	3:E:252:LEU:CD1	2.41	0.50
3:D:367:HIS:HD2	3:D:438:ILE:HD11	1.76	0.50
2:A:389:THR:OG1	2:A:449:VAL:HG21	2.11	0.50
3:D:131:GLU:N	3:D:131:GLU:OE1	2.45	0.50
8:L:25:ILE:HD12	8:L:54:PHE:CD1	2.45	0.50
3:E:187:GLY:O	3:E:260:ARG:NE	2.45	0.50
3:F:128:VAL:O	3:F:128:VAL:HG12	2.11	0.50
3:F:318:THR:O	3:F:318:THR:HG22	2.10	0.50
3:D:149:GLY:O	3:D:298:THR:OG1	2.24	0.49
3:D:374:VAL:O	3:D:377:ILE:HG22	2.12	0.49
3:E:408:ARG:NE	3:E:454:GLU:OE1	2.45	0.49
3:F:77:ASP:OD1	3:F:78:SER:N	2.45	0.49
3:F:279:VAL:O	3:F:279:VAL:HG23	2.12	0.49
4:G:73:SER:OG	4:G:74:ASP:N	2.45	0.49
8:K:42:LEU:HD21	8:R:40:PRO:HG3	1.94	0.49
2:B:169:GLY:O	2:B:329:THR:OG1	2.29	0.49
8:O:47:PHE:CE1	8:O:51:ILE:HD11	2.47	0.49
3:D:124:VAL:HG22	3:D:124:VAL:O	2.13	0.49
3:D:237:LEU:HD13	3:D:296:ILE:HG12	1.93	0.49
3:E:94:ILE:HD11	3:E:197:TYR:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:143:SER:OG	9:S:144:LYS:N	2.45	0.49
3:E:452:LEU:HD22	3:E:470:ALA:HB1	1.94	0.49
8:R:64:CYS:O	8:R:67:VAL:HG12	2.12	0.49
2:B:380:THR:O	2:B:384:LYS:N	2.44	0.49
3:D:146:TYR:OH	3:D:333:THR:HG21	2.12	0.49
3:E:150:GLY:O	3:E:152:ILE:HD12	2.12	0.49
6:I:28:THR:HG23	6:I:29:GLU:N	2.27	0.49
2:A:280:GLN:HE21	3:D:284:THR:HG22	1.77	0.49
2:B:180:ILE:HG22	2:B:184:ILE:HD12	1.93	0.49
8:K:54:PHE:CE1	8:L:56:LEU:HD23	2.48	0.49
3:D:45:LEU:HD13	3:D:64:ASP:HB3	1.95	0.48
8:N:54:PHE:HE1	8:O:56:LEU:HD21	1.72	0.48
8:Q:16:VAL:O	8:Q:16:VAL:HG12	2.13	0.48
2:A:406:PHE:O	2:A:408:SER:N	2.46	0.48
3:D:39:GLN:CG	3:D:76:LEU:HD23	2.43	0.48
2:C:400:VAL:O	2:C:400:VAL:HG23	2.14	0.48
3:E:394:ASP:OD1	3:E:395:GLU:N	2.47	0.48
4:G:40:PRO:O	4:G:43:VAL:HG12	2.13	0.48
3:D:200:MET:CE	3:D:215:VAL:HG11	2.43	0.48
3:F:66:THR:O	3:F:69:LEU:HD13	2.14	0.48
2:B:64:LEU:CD1	2:B:74:VAL:HG13	2.40	0.48
2:B:166:LEU:HD11	2:B:327:ILE:CG1	2.43	0.48
4:G:92:GLU:OE2	4:G:92:GLU:HA	2.14	0.48
1:8:38:GLU:OE1	1:8:40:THR:OG1	2.27	0.47
4:G:71:VAL:HG21	4:G:216:SER:OG	2.14	0.47
5:H:35:GLN:HE22	8:Q:41:SER:HB3	1.79	0.47
3:E:134:VAL:HG13	3:E:141:ASP:OD1	2.14	0.47
8:R:63:PHE:O	8:R:66:MET:HG3	2.15	0.47
3:D:391:LEU:HD12	4:G:23:MET:HE3	1.94	0.47
2:A:427:LEU:CD1	2:A:448:GLY:HA3	2.44	0.47
2:C:327:ILE:HD11	2:C:342:VAL:HG21	1.97	0.47
3:D:402:LEU:HD21	3:D:406:ARG:NH2	2.28	0.47
3:F:402:LEU:HD21	3:F:406:ARG:NH2	2.29	0.47
5:H:58:LEU:HD11	5:H:92:LEU:CD1	2.43	0.47
2:A:452:TYR:CD1	2:A:501:VAL:HG11	2.50	0.47
2:B:166:LEU:HD13	2:B:342:VAL:HG12	1.96	0.47
3:E:14:VAL:HG22	3:E:22:ASP:O	2.14	0.47
3:E:321:ALA:HB3	3:E:322:PRO:CD	2.45	0.47
4:G:80:ALA:O	4:G:171:TYR:OH	2.27	0.47
2:A:347:ASP:OD2	3:E:191:ARG:NE	2.44	0.47
2:B:489:ILE:O	2:B:489:ILE:HG22	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:371:VAL:HG22	2:C:372:SER:N	2.29	0.47
8:L:73:PHE:O	8:L:74:ALA:HB2	2.14	0.47
8:M:54:PHE:CZ	8:N:56:LEU:HD22	2.50	0.47
2:C:474:SER:OG	2:C:475:GLN:OE1	2.29	0.47
2:B:55:PHE:CD2	2:B:88:VAL:HG22	2.50	0.47
2:B:497:LEU:O	2:B:501:VAL:HG12	2.15	0.47
2:C:34:ILE:HD13	2:C:39:ALA:HB2	1.96	0.46
8:K:46:LEU:HD22	8:R:33:ILE:HG23	1.96	0.46
2:B:142:VAL:HB	2:B:374:VAL:CG1	2.45	0.46
2:C:170:ASP:OD1	2:C:332:GLY:N	2.48	0.46
2:C:249:SER:O	2:C:253:MET:HG3	2.16	0.46
8:Q:70:LEU:HD23	8:Q:70:LEU:C	2.36	0.46
3:D:9:THR:HG23	3:D:27:GLU:HB2	1.97	0.46
3:E:243:PHE:HB2	3:E:251:VAL:HG21	1.97	0.46
9:S:127:ASP:O	9:S:130:THR:OG1	2.27	0.46
2:B:373:ARG:CZ	21:F:600:ADP:H3'	2.45	0.46
2:B:442:VAL:HG13	2:B:489:ILE:HD11	1.96	0.46
2:C:224:ASP:OD1	2:C:224:ASP:O	2.34	0.46
3:F:164:VAL:HG11	21:F:600:ADP:N7	2.31	0.46
5:H:114:LYS:O	5:H:117:SER:HB3	2.16	0.46
8:N:25:ILE:HD12	8:O:60:MET:CE	2.45	0.46
8:R:58:GLU:OE1	8:R:58:GLU:HA	2.16	0.46
2:C:8:VAL:HG23	2:C:9:SER:N	2.31	0.46
3:D:224:GLU:O	3:D:229:ARG:NH1	2.49	0.46
2:A:449:VAL:HG22	2:A:449:VAL:O	2.15	0.46
2:C:423:ARG:NH2	2:C:456:LEU:O	2.37	0.46
3:E:97:VAL:HG13	3:E:98:ILE:HG23	1.97	0.46
3:E:206:ILE:HD11	3:E:217:LEU:CD1	2.40	0.46
3:F:186:VAL:HG23	3:F:232:VAL:CG1	2.46	0.46
3:F:333:THR:CG2	3:F:348:VAL:HG22	2.46	0.46
8:L:1:ASP:OD1	8:L:2:ILE:N	2.49	0.46
8:M:16:VAL:HG22	8:M:16:VAL:O	2.15	0.46
8:K:56:LEU:O	8:K:59:ALA:HB3	2.16	0.45
8:L:38:ARG:HD3	8:L:39:ASN:HB2	1.98	0.45
2:A:440:GLU:CG	2:A:473:ILE:HD11	2.47	0.45
3:F:97:VAL:HG21	3:F:228:ALA:HB1	1.97	0.45
4:G:148:LEU:HD23	4:G:148:LEU:O	2.16	0.45
3:E:155:PHE:CE1	3:E:332:THR:HG23	2.52	0.45
5:H:57:VAL:CG1	6:I:11:TYR:CZ	3.00	0.45
6:I:23:ARG:HA	6:I:26:LEU:CD1	2.46	0.45
9:S:14:ILE:HG23	9:S:15:GLU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:LEU:HD23	3:E:77:ASP:HA	1.97	0.45
5:H:132:GLN:NE2	6:I:3:TYR:CZ	2.85	0.45
6:I:45:VAL:HG23	6:I:45:VAL:O	2.16	0.45
8:K:27:THR:HA	8:L:27:THR:HG21	1.99	0.45
3:D:452:LEU:HD22	3:D:470:ALA:HB1	1.97	0.45
3:F:321:ALA:HB3	3:F:322:PRO:CD	2.47	0.45
8:L:25:ILE:O	8:L:28:VAL:HG12	2.16	0.45
2:A:327:ILE:HD11	2:A:342:VAL:HG21	1.99	0.45
3:F:224:GLU:O	3:F:229:ARG:NH1	2.50	0.45
3:E:212:THR:HG23	3:E:212:THR:O	2.17	0.45
3:F:32:ILE:HG22	3:F:33:LEU:HG	1.98	0.45
2:A:164:ARG:NH2	2:A:347:ASP:OD1	2.50	0.44
4:G:182:ASP:OD2	4:G:183:THR:N	2.49	0.44
8:P:54:PHE:CE1	8:Q:56:LEU:HD22	2.52	0.44
9:S:35:VAL:O	9:S:39:LEU:HD13	2.17	0.44
3:E:55:GLU:OE2	9:S:62:ARG:NH2	2.50	0.44
8:L:44:GLN:HA	8:L:44:GLN:OE1	2.17	0.44
2:B:165:GLU:OE1	2:B:349:GLN:N	2.51	0.44
2:B:373:ARG:HA	2:B:373:ARG:NE	2.33	0.44
2:C:327:ILE:HG22	2:C:328:GLU:N	2.32	0.44
2:C:496:LYS:O	2:C:499:GLU:HG3	2.18	0.44
3:D:285:LEU:C	3:D:285:LEU:HD23	2.38	0.44
5:H:40:THR:HG21	5:H:45:PHE:CE2	2.52	0.44
3:D:84:ILE:HG21	3:D:235:THR:HG23	2.00	0.44
3:D:391:LEU:CD1	4:G:23:MET:SD	3.06	0.44
3:E:321:ALA:HB3	3:E:322:PRO:HD3	1.99	0.44
9:S:39:LEU:HA	9:S:42:VAL:HG22	2.00	0.44
2:A:127:ARG:NH1	2:A:131:LEU:HD12	2.33	0.44
2:B:373:ARG:NH2	21:F:600:ADP:H3'	2.32	0.44
2:C:156:LEU:HD13	2:C:367:VAL:HG11	2.00	0.44
3:F:298:THR:O	3:F:298:THR:HG23	2.18	0.44
8:N:42:LEU:HD23	8:N:42:LEU:H	1.83	0.44
2:C:166:LEU:HD11	2:C:327:ILE:CG1	2.48	0.44
2:C:166:LEU:HD13	2:C:342:VAL:HG12	2.00	0.44
3:D:260:ARG:NH1	3:D:263:GLN:OE1	2.48	0.44
8:L:62:LEU:O	8:L:66:MET:HG2	2.18	0.44
2:C:41:VAL:HG11	2:C:44:LEU:HD12	1.99	0.44
3:E:15:ALA:HB3	3:E:22:ASP:HB2	1.99	0.44
3:E:384:LEU:O	3:E:388:ILE:HG12	2.17	0.44
3:F:359:ASP:OD1	3:F:360:PRO:HD2	2.17	0.44
2:C:14:GLU:HA	2:C:17:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:366:GLU:O	3:F:370:VAL:HG23	2.18	0.43
8:N:42:LEU:O	8:N:42:LEU:HG	2.18	0.43
2:C:41:VAL:HG11	2:C:44:LEU:CD1	2.48	0.43
8:R:16:VAL:HG22	8:R:16:VAL:O	2.18	0.43
3:E:237:LEU:HD11	3:E:292:MET:CG	2.47	0.43
2:A:270:ASP:OD1	2:A:271:LEU:N	2.52	0.43
3:D:39:GLN:HG3	3:D:76:LEU:HD23	2.01	0.43
3:D:310:ILE:HD13	3:D:325:THR:CG2	2.45	0.43
2:C:464:PHE:O	2:C:465:GLU:C	2.56	0.43
5:H:132:GLN:HA	5:H:135:ILE:HD13	2.01	0.43
8:Q:18:VAL:O	8:Q:18:VAL:HG12	2.17	0.43
2:B:25:LEU:O	2:B:25:LEU:HG	2.19	0.43
3:F:52:HIS:HD2	3:F:58:VAL:HG12	1.83	0.43
4:G:125:LEU:HD11	4:G:153:TYR:HB3	1.99	0.43
2:C:50:GLU:OE2	3:D:67:GLU:HG2	2.18	0.43
3:D:29:LEU:HD22	3:D:58:VAL:HG13	2.01	0.43
6:I:29:GLU:HG2	6:I:30:PHE:N	2.32	0.43
8:Q:37:ALA:O	8:R:39:ASN:ND2	2.47	0.43
3:D:374:VAL:HG13	3:D:410:ILE:HG21	1.99	0.43
3:E:237:LEU:HD23	3:E:253:LEU:CD2	2.49	0.43
8:N:66:MET:SD	8:N:67:VAL:HG23	2.58	0.43
8:Q:54:PHE:CZ	8:Q:58:GLU:OE2	2.72	0.43
9:S:22:LEU:HD13	9:S:85:LEU:HD22	2.00	0.43
3:D:170:ILE:HD11	3:D:183:PHE:CE2	2.54	0.43
4:G:148:LEU:HD23	4:G:148:LEU:C	2.39	0.43
4:G:173:THR:O	4:G:173:THR:HG23	2.19	0.43
2:B:156:LEU:HD21	2:B:394:LEU:HD13	2.00	0.43
2:C:388:GLY:O	2:C:392:LEU:HD23	2.19	0.43
3:F:370:VAL:HG21	3:F:442:GLN:HG3	2.00	0.43
3:F:41:ARG:NH1	3:F:69:LEU:HD12	2.33	0.42
3:F:52:HIS:CD2	3:F:58:VAL:HG12	2.53	0.42
4:G:194:ASP:OD2	4:G:195:ASP:N	2.52	0.42
3:F:205:VAL:HG12	3:F:205:VAL:O	2.19	0.42
3:F:310:ILE:HD13	3:F:325:THR:HG21	2.00	0.42
8:O:16:VAL:HG12	8:O:16:VAL:O	2.19	0.42
8:P:9:ILE:HD11	8:Q:6:ALA:O	2.19	0.42
2:B:164:ARG:NH1	2:B:345:ILE:O	2.52	0.42
3:E:406:ARG:NH1	3:E:450:ASP:OD2	2.53	0.42
4:G:89:MET:HE1	4:G:112:ILE:HD12	2.00	0.42
2:C:10:SER:O	2:C:14:GLU:HG2	2.18	0.42
2:C:103:LEU:HD13	2:C:253:MET:SD	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:SER:O	2:C:215:GLN:HG2	2.20	0.42
2:A:159:ILE:HD11	2:A:350:ILE:HD11	2.01	0.42
2:A:166:LEU:HD11	2:A:327:ILE:HD12	2.01	0.42
3:E:257:ASN:OD1	3:E:309:ALA:O	2.38	0.42
8:K:65:LEU:HB3	8:K:66:MET:HE3	2.00	0.42
2:A:13:GLU:O	2:A:17:LEU:CD2	2.67	0.42
3:F:277:SER:OG	3:F:278:ALA:N	2.49	0.42
5:H:139:GLU:HA	5:H:142:VAL:HG22	2.02	0.42
8:L:18:VAL:HG12	8:L:18:VAL:O	2.20	0.42
9:S:62:ARG:NH1	9:S:91:GLU:O	2.48	0.42
2:C:347:ASP:O	2:C:373:ARG:CD	2.68	0.42
2:C:434:SER:O	2:C:434:SER:OG	2.37	0.42
2:C:496:LYS:O	2:C:497:LEU:C	2.58	0.42
6:I:29:GLU:N	6:I:29:GLU:OE1	2.43	0.42
8:N:16:VAL:HG12	8:N:16:VAL:O	2.19	0.42
8:P:52:LEU:HD23	8:P:52:LEU:O	2.19	0.42
9:S:66:VAL:HG13	9:S:87:ASN:OD1	2.19	0.42
2:C:248:TYR:OH	2:C:301:LEU:O	2.33	0.42
8:Q:54:PHE:HE2	8:R:56:LEU:HD21	1.79	0.42
2:A:389:THR:O	2:A:393:GLU:HG2	2.20	0.42
2:A:464:PHE:O	2:A:465:GLU:C	2.57	0.42
2:C:237:SER:CB	3:F:294:GLU:OE2	2.68	0.42
3:D:139:VAL:HG13	3:D:140:VAL:N	2.35	0.42
3:F:29:LEU:HD22	3:F:58:VAL:CG1	2.49	0.42
8:M:69:PHE:O	8:M:72:LEU:N	2.53	0.42
2:B:127:ARG:NH2	2:B:131:LEU:HD23	2.34	0.41
2:C:148:THR:HG22	2:C:150:ILE:HD12	2.02	0.41
3:D:14:VAL:HG11	3:D:24:GLN:HB2	2.02	0.41
3:D:367:HIS:CD2	3:D:438:ILE:HD11	2.55	0.41
8:N:15:THR:O	8:N:15:THR:CG2	2.67	0.41
2:A:427:LEU:HD22	2:A:444:VAL:CG1	2.49	0.41
8:M:1:ASP:OD1	8:M:2:ILE:N	2.51	0.41
8:P:63:PHE:O	8:P:67:VAL:HG23	2.20	0.41
2:A:496:LYS:O	2:A:500:ILE:HG13	2.21	0.41
3:D:196:LEU:O	3:D:200:MET:HG2	2.19	0.41
3:E:431:LEU:O	3:E:431:LEU:HD23	2.20	0.41
3:F:207:ASN:OD1	3:F:212:THR:OG1	2.35	0.41
8:R:42:LEU:O	8:R:43:M3L:C	2.67	0.41
2:B:474:SER:OG	2:B:475:GLN:N	2.53	0.41
3:E:26:ASP:N	3:E:26:ASP:OD1	2.51	0.41
5:H:58:LEU:HD13	5:H:77:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:70:LEU:O	8:K:74:ALA:N	2.54	0.41
3:D:321:ALA:HB3	3:D:322:PRO:CD	2.51	0.41
3:F:374:VAL:HG13	3:F:410:ILE:HG21	2.01	0.41
6:I:3:TYR:CD2	6:I:4:TRP:N	2.88	0.41
8:K:15:THR:O	8:K:15:THR:HG22	2.19	0.41
2:A:502:THR:O	2:A:506:ALA:N	2.51	0.41
3:F:94:ILE:HD11	3:F:197:TYR:CD1	2.56	0.41
8:N:25:ILE:HD12	8:O:60:MET:HE1	2.02	0.41
2:A:286:ARG:NH1	3:D:273:GLY:O	2.54	0.41
2:A:439:GLU:HA	2:A:442:VAL:HG12	2.03	0.41
2:C:115:ILE:O	2:C:115:ILE:CG2	2.69	0.41
3:D:170:ILE:HD11	3:D:183:PHE:HE2	1.85	0.41
3:E:391:LEU:HD23	3:E:395:GLU:HG2	2.02	0.41
3:F:142:LEU:HD23	3:F:143:LEU:CD1	2.51	0.41
8:L:25:ILE:O	8:L:26:GLY:C	2.57	0.41
9:S:164:VAL:HG12	9:S:166:ILE:HD11	2.03	0.41
2:A:24:ASP:O	2:A:28:THR:OG1	2.33	0.41
2:A:251:CYS:SG	2:A:308:ARG:NE	2.94	0.41
2:C:30:ARG:HD2	2:C:87:ILE:HD13	2.02	0.41
3:D:64:ASP:OD1	3:D:65:GLY:N	2.48	0.41
3:F:255:ILE:HG21	3:F:258:ILE:CD1	2.50	0.41
4:G:168:VAL:O	4:G:226:SER:OG	2.35	0.41
5:H:26:VAL:HG13	5:H:26:VAL:O	2.21	0.41
5:H:101:ASP:OD1	5:H:102:MET:N	2.53	0.41
8:N:72:LEU:C	8:N:72:LEU:HD23	2.40	0.41
8:R:70:LEU:O	8:R:75:MET:N	2.54	0.41
2:B:156:LEU:CD2	2:B:367:VAL:HG11	2.50	0.41
2:B:164:ARG:HD3	2:B:306:LEU:O	2.21	0.41
2:C:390:MET:O	2:C:394:LEU:HD13	2.21	0.41
3:E:155:PHE:HE1	3:E:332:THR:HG23	1.85	0.41
4:G:160:ILE:HG22	4:G:176:LYS:HB2	2.03	0.40
5:H:132:GLN:HA	5:H:135:ILE:CD1	2.51	0.40
8:K:44:GLN:HA	8:K:44:GLN:OE1	2.21	0.40
3:F:233:ALA:O	3:F:237:LEU:HD13	2.20	0.40
8:N:52:LEU:HD23	8:N:52:LEU:C	2.41	0.40
2:C:450:ARG:O	2:C:452:TYR:N	2.54	0.40
4:G:52:TYR:CD1	4:G:52:TYR:N	2.88	0.40
2:A:133:ALA:HB2	2:A:308:ARG:HG3	2.03	0.40
2:A:175:LYS:HG2	2:A:352:LEU:HD12	2.02	0.40
3:D:66:THR:HB	3:D:69:LEU:HD12	2.03	0.40
8:M:1:ASP:HB3	8:M:4:THR:HG23	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:8:PHE:N	8:M:8:PHE:CD1	2.90	0.40
8:R:21:SER:O	8:R:25:ILE:HG12	2.21	0.40
9:S:5:VAL:O	9:S:5:VAL:HG23	2.19	0.40
9:S:39:LEU:HD22	9:S:105:PHE:CD2	2.57	0.40
3:D:103:ASP:OD1	3:D:103:ASP:N	2.49	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	8	39/66 (59%)	29 (74%)	10 (26%)	0	100	100
2	A	506/510 (99%)	474 (94%)	32 (6%)	0	100	100
2	B	473/510 (93%)	450 (95%)	23 (5%)	0	100	100
2	C	494/510 (97%)	461 (93%)	33 (7%)	0	100	100
3	D	467/482 (97%)	440 (94%)	27 (6%)	0	100	100
3	E	465/482 (96%)	434 (93%)	31 (7%)	0	100	100
3	F	465/482 (96%)	431 (93%)	34 (7%)	0	100	100
4	G	270/273 (99%)	259 (96%)	11 (4%)	0	100	100
5	H	130/146 (89%)	119 (92%)	11 (8%)	0	100	100
6	I	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
7	J	45/66 (68%)	44 (98%)	1 (2%)	0	100	100
8	K	71/75 (95%)	69 (97%)	2 (3%)	0	100	100
8	L	71/75 (95%)	66 (93%)	4 (6%)	1 (1%)	11	46
8	M	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	N	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	O	72/75 (96%)	70 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	P	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
8	Q	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
8	R	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
9	S	186/190 (98%)	177 (95%)	9 (5%)	0	100	100
10	a	224/226 (99%)	207 (92%)	17 (8%)	0	100	100
11	b	207/214 (97%)	201 (97%)	6 (3%)	0	100	100
12	d	154/160 (96%)	142 (92%)	12 (8%)	0	100	100
13	e	39/70 (56%)	37 (95%)	2 (5%)	0	100	100
14	f	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
15	g	77/102 (76%)	70 (91%)	7 (9%)	0	100	100
16	h	60/76 (79%)	48 (80%)	12 (20%)	0	100	100
17	j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
18	k	34/57 (60%)	32 (94%)	2 (6%)	0	100	100
All	All	5080/5419 (94%)	4774 (94%)	305 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	42	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8	41/66 (62%)	41 (100%)	0	100	100
2	A	411/413 (100%)	411 (100%)	0	100	100
2	B	387/413 (94%)	387 (100%)	0	100	100
2	C	403/413 (98%)	403 (100%)	0	100	100
3	D	379/386 (98%)	379 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	377/386 (98%)	377 (100%)	0	100 100
3	F	377/386 (98%)	377 (100%)	0	100 100
4	G	230/231 (100%)	230 (100%)	0	100 100
5	H	105/109 (96%)	104 (99%)	1 (1%)	76 86
6	I	38/41 (93%)	38 (100%)	0	100 100
7	J	34/50 (68%)	34 (100%)	0	100 100
8	K	49/50 (98%)	49 (100%)	0	100 100
8	L	49/50 (98%)	48 (98%)	1 (2%)	55 73
8	M	50/50 (100%)	50 (100%)	0	100 100
8	N	50/50 (100%)	50 (100%)	0	100 100
8	O	50/50 (100%)	50 (100%)	0	100 100
8	P	49/50 (98%)	49 (100%)	0	100 100
8	Q	50/50 (100%)	50 (100%)	0	100 100
8	R	50/50 (100%)	50 (100%)	0	100 100
9	S	163/165 (99%)	163 (100%)	0	100 100
10	a	200/200 (100%)	200 (100%)	0	100 100
11	b	186/190 (98%)	186 (100%)	0	100 100
12	d	140/142 (99%)	139 (99%)	1 (1%)	84 90
13	e	34/59 (58%)	34 (100%)	0	100 100
14	f	72/75 (96%)	72 (100%)	0	100 100
15	g	67/83 (81%)	67 (100%)	0	100 100
16	h	56/70 (80%)	56 (100%)	0	100 100
17	j	42/49 (86%)	42 (100%)	0	100 100
18	k	31/46 (67%)	31 (100%)	0	100 100
All	All	4170/4373 (95%)	4167 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	91	GLN
8	L	38	ARG
12	d	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	471	HIS
16	h	48	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)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	M3L	K	43	8	10,11,12	0.57	0	9,14,16	0.70	0
8	M3L	M	43	8	10,11,12	0.41	0	9,14,16	0.50	0
8	M3L	L	43	8	10,11,12	0.48	0	9,14,16	0.53	0
8	M3L	O	43	8	10,11,12	0.48	0	9,14,16	0.51	0
8	M3L	Q	43	8	10,11,12	0.43	0	9,14,16	0.56	0
8	M3L	N	43	8	10,11,12	0.50	0	9,14,16	0.59	0
8	M3L	P	43	8	10,11,12	0.50	0	9,14,16	0.50	0
8	M3L	R	43	8	10,11,12	0.44	0	9,14,16	0.40	0

