



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:37 AM UTC

PDB ID : 6ZQM / pdb_00006zqm
EMDB ID : EMD-11368
Title : bovine ATP synthase monomer state 2 (combined)
Authors : Spikes, T.E.; Montgomery, M.G.; Walker, J.E.
Deposited on : 2020-07-10
Resolution : 3.29 Å(reported)
Based on initial models : 2V7Q, 2CLY

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

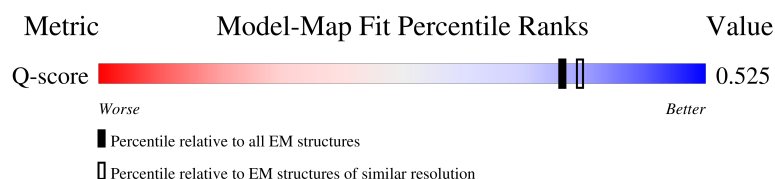
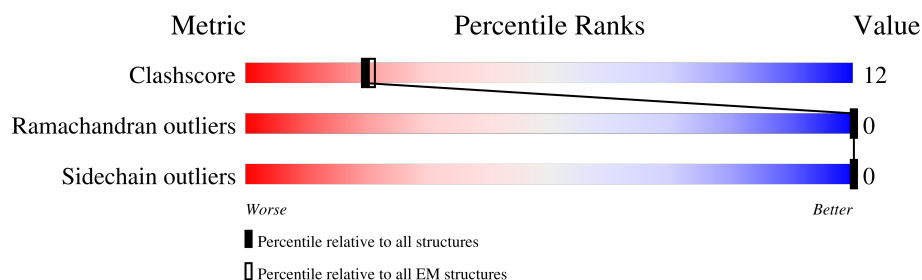
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.29 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	14466 (2.79 - 3.79)

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	510	 78% 17% 5%
1	B	510	 82% 15% 5%
1	C	510	 83% 15% 5%
2	D	482	 79% 18% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	482	
2	F	482	
3	G	273	
4	H	146	
5	I	50	
6	J	66	
7	K	75	
7	L	75	
7	M	75	
7	N	75	
7	O	75	
7	P	75	
7	Q	75	
7	R	75	
8	S	190	
9	8	66	
10	a	226	
11	d	160	
12	f	87	
13	g	102	
14	j	60	
15	b	214	
16	h	76	
17	k	57	
18	e	70	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 81155 atoms, of which 41153 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, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	486	Total	C	H	N	O	S	0	0
			7519	2338	3811	655	703	12		
1	B	495	Total	C	H	N	O	S	0	0
			7657	2377	3884	666	718	12		
1	C	501	Total	C	H	N	O	S	0	0
			7741	2402	3924	673	730	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	microheterogeneity	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	microheterogeneity	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	microheterogeneity	UNP P19483

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	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 7 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	L	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
7	M	74	Total	C	H	N	O	S	0	0
			1078	351	549	82	93	3		
7	N	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	O	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	P	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Q	74	Total	C	H	N	O	S	0	0
			1078	351	549	82	93	3		
7	R	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		

- Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

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

- Molecule 9 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	8	38	Total	C	H	N	O	S	0	0
			649	216	327	49	54	3		

- 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 subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	d	154	Total	C	H	N	O	S	0	0
			2534	817	1268	206	240	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	83	Total	C	H	N	O	S	0	0
			1411	456	718	120	114	3		

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

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

- Molecule 14 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

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

- Molecule 15 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	b	209	Total	C	H	N	O	S	0	0
			3457	1095	1756	292	308	6		

- 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		

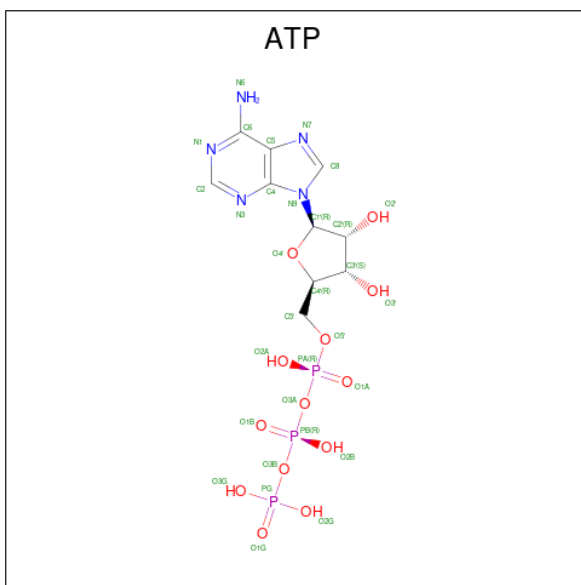
- Molecule 17 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	e	56	Total	C	H	N	O	S	0	0
			951	295	487	87	81	1		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

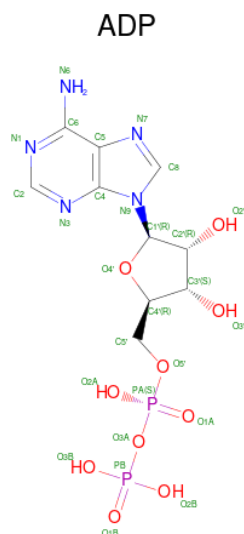


Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
19	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
19	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

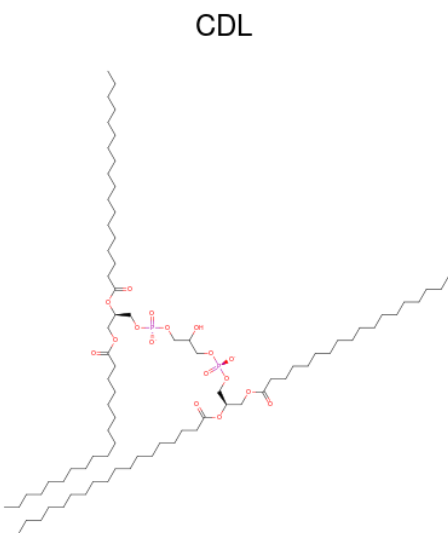
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	B	1	Total Mg 1 1	0
20	C	1	Total Mg 1 1	0
20	D	1	Total Mg 1 1	0
20	F	1	Total Mg 1 1	0

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



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

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



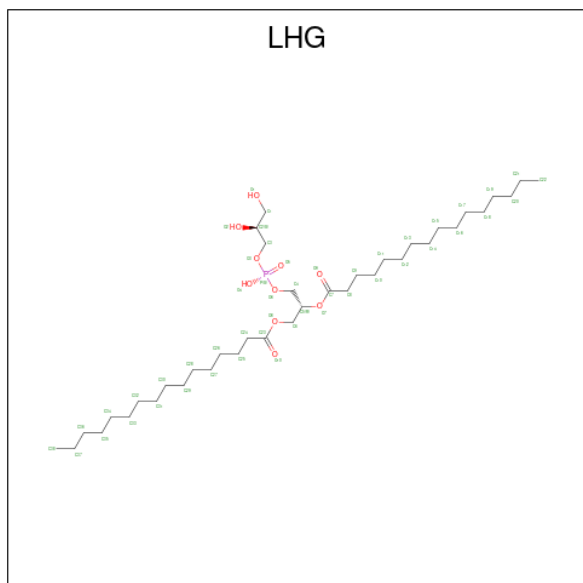
Mol	Chain	Residues	Atoms					AltConf
22	f	1	Total	C	H	O	P	0
			205	65	121	17	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	f	1	Total	C	H	O	P	0
			187	59	109	17	2	
22	b	1	Total	C	H	O	P	0
			202	64	119	17	2	

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



Mol	Chain	Residues	Atoms					AltConf
23	f	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	b	1	Total	C	H	O	P	0
			123	38	74	10	1	

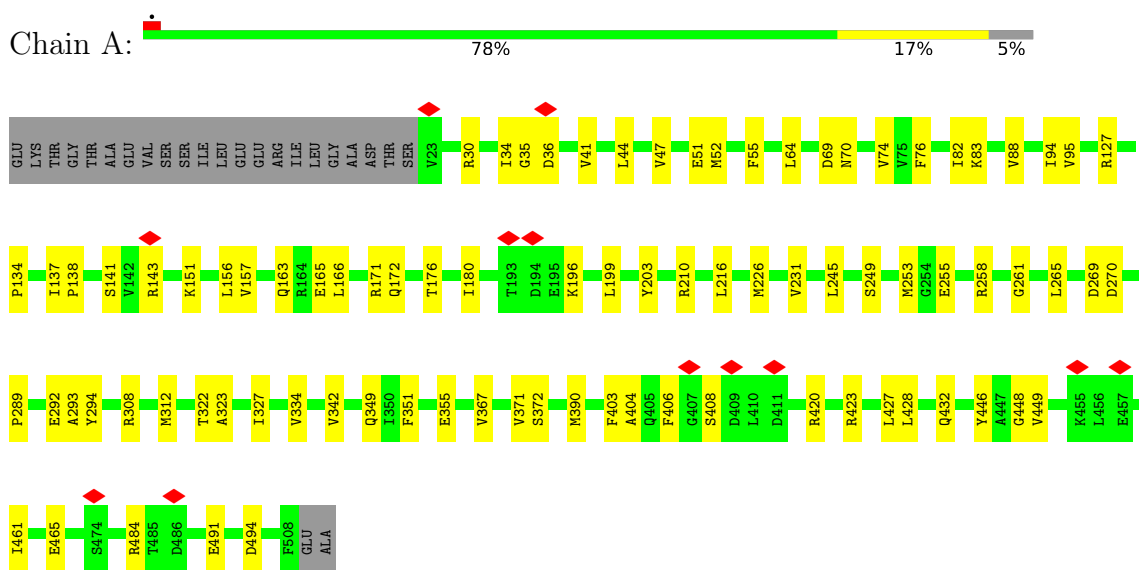
- Molecule 24 is water.

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	

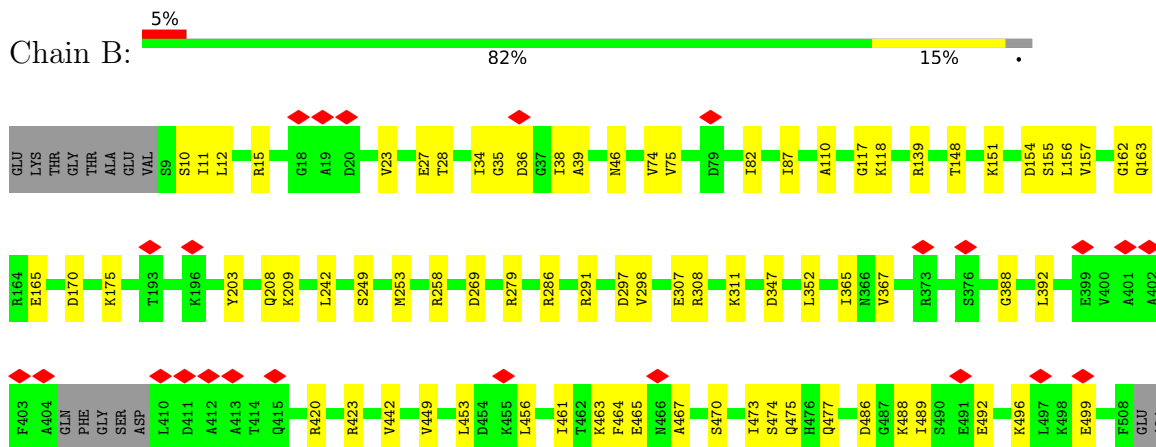
3 Residue-property plots

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.

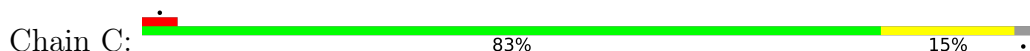
- Molecule 1: ATP synthase subunit alpha, mitochondrial

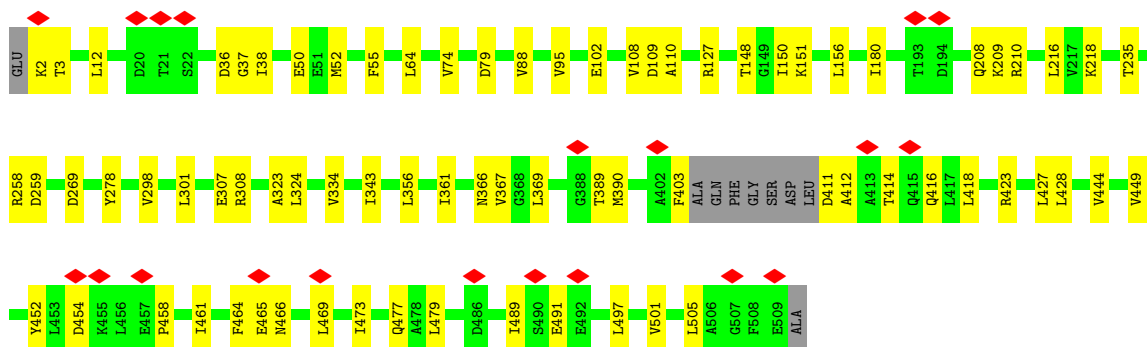


- Molecule 1: ATP synthase subunit alpha, mitochondrial

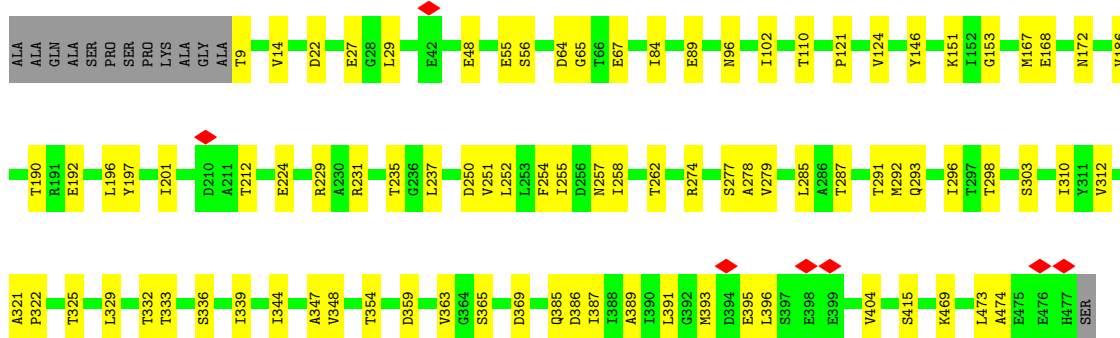
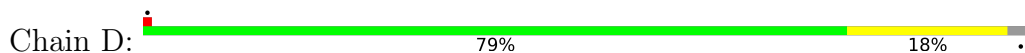


- Molecule 1: ATP synthase subunit alpha, mitochondrial

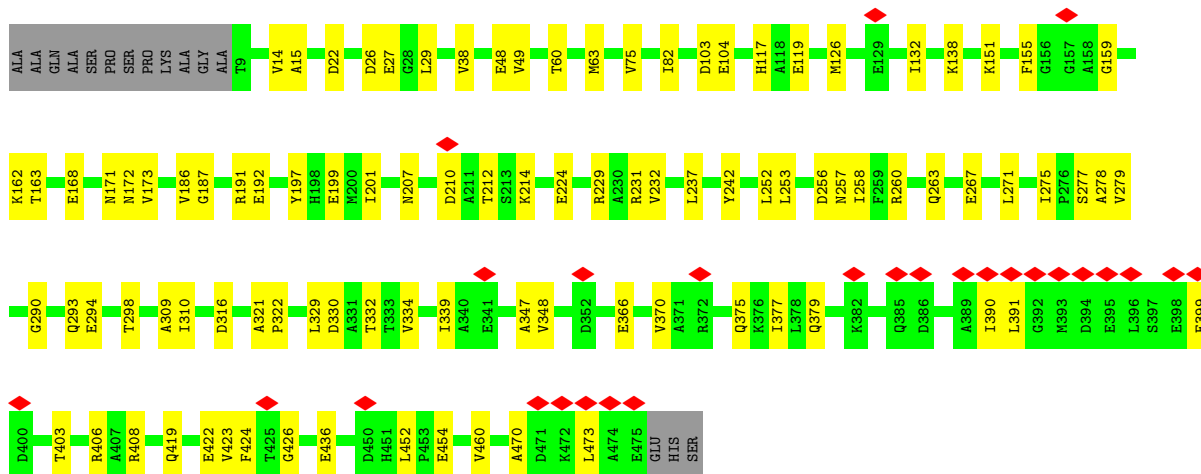
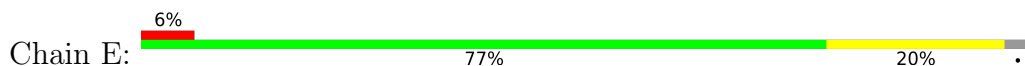




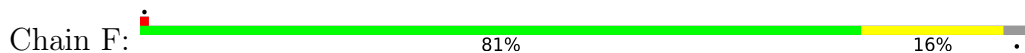
• Molecule 2: ATP synthase subunit beta, mitochondrial

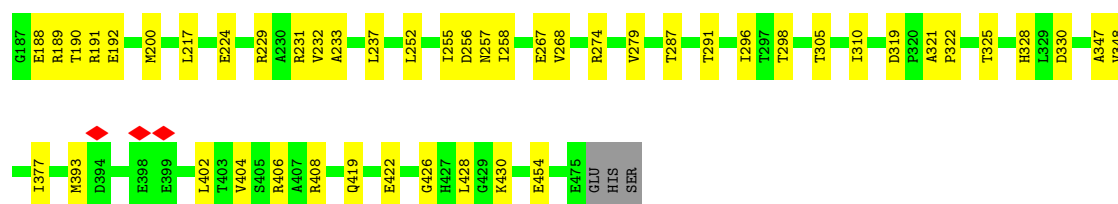


• Molecule 2: ATP synthase subunit beta, mitochondrial

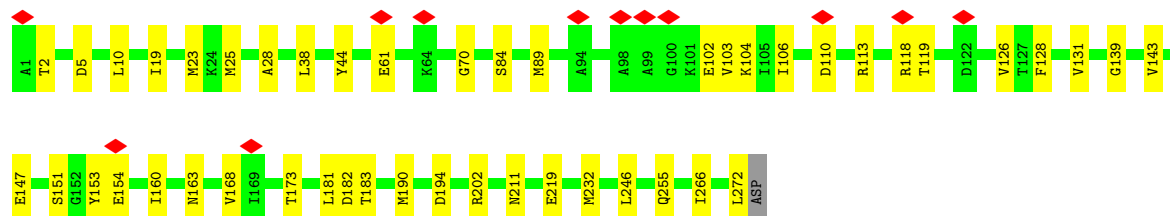
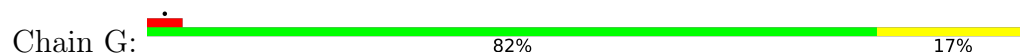


• Molecule 2: ATP synthase subunit beta, mitochondrial

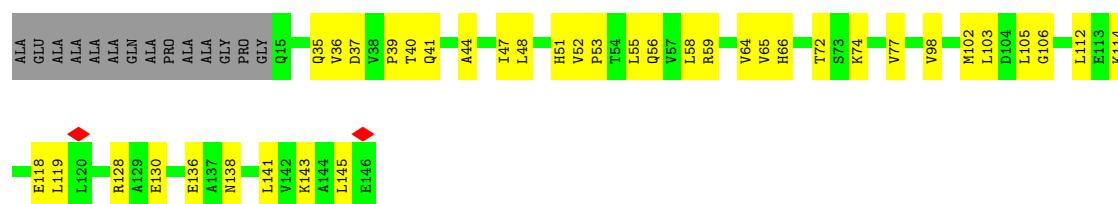




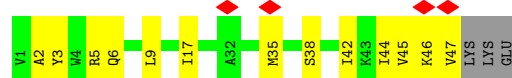
- Molecule 3: ATP synthase subunit gamma, mitochondrial



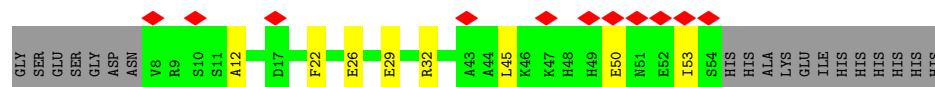
- Molecule 4: ATP synthase subunit delta, mitochondrial



- Molecule 5: ATP synthase subunit epsilon, mitochondrial



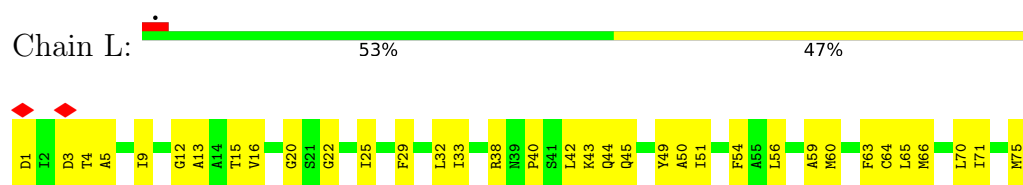
- Molecule 6: ATPase inhibitor, mitochondrial



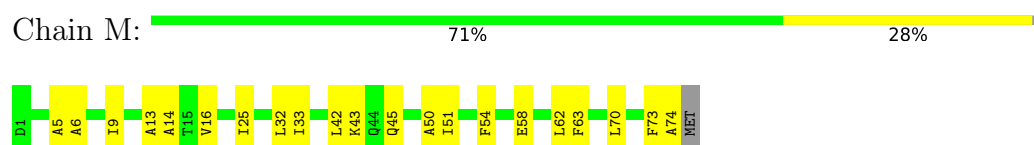
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



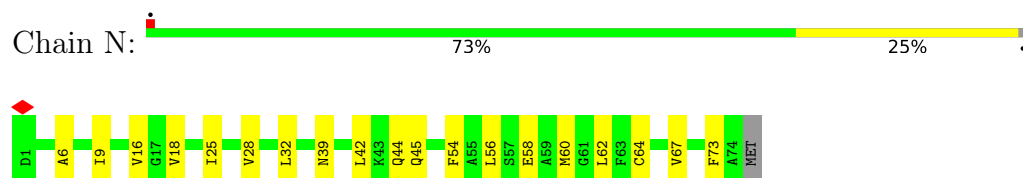
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



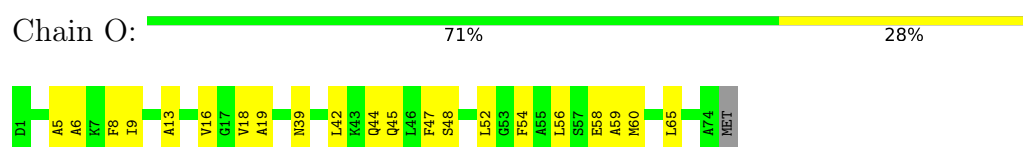
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



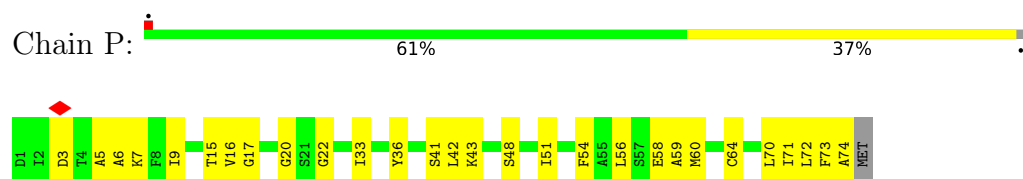
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



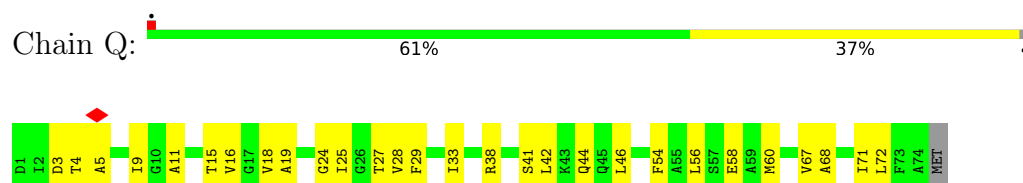
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



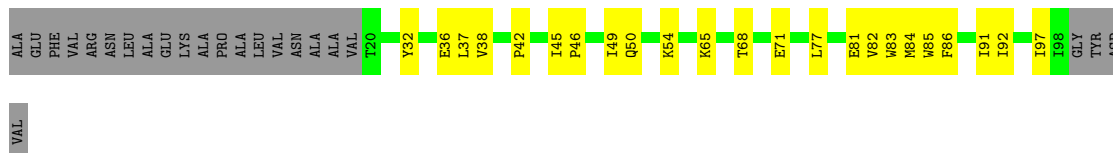
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial







- Molecule 13: ATP synthase subunit g, mitochondrial



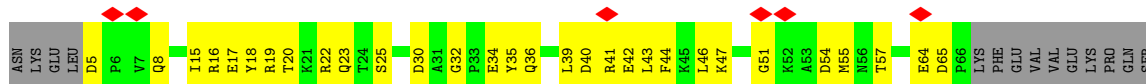
- Molecule 14: ATP synthase subunit ATP5MPL, mitochondrial



- Molecule 15: ATP synthase F(0) complex subunit B1, mitochondrial



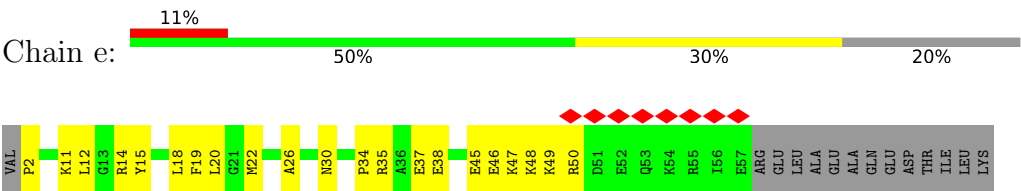
- Molecule 16: ATP synthase-coupling factor 6, mitochondrial



- Molecule 17: ATP synthase membrane subunit DAPIT, mitochondrial



- Molecule 18: ATP synthase subunit e, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90850	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 ($e^-/\text{\AA}^2$)	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	52.288	Depositor
Minimum map value	-26.711	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.097	Depositor
Recommended contour level	8.4	Depositor
Map size ($\text{\AA}$)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, M3L, MG, ADP, CDL, 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	0.41	0/3759	0.38	0/5071
1	B	0.39	0/3822	0.37	0/5155
1	C	0.40	0/3866	0.37	0/5214
2	D	0.41	0/3616	0.38	0/4906
2	E	0.38	0/3596	0.36	0/4879
2	F	0.42	0/3596	0.38	0/4879
3	G	0.37	0/2141	0.40	0/2876
4	H	0.41	0/991	0.42	0/1349
5	I	0.36	0/374	0.40	0/501
6	J	0.36	0/374	0.45	0/495
7	K	0.46	0/526	0.55	0/711
7	L	0.41	0/534	0.50	0/721
7	M	0.42	0/526	0.46	0/711
7	N	0.42	0/526	0.48	0/711
7	O	0.40	0/526	0.53	0/711
7	P	0.42	0/526	0.52	0/711
7	Q	0.46	0/526	0.58	0/711
7	R	0.47	0/526	0.53	1/711 (0.1%)
8	S	0.24	0/1464	0.36	0/1969
9	8	0.43	0/332	0.48	0/450
10	a	0.39	0/1779	0.44	0/2433
11	d	0.28	0/1297	0.47	0/1758
12	f	0.35	0/711	0.44	0/952
13	g	0.25	0/646	0.43	0/879
14	j	0.30	0/410	0.37	0/552
15	b	0.29	0/1733	0.47	0/2334
16	h	0.19	0/526	0.38	0/707
17	k	0.18	0/294	0.28	0/395
18	e	0.27	0/472	0.51	0/628
All	All	0.38	0/40015	0.41	1/54080 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	R	54	PHE	N-CA-C	5.06	117.19	111.02