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
8	M3L	K	43	8	-	1/9/10/12	-
8	M3L	M	43	8	-	1/9/10/12	-
8	M3L	L	43	8	-	3/9/10/12	-
8	M3L	O	43	8	-	1/9/10/12	-
8	M3L	Q	43	8	-	3/9/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	M3L	N	43	8	-	3/9/10/12	-
8	M3L	P	43	8	-	2/9/10/12	-
8	M3L	R	43	8	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	43	M3L	O-C-CA-CB
8	N	43	M3L	C-CA-CB-CG
8	P	43	M3L	O-C-CA-CB
8	Q	43	M3L	O-C-CA-CB
8	K	43	M3L	CG-CD-CE-NZ
8	Q	43	M3L	CG-CD-CE-NZ
8	Q	43	M3L	CA-CB-CG-CD
8	N	43	M3L	CE-CD-CG-CB
8	P	43	M3L	CG-CD-CE-NZ
8	L	43	M3L	CE-CD-CG-CB
8	R	43	M3L	C-CA-CB-CG
8	L	43	M3L	N-CA-CB-CG
8	N	43	M3L	N-CA-CB-CG
8	R	43	M3L	CE-CD-CG-CB
8	M	43	M3L	CE-CD-CG-CB
8	O	43	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	43	M3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	ATP	C	600	20	26,33,33	0.90	1 (3%)	31,52,52	1.66	5 (16%)
21	ADP	E	600	-	24,29,29	0.95	1 (4%)	29,45,45	1.54	5 (17%)
22	CDL	f	101	-	77,77,99	1.00	6 (7%)	83,89,111	1.10	5 (6%)
23	LHG	f	104	-	48,48,48	0.61	0	51,54,54	1.22	4 (7%)
19	ATP	A	600	20	26,33,33	0.90	1 (3%)	31,52,52	1.68	5 (16%)
22	CDL	b	301	-	82,82,99	0.98	6 (7%)	88,94,111	1.12	4 (4%)
21	ADP	F	600	20	24,29,29	0.94	1 (4%)	29,45,45	1.47	6 (20%)
19	ATP	B	600	20	26,33,33	0.91	1 (3%)	31,52,52	1.66	5 (16%)
23	LHG	f	103	-	38,38,48	0.60	0	41,44,54	1.25	4 (9%)
22	CDL	f	102	14	83,83,99	0.98	7 (8%)	89,95,111	1.10	4 (4%)
21	ADP	D	600	20	24,29,29	0.94	1 (4%)	29,45,45	1.50	5 (17%)