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	A	3708	3811	3812	63	0
1	B	3773	3884	3885	55	0
1	C	3817	3924	3925	57	0
2	D	3558	3605	3605	72	0
2	E	3539	3593	3593	73	0
2	F	3539	3592	3592	59	0
3	G	2115	2185	2185	43	0
4	H	979	978	978	35	0
5	I	369	395	395	11	0
6	J	370	361	361	12	0
7	K	529	550	550	54	0
7	L	537	559	559	46	0
7	M	529	549	550	27	0
7	N	529	550	550	26	0
7	O	529	550	550	30	0
7	P	529	550	550	33	0
7	Q	529	549	549	43	0
7	R	529	550	550	36	0
8	S	1447	1557	1557	45	0
9	8	322	327	327	25	0
10	a	1741	1870	1870	98	0
11	d	1266	1268	1268	70	0
12	f	693	718	718	33	0
13	g	629	662	662	31	0
14	j	400	428	428	18	0
15	b	1701	1756	1755	109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	h	514	495	495	29	0
17	k	289	307	307	7	0
18	e	464	487	487	25	0
19	A	31	12	12	1	0
19	B	31	12	12	1	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	1	0
21	F	27	12	12	2	0
22	b	83	119	113	2	0
22	f	162	230	218	10	0
23	b	49	74	74	1	0
23	f	39	48	48	8	0
24	A	3	0	0	0	0
24	B	3	0	0	2	0
24	C	3	0	0	0	0
24	D	4	0	0	2	0
24	F	4	0	0	4	0
All	All	40002	41153	41138	1013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1013) 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)
4:H:136:GLU:OE2	5:I:3:TYR:OH	1.79	1.00
7:K:56:LEU:HD21	7:R:54:PHE:CE1	2.02	0.95
2:E:390:ILE:HD11	3:G:25:MET:HE1	1.47	0.94
7:K:9:ILE:HG23	7:R:9:ILE:HD13	1.48	0.92
11:d:101:ALA:O	11:d:105:THR:HG22	1.69	0.92
13:g:38:VAL:O	18:e:11:LYS:NZ	2.00	0.92
7:K:1:ASP:N	7:L:3:ASP:OD2	2.06	0.89
11:d:37:LEU:HD23	15:b:134:MET:HE2	1.55	0.88
15:b:169:GLU:OE2	16:h:35:TYR:OH	1.91	0.88
1:A:83:LYS:NZ	2:D:29:LEU:O	2.07	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLU:OE1	2:F:190:THR:OG1	1.94	0.86
12:f:47:LYS:NZ	22:f:102:CDL:OA2	2.09	0.86
10:a:171:ILE:HD11	10:a:203:GLU:HG3	1.58	0.85
2:F:192:GLU:OE1	24:F:701:HOH:O	1.94	0.84
12:f:43:ARG:NH1	23:f:103:LHG:O2	2.10	0.84
22:b:301:CDL:O1	22:b:301:CDL:OA4	1.95	0.83
7:L:1:ASP:OD2	7:L:4:THR:N	2.12	0.83
12:f:13:GLU:N	12:f:13:GLU:OE1	2.13	0.82
8:S:69:LEU:HD12	8:S:86:ILE:HG21	1.61	0.82
1:B:420:ARG:NH1	1:B:449:VAL:O	2.12	0.82
1:A:390:MET:HE1	1:A:428:LEU:HD21	1.60	0.81
13:g:84:MET:HE1	15:b:40:GLY:C	2.05	0.81
1:C:209:LYS:NZ	2:F:330:ASP:OD1	2.13	0.81
12:f:78:LEU:HD21	15:b:52:VAL:HG22	1.63	0.81
2:F:188:GLU:OE2	24:F:701:HOH:O	1.96	0.81
2:E:390:ILE:HD11	3:G:25:MET:CE	2.11	0.80
7:K:9:ILE:HD13	7:L:9:ILE:HG23	1.61	0.80
1:C:258:ARG:NH1	1:C:308:ARG:O	2.14	0.80
22:f:101:CDL:OB3	22:f:101:CDL:O1	1.99	0.79
2:D:192:GLU:OE1	24:D:701:HOH:O	1.99	0.79
15:b:190:GLU:OE1	15:b:190:GLU:N	2.16	0.79
1:B:27:GLU:OE2	1:B:46:ASN:ND2	2.17	0.78
1:B:209:LYS:NZ	2:E:330:ASP:OD1	2.16	0.78
2:E:191:ARG:NH2	2:E:192:GLU:OE2	2.17	0.77
4:H:44:ALA:O	7:Q:38:ARG:NH2	2.17	0.77
12:f:8:GLU:N	12:f:8:GLU:OE1	2.18	0.77
8:S:173:MET:HE1	15:b:201:LEU:HD22	1.67	0.77
11:d:46:GLU:N	11:d:46:GLU:OE1	2.16	0.77
12:f:52:LYS:HG2	15:b:5:LEU:HD23	1.66	0.76
7:N:42:LEU:O	7:N:44:GLN:N	2.19	0.76
22:f:102:CDL:OA3	22:f:102:CDL:O1	2.01	0.76
8:S:76:GLU:OE1	8:S:76:GLU:N	2.19	0.75
15:b:143:ARG:NH2	16:h:64:GLU:O	2.20	0.75
4:H:39:PRO:O	4:H:40:THR:OG1	2.03	0.75
2:F:48:GLU:OE1	2:F:231:ARG:NE	2.19	0.74
1:C:36:ASP:OD1	2:F:274:ARG:NE	2.20	0.74
14:j:23:GLU:OE1	14:j:23:GLU:N	2.21	0.74
8:S:116:VAL:HG11	8:S:142:LEU:HD22	1.69	0.73
8:S:186:MET:HE1	15:b:174:ILE:HD12	1.69	0.73
2:E:171:ASN:OD1	2:E:214:LYS:NZ	2.21	0.73
2:E:173:VAL:HG11	2:E:252:LEU:HD23	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:54:PHE:CE1	7:L:56:LEU:HD13	2.23	0.73
8:S:33:GLU:N	8:S:33:GLU:OE1	2.21	0.73
9:8:1:MET:HE1	10:a:6:PHE:CE2	2.24	0.73
2:D:151:LYS:NZ	2:D:293:GLN:O	2.22	0.73
7:K:25:ILE:HD12	7:K:54:PHE:CD1	2.24	0.72
12:f:18:GLU:O	12:f:21:SER:OG	2.06	0.72
11:d:40:ARG:CZ	15:b:138:VAL:HG12	2.19	0.72
12:f:75:TYR:O	12:f:79:LYS:N	2.23	0.72
1:B:139:ARG:NH2	1:B:307:GLU:O	2.23	0.72
7:L:9:ILE:HD13	7:M:9:ILE:HG22	1.71	0.72
9:8:3:GLN:HB3	10:a:98:LEU:HD12	1.72	0.72
2:F:279:VAL:HG12	2:F:279:VAL:O	1.90	0.71
12:f:43:ARG:NH2	22:f:102:CDL:OA3	2.22	0.71
7:L:65:LEU:HD21	7:M:63:PHE:CE2	2.25	0.71
2:E:186:VAL:HG22	2:E:232:VAL:HG13	1.73	0.71
10:a:73:MET:HE3	10:a:73:MET:HA	1.73	0.71
11:d:46:GLU:O	15:b:141:ARG:NE	2.23	0.71
1:A:52:MET:HE2	1:A:95:VAL:HG22	1.73	0.71
1:B:279:ARG:NH1	2:E:277:SER:OG	2.23	0.71
22:f:102:CDL:O1	23:f:103:LHG:O4	2.09	0.70
1:B:151:LYS:NZ	1:B:465:GLU:OE1	2.24	0.70
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.71	0.70
9:8:21:PHE:O	14:j:17:TYR:OH	2.09	0.70
10:a:2:ASN:OD1	10:a:3:GLU:N	2.25	0.70
1:A:420:ARG:NH1	1:A:449:VAL:O	2.25	0.70
7:M:54:PHE:CZ	7:N:56:LEU:HD22	2.27	0.70
17:k:43:TYR:O	17:k:47:ARG:NH1	2.25	0.70
7:Q:25:ILE:HD12	7:Q:54:PHE:CE1	2.26	0.70
1:B:163:GLN:NE2	1:B:165:GLU:OE1	2.25	0.69
10:a:106:ILE:HG12	14:j:31:MET:HE1	1.74	0.69
11:d:56:TYR:CE2	15:b:155:LEU:HD13	2.27	0.69
8:S:22:LEU:HD22	8:S:85:LEU:HD22	1.73	0.69
2:F:287:THR:O	2:F:291:THR:HG23	1.92	0.69
3:G:61:GLU:OE1	3:G:61:GLU:N	2.25	0.69
2:D:391:LEU:HD23	2:D:395:GLU:CG	2.23	0.69
1:A:334:VAL:HG11	1:A:351:PHE:HE1	1.56	0.69
10:a:184:ILE:HG22	10:a:185:SER:H	1.57	0.69
1:A:258:ARG:NH1	1:A:308:ARG:O	2.25	0.69
1:C:218:LYS:HD3	2:F:128:VAL:HG21	1.75	0.68
17:k:19:ASN:OD1	17:k:21:TYR:N	2.26	0.68
8:S:39:LEU:HD22	8:S:102:ILE:HG22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:39:ARG:NH2	23:f:103:LHG:O1	2.25	0.68
7:L:45:GLN:OE1	7:L:45:GLN:N	2.27	0.68
2:D:287:THR:O	2:D:291:THR:HG23	1.94	0.68
3:G:194:ASP:OD1	7:L:38:ARG:NH1	2.27	0.68
2:D:391:LEU:HD23	2:D:395:GLU:HG3	1.76	0.67
2:E:399:GLU:O	2:E:403:THR:HG23	1.94	0.67
3:G:182:ASP:OD1	3:G:183:THR:N	2.27	0.67
7:L:42:LEU:O	7:L:44:GLN:N	2.27	0.67
7:O:45:GLN:N	7:O:45:GLN:OE1	2.28	0.67
8:S:122:THR:HG22	8:S:162:MET:HB3	1.76	0.67
1:C:52:MET:HE3	1:C:95:VAL:HG23	1.76	0.67
9:8:8:THR:O	9:8:11:THR:HG22	1.94	0.67
3:G:190:MET:HE2	3:G:190:MET:HA	1.76	0.67
1:B:23:VAL:HG21	8:S:173:MET:HE2	1.77	0.67
7:L:13:ALA:O	7:L:16:VAL:HG12	1.95	0.66
16:h:22:ARG:O	16:h:22:ARG:NE	2.27	0.66
1:C:491:GLU:OE1	1:C:491:GLU:N	2.27	0.66
11:d:29:SER:O	11:d:32:SER:OG	2.13	0.66
1:A:30:ARG:O	8:S:59:TYR:OH	2.14	0.66
8:S:69:LEU:HD12	8:S:86:ILE:CG2	2.25	0.66
15:b:137:GLU:O	15:b:140:TYR:HB2	1.95	0.66
1:A:36:ASP:OD2	2:D:274:ARG:NH2	2.29	0.65
2:F:237:LEU:HD11	2:F:296:ILE:HD11	1.77	0.65
13:g:45:ILE:HG22	13:g:49:ILE:HD11	1.76	0.65
13:g:85:TRP:HE3	18:e:18:LEU:HD21	1.61	0.65
1:A:491:GLU:OE1	1:A:491:GLU:N	2.28	0.65
1:C:109:ASP:OD1	1:C:110:ALA:N	2.30	0.65
7:L:25:ILE:HD12	7:L:54:PHE:HE1	1.61	0.65
1:B:291:ARG:NH1	2:F:319:ASP:OD1	2.29	0.65
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.79	0.65
13:g:92:ILE:CG2	18:e:22:MET:HE1	2.27	0.65
4:H:138:ASN:HA	4:H:141:LEU:HD12	1.78	0.65
12:f:78:LEU:HD21	15:b:52:VAL:CG2	2.27	0.65
1:B:170:ASP:O	1:B:175:LYS:NZ	2.29	0.65
19:B:600:ATP:O3G	24:B:701:HOH:O	2.15	0.65
2:D:389:ALA:HB2	6:J:26:GLU:OE2	1.96	0.65
8:S:22:LEU:HD21	8:S:39:LEU:HD11	1.79	0.64
15:b:177:VAL:O	15:b:181:VAL:HG13	1.97	0.64
2:D:192:GLU:OE2	24:D:702:HOH:O	2.13	0.64
12:f:61:MET:HE1	15:b:16:LEU:C	2.22	0.64
10:a:67:THR:HG22	14:j:21:TYR:OH	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:31:LYS:O	11:d:35:GLU:OE1	2.15	0.64
7:M:25:ILE:HD12	7:M:54:PHE:CD1	2.33	0.64
2:D:48:GLU:OE2	2:D:231:ARG:NE	2.30	0.64
1:A:427:LEU:HD11	1:A:448:GLY:HA3	1.79	0.63
10:a:209:ILE:O	10:a:213:VAL:HG23	1.98	0.63
8:S:186:MET:HE1	15:b:174:ILE:CD1	2.27	0.63
9:8:15:SER:OG	10:a:21:THR:OG1	2.06	0.63
10:a:216:LEU:O	10:a:220:LEU:HD23	1.98	0.63
4:H:55:LEU:O	4:H:56:GLN:NE2	2.32	0.63
7:Q:54:PHE:CE1	7:R:56:LEU:HD21	2.34	0.62
10:a:53:VAL:CG1	10:a:73:MET:HE1	2.29	0.62
7:L:16:VAL:HG23	7:M:16:VAL:HG13	1.80	0.62
7:O:16:VAL:HG23	7:P:16:VAL:HG13	1.81	0.62
4:H:102:MET:C	4:H:103:LEU:HD12	2.25	0.62
1:A:141:SER:OG	1:A:143:ARG:NH1	2.33	0.62
1:B:12:LEU:HD11	15:b:170:GLN:OE1	2.00	0.62
1:C:416:GLN:NE2	1:C:454:ASP:OD1	2.32	0.62
2:D:391:LEU:CD1	3:G:23:MET:HE1	2.30	0.62
7:L:32:LEU:HD12	7:L:50:ALA:CB	2.30	0.62
7:Q:25:ILE:HD12	7:Q:54:PHE:CD1	2.35	0.62
7:O:13:ALA:O	7:O:16:VAL:HG12	2.00	0.62
13:g:91:ILE:HD11	15:b:47:SER:HB2	1.82	0.62
1:A:165:GLU:OE2	1:A:349:GLN:N	2.33	0.62
7:O:16:VAL:CG2	7:P:16:VAL:HG13	2.30	0.61
15:b:157:TYR:OH	16:h:54:ASP:O	2.14	0.61
2:D:298:THR:HG23	2:D:303:SER:HA	1.80	0.61
2:F:186:VAL:HG23	2:F:232:VAL:CG1	2.30	0.61
4:H:35:GLN:NE2	7:Q:41:SER:OG	2.30	0.61
10:a:129:LEU:HD21	17:k:26:ARG:HB3	1.82	0.61
7:K:21:SER:OG	7:L:60:MET:HE1	2.00	0.61
7:K:55:ALA:HB2	10:a:213:VAL:HG21	1.81	0.61
10:a:159:ARG:O	10:a:163:ASN:ND2	2.32	0.61
7:K:55:ALA:CB	10:a:213:VAL:HG11	2.30	0.61
2:D:197:TYR:CZ	2:D:201:ILE:HD11	2.36	0.61
10:a:161:THR:O	10:a:165:THR:HG22	1.99	0.61
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.82	0.61
1:C:366:ASN:HD21	1:C:369:LEU:HD22	1.66	0.60
7:Q:11:ALA:HB2	7:Q:72:LEU:HD13	1.83	0.60
11:d:83:ASP:OD1	11:d:84:LYS:N	2.34	0.60
2:E:224:GLU:O	2:E:229:ARG:NH1	2.34	0.60
10:a:68:TRP:CD1	14:j:21:TYR:HH	2.18	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:131:GLN:NE2	17:k:21:TYR:O	2.33	0.60
13:g:81:GLU:OE2	15:b:37:LEU:N	2.34	0.60
21:F:600:ADP:O3A	24:F:702:HOH:O	2.16	0.60
9:8:28:VAL:HG23	10:a:70:LEU:HD11	1.82	0.60
1:A:166:LEU:HD11	1:A:327:ILE:CG1	2.32	0.60
2:E:275:ILE:HG23	3:G:266:ILE:HD12	1.84	0.60
7:K:16:VAL:HG13	7:R:16:VAL:CG2	2.31	0.60
2:D:277:SER:OG	2:D:278:ALA:N	2.35	0.60
2:F:255:ILE:HG21	2:F:258:ILE:HD13	1.83	0.60
7:Q:3:ASP:OD1	7:Q:4:THR:N	2.32	0.60
11:d:37:LEU:CD2	15:b:134:MET:HE2	2.30	0.60
13:g:91:ILE:HD11	15:b:47:SER:CB	2.31	0.60
4:H:35:GLN:NE2	4:H:37:ASP:OD2	2.34	0.60
4:H:130:GLU:OE1	5:I:9:LEU:HD11	2.00	0.60
10:a:57:MET:HE2	10:a:212:TYR:HE1	1.65	0.60
10:a:86:GLY:O	10:a:91:SER:OG	2.19	0.60
10:a:96:THR:O	10:a:161:THR:HG23	2.02	0.60
16:h:17:GLU:O	16:h:20:THR:OG1	2.20	0.60
15:b:32:THR:O	15:b:36:VAL:HG23	2.03	0.59
10:a:55:LYS:NZ	11:d:157:ILE:O	2.26	0.59
15:b:42:ILE:O	15:b:46:LEU:HD23	2.02	0.59
16:h:35:TYR:CE2	16:h:39:LEU:HD11	2.37	0.59
2:E:408:ARG:NE	2:E:454:GLU:OE2	2.35	0.59
7:M:32:LEU:HD12	7:M:50:ALA:HB2	1.85	0.59
9:8:6:THR:HG23	14:j:39:ARG:NH2	2.17	0.59
10:a:101:ASN:OD1	10:a:161:THR:OG1	2.15	0.59
18:e:34:PRO:O	18:e:38:GLU:OE1	2.20	0.59
1:C:473:ILE:O	1:C:477:GLN:NE2	2.35	0.59
2:D:167:MET:SD	2:D:196:LEU:HD13	2.43	0.59
11:d:15:PHE:O	11:d:18:ILE:HG22	2.03	0.59
1:B:208:GLN:NE2	24:B:702:HOH:O	2.32	0.59
1:B:453:LEU:HD22	1:B:461:ILE:HD13	1.85	0.59
7:K:16:VAL:HG13	7:R:16:VAL:HG23	1.85	0.59
7:M:54:PHE:CE1	7:N:56:LEU:HD22	2.38	0.59
2:E:390:ILE:HG22	2:E:391:LEU:HD12	1.83	0.59
10:a:15:LEU:O	10:a:17:LEU:N	2.35	0.59
1:A:127:ARG:NH2	1:A:255:GLU:OE1	2.36	0.59
1:A:163:GLN:NE2	1:A:165:GLU:OE1	2.35	0.59
9:8:1:MET:HA	9:8:1:MET:HE2	1.84	0.59
9:8:24:PHE:O	9:8:28:VAL:HG22	2.03	0.59
11:d:37:LEU:HD23	15:b:134:MET:CE	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:93:LEU:O	15:b:96:VAL:HG12	2.03	0.58
7:K:42:LEU:HD12	7:K:42:LEU:O	2.02	0.58
1:A:166:LEU:HD11	1:A:327:ILE:HG12	1.85	0.58
7:O:42:LEU:O	7:O:44:GLN:N	2.36	0.58
1:B:148:THR:OG1	1:B:154:ASP:OD1	2.20	0.58
1:C:12:LEU:HD22	8:S:88:LEU:HD21	1.84	0.58
7:P:71:ILE:HG22	7:P:71:ILE:O	2.03	0.58
1:B:11:ILE:HG13	1:B:12:LEU:HD12	1.84	0.58
2:F:428:LEU:O	2:F:430:LYS:NZ	2.36	0.58
11:d:38:THR:HA	15:b:134:MET:HE1	1.85	0.58
2:D:474:ALA:HB2	6:J:45:LEU:HD23	1.84	0.58
7:L:43:M3L:HM23	7:M:45:GLN:NE2	2.18	0.58
8:S:22:LEU:CD2	8:S:39:LEU:HD11	2.34	0.58
2:E:197:TYR:CZ	2:E:201:ILE:HD11	2.39	0.58
7:P:16:VAL:HG23	7:Q:16:VAL:HG13	1.86	0.58
11:d:157:ILE:H	11:d:157:ILE:HD12	1.68	0.58
1:B:203:TYR:OH	1:B:269:ASP:OD2	2.18	0.58
1:B:347:ASP:OD1	2:F:191:ARG:NE	2.36	0.58
2:E:310:ILE:CD1	2:E:329:LEU:HD21	2.34	0.58
1:C:366:ASN:ND2	1:C:369:LEU:HD22	2.19	0.58
1:A:69:ASP:OD1	1:A:70:ASN:ND2	2.37	0.57
2:E:132:ILE:HG23	2:E:132:ILE:O	2.04	0.57
3:G:84:SER:HB3	3:G:173:THR:HG21	1.85	0.57
7:K:10:GLY:HA2	7:R:9:ILE:HD12	1.86	0.57
7:O:39:ASN:OD1	7:O:42:LEU:HD12	2.04	0.57
7:L:32:LEU:HD12	7:L:50:ALA:HB2	1.85	0.57
15:b:26:TYR:OH	18:e:2:PRO:O	2.16	0.57
10:a:184:ILE:HG22	10:a:185:SER:N	2.18	0.57
11:d:113:GLU:O	11:d:116:LYS:HG2	2.04	0.57
15:b:81:PHE:CE1	15:b:85:LEU:HD11	2.39	0.57
1:C:37:GLY:N	1:C:79:ASP:OD2	2.36	0.57
4:H:103:LEU:HB3	4:H:145:LEU:HD11	1.85	0.57
1:C:64:LEU:HD12	1:C:74:VAL:HG11	1.86	0.57
2:E:298:THR:HG23	2:E:298:THR:O	2.03	0.57
7:K:9:ILE:HD13	7:L:9:ILE:CG2	2.34	0.57
7:O:58:GLU:CD	7:P:60:MET:HE1	2.29	0.57
15:b:182:VAL:O	15:b:185:ILE:HG22	2.04	0.57
1:C:452:TYR:CD2	1:C:501:VAL:HG11	2.39	0.57
2:D:168:GLU:OE2	2:D:172:ASN:ND2	2.38	0.57
2:E:210:ASP:OD1	2:E:212:THR:HG22	2.04	0.57
15:b:197:CYS:O	15:b:201:LEU:HD23	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:HG13	1:B:157:VAL:O	2.05	0.57
1:B:492:GLU:OE1	1:B:492:GLU:N	2.33	0.57
13:g:46:PRO:O	13:g:50:GLN:OE1	2.23	0.57
7:M:5:ALA:HB1	7:N:6:ALA:HB2	1.87	0.57
7:Q:9:ILE:CD1	7:R:9:ILE:HG23	2.34	0.57
8:S:22:LEU:HD22	8:S:85:LEU:CD2	2.34	0.57
2:F:170:ILE:HD11	2:F:183:PHE:CE1	2.40	0.57
7:N:18:VAL:O	7:N:18:VAL:HG22	2.04	0.57
8:S:116:VAL:HG13	8:S:116:VAL:O	2.04	0.57
8:S:178:LYS:O	8:S:182:LEU:HD23	2.05	0.57
10:a:30:LEU:HD22	12:f:59:LEU:HD11	1.86	0.57
12:f:43:ARG:NH2	23:f:103:LHG:O4	2.38	0.57
13:g:77:LEU:HD21	15:b:37:LEU:CD1	2.34	0.57
2:D:250:ASP:OD1	2:D:251:VAL:N	2.38	0.56
2:E:159:GLY:N	21:E:600:ADP:O1B	2.35	0.56
2:F:224:GLU:O	2:F:229:ARG:NH1	2.37	0.56
7:K:22:GLY:N	7:L:60:MET:HE3	2.20	0.56
7:K:25:ILE:HD12	7:K:54:PHE:CE1	2.40	0.56
8:S:34:GLN:O	8:S:38:GLU:OE1	2.22	0.56
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.86	0.56
2:D:389:ALA:HA	6:J:26:GLU:OE1	2.04	0.56
4:H:66:HIS:HD2	4:H:72:THR:HG22	1.70	0.56
7:P:70:LEU:O	7:P:74:ALA:N	2.34	0.56
9:8:38:GLU:N	9:8:38:GLU:OE1	2.36	0.56
2:F:393:MET:HE3	2:F:404:VAL:HG11	1.87	0.56
11:d:44:LEU:O	11:d:44:LEU:HD12	2.05	0.56
7:K:55:ALA:CB	10:a:213:VAL:HG21	2.35	0.56
7:L:9:ILE:CD1	7:M:9:ILE:HG22	2.36	0.56
7:K:54:PHE:CZ	7:L:56:LEU:HD13	2.39	0.56
1:C:102:GLU:OE1	1:C:102:GLU:N	2.36	0.56
4:H:98:VAL:HG21	4:H:103:LEU:HD11	1.86	0.56
7:Q:58:GLU:OE2	7:R:60:MET:HE1	2.06	0.56
15:b:83:ASP:O	15:b:87:GLU:OE1	2.24	0.56
1:C:411:ASP:OD2	1:C:412:ALA:N	2.34	0.56
7:L:38:ARG:O	7:L:38:ARG:NH2	2.37	0.56
7:P:72:LEU:HD23	7:P:73:PHE:CZ	2.40	0.56
16:h:34:GLU:OE1	16:h:34:GLU:N	2.35	0.56
7:Q:25:ILE:HD11	7:R:56:LEU:HD23	1.87	0.55
10:a:75:LEU:HD11	10:a:79:ILE:HD11	1.87	0.55
10:a:20:VAL:HG22	10:a:24:VAL:HG23	1.88	0.55
7:K:60:MET:HE1	7:R:58:GLU:OE1	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HD12	1:C:74:VAL:CG1	2.36	0.55
2:E:155:PHE:CE1	2:E:332:THR:HG23	2.42	0.55
15:b:83:ASP:O	15:b:86:ASN:N	2.40	0.55
15:b:87:GLU:HA	15:b:90:ILE:HG22	1.88	0.55
16:h:36:GLN:N	16:h:36:GLN:OE1	2.40	0.55
1:C:307:GLU:OE2	2:D:190:THR:OG1	2.18	0.55
7:Q:5:ALA:HB1	7:R:6:ALA:HB2	1.89	0.55
10:a:53:VAL:HG12	10:a:73:MET:HE1	1.87	0.55
1:A:371:VAL:HG22	1:A:372:SER:N	2.22	0.55
9:8:26:LEU:O	9:8:29:SER:N	2.40	0.55
12:f:61:MET:HE1	15:b:16:LEU:CA	2.37	0.55
13:g:85:TRP:CZ3	18:e:14:ARG:HD3	2.42	0.55
1:A:334:VAL:HG11	1:A:351:PHE:CE1	2.40	0.55
9:8:6:THR:HG23	14:j:39:ARG:HH21	1.71	0.55
16:h:47:LYS:O	16:h:51:GLY:N	2.35	0.55
2:E:275:ILE:HG23	3:G:266:ILE:CD1	2.36	0.55
7:K:47:PHE:HE1	7:L:49:TYR:HH	1.53	0.55
8:S:116:VAL:HG11	8:S:142:LEU:CD2	2.36	0.55
2:D:329:LEU:HD12	2:D:332:THR:HG22	1.89	0.54
10:a:38:VAL:HG13	10:a:38:VAL:O	2.06	0.54
1:C:356:LEU:CD1	1:C:361:ILE:HD13	2.37	0.54
2:D:279:VAL:HG12	2:D:279:VAL:O	2.07	0.54
2:D:336:SER:HB3	2:D:339:ILE:HD13	1.89	0.54
2:F:9:THR:HG22	2:F:27:GLU:HG3	1.88	0.54
2:F:255:ILE:HG21	2:F:258:ILE:CD1	2.37	0.54
7:Q:16:VAL:HG23	7:R:16:VAL:HG13	1.88	0.54
2:D:252:LEU:HD23	2:D:254:PHE:CZ	2.43	0.54
13:g:91:ILE:HD11	15:b:47:SER:OG	2.08	0.54
2:F:422:GLU:O	2:F:426:GLY:N	2.38	0.54
1:A:41:VAL:HG11	1:A:44:LEU:HD12	1.88	0.54
1:B:442:VAL:CG1	1:B:489:ILE:HD11	2.37	0.54
1:A:406:PHE:O	1:A:408:SER:N	2.40	0.54
4:H:64:VAL:HG22	4:H:74:LYS:HG2	1.90	0.54
11:d:80:ILE:HG22	15:b:140:TYR:OH	2.08	0.54
7:Q:58:GLU:OE2	7:R:60:MET:CE	2.56	0.54
2:F:95:MET:HE2	2:F:99:GLY:HA2	1.89	0.54
7:K:72:LEU:O	7:K:72:LEU:HD23	2.08	0.54
9:8:37:PRO:HB2	15:b:96:VAL:HG21	1.90	0.54
1:A:199:LEU:HD21	1:A:265:LEU:HB3	1.90	0.54
12:f:44:TYR:N	22:f:102:CDL:OA9	2.41	0.54
1:B:156:LEU:CD1	1:B:367:VAL:HG11	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ALA:O	1:C:324:LEU:HD12	2.08	0.53
7:M:58:GLU:OE1	7:M:58:GLU:HA	2.09	0.53
7:Q:11:ALA:CB	7:Q:72:LEU:HD13	2.37	0.53
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.90	0.53
7:P:72:LEU:HD23	7:P:73:PHE:CE2	2.42	0.53
11:d:92:GLU:OE2	15:b:125:PHE:HB2	2.08	0.53
11:d:129:GLN:OE1	15:b:2:VAL:O	2.26	0.53
1:A:432:GLN:OE1	19:A:600:ATP:C4	2.61	0.53
2:D:391:LEU:HD11	3:G:23:MET:CE	2.38	0.53
9:8:36:ASN:OD1	15:b:92:GLN:NE2	2.41	0.53
12:f:10:LYS:NZ	23:f:103:LHG:O6	2.42	0.53
1:B:473:ILE:O	1:B:477:GLN:NE2	2.40	0.53
7:P:33:ILE:HG23	7:Q:46:LEU:HD12	1.90	0.53
13:g:68:THR:N	13:g:71:GLU:OE2	2.39	0.53
1:C:489:ILE:O	1:C:489:ILE:HG23	2.08	0.53
2:D:391:LEU:HD11	3:G:23:MET:HE1	1.91	0.53
2:E:422:GLU:O	2:E:426:GLY:N	2.37	0.53
7:K:56:LEU:C	7:K:56:LEU:HD23	2.34	0.53
2:E:48:GLU:OE2	2:E:117:HIS:NE2	2.37	0.53
10:a:58:MET:HG3	10:a:69:THR:HG22	1.91	0.53
10:a:221:TYR:O	10:a:225:ASN:ND2	2.42	0.53
11:d:37:LEU:HD11	15:b:135:ALA:CB	2.39	0.53
2:D:224:GLU:O	2:D:229:ARG:NH1	2.42	0.53
7:L:12:GLY:HA2	7:M:14:ALA:HB2	1.89	0.53
10:a:62:ASN:OD1	10:a:63:SER:N	2.36	0.53
18:e:46:GLU:OE1	18:e:50:ARG:NH2	2.41	0.53
1:B:36:ASP:O	1:B:38:ILE:HD12	2.09	0.53
4:H:40:THR:O	4:H:59:ARG:NH1	2.41	0.53
1:C:52:MET:CE	1:C:95:VAL:HG23	2.39	0.53
2:E:377:ILE:HD11	2:E:406:ARG:HB2	1.91	0.53
2:E:452:LEU:HD22	2:E:470:ALA:HB1	1.91	0.53
7:Q:25:ILE:CD1	7:R:56:LEU:HD23	2.39	0.53
11:d:80:ILE:HG23	15:b:140:TYR:CE1	2.44	0.53
2:E:162:LYS:NZ	2:E:256:ASP:OD1	2.33	0.52
7:O:52:LEU:O	7:O:52:LEU:HD23	2.10	0.52
7:O:58:GLU:OE1	7:P:60:MET:HE1	2.09	0.52
5:I:35:MET:O	5:I:38:SER:OG	2.26	0.52
10:a:130:PRO:O	10:a:133:THR:OG1	2.19	0.52
13:g:84:MET:HE1	15:b:41:LEU:N	2.25	0.52
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.90	0.52
6:J:22:PHE:O	6:J:26:GLU:HG2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:33:ILE:HG23	7:Q:46:LEU:CD1	2.39	0.52
10:a:90:HIS:CG	15:b:56:GLU:OE2	2.62	0.52
7:M:25:ILE:HD12	7:M:54:PHE:HD1	1.73	0.52
10:a:29:LEU:HD23	22:f:101:CDL:H732	1.92	0.52
13:g:92:ILE:HG23	18:e:22:MET:HE1	1.91	0.52
1:A:423:ARG:HD2	1:A:461:ILE:HD11	1.91	0.52
1:C:2:LYS:O	8:S:94:ARG:NH1	2.42	0.52
2:F:189:ARG:NH1	24:F:703:HOH:O	2.32	0.52
9:8:20:LEU:HD23	9:8:20:LEU:O	2.10	0.52
9:8:20:LEU:HD23	9:8:21:PHE:CD2	2.45	0.52
13:g:85:TRP:CE3	18:e:18:LEU:HD21	2.42	0.52
2:D:393:MET:HA	2:D:396:LEU:HD23	1.90	0.52
3:G:131:VAL:HG22	5:I:42:ILE:CD1	2.40	0.52
7:K:52:LEU:C	7:K:52:LEU:HD23	2.34	0.52
7:M:32:LEU:HD12	7:M:50:ALA:CB	2.38	0.52
13:g:45:ILE:HG22	13:g:49:ILE:CD1	2.39	0.52
11:d:107:SER:O	11:d:111:ILE:HG13	2.09	0.52
12:f:59:LEU:O	12:f:62:VAL:HG12	2.10	0.52
1:A:180:ILE:CD1	1:A:216:LEU:HD11	2.39	0.52
2:E:186:VAL:HG22	2:E:232:VAL:CG1	2.38	0.52
2:F:124:VAL:HG22	2:F:124:VAL:O	2.10	0.52
22:b:301:CDL:H1O1	22:b:301:CDL:PA1	2.31	0.52
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.51
3:G:181:LEU:HD22	3:G:202:ARG:CB	2.39	0.51
11:d:19:ILE:HG21	11:d:24:LYS:HA	1.92	0.51
2:D:9:THR:HG22	2:D:27:GLU:CB	2.41	0.51
2:D:386:ASP:HB3	3:G:19:ILE:HD11	1.91	0.51
1:C:458:PRO:HA	1:C:461:ILE:HD12	1.92	0.51
7:P:15:THR:HG21	7:Q:67:VAL:HG11	1.93	0.51
7:Q:9:ILE:CD1	7:R:9:ILE:CG2	2.89	0.51
9:8:20:LEU:HD12	10:a:78:PHE:CD2	2.45	0.51
2:F:200:MET:HE1	2:F:217:LEU:HD21	1.92	0.51
10:a:103:GLY:HA2	14:j:31:MET:CE	2.41	0.51
18:e:14:ARG:O	18:e:18:LEU:HD23	2.09	0.51
1:B:474:SER:O	1:B:477:GLN:NE2	2.43	0.51
7:L:25:ILE:HD12	7:L:54:PHE:CE1	2.43	0.51
15:b:205:SER:O	15:b:209:GLN:NE2	2.44	0.51
7:N:64:CYS:O	7:N:67:VAL:HG12	2.10	0.51
7:P:16:VAL:O	7:P:16:VAL:HG22	2.11	0.51
7:Q:3:ASP:OD1	7:Q:4:THR:HG23	2.10	0.51
11:d:82:GLU:OE2	11:d:84:LYS:NZ	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:LEU:HD12	3:G:23:MET:HE1	1.92	0.51
2:E:168:GLU:OE2	2:E:172:ASN:ND2	2.44	0.51
11:d:99:SER:OG	15:b:118:VAL:HG13	2.11	0.51
1:B:365:ILE:HD12	1:B:365:ILE:H	1.76	0.51
1:C:444:VAL:CG1	1:C:469:LEU:HD21	2.41	0.51
11:d:89:VAL:HA	11:d:92:GLU:HG2	1.92	0.51
15:b:167:GLN:O	15:b:171:GLU:OE1	2.28	0.51
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.93	0.50
2:E:126:MET:HA	2:E:126:MET:HE3	1.93	0.50
7:K:60:MET:O	7:K:61:GLY:C	2.53	0.50
2:F:252:LEU:HD23	2:F:305:THR:HB	1.92	0.50
15:b:194:ILE:HA	15:b:197:CYS:SG	2.51	0.50
2:E:155:PHE:HE1	2:E:332:THR:HG23	1.75	0.50
11:d:56:TYR:CZ	15:b:155:LEU:HD13	2.46	0.50
7:P:7:LYS:NZ	7:P:74:ALA:O	2.44	0.50
1:B:423:ARG:NH2	1:B:456:LEU:O	2.43	0.50
1:C:50:GLU:OE1	2:D:67:GLU:HG3	2.12	0.50
11:d:56:TYR:OH	15:b:155:LEU:O	2.30	0.50
4:H:40:THR:HG22	4:H:41:GLN:N	2.27	0.50
4:H:105:LEU:HD22	4:H:145:LEU:HD13	1.93	0.50
7:K:26:GLY:O	7:K:30:GLY:N	2.44	0.50
1:C:479:LEU:HD21	1:C:497:LEU:HG	1.94	0.50
7:K:58:GLU:OE2	7:L:60:MET:SD	2.69	0.50
18:e:45:GLU:O	18:e:48:LYS:HG2	2.11	0.50
2:F:47:LEU:HD23	2:F:62:ALA:HA	1.93	0.50
7:M:5:ALA:O	7:N:6:ALA:HB1	2.11	0.50
10:a:106:ILE:N	10:a:107:PRO:CD	2.74	0.50
15:b:49:GLU:OE2	15:b:52:VAL:HG12	2.12	0.50
7:K:55:ALA:HB3	10:a:213:VAL:HG11	1.93	0.49
15:b:172:HIS:NE2	16:h:30:ASP:O	2.44	0.49
1:A:210:ARG:NH1	2:D:121:PRO:O	2.42	0.49
11:d:83:ASP:OD1	11:d:85:TYR:N	2.34	0.49
1:C:334:VAL:HG22	1:C:334:VAL:O	2.12	0.49
2:D:262:THR:HG23	2:D:285:LEU:HD13	1.95	0.49
2:E:279:VAL:HG12	2:E:279:VAL:O	2.11	0.49
4:H:52:VAL:HG22	4:H:53:PRO:HD2	1.94	0.49
7:P:9:ILE:CD1	7:Q:9:ILE:HB	2.42	0.49
11:d:80:ILE:HG23	15:b:140:TYR:HE1	1.76	0.49
13:g:37:LEU:O	18:e:15:TYR:OH	2.31	0.49
10:a:71:MET:HE1	14:j:21:TYR:HD2	1.77	0.49
10:a:155:ALA:O	10:a:156:LEU:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:184:SER:OG	16:h:16:ARG:NH2	2.44	0.49
7:K:54:PHE:CZ	7:L:56:LEU:HD22	2.48	0.49
7:M:58:GLU:OE2	7:N:60:MET:HE3	2.12	0.49
7:P:9:ILE:HD12	7:Q:9:ILE:HB	1.95	0.49
1:B:75:VAL:HG11	1:B:82:ILE:CD1	2.43	0.49
1:B:486:ASP:O	1:B:488:LYS:N	2.46	0.49
3:G:131:VAL:HG22	5:I:42:ILE:HD12	1.94	0.49
7:R:58:GLU:OE2	7:R:58:GLU:HA	2.12	0.49
8:S:173:MET:CE	15:b:201:LEU:HD22	2.41	0.49
10:a:115:THR:O	10:a:119:ASN:ND2	2.45	0.49
4:H:114:LYS:O	4:H:118:GLU:OE1	2.30	0.49
7:K:55:ALA:HB1	10:a:213:VAL:HG11	1.94	0.49
7:N:25:ILE:HG21	7:O:56:LEU:HD23	1.94	0.49
11:d:100:CYS:O	11:d:104:LEU:HB3	2.13	0.49
1:B:298:VAL:O	1:B:298:VAL:HG22	2.13	0.49
1:C:36:ASP:OD2	2:F:274:ARG:NH2	2.46	0.49
18:e:26:ALA:O	18:e:30:ASN:ND2	2.46	0.49
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.95	0.49
2:D:387:ILE:HG23	2:D:391:LEU:HD13	1.94	0.49
2:D:469:LYS:O	2:D:473:LEU:HD13	2.13	0.49
7:Q:54:PHE:CZ	7:R:56:LEU:HD21	2.47	0.49
1:B:15:ARG:NE	8:S:186:MET:O	2.46	0.49
2:D:212:THR:O	2:D:212:THR:HG22	2.12	0.49
2:F:170:ILE:HD11	2:F:183:PHE:HE1	1.75	0.49
7:K:73:PHE:O	7:K:74:ALA:HB2	2.13	0.49
3:G:154:GLU:HA	3:G:154:GLU:OE1	2.13	0.48
7:N:42:LEU:C	7:N:44:GLN:H	2.16	0.48
10:a:195:ILE:O	10:a:199:LEU:HD13	2.13	0.48
11:d:37:LEU:HD11	15:b:135:ALA:HA	1.95	0.48
12:f:29:THR:O	12:f:32:GLY:N	2.45	0.48
1:A:151:LYS:NZ	1:A:427:LEU:O	2.30	0.48
1:C:356:LEU:HD13	1:C:361:ILE:HD13	1.94	0.48
2:F:63:MET:HE1	2:F:231:ARG:CB	2.43	0.48
7:R:52:LEU:C	7:R:52:LEU:HD23	2.38	0.48
10:a:53:VAL:HG11	10:a:73:MET:HE1	1.96	0.48
7:K:58:GLU:O	7:K:59:ALA:C	2.56	0.48
10:a:61:HIS:O	10:a:66:GLN:NE2	2.46	0.48
10:a:78:PHE:O	10:a:82:THR:HG23	2.13	0.48
2:F:54:GLY:O	2:F:55:GLU:HB2	2.14	0.48
12:f:79:LYS:NZ	23:b:302:LHG:O5	2.42	0.48
2:D:333:THR:O	2:D:333:THR:OG1	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:VAL:HG22	2:E:22:ASP:O	2.13	0.48
4:H:47:ILE:C	4:H:48:LEU:HD22	2.38	0.48
1:B:474:SER:HG	1:B:475:GLN:CD	2.15	0.48
7:L:4:THR:O	7:L:4:THR:HG22	2.13	0.48
10:a:87:LEU:HD11	10:a:203:GLU:HB3	1.95	0.48
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.79	0.48
3:G:272:LEU:HD12	3:G:272:LEU:O	2.14	0.48
12:f:60:SER:O	12:f:61:MET:C	2.55	0.48
1:A:47:VAL:HG23	1:A:51:GLU:OE2	2.13	0.48
7:P:22:GLY:HA2	7:Q:60:MET:HE3	1.94	0.48
2:F:322:PRO:HA	2:F:325:THR:HG22	1.95	0.48
7:K:47:PHE:HE1	7:L:49:TYR:OH	1.96	0.48
7:K:72:LEU:HD22	7:K:73:PHE:CE2	2.49	0.48
18:e:34:PRO:O	18:e:37:GLU:HG2	2.14	0.48
4:H:119:LEU:HD11	4:H:128:ARG:HH11	1.79	0.48
7:L:29:PHE:O	7:L:33:ILE:HG12	2.14	0.48
11:d:40:ARG:NH1	15:b:138:VAL:HB	2.29	0.48
1:B:258:ARG:NH1	1:B:308:ARG:O	2.47	0.47
2:E:210:ASP:CG	2:E:212:THR:HG22	2.39	0.47
7:L:16:VAL:HG22	7:L:16:VAL:O	2.14	0.47
13:g:86:PHE:CE1	18:e:20:LEU:HD23	2.49	0.47
1:C:55:PHE:CD2	1:C:88:VAL:HG22	2.48	0.47
2:E:163:THR:HG21	2:E:199:GLU:OE1	2.14	0.47
4:H:102:MET:O	4:H:103:LEU:HD12	2.14	0.47
13:g:32:TYR:O	13:g:36:GLU:OE1	2.32	0.47
1:A:199:LEU:HD21	1:A:265:LEU:CB	2.44	0.47
1:C:148:THR:CG2	1:C:150:ILE:HD12	2.45	0.47
2:E:212:THR:HG23	2:E:212:THR:O	2.14	0.47
2:F:279:VAL:O	2:F:279:VAL:CG1	2.62	0.47
5:I:44:ILE:HG22	5:I:45:VAL:N	2.29	0.47
7:P:5:ALA:O	7:P:9:ILE:HG12	2.13	0.47
11:d:118:LEU:HD23	11:d:122:ARG:HG3	1.96	0.47
15:b:181:VAL:HG12	16:h:17:GLU:CD	2.40	0.47
1:A:196:LYS:NZ	1:A:261:GLY:O	2.48	0.47
1:C:38:ILE:CD1	1:C:74:VAL:HG12	2.45	0.47
7:Q:25:ILE:HD12	7:Q:54:PHE:HE1	1.74	0.47
8:S:186:MET:CE	15:b:174:ILE:HD12	2.41	0.47
10:a:44:THR:HG21	15:b:86:ASN:OD1	2.14	0.47
11:d:80:ILE:CG2	15:b:140:TYR:OH	2.63	0.47
1:C:151:LYS:HE3	1:C:427:LEU:O	2.14	0.47
2:D:389:ALA:HA	6:J:26:GLU:CD	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:40:THR:HG23	4:H:56:GLN:HB3	1.96	0.47
2:E:207:ASN:OD1	2:E:210:ASP:OD1	2.32	0.47
2:E:263:GLN:O	2:E:267:GLU:HG3	2.15	0.47
2:E:436:GLU:OE1	2:E:436:GLU:N	2.48	0.47
3:G:23:MET:SD	3:G:232:MET:SD	3.13	0.47
6:J:50:GLU:O	6:J:53:ILE:HG12	2.13	0.47
7:K:52:LEU:HD23	7:K:53:GLY:N	2.29	0.47
7:N:16:VAL:HG13	7:O:16:VAL:HG13	1.97	0.47
7:Q:33:ILE:HD11	7:R:50:ALA:HA	1.97	0.47
7:Q:54:PHE:CE1	7:R:56:LEU:CD2	2.97	0.47
9:8:28:VAL:HG23	10:a:70:LEU:CD1	2.44	0.47
10:a:131:GLN:OE1	10:a:131:GLN:HA	2.15	0.47
12:f:8:GLU:CD	12:f:25:MET:HE1	2.39	0.47
15:b:200:ASP:O	15:b:204:LEU:HD23	2.14	0.47
2:D:9:THR:HG22	2:D:27:GLU:HB3	1.95	0.47
7:N:9:ILE:HD11	7:O:6:ALA:HA	1.95	0.47
11:d:57:LYS:HG2	11:d:63:ALA:HB1	1.97	0.47
2:E:38:VAL:HG22	2:E:75:VAL:HG22	1.96	0.47
7:K:60:MET:SD	7:K:60:MET:N	2.88	0.47
7:Q:29:PHE:CE2	7:R:52:LEU:HD22	2.50	0.47
15:b:126:ASP:O	15:b:129:ARG:HG2	2.15	0.47
1:A:134:PRO:HB3	1:A:312:MET:HE1	1.96	0.47
2:D:393:MET:N	6:J:29:GLU:OE2	2.37	0.47
11:d:81:PRO:HG2	15:b:140:TYR:CE2	2.50	0.47
11:d:89:VAL:O	11:d:92:GLU:HB2	2.15	0.47
15:b:158:HIS:NE2	16:h:55:MET:O	2.46	0.47
1:A:55:PHE:CD1	1:A:88:VAL:HG22	2.50	0.46
1:A:403:PHE:O	1:A:404:ALA:C	2.58	0.46
2:E:63:MET:HE1	2:E:231:ARG:HG3	1.96	0.46
7:O:47:PHE:O	7:O:48:SER:C	2.58	0.46
8:S:186:MET:SD	8:S:187:ARG:N	2.88	0.46
10:a:140:MET:O	10:a:144:ILE:HD12	2.14	0.46
15:b:164:MET:O	15:b:167:GLN:NE2	2.48	0.46
16:h:19:ARG:O	16:h:23:GLN:OE1	2.32	0.46
18:e:46:GLU:OE1	18:e:50:ARG:NE	2.48	0.46
1:C:390:MET:CE	1:C:428:LEU:HD21	2.43	0.46
8:S:150:LEU:HD23	8:S:151:GLU:N	2.30	0.46
11:d:113:GLU:O	11:d:117:GLU:OE1	2.34	0.46
2:D:391:LEU:HD12	2:D:391:LEU:N	2.31	0.46
2:E:26:ASP:OD1	2:E:27:GLU:N	2.49	0.46
7:K:52:LEU:O	7:K:53:GLY:C	2.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:9:ILE:CD1	7:P:9:ILE:HB	2.45	0.46
11:d:81:PRO:HD2	15:b:140:TYR:CE1	2.50	0.46
13:g:77:LEU:HD23	13:g:77:LEU:O	2.15	0.46
15:b:181:VAL:HG12	16:h:17:GLU:OE1	2.15	0.46
1:A:64:LEU:HD12	1:A:74:VAL:HG11	1.97	0.46
1:C:278:TYR:CD2	1:C:301:LEU:HD22	2.50	0.46
2:D:55:GLU:O	2:D:56:SER:OG	2.32	0.46
2:D:258:ILE:HD11	2:D:292:MET:HE1	1.96	0.46
2:F:151:LYS:NZ	2:F:296:ILE:O	2.39	0.46
3:G:2:THR:HG23	3:G:5:ASP:H	1.79	0.46
7:Q:42:LEU:O	7:Q:44:GLN:N	2.38	0.46
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.97	0.46
2:E:290:GLY:O	2:E:294:GLU:HB2	2.16	0.46
2:F:77:ASP:OD1	2:F:78:SER:N	2.49	0.46
7:N:58:GLU:HG3	7:N:62:LEU:HD23	1.97	0.46
1:B:453:LEU:HD22	1:B:461:ILE:CD1	2.45	0.46
2:D:89:GLU:HB2	2:D:110:THR:HG22	1.96	0.46
7:M:43:M3L:HM22	7:N:45:GLN:NE2	2.31	0.46
11:d:82:GLU:OE1	11:d:82:GLU:N	2.46	0.46
14:j:20:ALA:C	14:j:21:TYR:HD1	2.24	0.46
1:A:403:PHE:O	1:A:406:PHE:N	2.48	0.46
2:E:423:VAL:HG23	2:E:424:PHE:CD1	2.51	0.46
2:F:146:TYR:HE2	2:F:169:LEU:HD21	1.79	0.46
7:K:6:ALA:O	7:K:7:LYS:C	2.59	0.46
7:K:25:ILE:O	7:K:26:GLY:C	2.59	0.46
7:L:22:GLY:O	7:L:25:ILE:HG22	2.14	0.46
8:S:55:LEU:HD13	8:S:95:LEU:HD12	1.97	0.46
13:g:97:ILE:O	13:g:97:ILE:HG22	2.16	0.46
1:B:10:SER:N	16:h:18:TYR:OH	2.49	0.46
1:B:249:SER:O	1:B:253:MET:HG3	2.15	0.46
2:E:138:LYS:NZ	2:E:460:VAL:O	2.49	0.46
7:K:51:ILE:O	7:K:52:LEU:C	2.57	0.46
7:M:73:PHE:O	7:M:74:ALA:HB2	2.16	0.46
7:N:25:ILE:HG21	7:O:56:LEU:CD2	2.46	0.46
2:E:119:GLU:N	2:E:119:GLU:OE1	2.49	0.46
4:H:119:LEU:HD11	4:H:128:ARG:NH1	2.31	0.46
7:K:6:ALA:HB2	7:R:5:ALA:HB1	1.98	0.46
7:K:57:SER:O	7:K:58:GLU:C	2.58	0.46
7:L:65:LEU:HD21	7:M:63:PHE:CZ	2.50	0.46
7:Q:68:ALA:O	7:Q:71:ILE:HG22	2.16	0.46
10:a:169:LEU:O	10:a:173:LEU:HD13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ILE:HG22	2:D:310:ILE:HG12	1.97	0.45
2:F:377:ILE:HD11	2:F:406:ARG:HB2	1.98	0.45
15:b:83:ASP:O	15:b:84:LYS:C	2.59	0.45
1:A:322:THR:HG22	1:A:323:ALA:N	2.31	0.45
2:D:393:MET:HE3	2:D:404:VAL:HG11	1.98	0.45
8:S:162:MET:HE2	15:b:197:CYS:SG	2.56	0.45
16:h:39:LEU:HA	16:h:42:GLU:OE1	2.16	0.45
1:A:172:GLN:HG2	2:D:354:THR:HG21	1.98	0.45
7:N:58:GLU:OE2	7:O:60:MET:HE1	2.16	0.45
7:O:52:LEU:HD23	7:O:52:LEU:C	2.41	0.45
2:D:391:LEU:HD23	2:D:395:GLU:HG2	1.97	0.45
2:F:25:PHE:O	2:F:56:SER:HB3	2.16	0.45
3:G:102:GLU:OE2	3:G:102:GLU:HA	2.16	0.45
4:H:105:LEU:O	4:H:106:GLY:C	2.60	0.45
11:d:11:ASP:O	11:d:11:ASP:CG	2.59	0.45
11:d:56:TYR:HE1	15:b:159:ILE:CG1	2.29	0.45
1:B:286:ARG:NH2	2:E:275:ILE:HD11	2.31	0.45
2:E:29:LEU:N	2:E:29:LEU:HD12	2.32	0.45
11:d:37:LEU:HD11	15:b:135:ALA:HB2	1.97	0.45
2:F:10:THR:N	2:F:27:GLU:OE2	2.48	0.45
3:G:44:TYR:CE2	3:G:211:ASN:OD1	2.69	0.45
7:O:54:PHE:CE1	7:P:56:LEU:HD23	2.51	0.45
10:a:106:ILE:HG12	14:j:31:MET:CE	2.44	0.45
3:G:190:MET:HE2	3:G:190:MET:CA	2.46	0.45
4:H:143:LYS:O	4:H:143:LYS:HG2	2.17	0.45
7:M:13:ALA:O	7:M:16:VAL:HG12	2.16	0.45
7:Q:15:THR:HG21	7:R:14:ALA:HB1	1.98	0.45
1:A:203:TYR:OH	1:A:269:ASP:OD1	2.24	0.45
2:D:385:GLN:O	6:J:26:GLU:OE2	2.35	0.45
2:F:163:THR:HA	2:F:166:ILE:HG22	1.99	0.45
2:F:233:ALA:O	2:F:237:LEU:HD13	2.17	0.45
7:R:38:ARG:NH1	7:R:38:ARG:HB3	2.32	0.45
7:R:56:LEU:HD23	7:R:56:LEU:O	2.16	0.45
10:a:71:MET:SD	14:j:21:TYR:CE2	3.09	0.45
11:d:6:ALA:C	11:d:7:LEU:HD22	2.42	0.45
1:A:249:SER:O	1:A:253:MET:HG3	2.17	0.45
11:d:98:LYS:O	11:d:102:GLU:OE2	2.35	0.45
15:b:84:LYS:HA	15:b:87:GLU:OE2	2.17	0.45
8:S:98:THR:N	8:S:99:PRO:HD2	2.32	0.45
16:h:5:ASP:O	16:h:8:GLN:NE2	2.48	0.45
2:D:64:ASP:OD1	2:D:65:GLY:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:70:GLY:HA3	3:G:89:MET:SD	2.57	0.44
7:K:53:GLY:O	7:K:54:PHE:C	2.58	0.44
1:B:464:PHE:O	1:B:465:GLU:C	2.60	0.44
1:C:423:ARG:HG3	1:C:461:ILE:HD11	1.99	0.44
2:E:237:LEU:HD23	2:E:253:LEU:CD1	2.48	0.44
6:J:29:GLU:C	6:J:29:GLU:OE1	2.60	0.44
11:d:100:CYS:O	11:d:101:ALA:C	2.60	0.44
15:b:58:PHE:HA	15:b:61:ILE:HG22	1.99	0.44
7:R:58:GLU:O	7:R:59:ALA:C	2.58	0.44
8:S:171:VAL:HG21	8:S:173:MET:HE3	1.99	0.44
8:S:173:MET:SD	15:b:197:CYS:HB2	2.58	0.44
10:a:129:LEU:HD22	17:k:30:VAL:HG23	1.99	0.44
11:d:158:GLU:OE1	11:d:158:GLU:N	2.37	0.44
15:b:178:GLU:HA	15:b:181:VAL:HG22	1.98	0.44
7:K:72:LEU:CD1	7:L:71:ILE:HD11	2.47	0.44
16:h:25:SER:O	16:h:25:SER:OG	2.31	0.44
2:F:229:ARG:NH2	2:F:267:GLU:OE2	2.50	0.44
7:P:54:PHE:CZ	7:Q:56:LEU:HD12	2.52	0.44
7:R:42:LEU:O	7:R:43:M3L:C	2.66	0.44
9:8:2:PRO:HB3	10:a:10:ILE:HD13	1.98	0.44
10:a:154:MET:O	10:a:158:VAL:HG12	2.18	0.44
1:B:117:GLY:O	1:B:118:LYS:C	2.61	0.44
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.48	0.44
11:d:45:PRO:O	15:b:141:ARG:HD3	2.18	0.44
1:B:297:ASP:OD1	1:B:297:ASP:O	2.35	0.44
2:D:124:VAL:HG22	2:D:124:VAL:O	2.17	0.44
2:D:255:ILE:HG21	2:D:258:ILE:CD1	2.47	0.44
2:E:375:GLN:O	2:E:379:GLN:HG3	2.18	0.44
2:F:258:ILE:HG22	2:F:310:ILE:HG13	2.00	0.44
7:K:18:VAL:HB	7:L:64:CYS:SG	2.58	0.44
7:N:16:VAL:HG12	7:N:16:VAL:O	2.16	0.44
7:N:25:ILE:HD12	7:N:54:PHE:HD1	1.82	0.44
8:S:159:MET:HB2	15:b:185:ILE:HD11	1.99	0.44
15:b:158:HIS:CD2	16:h:55:MET:HE3	2.53	0.44
1:B:496:LYS:O	1:B:499:GLU:HG3	2.17	0.44
1:C:361:ILE:H	1:C:361:ILE:HD12	1.83	0.44
1:C:464:PHE:O	1:C:465:GLU:C	2.60	0.44
21:D:600:ADP:O1A	21:D:600:ADP:O1B	2.36	0.44
2:E:256:ASP:HA	2:E:257:ASN:HA	1.83	0.44
2:E:347:ALA:O	2:E:348:VAL:C	2.61	0.44
6:J:26:GLU:OE1	6:J:26:GLU:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:54:PHE:CE1	7:O:56:LEU:HD21	2.53	0.44
7:P:3:ASP:O	7:P:7:LYS:HG2	2.18	0.44
10:a:66:GLN:OE1	11:d:157:ILE:HD13	2.17	0.44
11:d:18:ILE:HD12	15:b:117:LEU:HD21	2.00	0.44
14:j:16:TYR:HA	14:j:20:ALA:HB3	1.99	0.44
15:b:189:GLN:N	15:b:190:GLU:OE1	2.50	0.44
1:B:74:VAL:HG23	1:B:74:VAL:O	2.17	0.44
11:d:41:LEU:HD12	15:b:138:VAL:CG2	2.48	0.44
2:D:14:VAL:HG22	2:D:22:ASP:O	2.17	0.43
4:H:36:VAL:HG23	4:H:65:VAL:HG22	2.01	0.43
7:L:43:M3L:HM23	7:M:45:GLN:HE22	1.82	0.43
8:S:184:ARG:HA	8:S:184:ARG:NE	2.33	0.43
2:F:183:PHE:HB3	2:F:217:LEU:HD23	2.01	0.43
3:G:181:LEU:HD22	3:G:202:ARG:HB3	2.00	0.43
7:L:50:ALA:O	7:L:51:ILE:C	2.60	0.43
10:a:25:LEU:HD23	10:a:25:LEU:O	2.18	0.43
10:a:41:ARG:O	10:a:44:THR:OG1	2.32	0.43
10:a:122:LYS:HA	17:k:27:MET:HE2	2.00	0.43
13:g:83:TRP:CD1	13:g:83:TRP:C	2.96	0.43
2:E:339:ILE:HG22	2:E:339:ILE:O	2.18	0.43
2:F:408:ARG:NH2	2:F:454:GLU:OE1	2.50	0.43
7:K:67:VAL:O	7:K:68:ALA:C	2.61	0.43
7:L:63:PHE:O	7:L:66:MET:HG3	2.17	0.43
7:Q:25:ILE:HA	7:Q:28:VAL:HG12	1.99	0.43
7:R:41:SER:O	7:R:41:SER:OG	2.32	0.43
12:f:65:ALA:O	12:f:69:LEU:HD23	2.18	0.43
15:b:9:GLY:O	15:b:10:GLY:C	2.61	0.43
15:b:168:LYS:HZ2	16:h:35:TYR:HD1	1.64	0.43
18:e:46:GLU:HA	18:e:49:LYS:HG2	2.00	0.43
1:C:390:MET:HE1	1:C:428:LEU:CD2	2.46	0.43
2:E:48:GLU:OE1	2:E:231:ARG:NE	2.50	0.43
3:G:163:ASN:ND2	3:G:173:THR:HG22	2.33	0.43
7:Q:5:ALA:O	7:Q:9:ILE:HG12	2.19	0.43
9:8:8:THR:O	9:8:9:TRP:C	2.60	0.43
2:D:84:ILE:HD13	2:D:235:THR:HG23	2.00	0.43
3:G:139:GLY:O	3:G:143:VAL:HG23	2.18	0.43
4:H:39:PRO:C	4:H:40:THR:HG1	2.11	0.43
7:L:5:ALA:HB1	7:M:6:ALA:HB3	1.99	0.43
7:O:8:PHE:HB2	7:P:6:ALA:HB1	2.00	0.43
8:S:150:LEU:HD21	8:S:152:VAL:HG23	2.01	0.43
11:d:109:THR:O	11:d:113:GLU:OE1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:10:LYS:HD2	23:f:103:LHG:O5	2.18	0.43
12:f:86:TYR:CD1	12:f:86:TYR:O	2.71	0.43
1:A:74:VAL:O	1:A:74:VAL:HG23	2.19	0.43
1:B:162:GLY:HA3	1:B:311:LYS:HB2	2.00	0.43
2:E:171:ASN:ND2	2:E:419:GLN:OE1	2.52	0.43
3:G:110:ASP:OD1	3:G:113:ARG:NH2	2.43	0.43
7:Q:18:VAL:HG12	7:Q:18:VAL:O	2.17	0.43
7:Q:27:THR:HA	7:R:27:THR:HG21	2.01	0.43
8:S:131:LEU:HD11	8:S:152:VAL:HG21	2.01	0.43
13:g:42:PRO:HA	13:g:45:ILE:HG12	2.01	0.43
15:b:168:LYS:HA	15:b:171:GLU:OE1	2.18	0.43
1:C:389:THR:OG1	1:C:449:VAL:HG21	2.18	0.43
2:F:419:GLN:NE2	2:F:422:GLU:OE2	2.48	0.43
3:G:151:SER:O	3:G:153:TYR:N	2.44	0.43
7:L:15:THR:O	7:L:15:THR:HG22	2.17	0.43
7:O:16:VAL:HG22	7:O:16:VAL:O	2.19	0.43
7:P:36:TYR:O	7:P:36:TYR:CG	2.72	0.43
7:P:42:LEU:O	7:P:43:M3L:C	2.65	0.43
10:a:29:LEU:HD12	10:a:29:LEU:C	2.44	0.43
12:f:43:ARG:NH1	23:f:103:LHG:H02	2.13	0.43
1:A:157:VAL:O	1:A:157:VAL:HG22	2.18	0.43
1:A:166:LEU:HD11	1:A:327:ILE:HG13	2.01	0.43
1:A:355:GLU:OE2	6:J:12:ALA:N	2.52	0.43
3:G:103:VAL:HG12	3:G:104:LYS:N	2.33	0.43
9:8:3:GLN:HB3	10:a:98:LEU:CD1	2.47	0.43
11:d:109:THR:HG23	11:d:110:ARG:N	2.34	0.43
1:C:356:LEU:HD12	1:C:361:ILE:HD13	2.01	0.43
7:Q:19:ALA:O	7:R:20:GLY:HA3	2.19	0.43
10:a:73:MET:HA	10:a:73:MET:CE	2.47	0.43
11:d:130:MET:HG2	11:d:134:ASP:HB2	2.00	0.43
16:h:54:ASP:HB3	16:h:57:THR:HG23	2.00	0.43
1:B:467:ALA:O	1:B:470:SER:OG	2.29	0.43
4:H:112:LEU:HD23	4:H:112:LEU:O	2.19	0.43
7:K:5:ALA:O	7:K:9:ILE:HG22	2.19	0.43
10:a:94:PRO:HB2	10:a:100:MET:SD	2.59	0.43
11:d:81:PRO:HD2	15:b:140:TYR:CZ	2.54	0.43
16:h:15:ILE:O	16:h:19:ARG:HG2	2.19	0.43
1:A:52:MET:HE1	1:A:76:PHE:HE1	1.84	0.42
2:D:146:TYR:OH	2:D:333:THR:HG21	2.19	0.42
2:E:15:ALA:HB3	2:E:22:ASP:HB2	2.01	0.42
7:K:60:MET:HE1	7:R:58:GLU:CD	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:42:LEU:C	7:L:44:GLN:H	2.25	0.42
7:L:59:ALA:HB2	10:a:202:LEU:CD2	2.49	0.42
7:N:25:ILE:HD12	7:N:54:PHE:CD1	2.54	0.42
7:O:58:GLU:OE2	7:P:60:MET:HE1	2.19	0.42
9:8:16:MET:SD	9:8:16:MET:C	3.02	0.42
11:d:31:LYS:O	11:d:34:ASN:HB3	2.18	0.42
22:f:101:CDL:H1O1	22:f:101:CDL:PB2	2.39	0.42
15:b:199:ALA:O	15:b:203:LEU:HG	2.18	0.42
1:B:442:VAL:HG11	1:B:489:ILE:HD11	2.02	0.42
1:C:108:VAL:HG22	1:C:109:ASP:N	2.34	0.42
2:D:359:ASP:O	2:D:363:VAL:HG22	2.19	0.42
2:E:316:ASP:OD2	3:G:255:GLN:NE2	2.52	0.42
3:G:202:ARG:NH1	5:I:5:ARG:CZ	2.82	0.42
10:a:135:THR:N	10:a:136:PRO:HD2	2.35	0.42
10:a:152:GLN:HB2	10:a:153:PRO:HD3	1.99	0.42
15:b:160:SER:HB3	16:h:46:LEU:HD11	2.02	0.42
16:h:41:ARG:HG3	16:h:42:GLU:N	2.34	0.42
2:D:393:MET:CE	2:D:404:VAL:HG11	2.49	0.42
3:G:118:ARG:HG3	3:G:119:THR:H	1.84	0.42
4:H:51:HIS:ND1	4:H:52:VAL:O	2.46	0.42
7:K:56:LEU:HD21	7:R:54:PHE:CZ	2.52	0.42
7:M:70:LEU:O	7:M:74:ALA:N	2.52	0.42
7:O:18:VAL:HG11	7:O:65:LEU:HD13	2.01	0.42
8:S:15:GLU:CG	8:S:16:GLY:N	2.82	0.42
10:a:68:TRP:O	10:a:69:THR:C	2.63	0.42
15:b:93:LEU:HD23	15:b:93:LEU:HA	1.93	0.42
17:k:38:ALA:HA	17:k:41:VAL:HG12	2.02	0.42
3:G:10:LEU:HD13	3:G:246:LEU:HB3	2.01	0.42
7:N:39:ASN:CG	7:N:42:LEU:HD13	2.44	0.42
22:f:102:CDL:H1O1	22:f:102:CDL:PA1	2.29	0.42
1:A:176:THR:O	1:A:180:ILE:HG12	2.20	0.42
2:F:29:LEU:HD12	2:F:29:LEU:H	1.84	0.42
2:F:268:VAL:HG22	2:F:268:VAL:O	2.19	0.42
7:N:9:ILE:HD12	7:O:9:ILE:HB	2.02	0.42
10:a:71:MET:SD	14:j:21:TYR:CD2	3.12	0.42
10:a:217:LEU:HD12	10:a:221:TYR:OH	2.18	0.42
11:d:92:GLU:OE2	15:b:125:PHE:CB	2.68	0.42
7:K:4:THR:OG1	7:L:3:ASP:OD1	2.34	0.42
7:K:19:ALA:O	7:L:20:GLY:HA3	2.19	0.42
7:K:65:LEU:O	7:K:68:ALA:HB3	2.20	0.42
10:a:66:GLN:HA	10:a:69:THR:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:65:LEU:HD11	11:d:69:PHE:CE2	2.55	0.42
11:d:135:LEU:C	11:d:135:LEU:HD23	2.44	0.42
1:A:34:ILE:HG13	1:A:35:GLY:N	2.35	0.42
1:A:95:VAL:HG11	1:A:245:LEU:HD21	2.01	0.42
1:C:127:ARG:NH1	1:C:259:ASP:OD2	2.49	0.42
1:C:210:ARG:HG2	1:C:235:THR:HG21	2.02	0.42
2:E:267:GLU:O	2:E:271:LEU:HG	2.19	0.42
3:G:147:GLU:OE1	3:G:147:GLU:HA	2.18	0.42
10:a:9:PHE:N	10:a:9:PHE:CD1	2.87	0.42
10:a:137:LEU:O	10:a:137:LEU:HD12	2.19	0.42
18:e:47:LYS:HD2	18:e:50:ARG:HH12	1.84	0.42
1:A:226:MET:HE1	1:A:231:VAL:HG23	2.02	0.42
2:D:186:VAL:HB	2:D:257:ASN:O	2.20	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.50	0.42
7:R:13:ALA:O	7:R:16:VAL:HG12	2.19	0.42
10:a:152:GLN:OE1	10:a:221:TYR:CE1	2.73	0.42
13:g:50:GLN:HB3	13:g:54:LYS:NZ	2.35	0.42
13:g:77:LEU:HD21	15:b:37:LEU:HD13	2.01	0.42
2:E:151:LYS:HG2	2:E:293:GLN:OE1	2.20	0.42
2:E:242:TYR:CD2	2:E:242:TYR:C	2.98	0.42
2:E:258:ILE:HG22	2:E:309:ALA:O	2.20	0.42
4:H:58:LEU:HD13	4:H:77:VAL:HG21	2.02	0.42
10:a:24:VAL:O	10:a:24:VAL:HG12	2.19	0.42
12:f:77:GLU:OE1	12:f:77:GLU:N	2.52	0.42
1:B:155:SER:OG	1:B:156:LEU:N	2.53	0.41
1:C:3:THR:HG21	8:S:17:ARG:NH1	2.35	0.41
1:C:208:GLN:NE2	1:C:269:ASP:O	2.53	0.41
1:C:334:VAL:CG2	1:C:343:ILE:HD11	2.49	0.41
2:F:159:GLY:N	21:F:600:ADP:O3B	2.46	0.41
3:G:38:LEU:HD11	3:G:219:GLU:OE2	2.20	0.41
4:H:37:ASP:OD2	7:Q:41:SER:OG	2.32	0.41
7:K:60:MET:CE	7:R:58:GLU:OE2	2.68	0.41
8:S:150:LEU:CD2	8:S:152:VAL:HG23	2.50	0.41
10:a:1:MET:O	10:a:1:MET:HG2	2.20	0.41
10:a:107:PRO:HD3	14:j:31:MET:HE1	2.01	0.41
10:a:177:ALA:O	10:a:181:LEU:HD13	2.20	0.41
15:b:170:GLN:O	15:b:174:ILE:HG12	2.20	0.41
15:b:175:ASN:O	15:b:178:GLU:HG3	2.20	0.41
16:h:39:LEU:O	16:h:43:LEU:HD23	2.20	0.41
2:D:365:SER:O	2:D:369:ASP:OD2	2.38	0.41
2:F:63:MET:CE	2:F:97:VAL:HG21	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:54:PHE:CD1	7:O:56:LEU:HD21	2.55	0.41
7:O:5:ALA:O	7:O:9:ILE:HG12	2.20	0.41
7:P:54:PHE:CE1	7:Q:56:LEU:HD12	2.56	0.41
7:Q:24:GLY:O	7:Q:27:THR:HG22	2.20	0.41
8:S:186:MET:HE1	15:b:174:ILE:CG1	2.50	0.41
10:a:149:LEU:HA	10:a:152:GLN:HE21	1.86	0.41
11:d:41:LEU:HB2	15:b:138:VAL:HG21	2.02	0.41
15:b:152:LYS:O	15:b:155:LEU:HG	2.20	0.41
1:A:371:VAL:HG22	1:A:372:SER:H	1.83	0.41
1:B:35:GLY:O	1:B:36:ASP:HB2	2.20	0.41
1:C:298:VAL:HG22	1:C:298:VAL:O	2.20	0.41
2:E:48:GLU:HB2	2:E:63:MET:HE2	2.02	0.41
7:K:62:LEU:O	7:K:63:PHE:C	2.64	0.41
8:S:168:GLU:OE1	8:S:168:GLU:N	2.52	0.41
11:d:118:LEU:HD23	11:d:118:LEU:C	2.45	0.41
1:A:342:VAL:HG12	1:A:342:VAL:O	2.20	0.41
1:B:156:LEU:HD12	1:B:367:VAL:HG11	2.02	0.41
1:C:414:THR:O	1:C:418:LEU:HD13	2.20	0.41
2:D:347:ALA:O	2:D:348:VAL:C	2.63	0.41
2:F:347:ALA:O	2:F:348:VAL:C	2.63	0.41
7:M:58:GLU:O	7:M:62:LEU:HD23	2.20	0.41
7:O:19:ALA:HA	7:P:20:GLY:HA3	2.02	0.41
10:a:26:PHE:CD2	10:a:26:PHE:C	2.98	0.41
11:d:37:LEU:HD11	15:b:135:ALA:CA	2.51	0.41
13:g:82:VAL:HG13	13:g:83:TRP:N	2.36	0.41
1:B:388:GLY:O	1:B:392:LEU:HD13	2.20	0.41
2:D:312:VAL:O	2:D:312:VAL:HG12	2.21	0.41
2:E:473:LEU:HD12	2:E:473:LEU:C	2.45	0.41
3:G:128:PHE:HB3	5:I:42:ILE:CG2	2.50	0.41
10:a:61:HIS:HB3	10:a:65:GLY:HA3	2.02	0.41
10:a:90:HIS:HA	15:b:56:GLU:OE2	2.19	0.41
13:g:92:ILE:HG22	18:e:22:MET:HE1	2.01	0.41
16:h:64:GLU:OE1	16:h:65:ASP:O	2.38	0.41
18:e:34:PRO:O	18:e:37:GLU:N	2.54	0.41
1:A:446:TYR:OH	1:A:494:ASP:OD1	2.19	0.41
1:B:463:LYS:O	1:B:464:PHE:C	2.63	0.41
3:G:168:VAL:O	3:G:168:VAL:HG22	2.20	0.41
7:L:40:PRO:HG3	7:M:42:LEU:HD11	2.02	0.41
11:d:94:LYS:O	11:d:97:VAL:HG22	2.20	0.41
2:D:387:ILE:CG2	2:D:391:LEU:HD13	2.50	0.41
7:K:20:GLY:HA3	7:R:19:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:25:ILE:HD11	7:R:56:LEU:CD2	2.49	0.41
9:8:12:MET:HE2	9:8:12:MET:HB2	1.96	0.41
10:a:75:LEU:CD1	10:a:79:ILE:HD11	2.48	0.41
1:A:34:ILE:HG21	1:A:82:ILE:O	2.21	0.41
1:A:151:LYS:NZ	1:A:465:GLU:OE1	2.53	0.41
2:D:96:ASN:OD1	2:D:102:ILE:HG21	2.20	0.41
3:G:160:ILE:HG23	3:G:160:ILE:O	2.20	0.41
9:8:12:MET:SD	10:a:20:VAL:HG21	2.61	0.41
10:a:13:VAL:O	10:a:13:VAL:HG23	2.20	0.41
13:g:50:GLN:HB3	13:g:54:LYS:HZ2	1.86	0.41
15:b:71:VAL:HG13	15:b:72:LYS:N	2.36	0.41
18:e:34:PRO:C	18:e:38:GLU:OE1	2.63	0.41
1:A:289:PRO:O	1:A:294:TYR:O	2.39	0.41
1:A:390:MET:HE1	1:A:428:LEU:CD2	2.41	0.41
2:D:386:ASP:O	2:D:389:ALA:HB3	2.20	0.41
2:E:49:VAL:HA	2:E:60:THR:HG22	2.03	0.41
2:E:186:VAL:HA	2:E:232:VAL:HG11	2.03	0.41
2:E:187:GLY:O	2:E:260:ARG:NE	2.54	0.41
2:E:334:VAL:O	2:E:334:VAL:HG12	2.21	0.41
2:F:298:THR:O	2:F:298:THR:HG23	2.21	0.41
4:H:35:GLN:NE2	7:Q:41:SER:HG	2.19	0.41
7:O:54:PHE:CD2	7:O:54:PHE:C	2.97	0.41
7:O:59:ALA:HB3	7:O:60:MET:HE2	2.03	0.41
7:P:48:SER:O	7:P:51:ILE:HG12	2.21	0.41
7:P:58:GLU:O	7:P:59:ALA:C	2.63	0.41
8:S:39:LEU:HD12	8:S:105:PHE:CD1	2.56	0.41
10:a:30:LEU:CD2	12:f:59:LEU:HD11	2.50	0.41
10:a:71:MET:HA	10:a:74:SER:OG	2.21	0.41
10:a:103:GLY:HA2	14:j:31:MET:HE3	2.03	0.41
10:a:103:GLY:O	10:a:107:PRO:HG3	2.20	0.41
11:d:106:GLN:HA	11:d:109:THR:HG22	2.02	0.41
11:d:134:ASP:O	11:d:138:VAL:HG23	2.21	0.41
14:j:28:THR:O	14:j:31:MET:HB3	2.21	0.41
15:b:129:ARG:HG3	15:b:130:ASN:N	2.36	0.41
16:h:32:GLY:O	16:h:35:TYR:HB3	2.21	0.41
1:B:110:ALA:HB3	1:B:242:LEU:HD22	2.03	0.41
1:C:156:LEU:HD22	1:C:367:VAL:HG11	2.02	0.41
2:F:256:ASP:HA	2:F:257:ASN:HA	1.88	0.41
2:F:402:LEU:HD11	2:F:406:ARG:CZ	2.51	0.41
10:a:78:PHE:CE1	10:a:82:THR:HG21	2.56	0.41
11:d:91:ALA:O	11:d:92:GLU:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:20:GLU:OE1	15:b:24:PHE:CE2	2.74	0.41
2:D:9:THR:HG22	2:D:27:GLU:HB2	2.03	0.40
2:E:452:LEU:HD22	2:E:470:ALA:CB	2.51	0.40
7:M:51:ILE:HD13	7:M:51:ILE:HA	1.95	0.40
7:O:18:VAL:HG23	7:P:64:CYS:SG	2.61	0.40
7:P:17:GLY:HA3	7:P:64:CYS:SG	2.61	0.40
8:S:109:MET:HE3	8:S:109:MET:CA	2.50	0.40
15:b:52:VAL:O	15:b:52:VAL:HG23	2.20	0.40
15:b:155:LEU:HD12	15:b:156:ASP:N	2.36	0.40
18:e:19:PHE:O	18:e:22:MET:HB2	2.21	0.40
18:e:34:PRO:O	18:e:35:ARG:C	2.61	0.40
1:C:452:TYR:O	1:C:505:LEU:HD22	2.22	0.40
1:C:465:GLU:O	1:C:466:ASN:C	2.65	0.40
2:D:153:GLY:HA3	2:D:329:LEU:HD13	2.03	0.40
2:E:63:MET:HE3	2:E:82:ILE:HD11	2.03	0.40
2:E:277:SER:OG	2:E:278:ALA:N	2.49	0.40
2:E:390:ILE:HG23	3:G:28:ALA:HB1	2.02	0.40
2:F:26:ASP:OD1	2:F:27:GLU:OE1	2.39	0.40
3:G:106:ILE:HG23	3:G:126:VAL:O	2.21	0.40
4:H:143:LYS:NZ	7:P:41:SER:HA	2.36	0.40
7:M:33:ILE:HG21	7:N:32:LEU:HA	2.04	0.40
8:S:109:MET:HE3	8:S:109:MET:HA	2.02	0.40
12:f:43:ARG:NH1	23:f:103:LHG:O4	2.54	0.40
18:e:11:LYS:O	18:e:14:ARG:HB3	2.21	0.40
1:A:52:MET:HE1	1:A:76:PHE:CE1	2.56	0.40
1:A:94:ILE:HG22	1:A:95:VAL:N	2.36	0.40
1:A:137:ILE:N	1:A:138:PRO:CD	2.85	0.40
1:A:292:GLU:O	1:A:293:ALA:HB3	2.22	0.40
1:C:180:ILE:HD11	1:C:216:LEU:HD11	2.02	0.40
1:C:403:PHE:CZ	6:J:32:ARG:HB2	2.56	0.40
3:G:194:ASP:OD2	4:H:52:VAL:HG21	2.22	0.40
8:S:102:ILE:HG13	8:S:103:SER:N	2.36	0.40
10:a:26:PHE:O	10:a:27:PRO:C	2.64	0.40
12:f:16:LEU:HD21	13:g:65:LYS:C	2.47	0.40
1:A:171:ARG:O	1:A:172:GLN:C	2.64	0.40
1:A:269:ASP:HA	1:A:270:ASP:HA	1.87	0.40
2:E:103:ASP:O	2:E:104:GLU:C	2.65	0.40
2:E:366:GLU:O	2:E:370:VAL:HG23	2.21	0.40
2:F:151:LYS:HD2	2:F:328:HIS:O	2.22	0.40
2:F:188:GLU:HG3	2:F:189:ARG:N	2.37	0.40
5:I:46:LYS:NZ	5:I:47:VAL:O	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:32:LEU:C	7:L:32:LEU:HD23	2.46	0.40
9:8:31:HIS:HB2	11:d:152:TRP:HH2	1.85	0.40
12:f:63:LEU:O	12:f:64:ALA:C	2.63	0.40
22:f:101:CDL:OA2	14:j:8:LYS:NZ	2.52	0.40
15:b:68:VAL:HA	15:b:71:VAL:HG12	2.02	0.40
16:h:40:ASP:O	16:h:44:PHE:CG	2.74	0.40
1:B:28:THR:OG1	1:B:87:ILE:HG23	2.22	0.40
1:B:75:VAL:HG11	1:B:82:ILE:HD11	2.03	0.40
4:H:130:GLU:HG3	5:I:17:ILE:HD11	2.04	0.40
5:I:2:ALA:O	5:I:6:GLN:HG2	2.21	0.40
7:L:70:LEU:O	7:L:75:MET:N	2.54	0.40
7:N:25:ILE:HA	7:N:28:VAL:HG12	2.04	0.40
7:N:73:PHE:N	7:N:73:PHE:CD1	2.89	0.40
10:a:184:ILE:O	10:a:185:SER:C	2.63	0.40
11:d:104:LEU:O	11:d:108:LYS:HG3	2.22	0.40
12:f:51:VAL:HG23	12:f:54:GLY:N	2.37	0.40
12:f:52:LYS:CG	15:b:5:LEU:HD23	2.44	0.40
13:g:45:ILE:CD1	18:e:12:LEU:HD11	2.51	0.40
15:b:67:LEU:HD23	15:b:67:LEU:HA	1.96	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	484/510 (95%)	444 (92%)	40 (8%)	0	100	100
1	B	491/510 (96%)	451 (92%)	40 (8%)	0	100	100
1	C	497/510 (98%)	461 (93%)	36 (7%)	0	100	100
2	D	467/482 (97%)	419 (90%)	48 (10%)	0	100	100
2	E	465/482 (96%)	432 (93%)	33 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	465/482 (96%)	422 (91%)	43 (9%)	0	100	100
3	G	270/273 (99%)	256 (95%)	14 (5%)	0	100	100
4	H	130/146 (89%)	115 (88%)	15 (12%)	0	100	100
5	I	45/50 (90%)	41 (91%)	4 (9%)	0	100	100
6	J	45/66 (68%)	42 (93%)	3 (7%)	0	100	100
7	K	71/75 (95%)	60 (84%)	11 (16%)	0	100	100
7	L	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
7	M	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
7	N	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
7	O	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
7	P	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
7	Q	71/75 (95%)	65 (92%)	6 (8%)	0	100	100
7	R	71/75 (95%)	66 (93%)	5 (7%)	0	100	100
8	S	186/190 (98%)	175 (94%)	11 (6%)	0	100	100
9	8	36/66 (54%)	29 (81%)	7 (19%)	0	100	100
10	a	224/226 (99%)	201 (90%)	23 (10%)	0	100	100
11	d	152/160 (95%)	133 (88%)	19 (12%)	0	100	100
12	f	81/87 (93%)	73 (90%)	8 (10%)	0	100	100
13	g	77/102 (76%)	68 (88%)	9 (12%)	0	100	100
14	j	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
15	b	207/214 (97%)	200 (97%)	7 (3%)	0	100	100
16	h	60/76 (79%)	49 (82%)	11 (18%)	0	100	100
17	k	34/57 (60%)	33 (97%)	1 (3%)	0	100	100
18	e	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
All	All	5085/5419 (94%)	4670 (92%)	415 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	393/412 (95%)	393 (100%)	0	100	100
1	B	401/412 (97%)	401 (100%)	0	100	100
1	C	406/412 (98%)	406 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	377/386 (98%)	377 (100%)	0	100	100
2	F	377/386 (98%)	377 (100%)	0	100	100
3	G	230/231 (100%)	230 (100%)	0	100	100
4	H	105/109 (96%)	105 (100%)	0	100	100
5	I	38/41 (93%)	38 (100%)	0	100	100
6	J	34/50 (68%)	34 (100%)	0	100	100
7	K	49/50 (98%)	49 (100%)	0	100	100
7	L	50/50 (100%)	50 (100%)	0	100	100
7	M	49/50 (98%)	49 (100%)	0	100	100
7	N	49/50 (98%)	49 (100%)	0	100	100
7	O	49/50 (98%)	49 (100%)	0	100	100
7	P	49/50 (98%)	49 (100%)	0	100	100
7	Q	49/50 (98%)	49 (100%)	0	100	100
7	R	49/50 (98%)	49 (100%)	0	100	100
8	S	163/165 (99%)	163 (100%)	0	100	100
9	8	38/66 (58%)	38 (100%)	0	100	100
10	a	200/200 (100%)	200 (100%)	0	100	100
11	d	138/142 (97%)	138 (100%)	0	100	100
12	f	72/75 (96%)	72 (100%)	0	100	100
13	g	67/83 (81%)	67 (100%)	0	100	100
14	j	42/49 (86%)	42 (100%)	0	100	100
15	b	186/190 (98%)	186 (100%)	0	100	100
16	h	56/70 (80%)	56 (100%)	0	100	100
17	k	31/46 (67%)	31 (100%)	0	100	100
18	e	47/59 (80%)	47 (100%)	0	100	100
All	All	4173/4370 (96%)	4173 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	B	172	GLN
1	B	302	HIS
1	C	302	HIS
1	C	366	ASN
1	C	396	GLN
1	C	475	GLN
1	C	476	HIS
2	D	207	ASN
2	D	411	GLN
2	D	451	HIS
2	D	455	GLN
2	F	39	GLN
2	F	246	GLN
4	H	15	GLN
4	H	66	HIS
4	H	138	ASN
8	S	34	GLN
10	a	56	GLN
10	a	152	GLN
12	f	70	ASN
15	b	209	GLN
18	e	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
7	M3L	O	43	7	10,11,12	0.46	0	9,14,16	0.69	0
7	M3L	R	43	7	10,11,12	0.55	0	9,14,16	0.56	0
7	M3L	K	43	7	10,11,12	0.52	0	9,14,16	0.61	0
7	M3L	Q	43	7	10,11,12	0.51	0	9,14,16	0.56	0
7	M3L	N	43	7	10,11,12	0.45	0	9,14,16	0.43	0
7	M3L	P	43	7	10,11,12	0.51	0	9,14,16	0.55	0
7	M3L	L	43	7	10,11,12	0.43	0	9,14,16	0.61	0
7	M3L	M	43	7	10,11,12	0.61	0	9,14,16	0.50	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
7	M3L	O	43	7	-	7/9/10/12	-
7	M3L	R	43	7	-	1/9/10/12	-
7	M3L	K	43	7	-	5/9/10/12	-
7	M3L	Q	43	7	-	0/9/10/12	-
7	M3L	N	43	7	-	3/9/10/12	-
7	M3L	P	43	7	-	2/9/10/12	-
7	M3L	L	43	7	-	3/9/10/12	-
7	M3L	M	43	7	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	43	M3L	C-CA-CB-CG
7	N	43	M3L	O-C-CA-CB
7	O	43	M3L	C-CA-CB-CG
7	O	43	M3L	O-C-CA-CB
7	O	43	M3L	CG-CD-CE-NZ
7	O	43	M3L	CD-CE-NZ-CM3
7	O	43	M3L	CD-CE-NZ-CM1
7	N	43	M3L	CA-CB-CG-CD
7	K	43	M3L	CE-CD-CG-CB
7	O	43	M3L	CD-CE-NZ-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	43	M3L	CE-CD-CG-CB
7	P	43	M3L	CE-CD-CG-CB
7	O	43	M3L	CE-CD-CG-CB
7	K	43	M3L	CD-CE-NZ-CM1
7	N	43	M3L	CE-CD-CG-CB
7	L	43	M3L	N-CA-CB-CG
7	R	43	M3L	N-CA-CB-CG
7	K	43	M3L	CD-CE-NZ-CM3
7	K	43	M3L	CD-CE-NZ-CM2
7	L	43	M3L	CG-CD-CE-NZ
7	P	43	M3L	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	43	M3L	1	0
7	P	43	M3L	1	0
7	L	43	M3L	2	0
7	M	43	M3L	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
22	CDL	f	101	-	83,83,99	1.00	7 (8%)	89,95,111	1.08	4 (4%)
22	CDL	b	301	-	82,82,99	1.00	6 (7%)	88,94,111	1.16	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	f	103	-	38,38,48	0.75	1 (2%)	41,44,54	1.30	4 (9%)
19	ATP	C	600	20	32,33,33	1.29	6 (18%)	48,52,52	1.84	11 (22%)
23	LHG	b	302	-	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
21	ADP	E	600	-	28,29,29	1.40	5 (17%)	43,45,45	1.85	12 (27%)
21	ADP	D	600	20	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
19	ATP	A	600	20	32,33,33	1.27	5 (15%)	48,52,52	1.86	11 (22%)
21	ADP	F	600	20	28,29,29	1.40	5 (17%)	43,45,45	1.87	10 (23%)
19	ATP	B	600	20	32,33,33	1.28	5 (15%)	48,52,52	1.83	12 (25%)
22	CDL	f	102	-	77,77,99	1.02	7 (9%)	83,89,111	1.15	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	f	101	-	-	30/94/94/110	-
22	CDL	b	301	-	-	38/93/93/110	-
23	LHG	f	103	-	-	21/43/43/53	-
19	ATP	C	600	20	-	5/22/38/38	0/3/3/3
23	LHG	b	302	-	-	17/53/53/53	-
21	ADP	E	600	-	-	5/16/32/32	0/3/3/3
21	ADP	D	600	20	-	8/16/32/32	0/3/3/3
19	ATP	A	600	20	-	0/22/38/38	0/3/3/3
21	ADP	F	600	20	-	6/16/32/32	0/3/3/3
19	ATP	B	600	20	-	4/22/38/38	0/3/3/3
22	CDL	f	102	-	-	35/88/88/110	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	600	ADP	C5-C4	4.32	1.46	1.39
19	B	600	ATP	C5-C4	4.10	1.46	1.39
21	F	600	ADP	C5-C4	4.02	1.46	1.39
19	C	600	ATP	C5-C4	4.00	1.46	1.39
21	D	600	ADP	C5-C4	4.00	1.46	1.39
19	A	600	ATP	C5-C4	3.99	1.46	1.39
22	b	301	CDL	OA6-CA4	-3.08	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	600	ADP	C5-N7	-3.03	1.33	1.39
21	F	600	ADP	C5-N7	-3.00	1.33	1.39
22	f	102	CDL	OA6-CA4	-2.84	1.39	1.46
22	f	101	CDL	OA6-CA4	-2.80	1.40	1.46
22	f	101	CDL	OB6-CB4	-2.80	1.40	1.46
22	b	301	CDL	OB8-CB7	2.76	1.41	1.33
23	f	103	LHG	O7-C5	-2.75	1.40	1.46
22	f	102	CDL	OB8-CB7	2.75	1.41	1.33
19	A	600	ATP	C5-N7	-2.75	1.34	1.39
19	B	600	ATP	C5-N7	-2.74	1.34	1.39
22	b	301	CDL	OB6-CB4	-2.71	1.40	1.46
19	C	600	ATP	C5-N7	-2.70	1.34	1.39
22	f	101	CDL	OB8-CB7	2.68	1.41	1.33
21	E	600	ADP	C5-N7	-2.64	1.34	1.39
22	f	102	CDL	OB6-CB4	-2.63	1.40	1.46
22	f	102	CDL	OA8-CA6	-2.49	1.39	1.45
21	D	600	ADP	C4-N9	-2.46	1.32	1.37
22	f	102	CDL	OB6-CB5	2.43	1.41	1.34
21	E	600	ADP	C5-C6	2.43	1.47	1.41
22	b	301	CDL	OB6-CB5	2.39	1.41	1.34
23	b	302	LHG	O7-C5	-2.36	1.41	1.46
22	f	101	CDL	OA8-CA6	-2.32	1.40	1.45
22	f	101	CDL	OB6-CB5	2.32	1.40	1.34
19	C	600	ATP	C4-N9	-2.31	1.32	1.37
19	C	600	ATP	C5-C6	2.30	1.47	1.41
21	F	600	ADP	C5-C6	2.28	1.47	1.41
19	B	600	ATP	C4-N9	-2.27	1.33	1.37
21	E	600	ADP	C4-N9	-2.26	1.33	1.37
22	f	101	CDL	OA8-CA7	2.26	1.39	1.33
22	b	301	CDL	OA8-CA7	2.25	1.39	1.33
21	E	600	ADP	C8-N7	2.22	1.36	1.31
21	F	600	ADP	C4-N9	-2.19	1.33	1.37
19	B	600	ATP	C5-C6	2.18	1.47	1.41
22	f	102	CDL	OA8-CA7	2.18	1.39	1.33
19	C	600	ATP	C8-N7	2.16	1.35	1.31
22	b	301	CDL	OA8-CA6	-2.16	1.40	1.45
19	A	600	ATP	C5-C6	2.13	1.46	1.41
19	A	600	ATP	C4-N9	-2.12	1.33	1.37
21	F	600	ADP	C8-N9	-2.11	1.34	1.37
19	B	600	ATP	C8-N7	2.10	1.35	1.31
19	C	600	ATP	C8-N9	-2.07	1.34	1.37
21	D	600	ADP	C8-N9	-2.07	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	600	ADP	C5-C6	2.06	1.46	1.41
22	f	101	CDL	OA6-CA5	2.06	1.40	1.34
22	f	102	CDL	OA6-CA5	2.02	1.40	1.34
19	A	600	ATP	C8-N7	2.01	1.35	1.31

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	600	ATP	C5-C4-N3	-6.08	118.34	126.72
21	F	600	ADP	C5-C4-N3	-6.06	118.38	126.72
19	C	600	ATP	C5-C4-N3	-5.76	118.78	126.72
21	D	600	ADP	C5-C4-N3	-5.62	118.97	126.72
19	B	600	ATP	C5-C4-N3	-5.59	119.02	126.72
21	E	600	ADP	C5-C4-N3	-5.38	119.31	126.72
19	A	600	ATP	N3-C4-N9	4.91	135.52	127.17
21	F	600	ADP	N3-C4-N9	4.84	135.40	127.17
21	D	600	ADP	N3-C4-N9	4.61	135.00	127.17
19	B	600	ATP	N3-C4-N9	4.54	134.90	127.17
23	b	302	LHG	O4-P-O5	4.47	133.23	112.44
19	C	600	ATP	N3-C4-N9	4.42	134.68	127.17
23	f	103	LHG	O4-P-O5	4.38	132.80	112.44
22	b	301	CDL	OB6-CB5-C51	4.28	120.73	111.48
21	E	600	ADP	N3-C4-N9	4.18	134.28	127.17
22	f	102	CDL	OA6-CA5-C11	4.16	120.47	111.48
22	f	101	CDL	OA6-CA5-C11	4.00	120.14	111.48
22	f	102	CDL	OB6-CB5-C51	3.92	119.96	111.48
21	F	600	ADP	C2-N3-C4	3.85	121.24	111.83
21	D	600	ADP	N3-C2-N1	-3.82	122.80	128.58
19	A	600	ATP	C2-N3-C4	3.81	121.14	111.83
19	C	600	ATP	C2-N3-C4	3.78	121.06	111.83
21	E	600	ADP	N3-C2-N1	-3.75	122.90	128.58
21	D	600	ADP	C2-N3-C4	3.75	120.98	111.83
22	b	301	CDL	OA6-CA5-C11	3.74	119.57	111.48
21	E	600	ADP	C2-N3-C4	3.68	120.83	111.83
19	C	600	ATP	N3-C2-N1	-3.65	123.06	128.58
21	F	600	ADP	N3-C2-N1	-3.62	123.10	128.58
19	B	600	ATP	C2-N3-C4	3.61	120.65	111.83
22	f	101	CDL	OB6-CB5-C51	3.61	119.28	111.48
19	C	600	ATP	C4-C5-N7	-3.58	106.49	110.58
21	E	600	ADP	C4-C5-N7	-3.57	106.50	110.58
19	B	600	ATP	N3-C2-N1	-3.54	123.22	128.58
19	A	600	ATP	N3-C2-N1	-3.51	123.28	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	600	ADP	C4-C5-N7	-3.41	106.68	110.58
19	A	600	ATP	C4-C5-N7	-3.28	106.84	110.58
19	B	600	ATP	C4-C5-N7	-3.26	106.86	110.58
22	b	301	CDL	OA8-CA7-C31	3.16	121.46	111.83
21	D	600	ADP	C4-C5-N7	-3.09	107.05	110.58
19	B	600	ATP	C4-N9-C8	3.00	108.89	105.74
21	D	600	ADP	C4-N9-C8	2.89	108.77	105.74
19	A	600	ATP	C4-N9-C8	2.83	108.71	105.74
21	E	600	ADP	C4-N9-C8	2.83	108.70	105.74
23	b	302	LHG	O8-C23-C24	2.80	120.38	111.83
23	f	103	LHG	O8-C23-C24	2.76	120.25	111.83
19	C	600	ATP	C4-N9-C8	2.75	108.63	105.74
21	F	600	ADP	C4-N9-C8	2.72	108.59	105.74
22	f	102	CDL	OB8-CB7-C71	2.69	120.02	111.83
22	f	101	CDL	OA8-CA7-C31	2.67	119.97	111.83
21	F	600	ADP	C5-N7-C8	2.66	107.63	103.45
22	f	102	CDL	OA8-CA7-C31	2.64	119.89	111.83
21	E	600	ADP	C5-N7-C8	2.59	107.52	103.45
19	C	600	ATP	C5-N7-C8	2.58	107.51	103.45
19	A	600	ATP	C5-N7-C8	2.55	107.46	103.45
19	A	600	ATP	C3'-C2'-C1'	2.54	106.27	101.46
19	B	600	ATP	C5-N7-C8	2.50	107.39	103.45
22	b	301	CDL	OB8-CB7-C71	2.50	119.44	111.83
21	E	600	ADP	C3'-C2'-C1'	2.42	106.03	101.46
19	C	600	ATP	C3'-C2'-C1'	2.40	106.01	101.46
21	D	600	ADP	C5-N7-C8	2.39	107.21	103.45
23	b	302	LHG	C11-C10-C9	-2.39	102.30	114.37
19	B	600	ATP	C3'-C2'-C1'	2.36	105.93	101.46
21	E	600	ADP	C2-N1-C6	2.35	122.60	118.73
22	f	101	CDL	OB8-CB7-C71	2.31	118.87	111.83
19	B	600	ATP	O4'-C1'-N9	2.27	112.45	108.09
21	E	600	ADP	C6-C5-N7	2.25	136.43	132.09
19	B	600	ATP	N9-C8-N7	-2.22	110.78	113.94
21	D	600	ADP	C2-N1-C6	2.22	122.38	118.73
21	E	600	ADP	C2'-C1'-N9	-2.21	107.82	113.30
21	D	600	ADP	C2'-C1'-N9	-2.20	107.84	113.30
19	C	600	ATP	N9-C8-N7	-2.19	110.83	113.94
19	B	600	ATP	C2'-C1'-N9	-2.17	107.90	113.30
22	b	301	CDL	CB4-OB6-CB5	-2.17	112.61	117.80
23	f	103	LHG	C27-C26-C25	-2.17	103.42	114.37
21	E	600	ADP	N9-C8-N7	-2.17	110.86	113.94
23	b	302	LHG	C20-C19-C18	-2.17	103.42	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	600	ATP	N9-C8-N7	-2.16	110.87	113.94
19	A	600	ATP	O4'-C1'-N9	2.16	112.24	108.09
22	f	102	CDL	CB4-OB6-CB5	-2.16	112.64	117.80
23	f	103	LHG	C5-O7-C7	-2.16	112.64	117.80
21	F	600	ADP	N9-C8-N7	-2.15	110.88	113.94
19	C	600	ATP	C6-C5-N7	2.15	136.23	132.09
19	A	600	ATP	C2'-C1'-N9	-2.11	108.06	113.30
21	D	600	ADP	N9-C8-N7	-2.11	110.95	113.94
21	F	600	ADP	C2'-C1'-N9	-2.10	108.09	113.30
23	b	302	LHG	C18-C17-C16	-2.10	103.76	114.37
19	C	600	ATP	C2-N1-C6	2.10	122.17	118.73
23	b	302	LHG	C27-C26-C25	-2.06	103.97	114.37
21	F	600	ADP	C2-N1-C6	2.02	122.05	118.73
19	B	600	ATP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	600	ATP	C5'-O5'-PA-O1A
19	C	600	ATP	C5'-O5'-PA-O1A
19	C	600	ATP	C5'-O5'-PA-O3A
21	D	600	ADP	C5'-O5'-PA-O1A
21	D	600	ADP	C5'-O5'-PA-O3A
21	E	600	ADP	C5'-O5'-PA-O1A
21	E	600	ADP	C5'-O5'-PA-O2A
21	E	600	ADP	C5'-O5'-PA-O3A
22	f	101	CDL	CA2-OA2-PA1-OA4
22	f	101	CDL	CA2-OA2-PA1-OA5
22	f	102	CDL	C1-CA2-OA2-PA1
22	f	102	CDL	CA2-OA2-PA1-OA4
22	f	102	CDL	CA2-OA2-PA1-OA5
22	f	102	CDL	CB2-OB2-PB2-OB3
22	f	102	CDL	CB2-OB2-PB2-OB4
22	f	102	CDL	CB2-OB2-PB2-OB5
22	f	102	CDL	CB3-OB5-PB2-OB3
22	f	102	CDL	C51-CB5-OB6-CB4
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	CA3-OA5-PA1-OA2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	b	301	CDL	CA3-OA5-PA1-OA3
22	b	301	CDL	CB2-OB2-PB2-OB3
22	b	301	CDL	CB2-OB2-PB2-OB5
22	b	301	CDL	OB6-CB4-CB6-OB8
23	f	103	LHG	C3-O3-P-O5
23	f	103	LHG	C4-O6-P-O3
23	f	103	LHG	C4-O6-P-O4
23	b	302	LHG	C1-C2-C3-O3
23	f	103	LHG	O10-C23-O8-C6
22	f	102	CDL	OB7-CB5-OB6-CB4
22	f	101	CDL	C31-CA7-OA8-CA6
22	f	102	CDL	C31-CA7-OA8-CA6
23	f	103	LHG	C24-C23-O8-C6
22	f	101	CDL	OA9-CA7-OA8-CA6
22	f	102	CDL	OA9-CA7-OA8-CA6
23	f	103	LHG	O2-C2-C3-O3
23	b	302	LHG	O2-C2-C3-O3
19	C	600	ATP	O4'-C4'-C5'-O5'
23	f	103	LHG	C1-C2-C3-O3
22	f	101	CDL	CB5-C51-C52-C53
19	B	600	ATP	O4'-C4'-C5'-O5'
22	f	101	CDL	CA5-C11-C12-C13
22	f	102	CDL	CB5-C51-C52-C53
23	b	302	LHG	C7-C8-C9-C10
22	b	301	CDL	O1-C1-CB2-OB2
23	f	103	LHG	C8-C7-O7-C5
22	b	301	CDL	CA2-C1-CB2-OB2
21	E	600	ADP	O4'-C4'-C5'-O5'
21	F	600	ADP	O4'-C4'-C5'-O5'
22	f	101	CDL	C1-CB2-OB2-PB2
23	b	302	LHG	O1-C1-C2-C3
22	f	101	CDL	C52-C53-C54-C55
22	f	101	CDL	C11-CA5-OA6-CA4
21	D	600	ADP	O4'-C4'-C5'-O5'
22	f	102	CDL	C40-C41-C42-C43
22	b	301	CDL	CB5-C51-C52-C53
22	b	301	CDL	C60-C61-C62-C63
22	f	102	CDL	C37-C38-C39-C40
22	f	101	CDL	OA7-CA5-OA6-CA4
23	f	103	LHG	C11-C10-C9-C8
22	f	101	CDL	C75-C76-C77-C78
22	b	301	CDL	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	f	101	CDL	C57-C58-C59-C60
22	f	101	CDL	C12-C13-C14-C15
23	b	302	LHG	C31-C32-C33-C34
22	f	101	CDL	CA7-C31-C32-C33
23	b	302	LHG	C28-C29-C30-C31
22	f	101	CDL	C71-CB7-OB8-CB6
22	b	301	CDL	CB4-CB3-OB5-PB2
22	f	102	CDL	C42-C43-C44-C45
23	f	103	LHG	C13-C14-C15-C16
22	b	301	CDL	C54-C55-C56-C57
23	f	103	LHG	C12-C13-C14-C15
23	f	103	LHG	O9-C7-O7-C5
22	f	101	CDL	OB9-CB7-OB8-CB6
23	f	103	LHG	C4-C5-C6-O8
22	f	102	CDL	O1-C1-CB2-OB2
23	b	302	LHG	C23-C24-C25-C26
22	f	101	CDL	C74-C75-C76-C77
22	f	101	CDL	C54-C55-C56-C57
22	b	301	CDL	C14-C15-C16-C17
19	C	600	ATP	C3'-C4'-C5'-O5'
22	f	102	CDL	C71-CB7-OB8-CB6
22	f	102	CDL	C12-C13-C14-C15
22	f	102	CDL	C13-C14-C15-C16
22	b	301	CDL	C53-C54-C55-C56
23	f	103	LHG	C11-C12-C13-C14
23	b	302	LHG	C5-C4-O6-P
23	b	302	LHG	C13-C14-C15-C16
22	f	102	CDL	OA5-CA3-CA4-CA6
23	b	302	LHG	O6-C4-C5-C6
22	f	102	CDL	C17-C18-C19-C20
22	f	102	CDL	C32-C33-C34-C35
23	b	302	LHG	C15-C16-C17-C18
22	f	102	CDL	CA2-C1-CB2-OB2
22	f	102	CDL	OB9-CB7-OB8-CB6
19	B	600	ATP	C3'-C4'-C5'-O5'
21	F	600	ADP	C3'-C4'-C5'-O5'
22	b	301	CDL	C73-C74-C75-C76
22	f	101	CDL	C14-C15-C16-C17
22	f	102	CDL	C20-C21-C22-C23
22	f	102	CDL	C52-C53-C54-C55
19	B	600	ATP	PB-O3B-PG-O1G
21	D	600	ADP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	F	600	ADP	PA-O3A-PB-O1B
22	f	102	CDL	OA5-CA3-CA4-OA6
22	f	102	CDL	C74-C75-C76-C77
22	b	301	CDL	CB3-CB4-CB6-OB8
22	f	101	CDL	C16-C17-C18-C19
22	f	102	CDL	C18-C19-C20-C21
22	f	101	CDL	C13-C14-C15-C16
22	f	101	CDL	C77-C78-C79-C80
22	b	301	CDL	CA5-C11-C12-C13
22	b	301	CDL	C71-C72-C73-C74
22	f	101	CDL	OB5-CB3-CB4-CB6
22	f	101	CDL	OB5-CB3-CB4-OB6
23	b	302	LHG	O6-C4-C5-O7
23	f	103	LHG	O7-C5-C6-O8
19	C	600	ATP	C5'-O5'-PA-O2A
21	D	600	ADP	C5'-O5'-PA-O2A
22	f	101	CDL	CA3-OA5-PA1-OA3
22	f	102	CDL	CA3-OA5-PA1-OA3
22	b	301	CDL	CB2-OB2-PB2-OB4
23	f	103	LHG	C4-O6-P-O5
22	f	102	CDL	C1-CB2-OB2-PB2
22	f	102	CDL	CA7-C31-C32-C33
22	b	301	CDL	OB9-CB7-OB8-CB6
22	b	301	CDL	C13-C14-C15-C16
21	E	600	ADP	C3'-C4'-C5'-O5'
22	b	301	CDL	OB7-CB5-OB6-CB4
22	b	301	CDL	C51-CB5-OB6-CB4
22	b	301	CDL	C71-CB7-OB8-CB6
23	b	302	LHG	C11-C12-C13-C14
23	b	302	LHG	C34-C35-C36-C37
23	f	103	LHG	C9-C10-C11-C12
23	b	302	LHG	C27-C28-C29-C30
23	b	302	LHG	C32-C33-C34-C35
21	D	600	ADP	C3'-C4'-C5'-O5'
23	b	302	LHG	C14-C15-C16-C17
22	f	101	CDL	C33-C34-C35-C36
22	f	101	CDL	CA4-CA3-OA5-PA1
22	b	301	CDL	CA4-CA3-OA5-PA1
22	b	301	CDL	C64-C65-C66-C67
22	b	301	CDL	OA7-CA5-OA6-CA4
22	f	102	CDL	C72-C73-C74-C75
22	b	301	CDL	C72-C73-C74-C75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	b	301	CDL	C32-C31-CA7-OA8
22	f	101	CDL	C55-C56-C57-C58
22	b	301	CDL	C37-C38-C39-C40
21	D	600	ADP	PA-O3A-PB-O2B
21	D	600	ADP	PA-O3A-PB-O3B
21	F	600	ADP	PA-O3A-PB-O2B
21	F	600	ADP	PA-O3A-PB-O3B
22	f	101	CDL	C1-CA2-OA2-PA1
23	f	103	LHG	C23-C24-C25-C26
22	b	301	CDL	C11-CA5-OA6-CA4
22	b	301	CDL	C12-C13-C14-C15
23	f	103	LHG	C25-C26-C27-C28
22	f	102	CDL	OB5-CB3-CB4-OB6
22	b	301	CDL	C39-C40-C41-C42
23	f	103	LHG	C16-C17-C18-C19
22	f	101	CDL	C53-C54-C55-C56
23	f	103	LHG	C14-C15-C16-C17
22	f	102	CDL	C43-C44-C45-C46
22	b	301	CDL	C59-C60-C61-C62
21	F	600	ADP	PB-O3A-PA-O2A