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	ATP	C	600	20	-	0/18/38/38	0/3/3/3
21	ADP	E	600	-	-	3/12/32/32	0/3/3/3
22	CDL	f	101	-	-	29/88/88/110	-
23	LHG	f	104	-	-	12/53/53/53	-
19	ATP	A	600	20	-	1/18/38/38	0/3/3/3
22	CDL	b	301	-	-	32/93/93/110	-
21	ADP	F	600	20	-	2/12/32/32	0/3/3/3
19	ATP	B	600	20	-	0/18/38/38	0/3/3/3
23	LHG	f	103	-	-	15/43/43/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	f	102	14	-	28/94/94/110	-
21	ADP	D	600	20	-	2/12/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	f	101	CDL	OA6-CA4	-2.77	1.39	1.46
22	f	102	CDL	OB8-CB7	2.73	1.41	1.33
22	b	301	CDL	OA6-CA4	-2.73	1.39	1.46
22	f	101	CDL	OB8-CB7	2.66	1.41	1.33
22	b	301	CDL	OB8-CB7	2.61	1.41	1.33
22	f	102	CDL	OA6-CA4	-2.55	1.40	1.46
22	f	102	CDL	OB6-CB4	-2.54	1.40	1.46
22	f	101	CDL	OB6-CB5	2.48	1.41	1.34
22	f	101	CDL	OB6-CB4	-2.47	1.40	1.46
22	f	102	CDL	OB6-CB5	2.42	1.41	1.34
22	b	301	CDL	OB6-CB5	2.39	1.41	1.34
21	E	600	ADP	C5-C4	2.39	1.47	1.40
22	b	301	CDL	OB6-CB4	-2.38	1.40	1.46
22	b	301	CDL	OA8-CA7	2.33	1.40	1.33
22	f	102	CDL	OA8-CA7	2.28	1.40	1.33
22	f	102	CDL	OA8-CA6	-2.26	1.40	1.45
21	D	600	ADP	C5-C4	2.25	1.46	1.40
22	f	101	CDL	OA8-CA7	2.22	1.39	1.33
19	C	600	ATP	C5-C4	2.18	1.46	1.40
19	A	600	ATP	C5-C4	2.17	1.46	1.40
22	f	101	CDL	OA8-CA6	-2.16	1.40	1.45
21	F	600	ADP	C5-C4	2.15	1.46	1.40
19	B	600	ATP	C5-C4	2.15	1.46	1.40
22	f	102	CDL	OA6-CA5	2.14	1.40	1.34
22	b	301	CDL	OA8-CA6	-2.12	1.40	1.45

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	600	ATP	PB-O3B-PG	-4.87	116.12	132.83
22	b	301	CDL	OA6-CA5-C11	4.57	121.35	111.50
19	C	600	ATP	PB-O3B-PG	-4.35	117.89	132.83
19	B	600	ATP	PA-O3A-PB	-4.34	117.95	132.83
23	f	104	LHG	O4-P-O5	4.18	132.93	112.24
23	f	103	LHG	O4-P-O5	4.17	132.86	112.24
22	b	301	CDL	OB6-CB5-C51	4.09	120.31	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	f	102	CDL	OA6-CA5-C11	4.07	120.27	111.50
22	f	101	CDL	OA6-CA5-C11	3.99	120.10	111.50
22	f	102	CDL	OB6-CB5-C51	3.90	119.90	111.50
21	E	600	ADP	PA-O3A-PB	-3.85	119.60	132.83
22	f	101	CDL	OB6-CB5-C51	3.78	119.64	111.50
21	F	600	ADP	N3-C2-N1	-3.76	122.80	128.68
21	E	600	ADP	N3-C2-N1	-3.66	122.96	128.68
19	B	600	ATP	N3-C2-N1	-3.62	123.01	128.68
19	A	600	ATP	N3-C2-N1	-3.60	123.06	128.68
19	C	600	ATP	N3-C2-N1	-3.57	123.09	128.68
21	D	600	ADP	N3-C2-N1	-3.56	123.11	128.68
21	D	600	ADP	C3'-C2'-C1'	3.53	106.29	100.98
19	B	600	ATP	C3'-C2'-C1'	3.43	106.14	100.98
21	E	600	ADP	C3'-C2'-C1'	3.42	106.12	100.98
19	C	600	ATP	C3'-C2'-C1'	3.35	106.02	100.98
19	B	600	ATP	PB-O3B-PG	-3.34	121.36	132.83
21	F	600	ADP	PA-O3A-PB	-3.34	121.38	132.83
19	C	600	ATP	PA-O3A-PB	-3.28	121.56	132.83
19	A	600	ATP	PA-O3A-PB	-3.28	121.57	132.83
21	D	600	ADP	PA-O3A-PB	-2.86	123.01	132.83
19	A	600	ATP	C4-C5-N7	-2.76	106.52	109.40
22	b	301	CDL	OA8-CA7-C31	2.76	120.57	111.91
23	f	104	LHG	O8-C23-C24	2.76	120.56	111.91
21	E	600	ADP	C4-C5-N7	-2.72	106.56	109.40
19	C	600	ATP	C4-C5-N7	-2.67	106.61	109.40
22	f	101	CDL	OA8-CA7-C31	2.67	120.28	111.91
21	D	600	ADP	C4-C5-N7	-2.64	106.64	109.40
23	f	103	LHG	O8-C23-C24	2.61	120.11	111.91
21	F	600	ADP	C4-C5-N7	-2.57	106.72	109.40
19	B	600	ATP	C4-C5-N7	-2.55	106.74	109.40
19	A	600	ATP	C3'-C2'-C1'	2.45	104.67	100.98
22	f	102	CDL	OA8-CA7-C31	2.44	119.58	111.91
21	F	600	ADP	C3'-C2'-C1'	2.44	104.65	100.98
23	f	103	LHG	C11-C10-C9	-2.40	102.25	114.42
22	f	102	CDL	OB8-CB7-C71	2.37	119.35	111.91
23	f	104	LHG	C11-C10-C9	-2.31	102.68	114.42
22	b	301	CDL	OB8-CB7-C71	2.31	119.14	111.91
22	f	101	CDL	OB8-CB7-C71	2.20	118.82	111.91
23	f	103	LHG	C27-C26-C25	-2.18	103.37	114.42
23	f	104	LHG	C20-C19-C18	-2.15	103.51	114.42
21	F	600	ADP	C2'-C3'-C4'	2.11	106.75	102.64
21	E	600	ADP	C2-N1-C6	2.08	122.32	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	F	600	ADP	C2-N1-C6	2.07	122.30	118.75
21	D	600	ADP	C2-N1-C6	2.05	122.26	118.75
22	f	101	CDL	CA4-OA6-CA5	-2.02	112.81	117.79