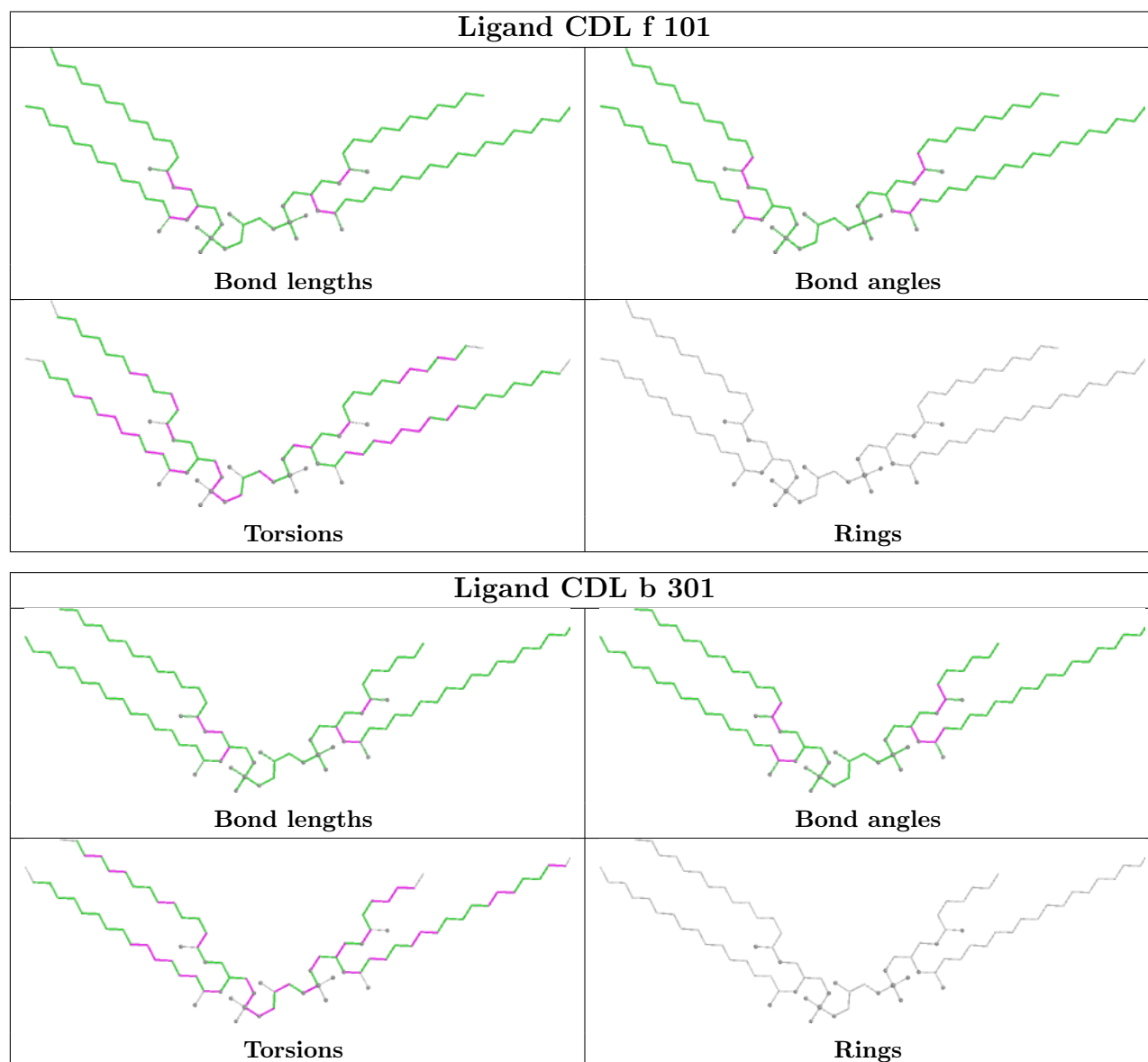
There are no ring outliers.