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	D	600	ADP	C5'-O5'-PA-O3A
21	E	600	ADP	C5'-O5'-PA-O1A
21	E	600	ADP	C5'-O5'-PA-O3A
21	F	600	ADP	C5'-O5'-PA-O3A
22	b	301	CDL	C1-CA2-OA2-PA1
22	b	301	CDL	CA2-OA2-PA1-OA3
22	b	301	CDL	CA2-OA2-PA1-OA4
22	b	301	CDL	CA2-OA2-PA1-OA5
22	b	301	CDL	CB2-OB2-PB2-OB3
22	b	301	CDL	CB2-OB2-PB2-OB4
22	f	101	CDL	O1-C1-CA2-OA2
22	f	101	CDL	CA2-C1-CB2-OB2
22	f	101	CDL	C11-CA5-OA6-CA4
22	f	101	CDL	OB5-CB3-CB4-OB6
22	f	102	CDL	CB2-OB2-PB2-OB3
23	f	103	LHG	C3-O3-P-O5
23	f	103	LHG	C6-C5-O7-C7
23	f	103	LHG	C8-C7-O7-C5
23	f	104	LHG	C1-C2-C3-O3
22	f	101	CDL	OA7-CA5-OA6-CA4
23	f	103	LHG	O9-C7-O7-C5
22	f	102	CDL	C31-CA7-OA8-CA6
22	f	102	CDL	OA9-CA7-OA8-CA6
22	f	101	CDL	O1-C1-CB2-OB2
23	f	104	LHG	O2-C2-C3-O3
22	f	101	CDL	CB2-C1-CA2-OA2
22	b	301	CDL	CA5-C11-C12-C13
22	f	101	CDL	CB5-C51-C52-C53
22	b	301	CDL	C71-C72-C73-C74
22	f	102	CDL	CA5-C11-C12-C13
22	f	102	CDL	CA7-C31-C32-C33
23	f	104	LHG	C7-C8-C9-C10
22	f	102	CDL	CB5-C51-C52-C53
22	b	301	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	f	103	LHG	C3-O3-P-O6
23	f	103	LHG	C4-O6-P-O3
23	f	104	LHG	C28-C29-C30-C31
23	f	103	LHG	C13-C14-C15-C16
22	b	301	CDL	CB4-CB3-OB5-PB2
23	f	104	LHG	C5-C4-O6-P
23	f	103	LHG	C24-C25-C26-C27
22	f	101	CDL	C40-C41-C42-C43
23	f	103	LHG	C23-C24-C25-C26
22	f	101	CDL	C21-C22-C23-C24
23	f	104	LHG	C15-C16-C17-C18
22	b	301	CDL	C13-C14-C15-C16
22	f	101	CDL	C19-C20-C21-C22
22	b	301	CDL	C51-C52-C53-C54
22	f	102	CDL	C11-CA5-OA6-CA4
22	b	301	CDL	C60-C61-C62-C63
22	b	301	CDL	C73-C74-C75-C76
22	f	101	CDL	OB7-CB5-OB6-CB4
22	f	102	CDL	OA7-CA5-OA6-CA4
22	b	301	CDL	C53-C54-C55-C56
22	b	301	CDL	C11-CA5-OA6-CA4
22	f	101	CDL	C51-CB5-OB6-CB4
22	b	301	CDL	OA7-CA5-OA6-CA4
22	b	301	CDL	OB6-CB4-CB6-OB8
22	f	102	CDL	C1-CB2-OB2-PB2
22	f	101	CDL	OB5-CB3-CB4-CB6
22	f	102	CDL	OB5-CB3-CB4-CB6
23	f	104	LHG	O6-C4-C5-C6
22	b	301	CDL	C54-C55-C56-C57
22	f	101	CDL	C37-C38-C39-C40
23	f	104	LHG	C11-C12-C13-C14
23	f	103	LHG	C27-C28-C29-C30
22	f	102	CDL	C13-C14-C15-C16
22	f	101	CDL	OA5-CA3-CA4-OA6
23	f	104	LHG	C29-C30-C31-C32
22	b	301	CDL	C33-C34-C35-C36
22	f	102	CDL	C54-C55-C56-C57
22	f	102	CDL	C71-CB7-OB8-CB6
23	f	103	LHG	C2-C3-O3-P
22	f	101	CDL	C17-C18-C19-C20
22	f	101	CDL	C74-C75-C76-C77
22	b	301	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	101	CDL	C13-C14-C15-C16
22	f	102	CDL	C12-C13-C14-C15
22	f	101	CDL	OA5-CA3-CA4-CA6
22	f	102	CDL	C74-C75-C76-C77
19	A	600	ATP	PB-O3B-PG-O1G
22	f	101	CDL	C31-CA7-OA8-CA6
22	f	102	CDL	OB9-CB7-OB8-CB6
22	f	102	CDL	OB5-CB3-CB4-OB6
23	f	104	LHG	O6-C4-C5-O7
22	b	301	CDL	C71-CB7-OB8-CB6
23	f	104	LHG	C31-C32-C33-C34
22	f	101	CDL	C32-C33-C34-C35
22	b	301	CDL	C16-C17-C18-C19
23	f	103	LHG	C11-C10-C9-C8
22	b	301	CDL	CA3-OA5-PA1-OA2
21	D	600	ADP	C5'-O5'-PA-O1A
21	E	600	ADP	C5'-O5'-PA-O2A
21	F	600	ADP	C5'-O5'-PA-O1A
23	f	103	LHG	C4-O6-P-O5
23	f	104	LHG	C14-C15-C16-C17
22	f	101	CDL	OA9-CA7-OA8-CA6
22	f	102	CDL	C52-C53-C54-C55
22	b	301	CDL	OB9-CB7-OB8-CB6
22	f	102	CDL	C60-C61-C62-C63
22	f	102	CDL	C73-C74-C75-C76
22	f	102	CDL	C56-C57-C58-C59
22	f	102	CDL	C53-C54-C55-C56
23	f	103	LHG	C10-C11-C12-C13
22	b	301	CDL	C12-C11-CA5-OA6
22	f	102	CDL	CA2-OA2-PA1-OA5
22	f	102	CDL	CB3-OB5-PB2-OB2
22	f	101	CDL	C42-C43-C44-C45
22	f	101	CDL	CA3-CA4-CA6-OA8
22	b	301	CDL	C58-C59-C60-C61
22	f	102	CDL	C14-C15-C16-C17
22	f	102	CDL	C1-CA2-OA2-PA1
22	f	101	CDL	C36-C37-C38-C39
23	f	103	LHG	O6-C4-C5-C6
22	b	301	CDL	CA4-CA3-OA5-PA1
22	f	102	CDL	C33-C34-C35-C36
22	f	101	CDL	C52-C53-C54-C55
22	b	301	CDL	C57-C58-C59-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	102	CDL	CA4-CA3-OA5-PA1
22	b	301	CDL	CB3-OB5-PB2-OB3
22	f	101	CDL	CB3-OB5-PB2-OB3
22	b	301	CDL	CB2-C1-CA2-OA2
22	b	301	CDL	C52-C51-CB5-OB6
22	f	101	CDL	C32-C31-CA7-OA8

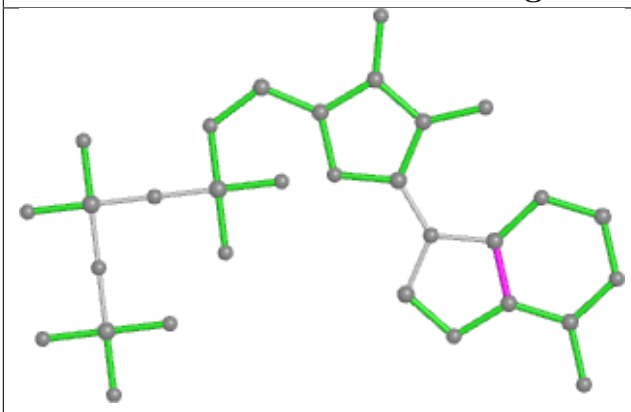
There are no ring outliers.

2 monomers are involved in 4 short contacts:

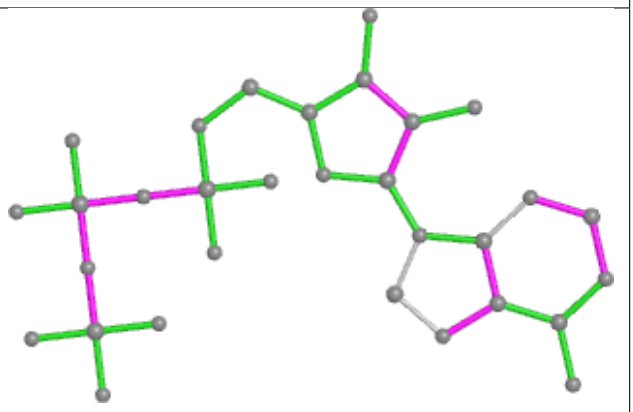
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	600	ADP	3	0
21	D	600	ADP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

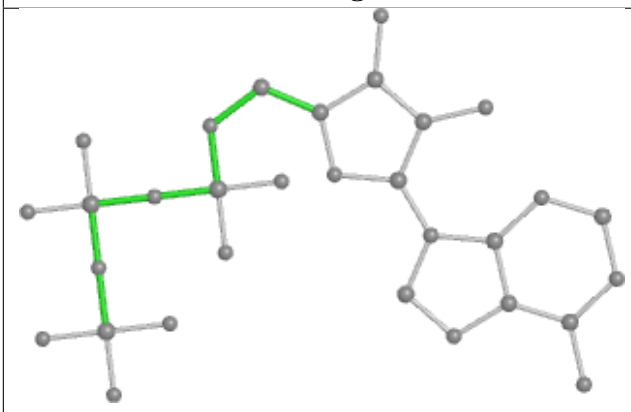
Ligand ATP C 600



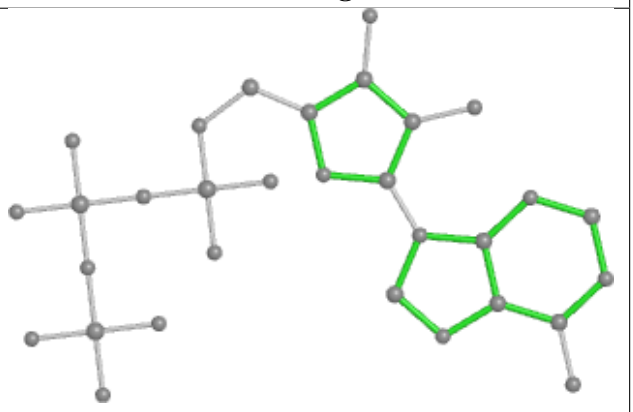
Bond lengths



Bond angles

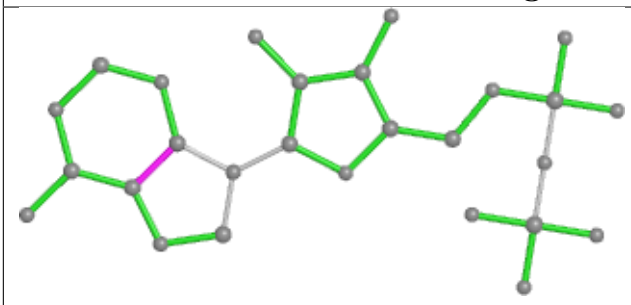


Torsions

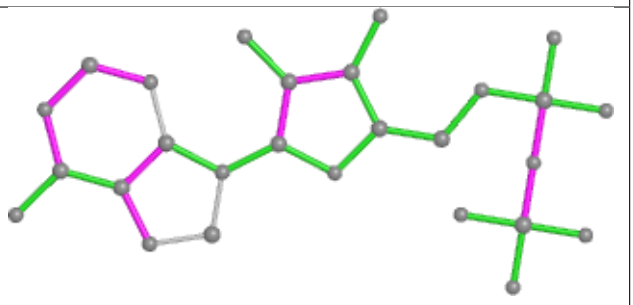


Rings

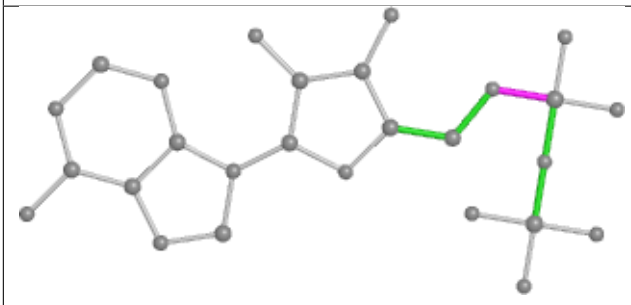
Ligand ADP E 600



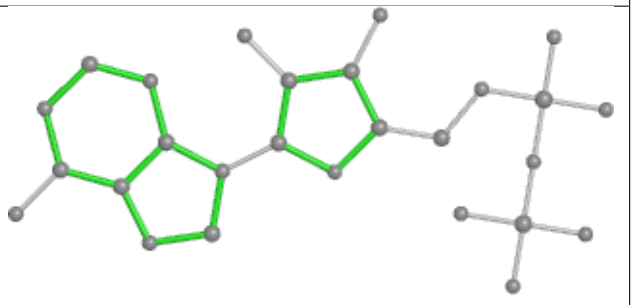
Bond lengths



Bond angles

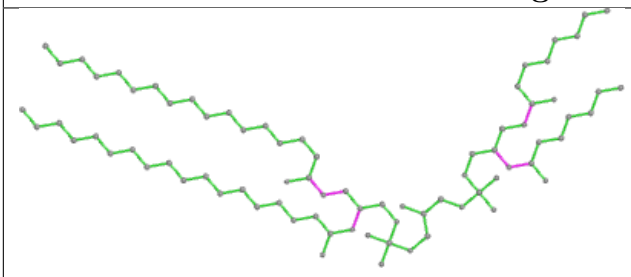


Torsions

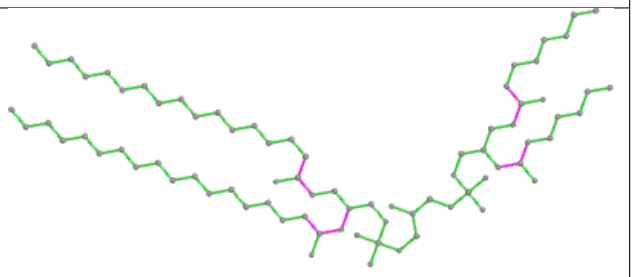


Rings

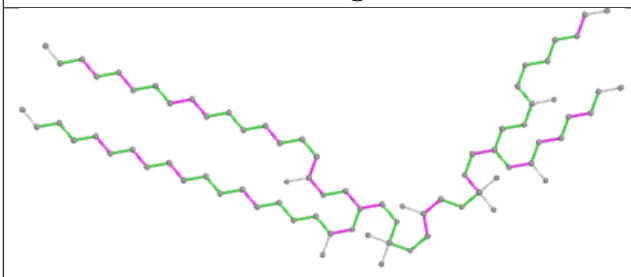
Ligand CDL f 101



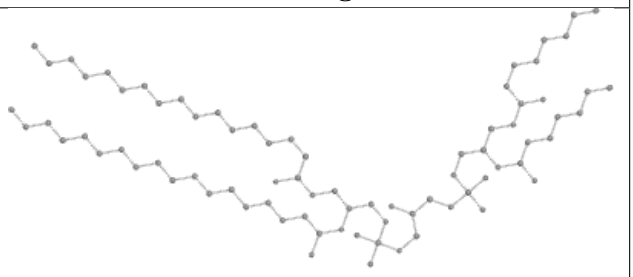
Bond lengths



Bond angles

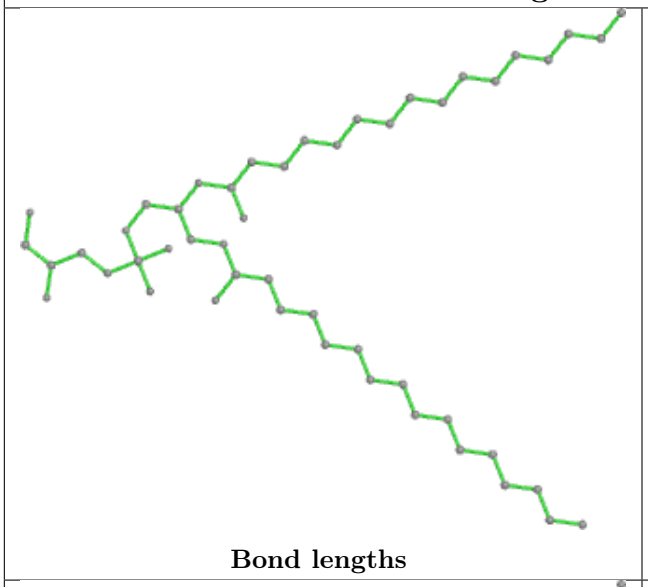


Torsions

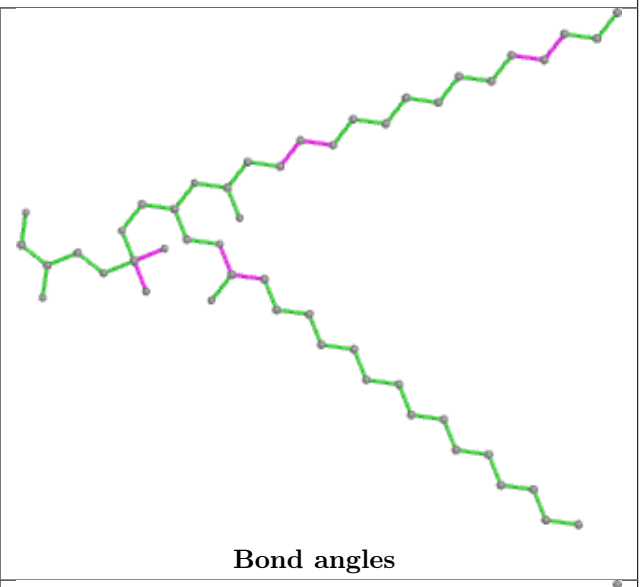


Rings

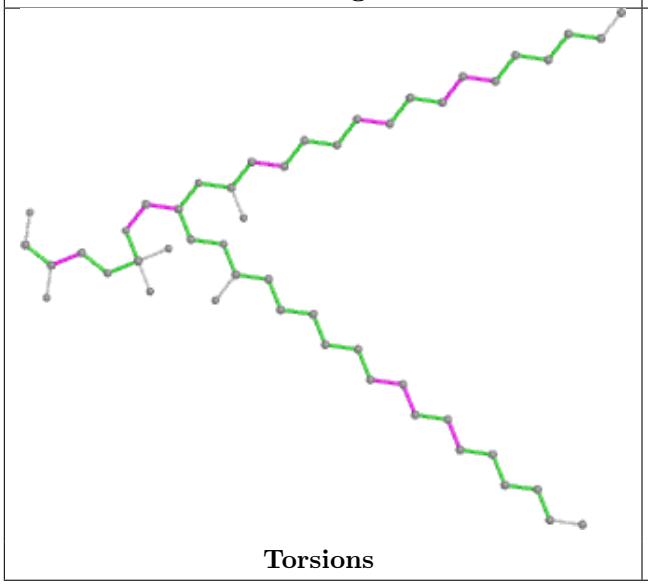
Ligand LHG f 104



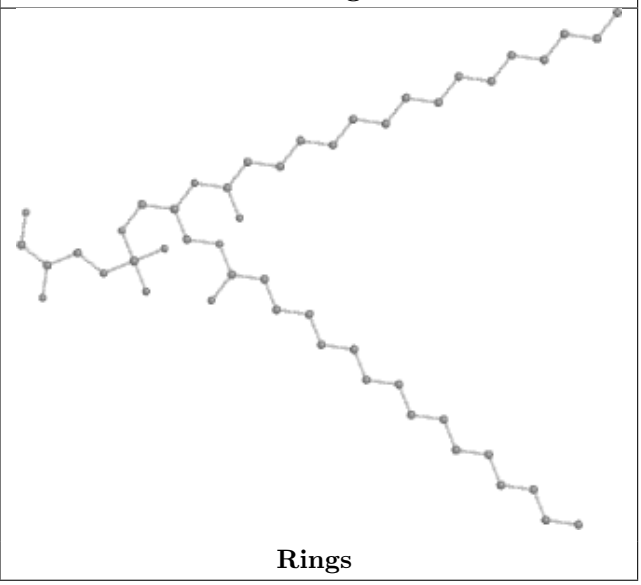
Bond lengths



Bond angles

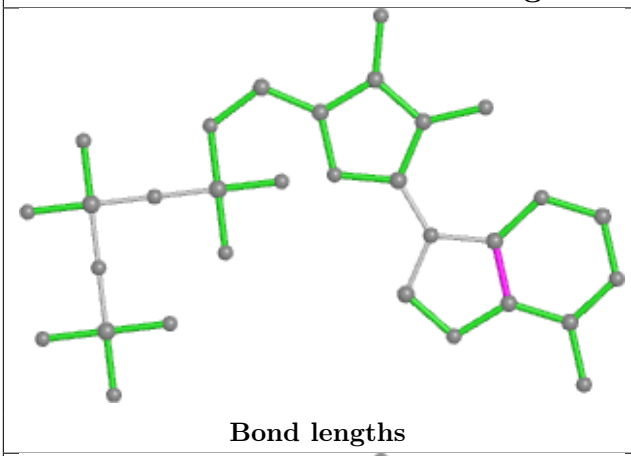


Torsions

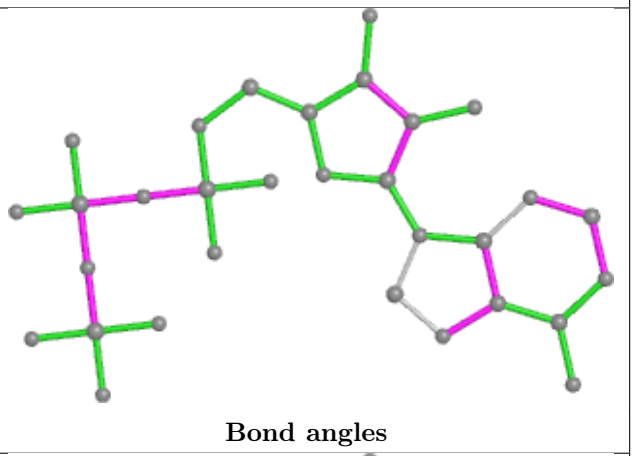


Rings

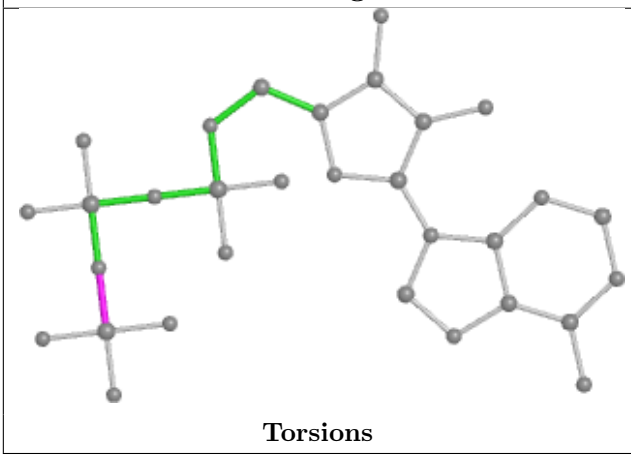
Ligand ATP A 600



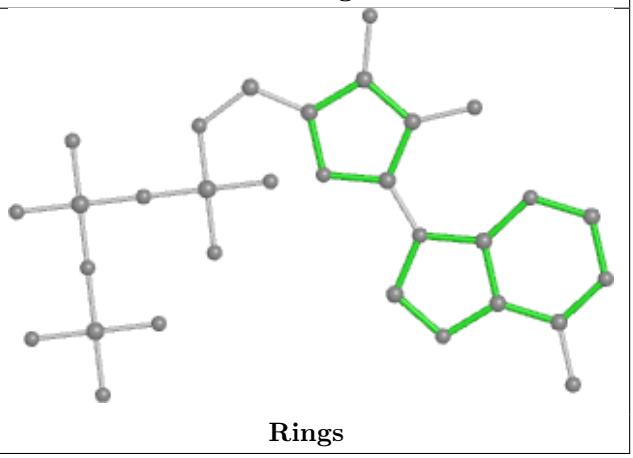
Bond lengths



Bond angles

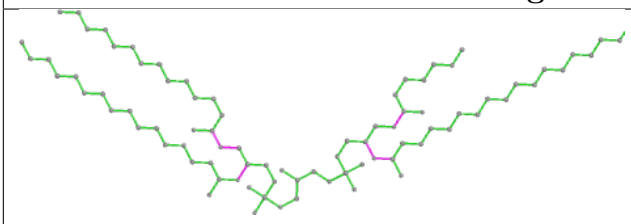


Torsions

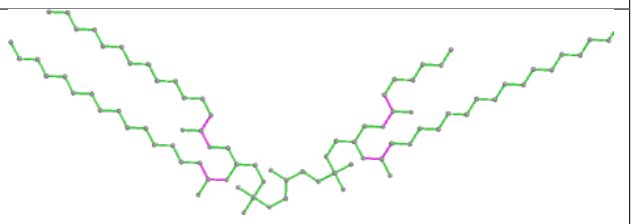


Rings