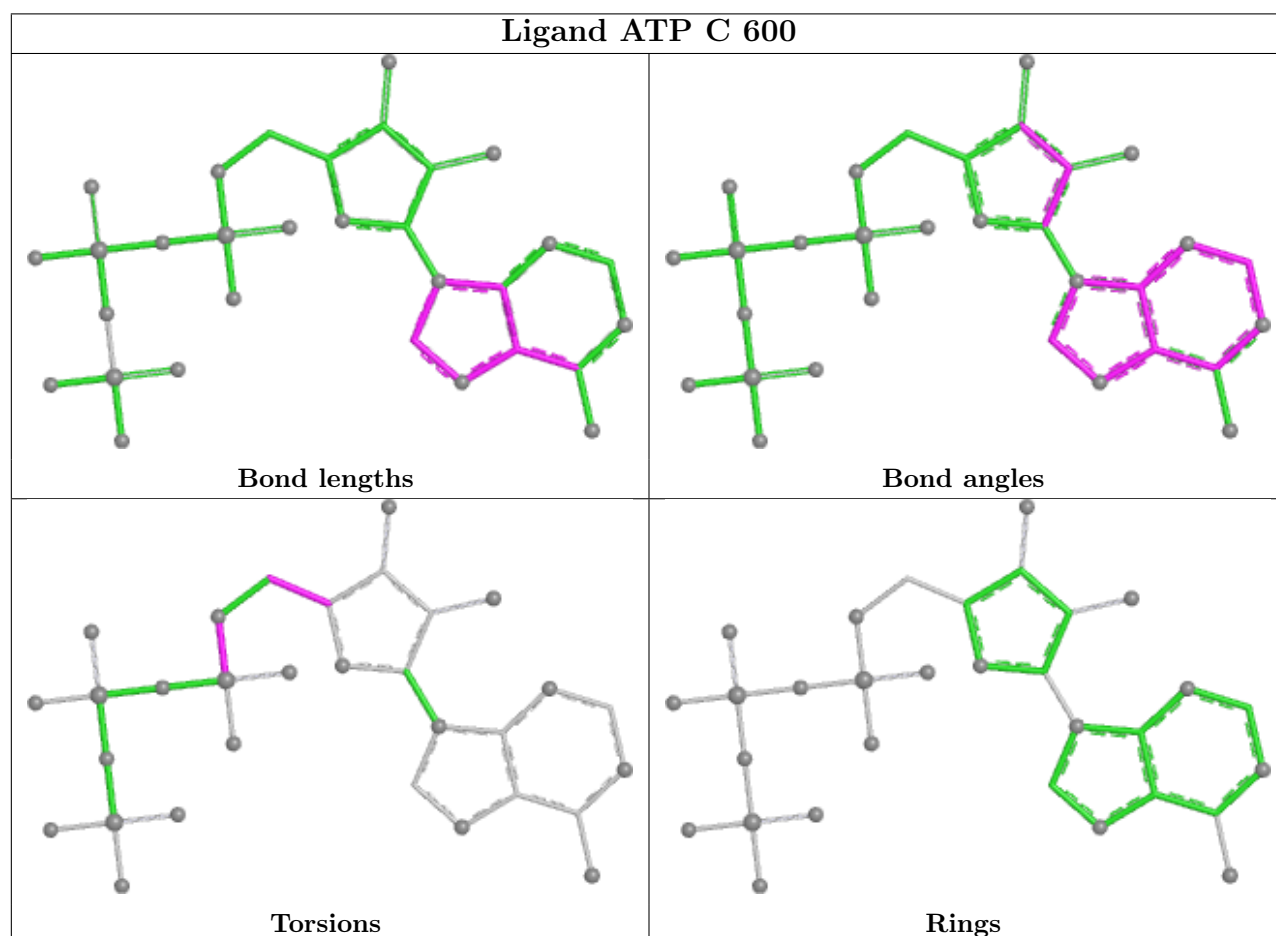
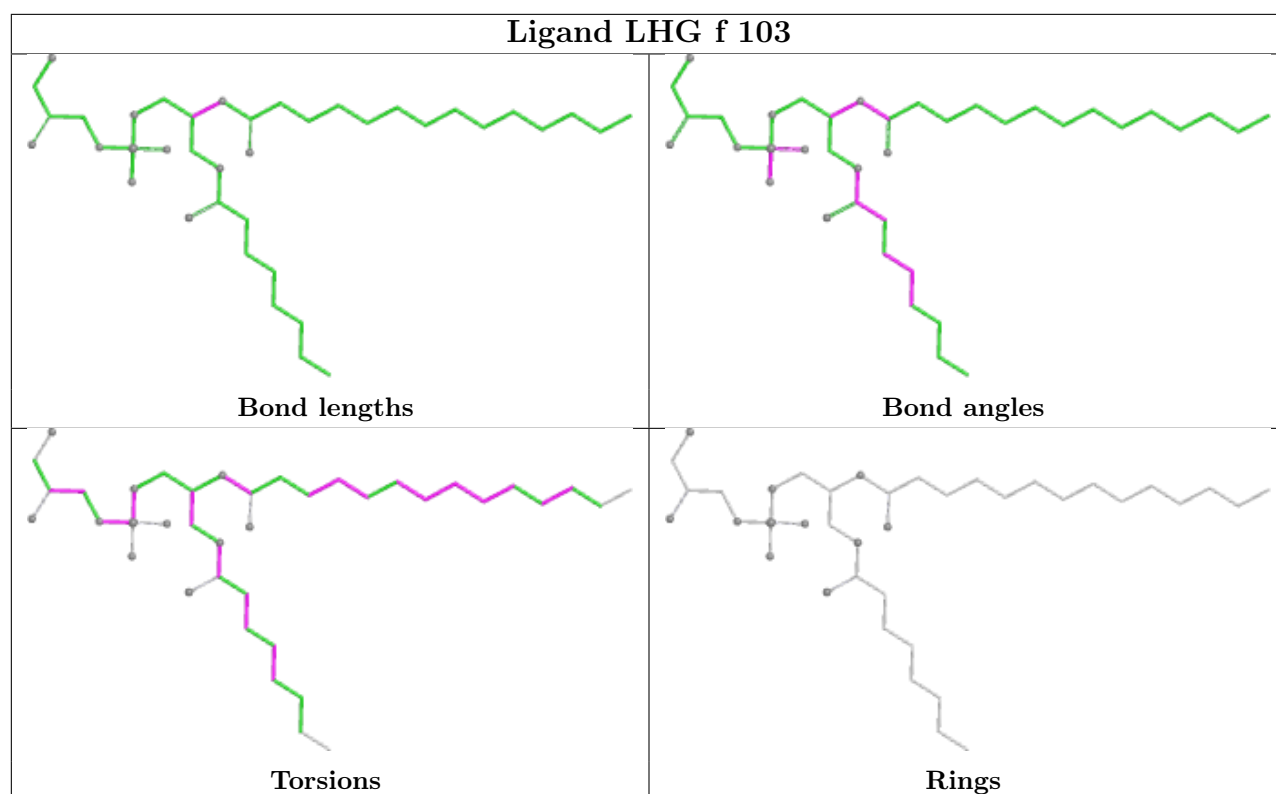
10 monomers are involved in 26 short contacts:

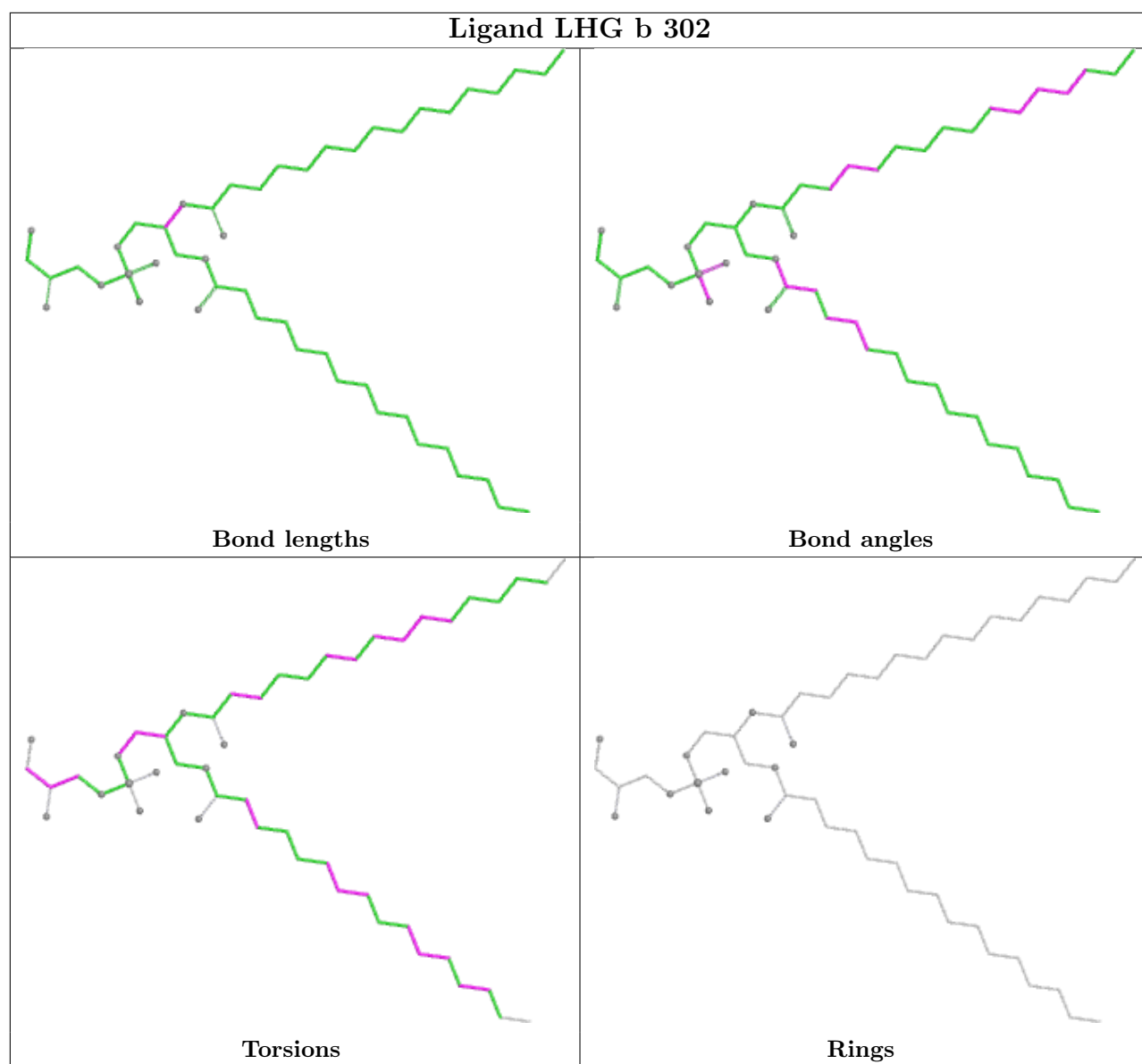
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	f	101	CDL	4	0
22	b	301	CDL	2	0
23	f	103	LHG	8	0
23	b	302	LHG	1	0
21	E	600	ADP	1	0
21	D	600	ADP	1	0
19	A	600	ATP	1	0
21	F	600	ADP	2	0
19	B	600	ATP	1	0
22	f	102	CDL	6	0

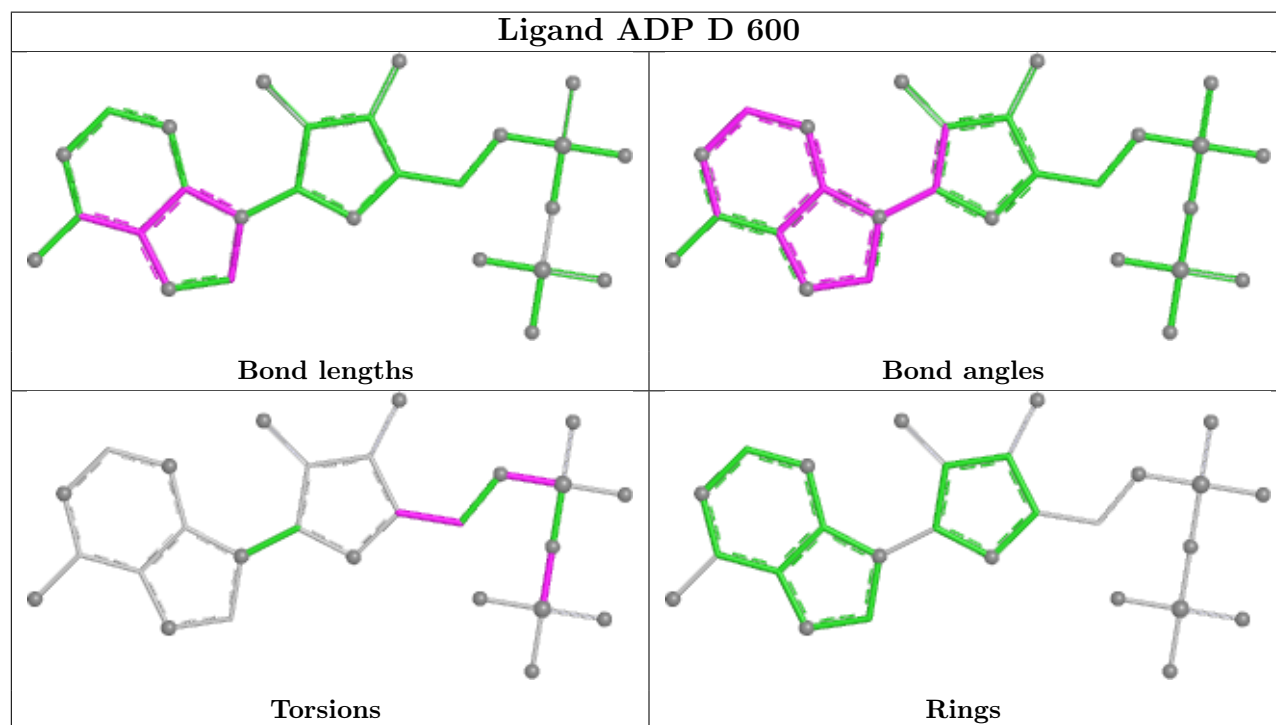
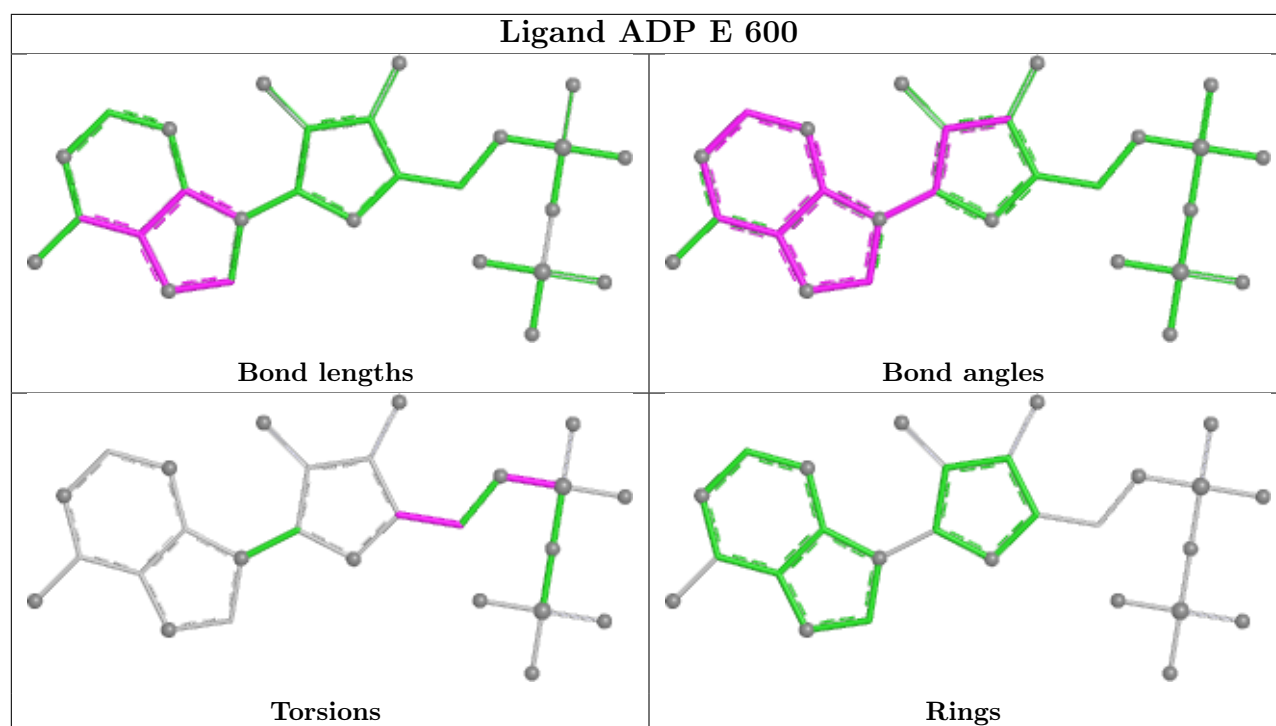
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

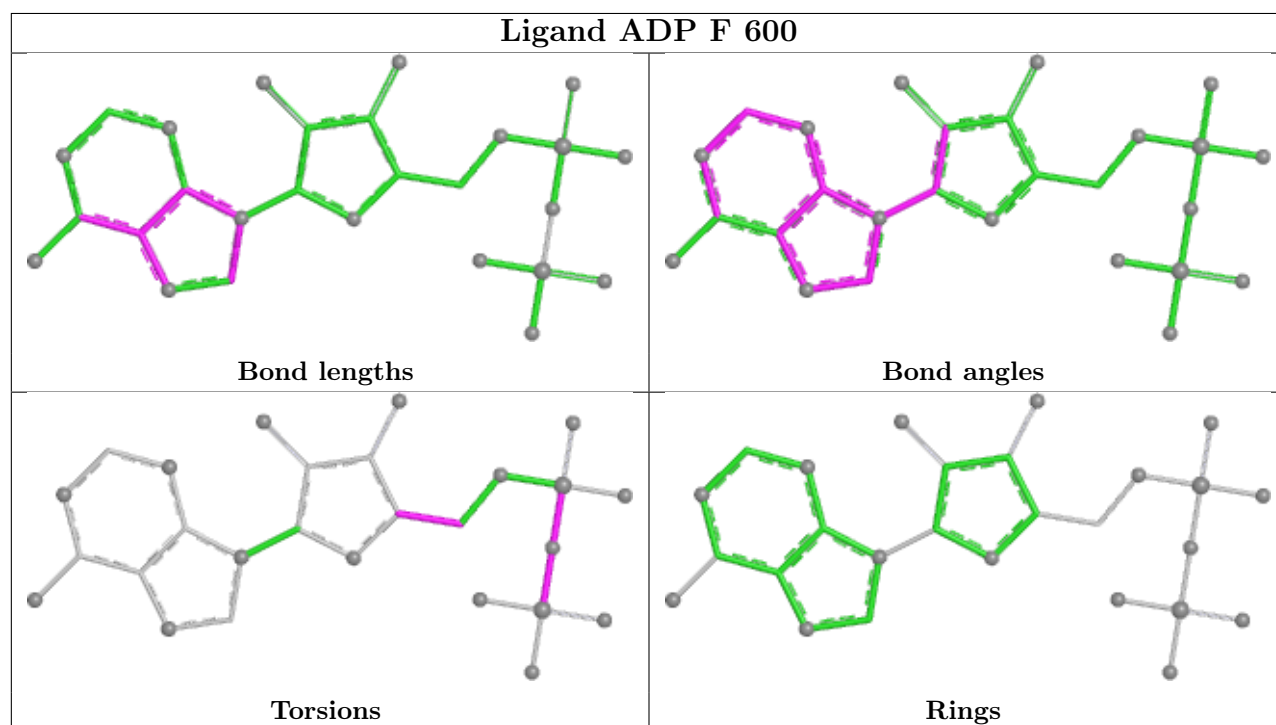
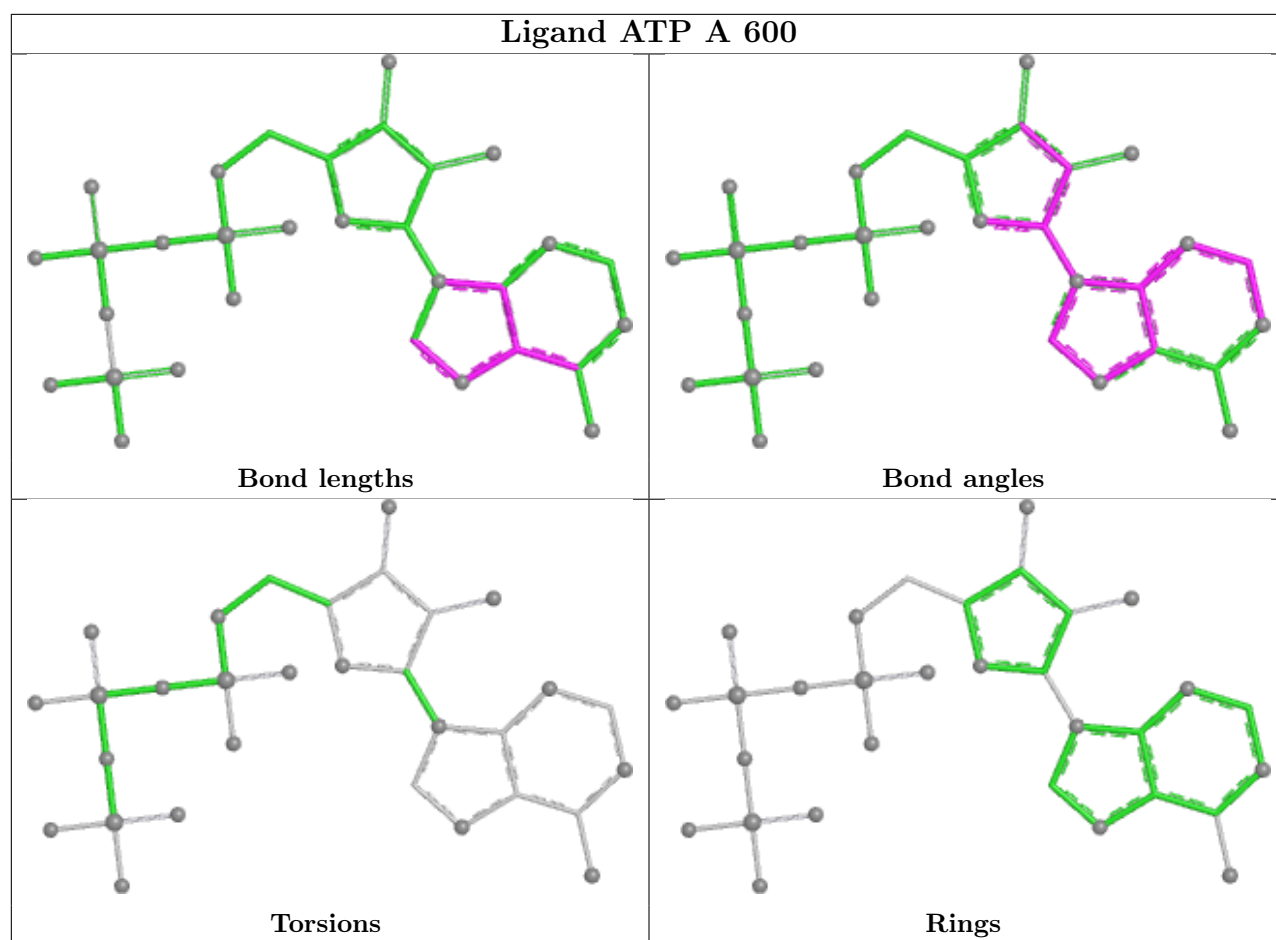
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

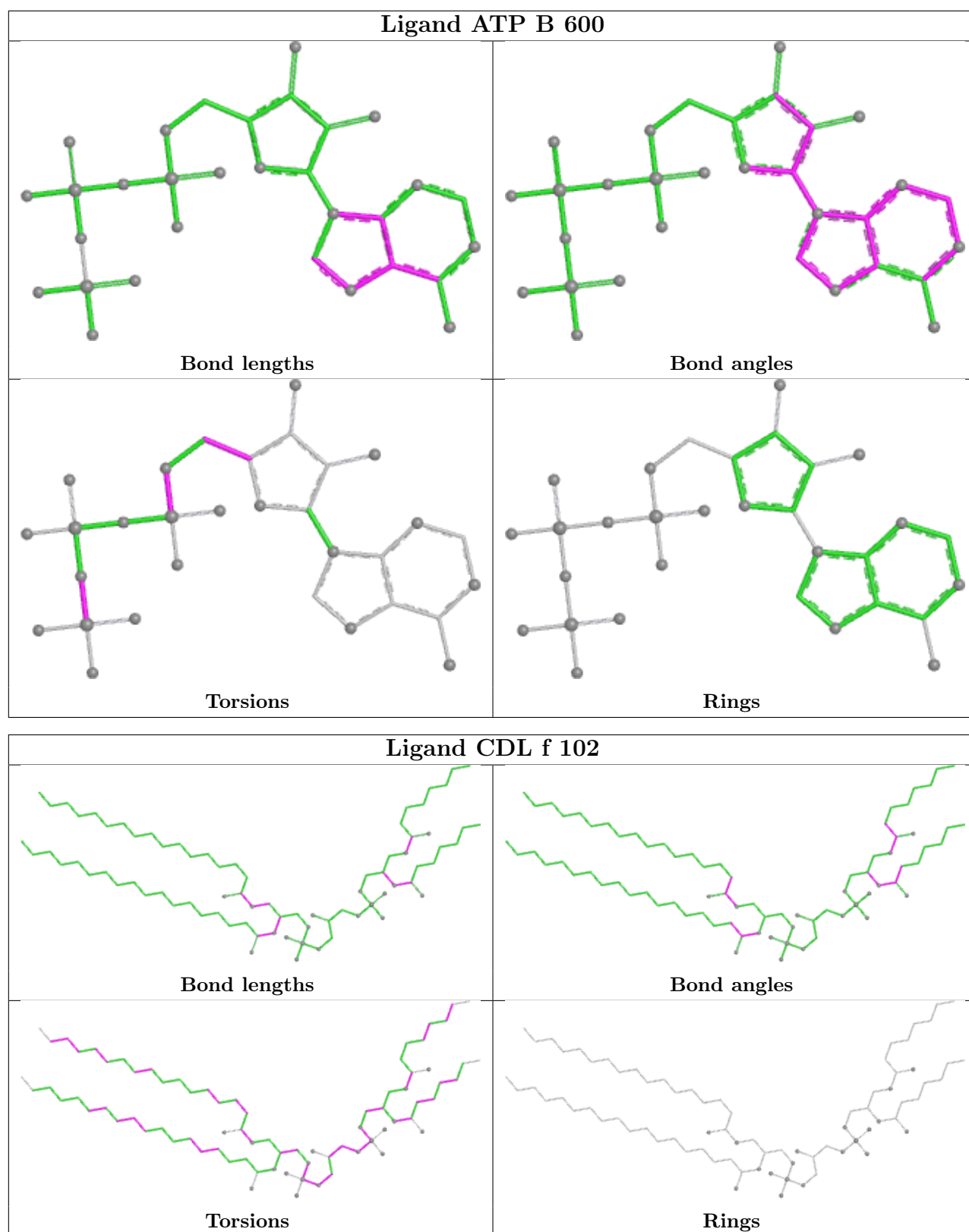












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

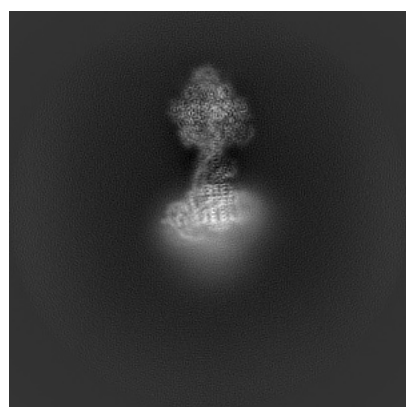
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11368. These allow visual inspection of the internal detail of the map and identification of artifacts.

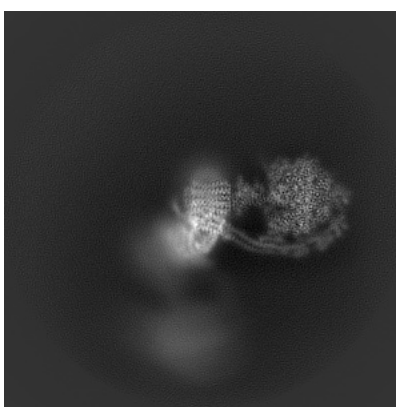
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

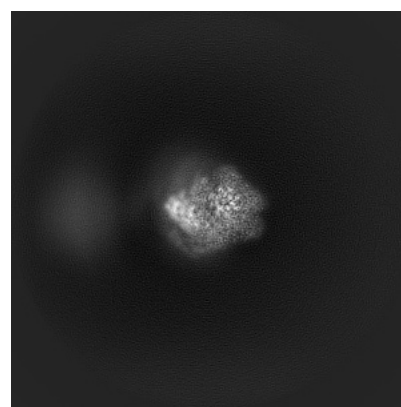
6.1.1 Primary map



X



Y

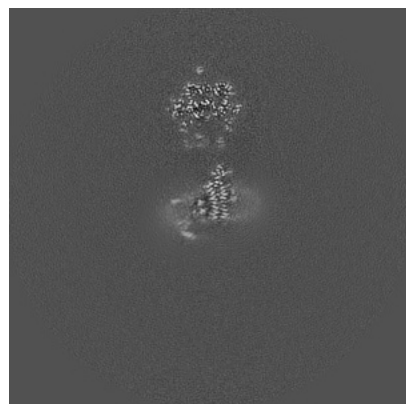


Z

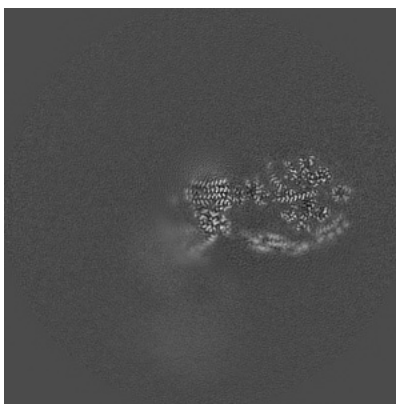
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

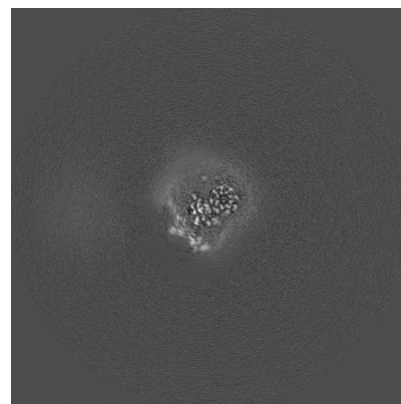
6.2.1 Primary map



X Index: 250



Y Index: 250

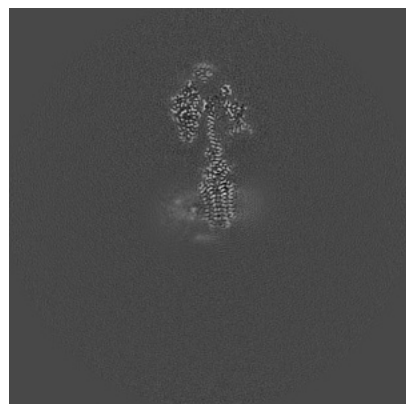


Z Index: 250

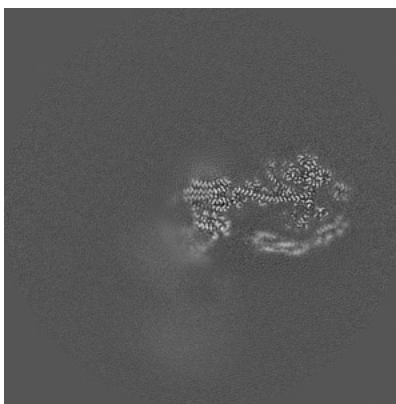
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

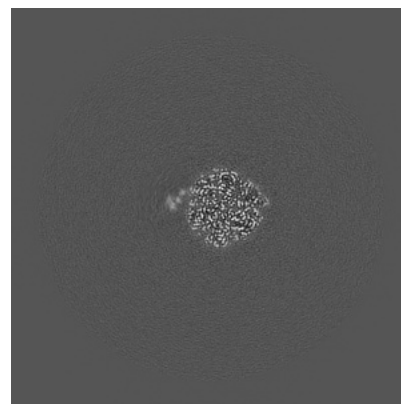
6.3.1 Primary map



X Index: 260



Y Index: 253

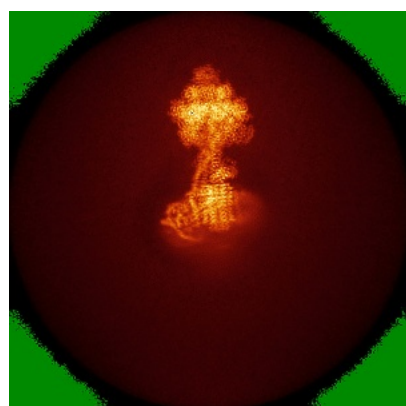


Z Index: 378

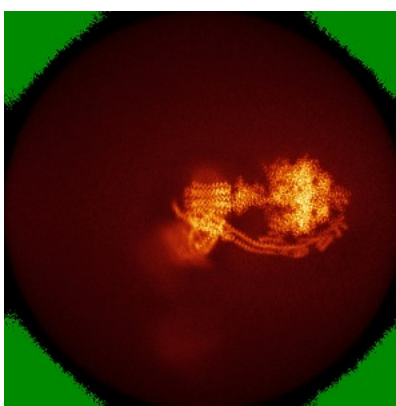
The images above show the largest variance slices of the map in three orthogonal directions.