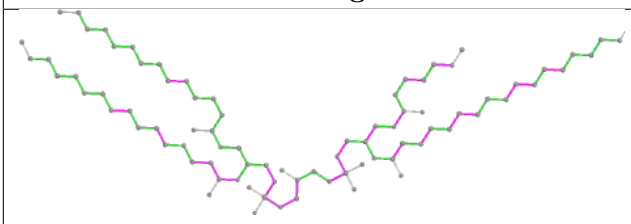
Ligand CDL b 301



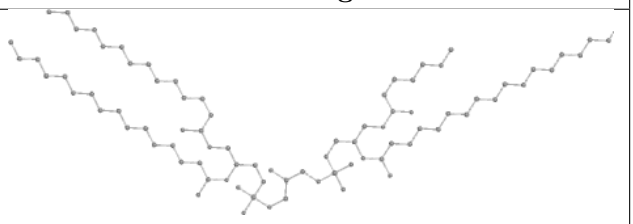
Bond lengths



Bond angles

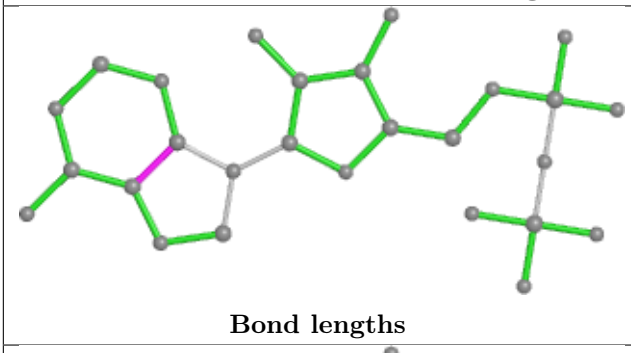


Torsions

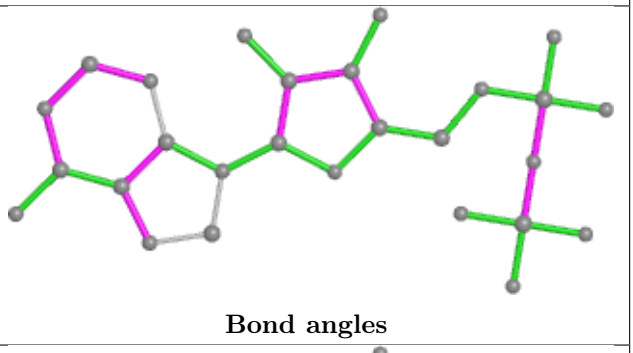


Rings

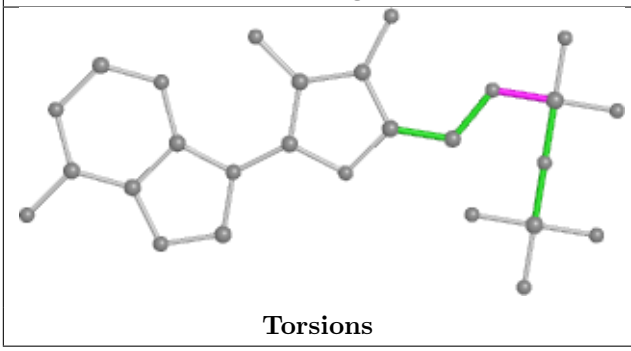
Ligand ADP F 600



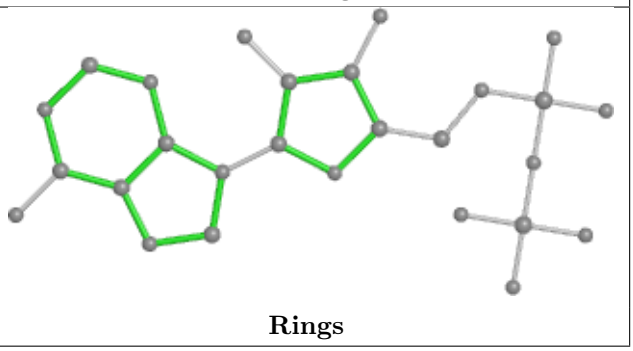
Bond lengths



Bond angles

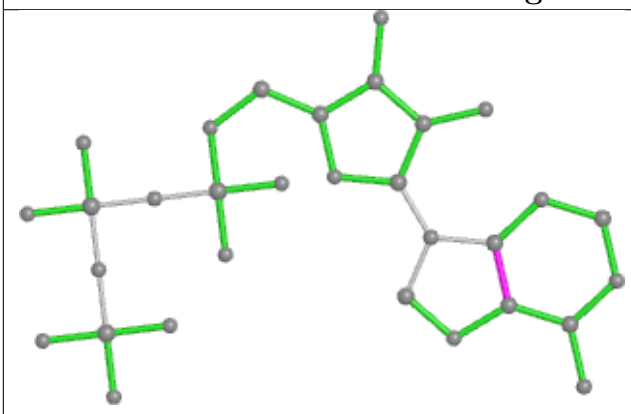


Torsions

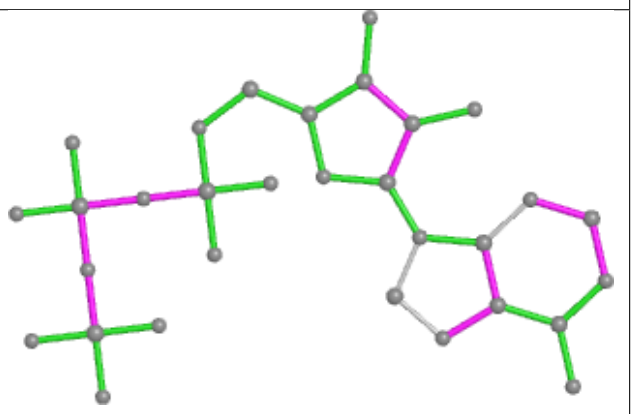


Rings

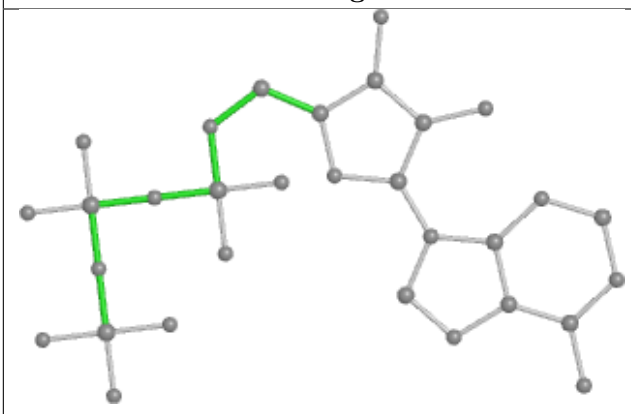
Ligand ATP B 600



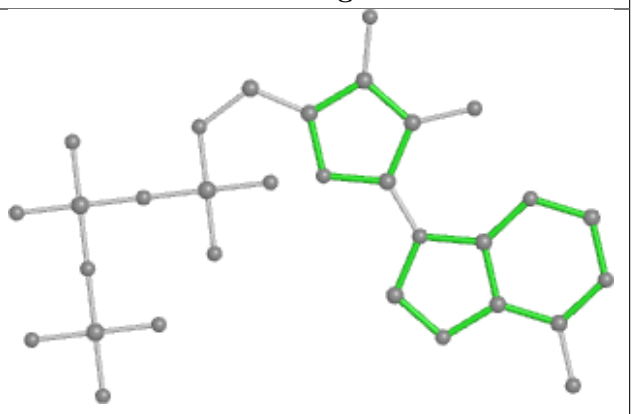
Bond lengths



Bond angles

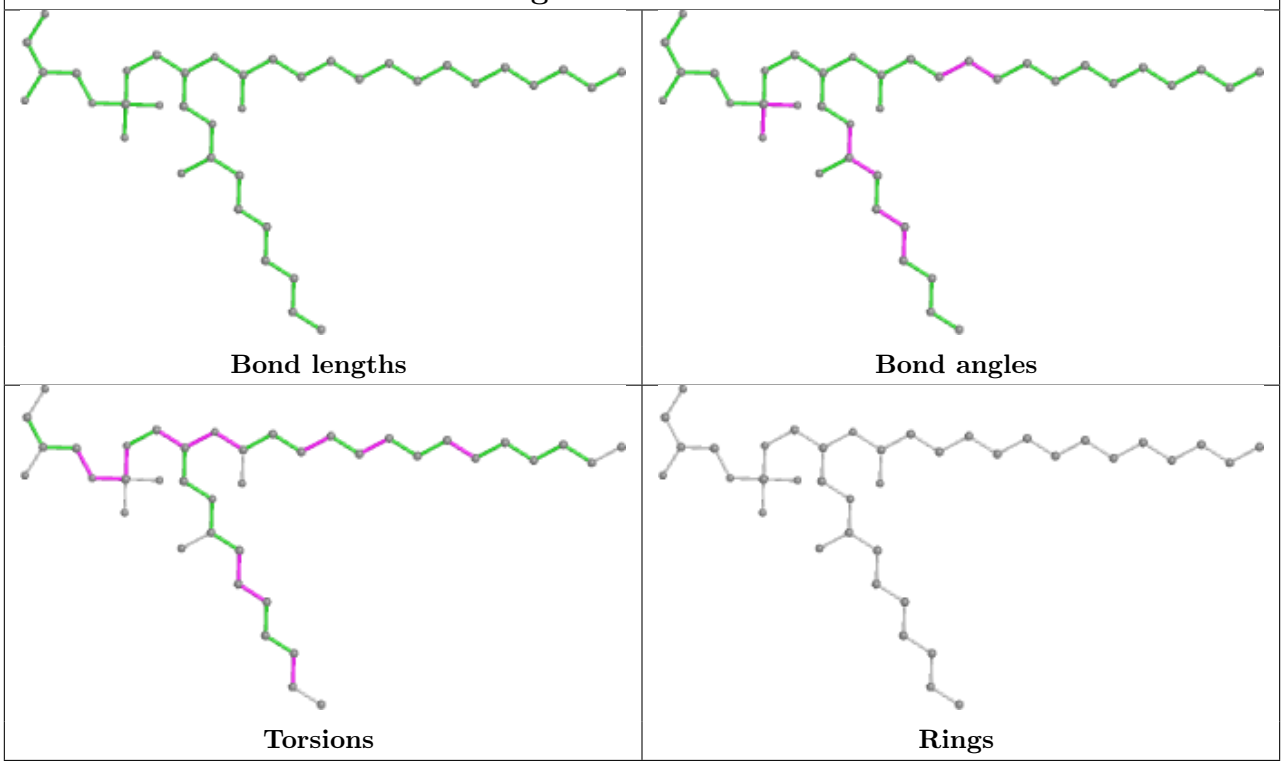


Torsions

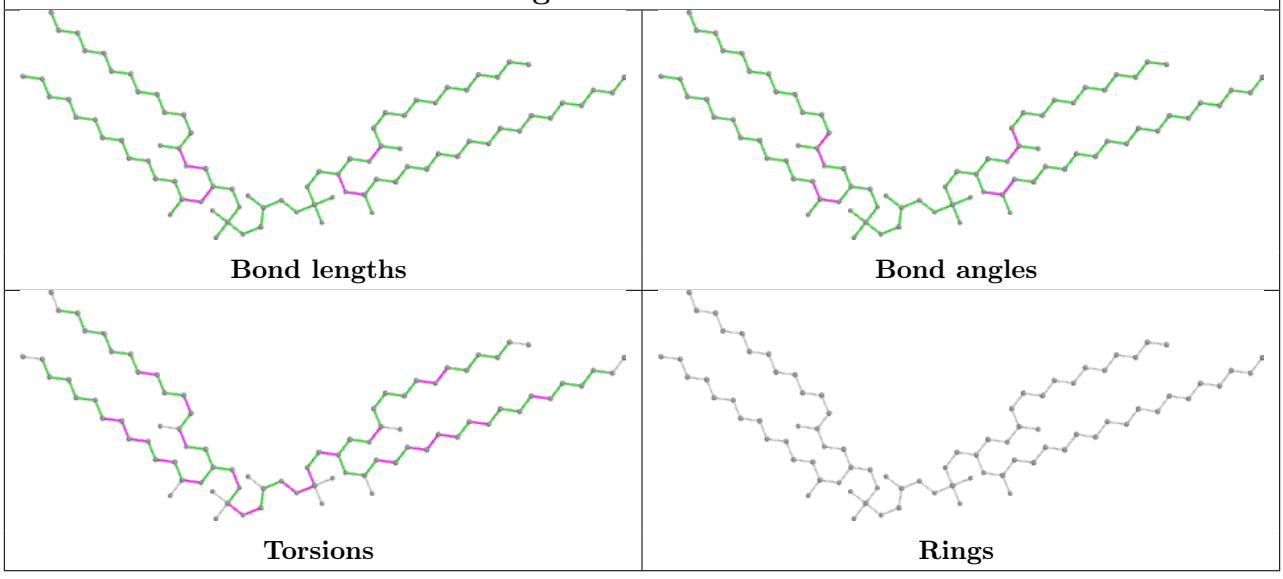


Rings

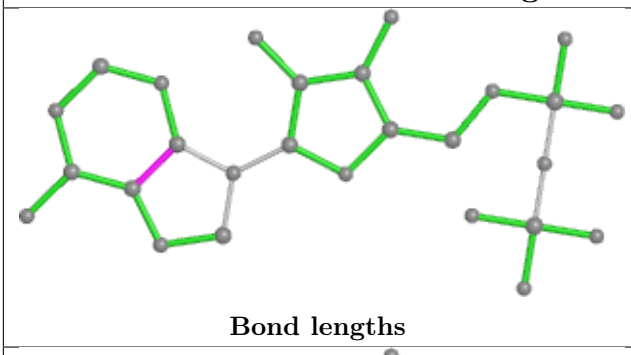
Ligand LHG f 103



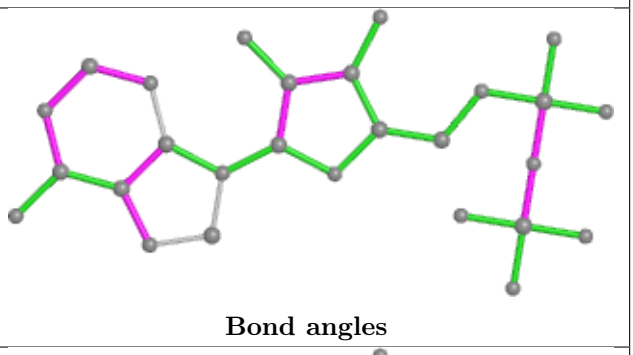
Ligand CDL f 102



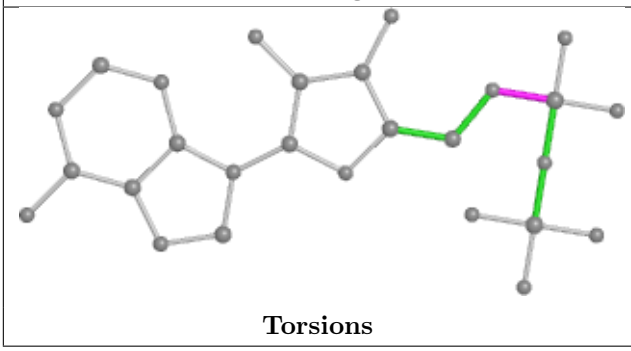
Ligand ADP D 600



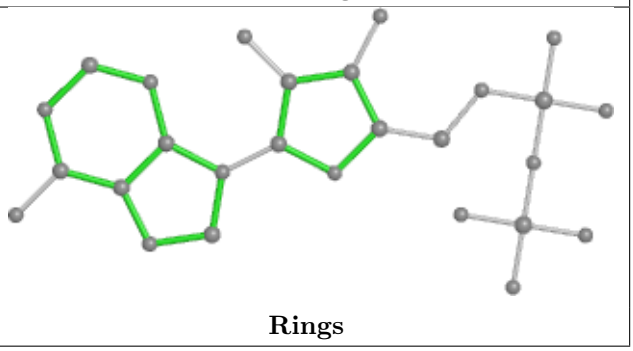
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

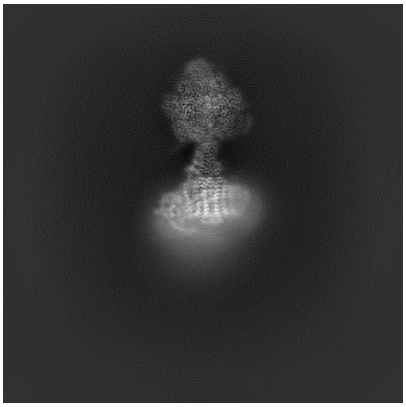
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11342. These allow visual inspection of the internal detail of the map and identification of artifacts.

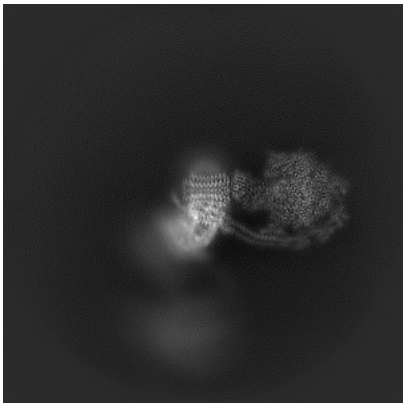
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

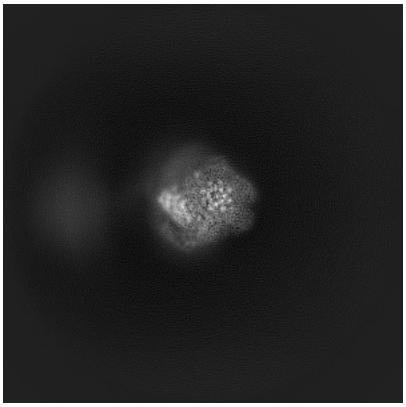
6.1.1 Primary map



X



Y

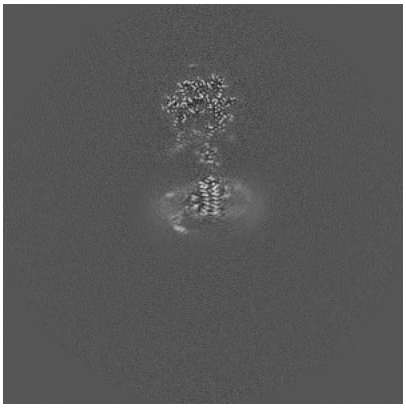


Z

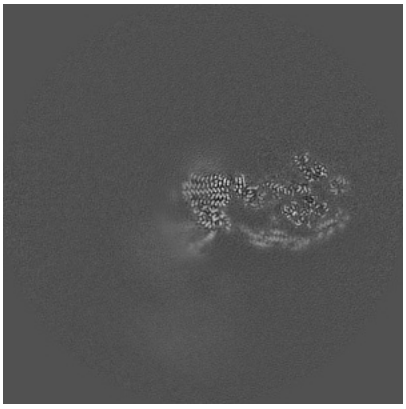
The images above show the map projected in three orthogonal directions.

6.2 Central slices

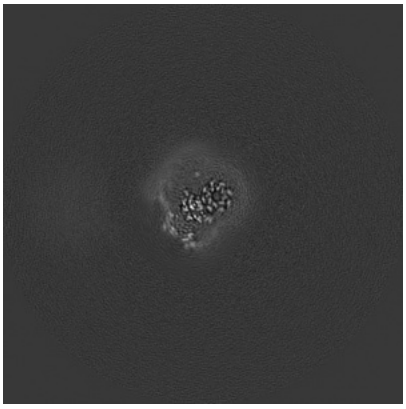
6.2.1 Primary map



X Index: 250



Y Index: 250

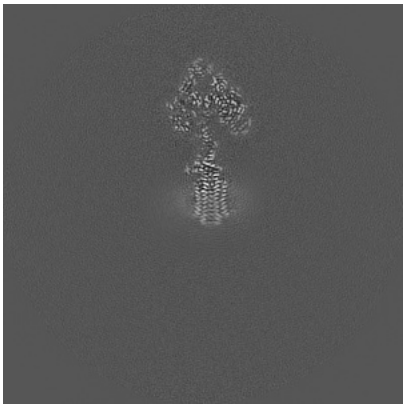


Z Index: 250

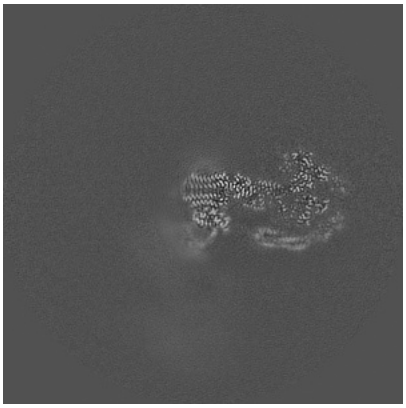
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

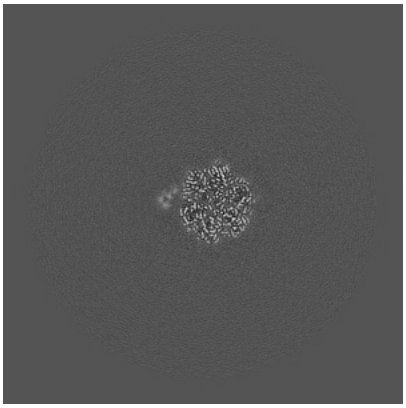
6.3.1 Primary map



X Index: 273



Y Index: 254



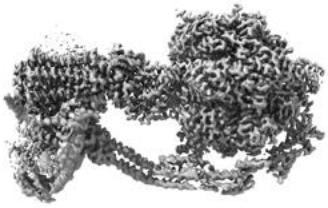
Z Index: 376

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 8.86. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

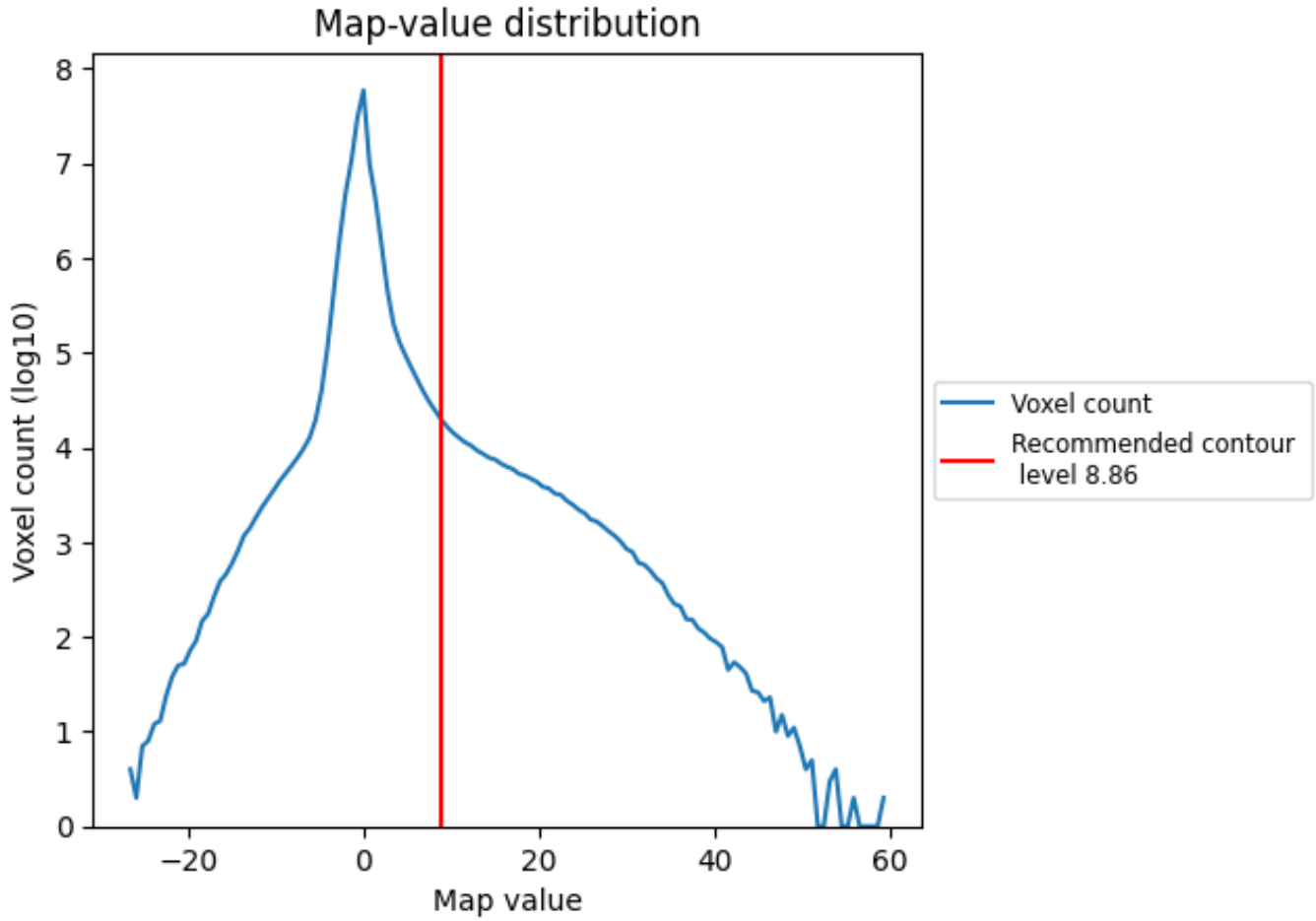
6.5 Mask visualisation (i)

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

7 Map analysis

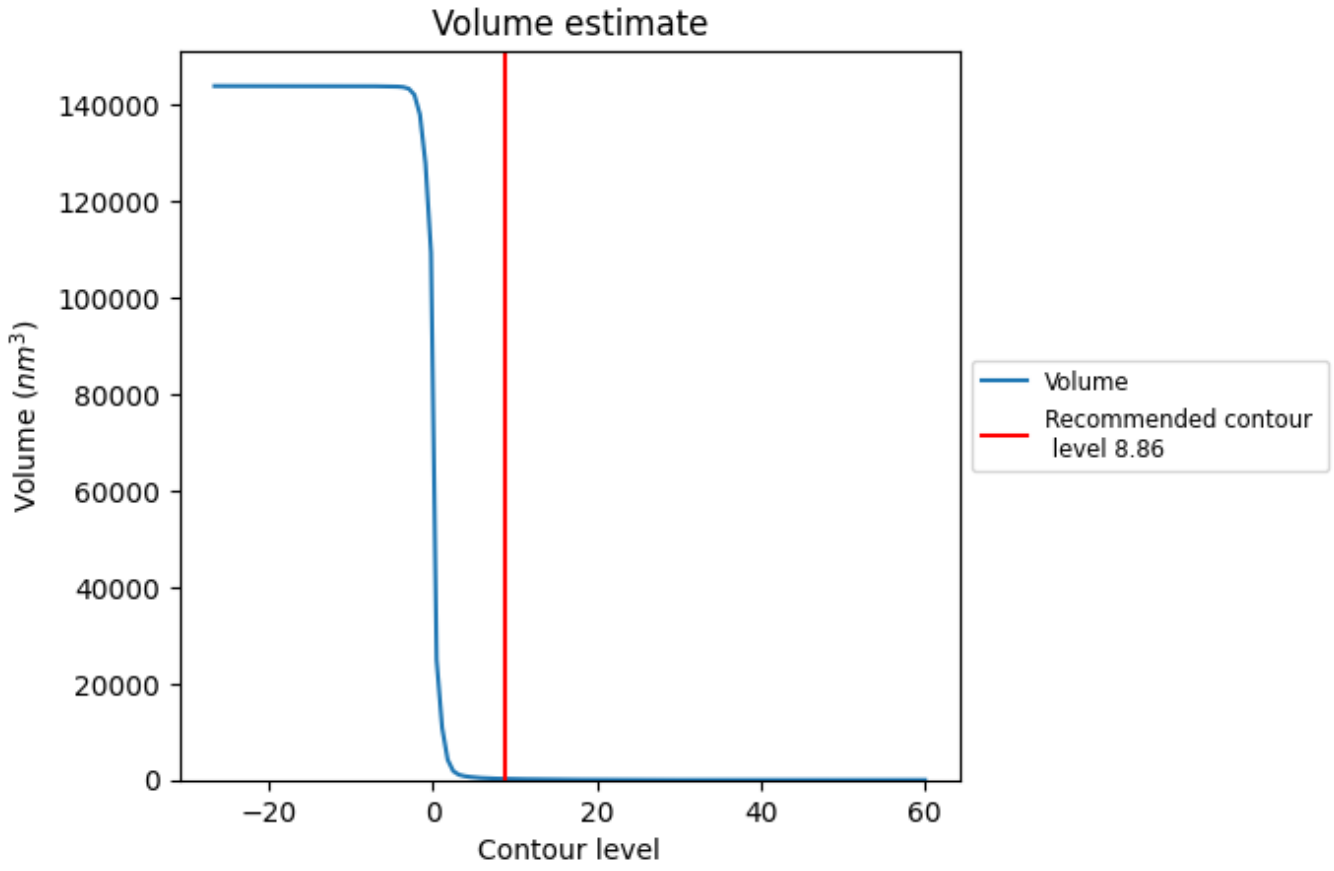
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