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

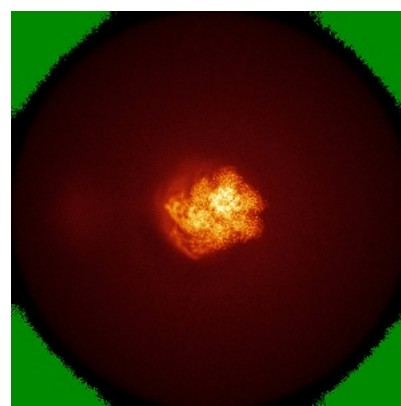
6.4.1 Primary map



X



Y



Z

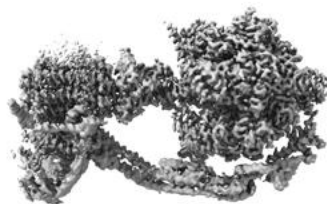
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

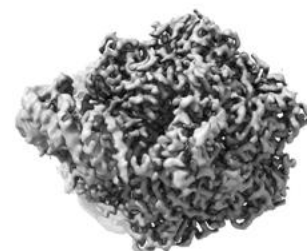
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

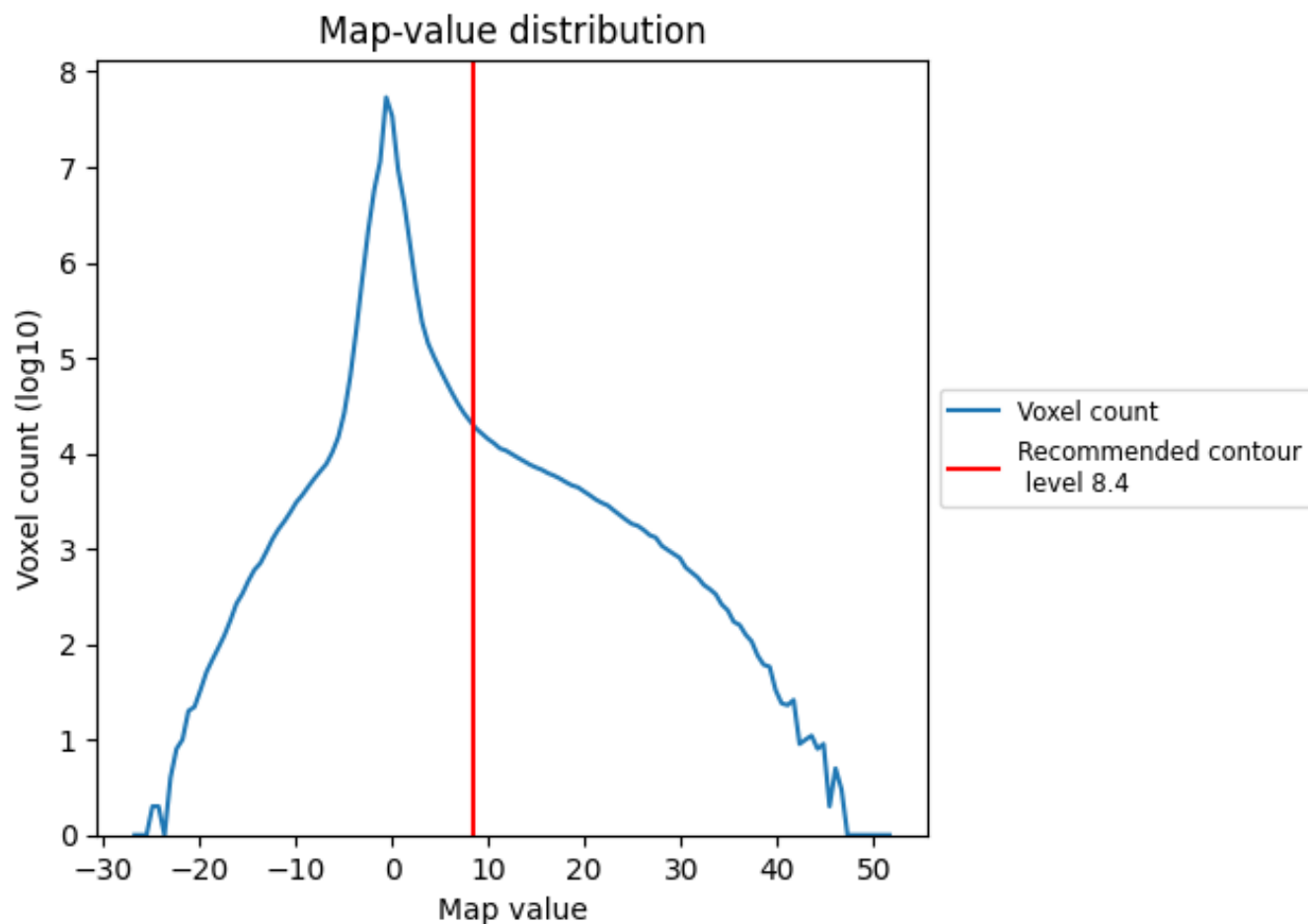
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

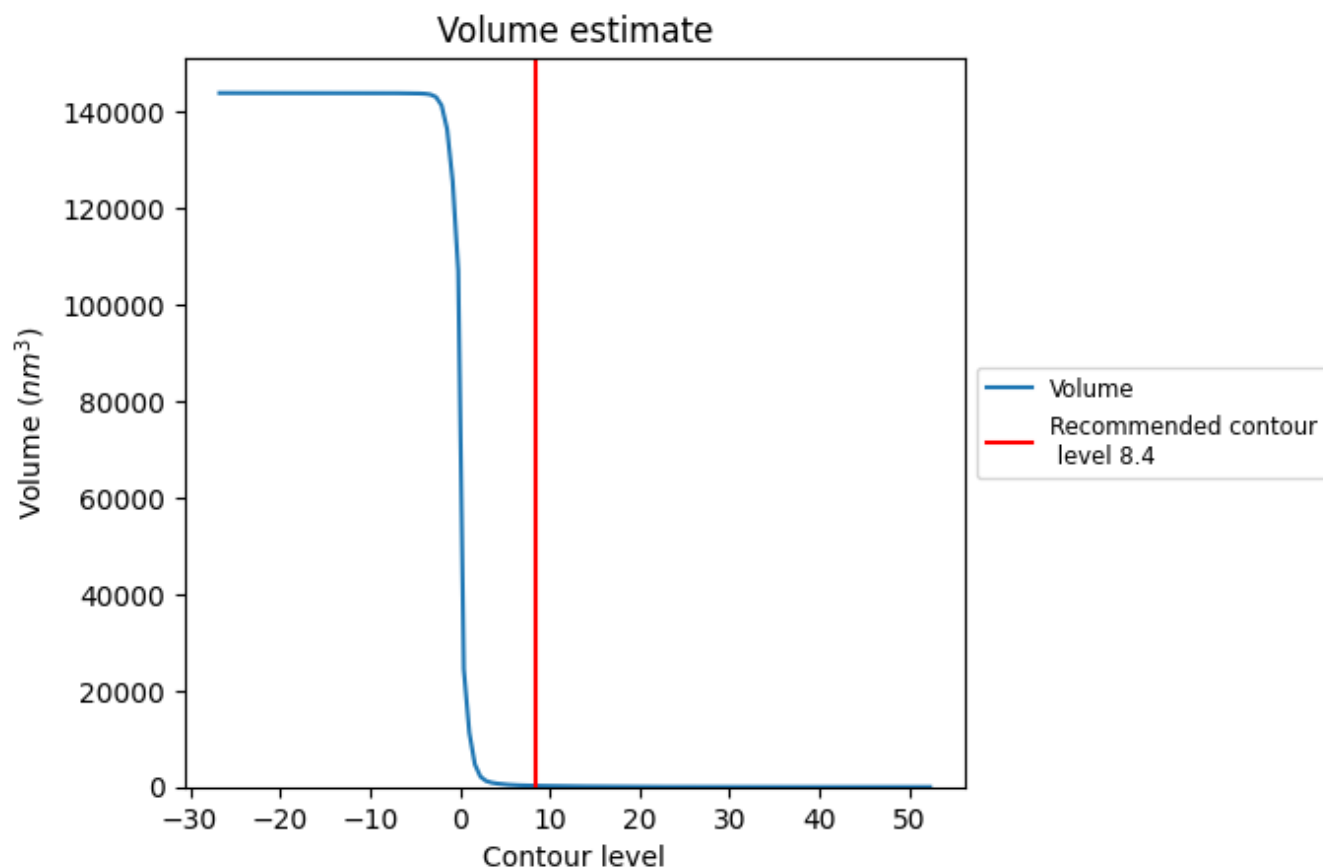
This section contains the results of statistical analysis of the map.

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.

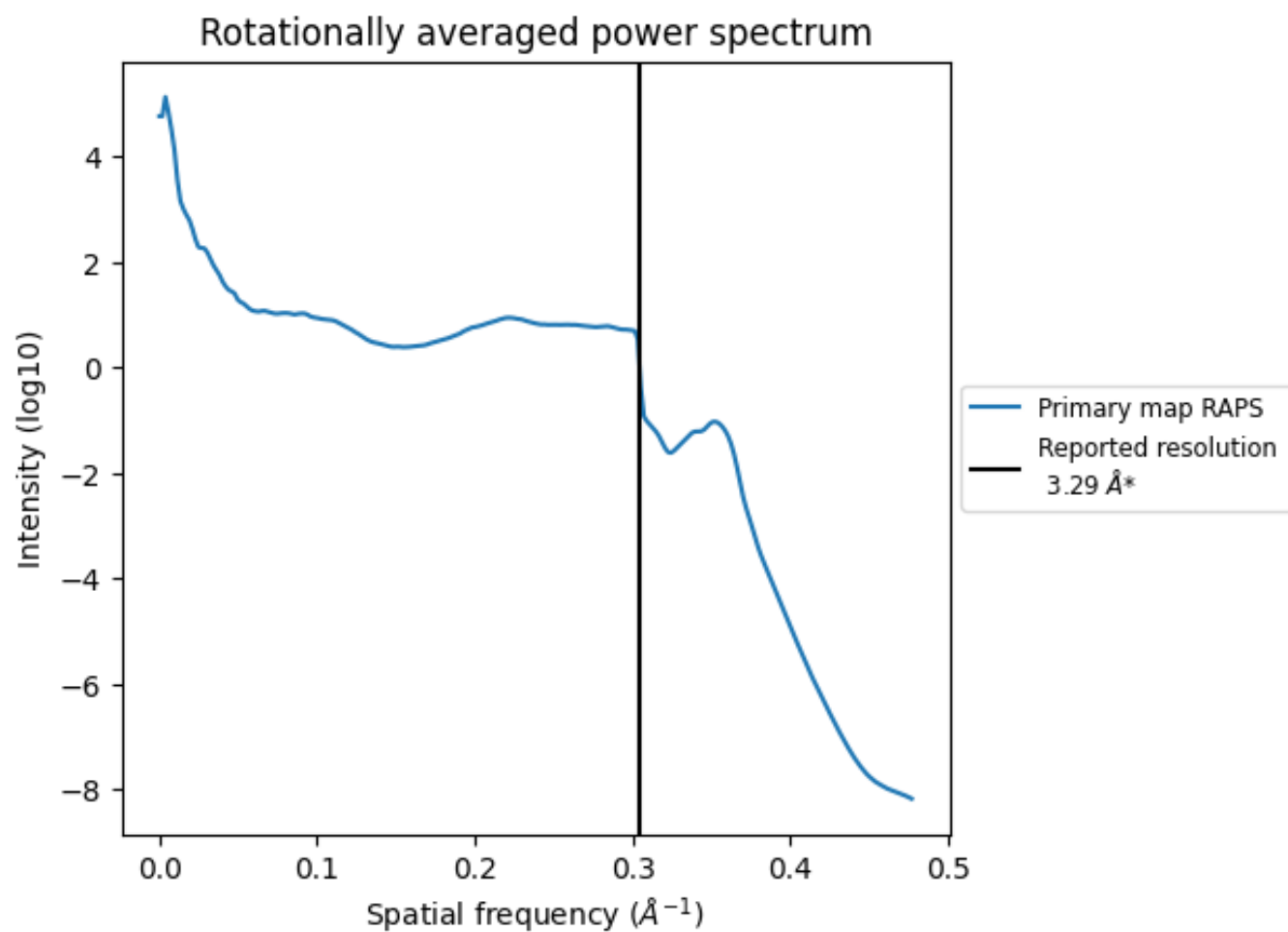
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

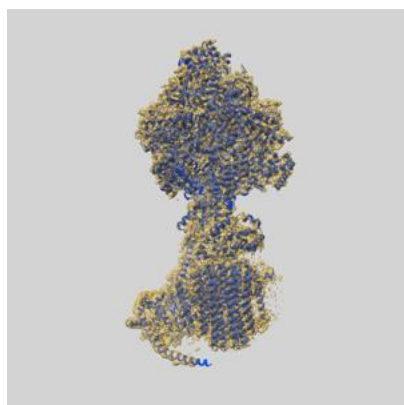
8 Fourier-Shell correlation

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

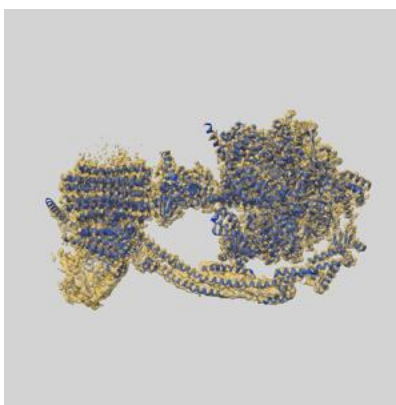
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11368 and PDB model 6ZQM. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

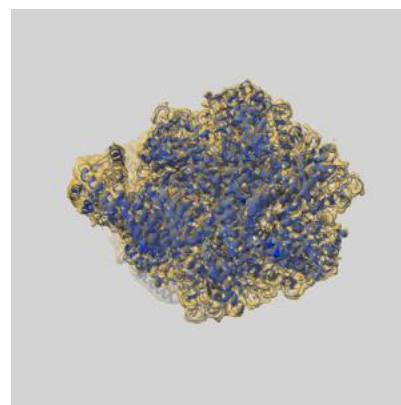
9.1 Map-model overlay [i](#)



X



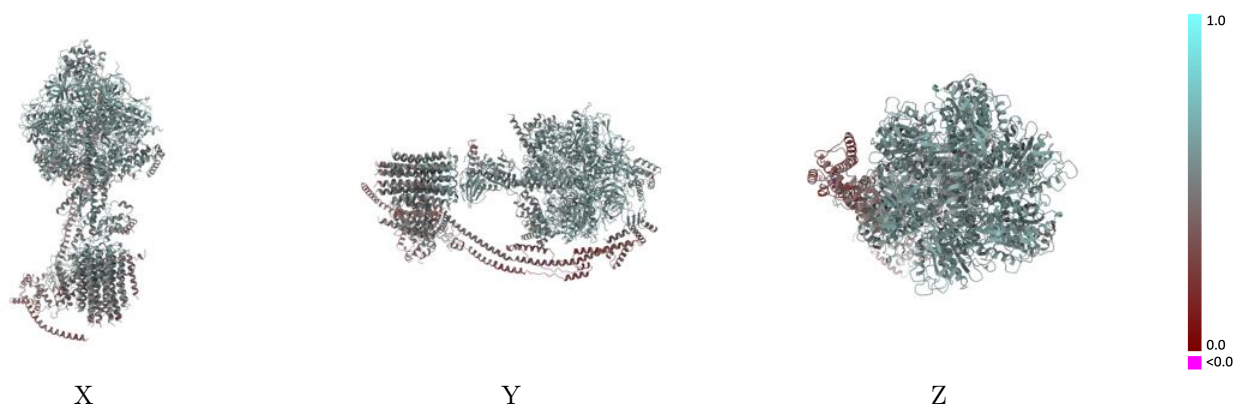
Y



Z

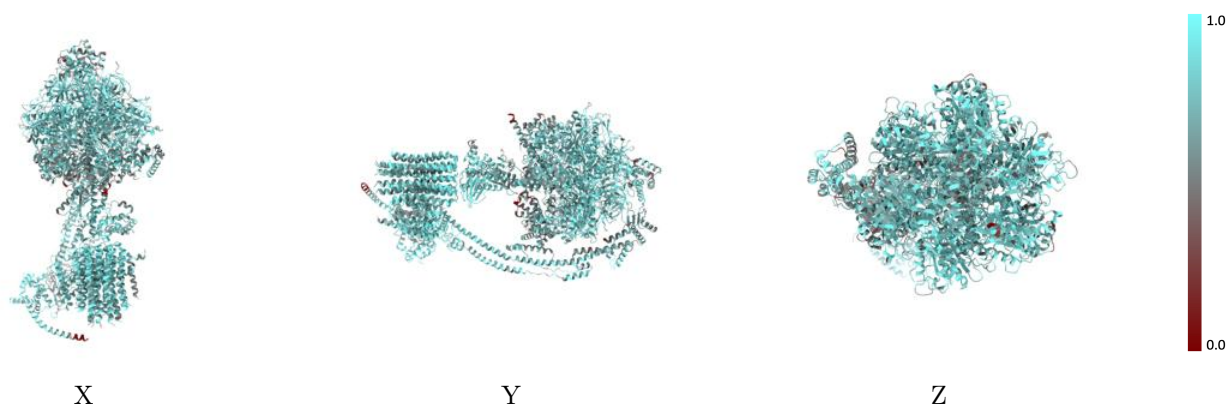
The images above show the 3D surface view of the map at the recommended contour level 8.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



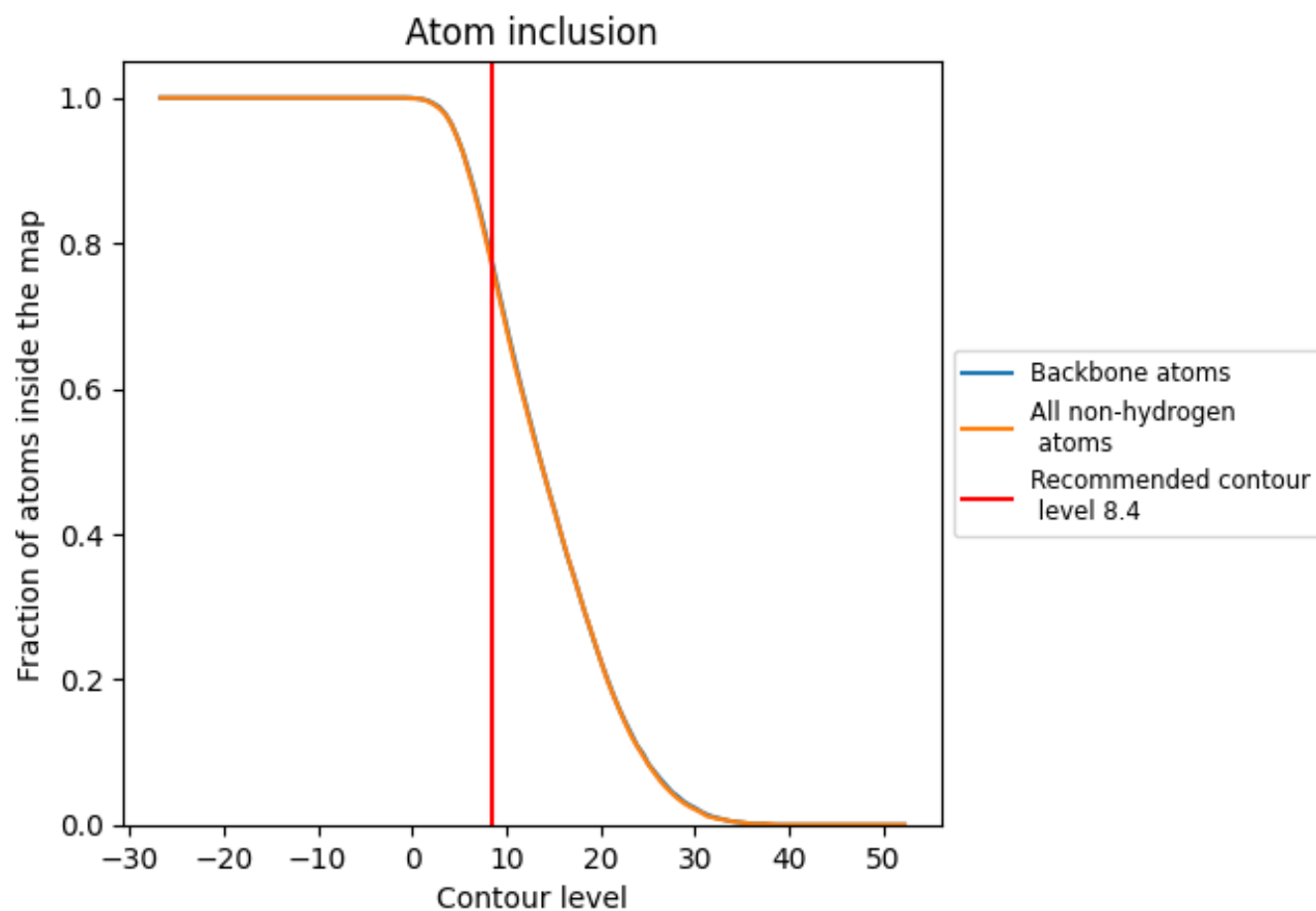
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (8.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.5250
8	 0.9190	 0.5220
A	 0.7960	 0.5760
B	 0.7570	 0.5580
C	 0.7710	 0.5670
D	 0.8010	 0.5750
E	 0.7600	 0.5670
F	 0.7990	 0.5760
G	 0.7360	 0.5470
H	 0.8180	 0.5330
I	 0.7470	 0.5300
J	 0.5880	 0.5210
K	 0.8210	 0.5190
L	 0.7940	 0.5050
M	 0.8060	 0.5050
N	 0.8060	 0.5030
O	 0.8250	 0.5090
P	 0.8250	 0.5110
Q	 0.8170	 0.5010
R	 0.8310	 0.5140
S	 0.6590	 0.5150
a	 0.8300	 0.4690
b	 0.7790	 0.4030
d	 0.7620	 0.3610
e	 0.7040	 0.3540
f	 0.8340	 0.4650
g	 0.8560	 0.3430
h	 0.6560	 0.3070
j	 0.8050	 0.4210
k	 0.6620	 0.3660