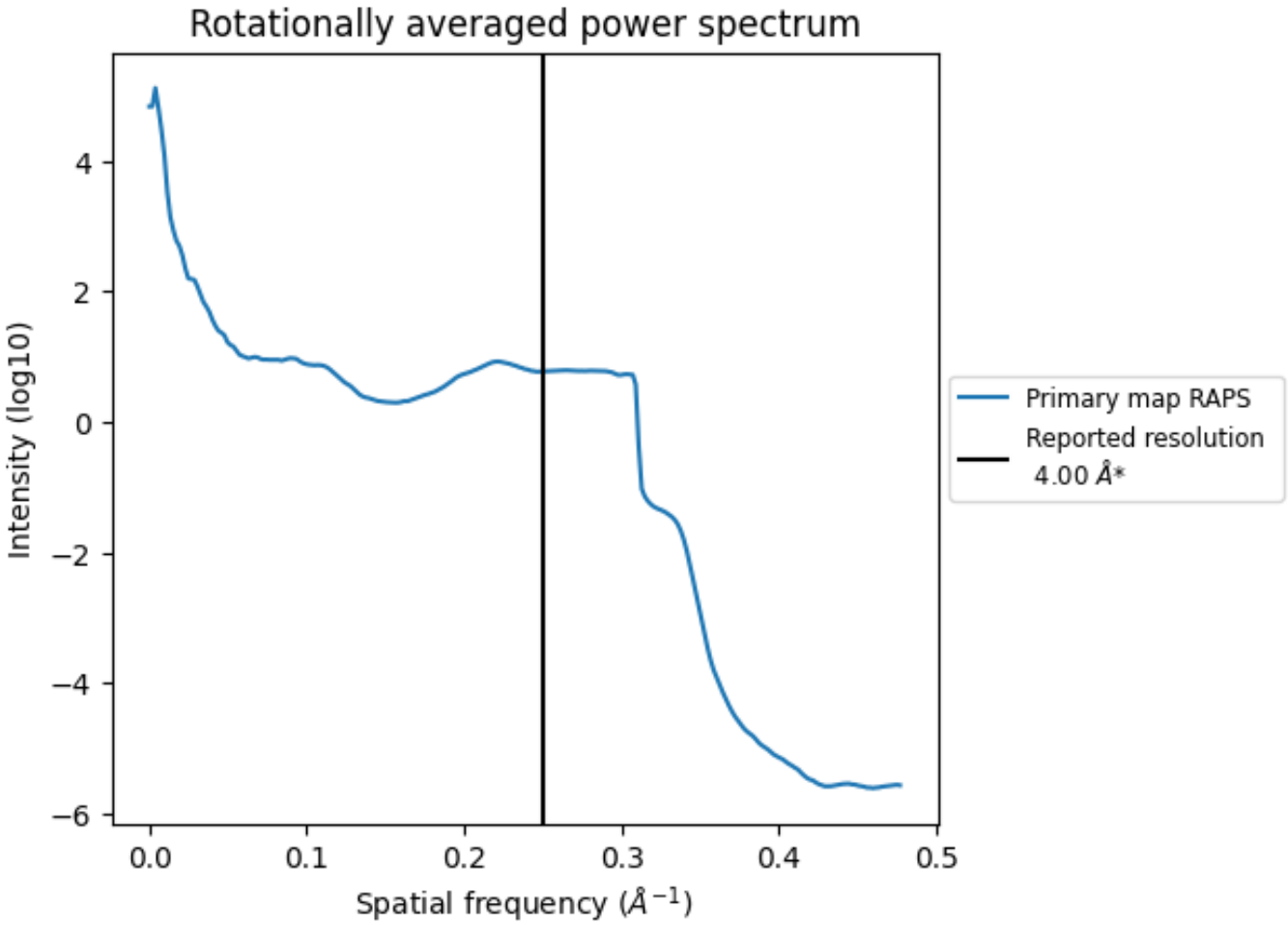
7.2 Volume estimate



The volume at the recommended contour level is 224 nm^3; this corresponds to an approximate mass of 202 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

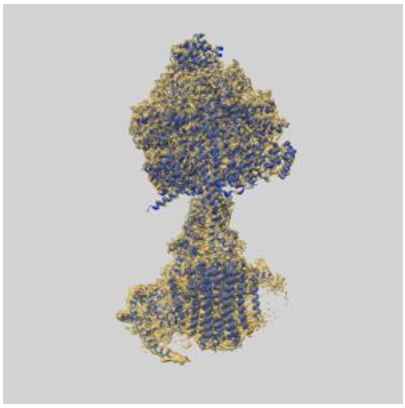
8 Fourier-Shell correlation

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

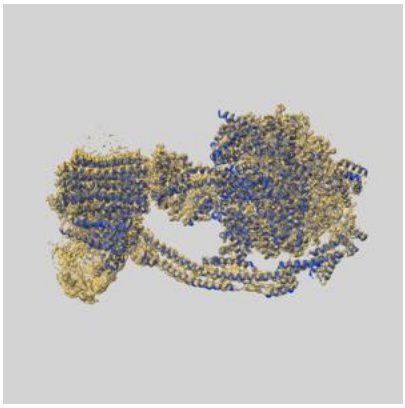
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11342 and PDB model 6ZPO. Per-residue inclusion information can be found in section 3 on page 11.

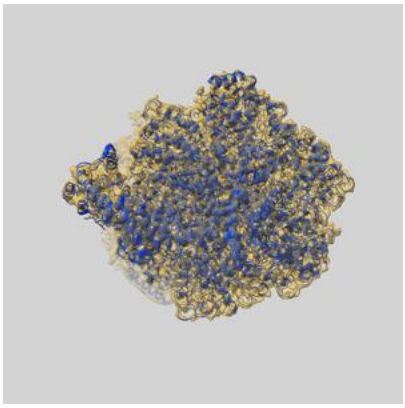
9.1 Map-model overlay



X



Y



Z

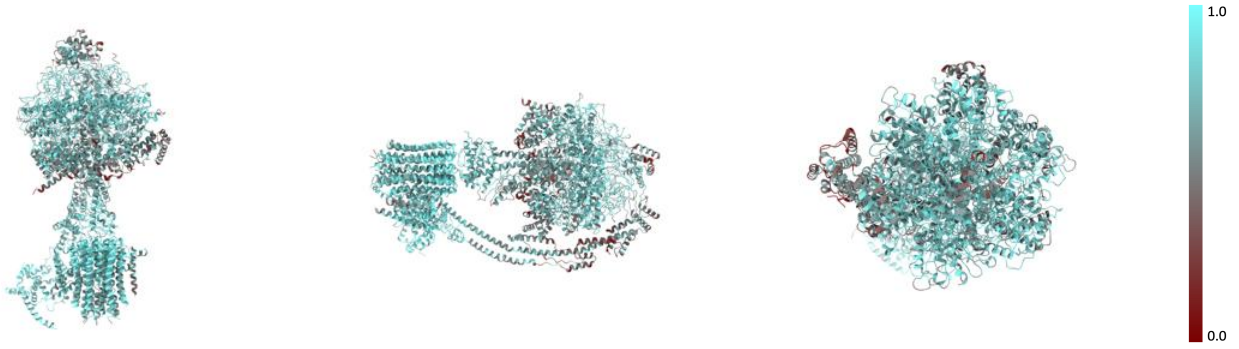
The images above show the 3D surface view of the map at the recommended contour level 8.86 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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

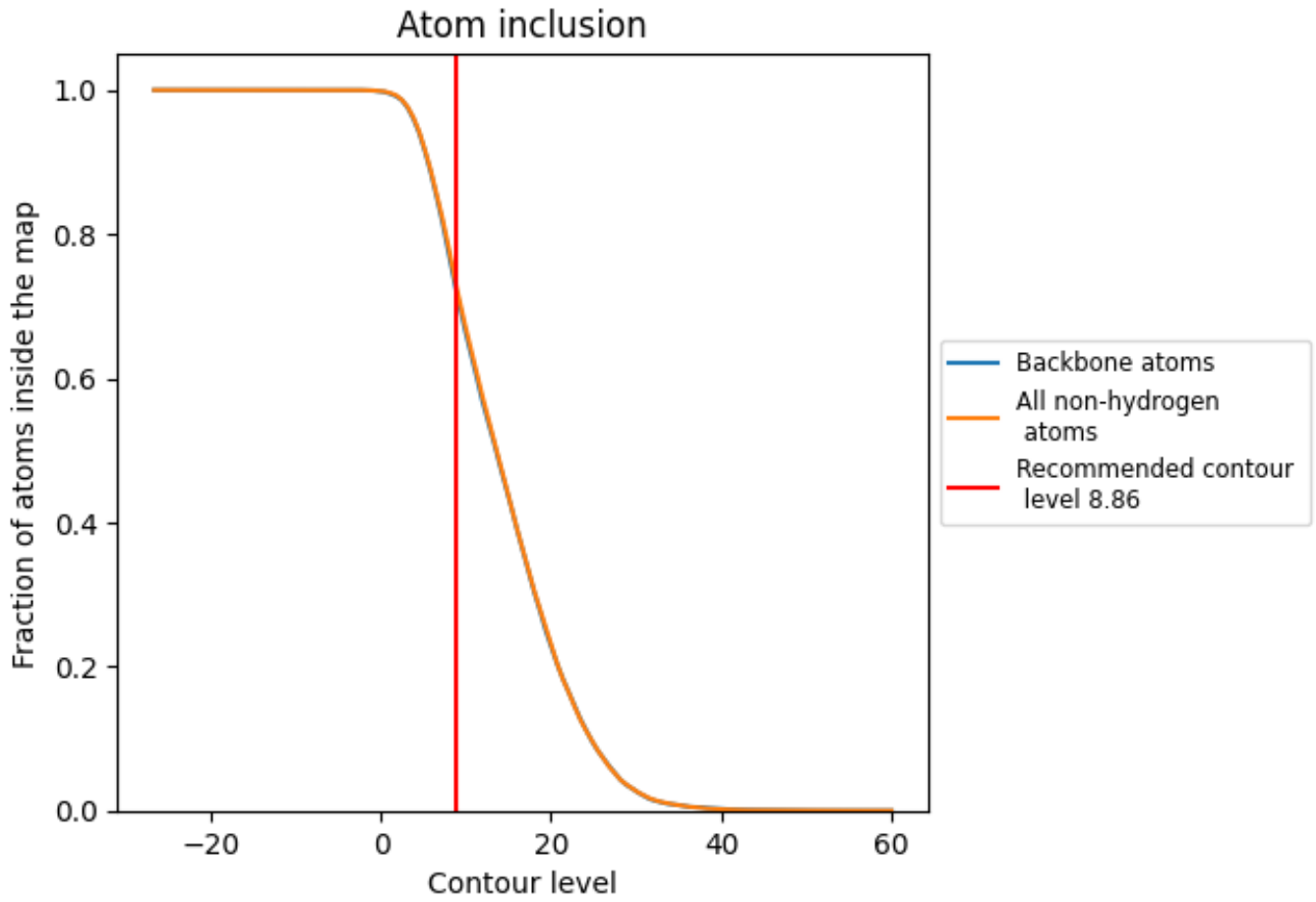
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (8.86).

9.4 Atom inclusion (i)



At the recommended contour level, 72% 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 (8.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7291	0.5290
8	0.8480	0.4980
A	0.7442	0.5810
B	0.7210	0.5750
C	0.7082	0.5640
D	0.7637	0.5840
E	0.7202	0.5730
F	0.7502	0.5840
G	0.7197	0.5460
H	0.8155	0.5340
I	0.7577	0.5290
J	0.5294	0.5320
K	0.8229	0.5020
L	0.8133	0.5020
M	0.8443	0.5060
N	0.8255	0.5030
O	0.8011	0.4990
P	0.8076	0.5030
Q	0.7786	0.4610
R	0.8199	0.4810
S	0.5695	0.5260
a	0.8223	0.4680
b	0.7182	0.4220
d	0.6109	0.3770
e	0.8692	0.3740
f	0.8100	0.4670
g	0.8479	0.3420
h	0.3698	0.3440
j	0.7635	0.4080
k	0.6157	0.3130