



Full wwPDB EM Validation Report ⓘ

Nov 3, 2022 – 01:06 pm GMT

PDB ID : 7QV9
EMDB ID : EMD-14171
Title : CryoEM structure of bacterial transcription intermediate complex mediated by activator PspF
Authors : Ye, F.Z.; Zhang, X.D.
Deposited on : 2022-01-20
Resolution : 3.50 Å(reported)
Based on initial model : 5NSS

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

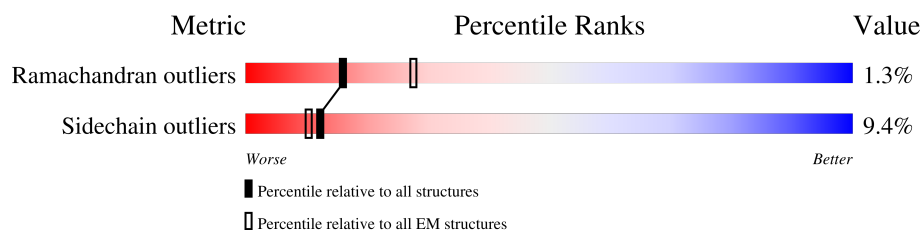
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

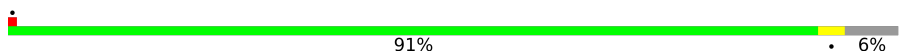

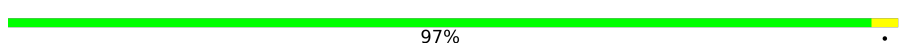
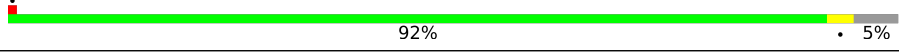

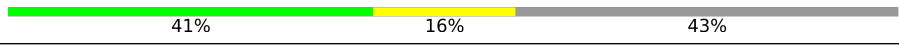
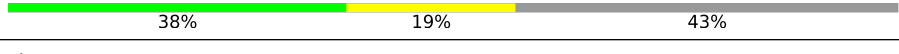


The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	N	63	
6	T	63	
7	a	295	
7	b	295	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	c	295	<div><div></div><div>9%</div><div>69%</div><div>16%</div><div>•</div><div>13%</div></div>
7	d	295	<div><div></div><div>5%</div><div>68%</div><div>16%</div><div>•</div><div>13%</div></div>
7	e	295	<div><div></div><div>5%</div><div>61%</div><div>23%</div><div>•</div><div>12%</div></div>
7	f	295	<div><div></div><div>6%</div><div>63%</div><div>21%</div><div>•</div><div>12%</div></div>
8	M	477	<div><div></div><div>53%</div><div>28%</div><div>6%</div><div>13%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 41491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total	C	N	O	S	0	0
			2322	1453	407	455	7		
1	B	223	Total	C	N	O	S	0	0
			1676	1045	294	332	5		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10125	6360	1761	1964	40		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			9634	6052	1730	1814	38		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total	C	N	O	S	0	0
			546	335	109	101	1		

- Molecule 5 is a DNA chain called Non-template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

- Molecule 6 is a DNA chain called Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

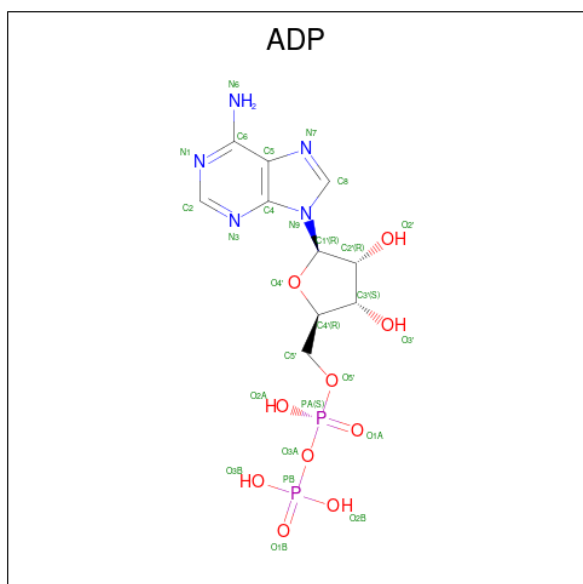
- Molecule 7 is a protein called Transcription activator PspF.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	259	Total	C	N	O	S	0	0
			2052	1301	361	380	10		
7	b	258	Total	C	N	O	S	0	0
			2052	1302	360	380	10		
7	c	256	Total	C	N	O	S	0	0
			2000	1270	349	372	9		
7	d	256	Total	C	N	O	S	0	0
			2041	1295	361	376	9		
7	f	259	Total	C	N	O	S	0	0
			2053	1304	358	381	10		
7	e	259	Total	C	N	O	S	0	0
			2062	1308	364	381	9		

- Molecule 8 is a protein called RNA polymerase sigma-54 factor.

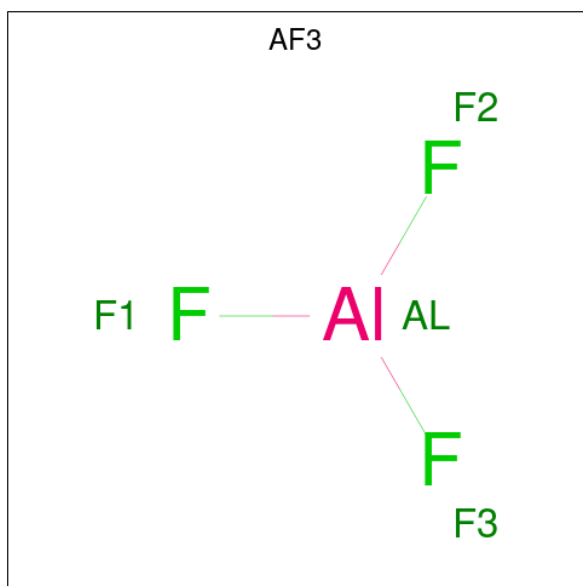
Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	417	Total	C	N	O	S	0	0
			3301	2071	572	646	12		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



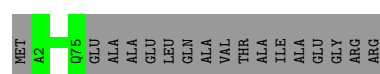
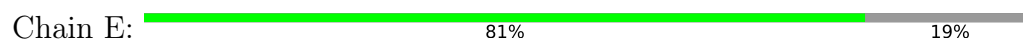
Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	f	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	a	1	Total	Al	F	0
			4	1	3	
10	b	1	Total	Al	F	0
			4	1	3	
10	f	1	Total	Al	F	0
			4	1	3	
10	e	1	Total	Al	F	0
			4	1	3	

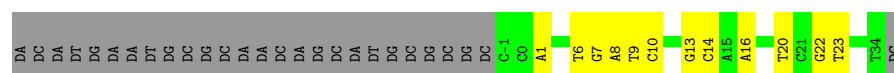
- Molecule 4: DNA-directed RNA polymerase subunit omega



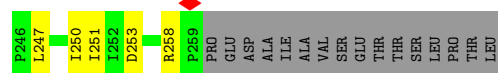
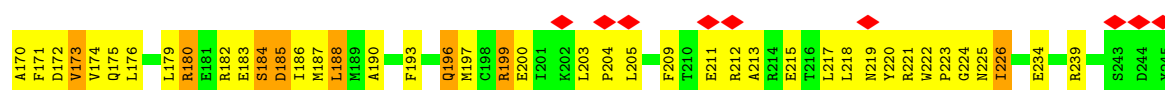
- Molecule 5: Non-template promoter DNA



- Molecule 6: Template promoter DNA

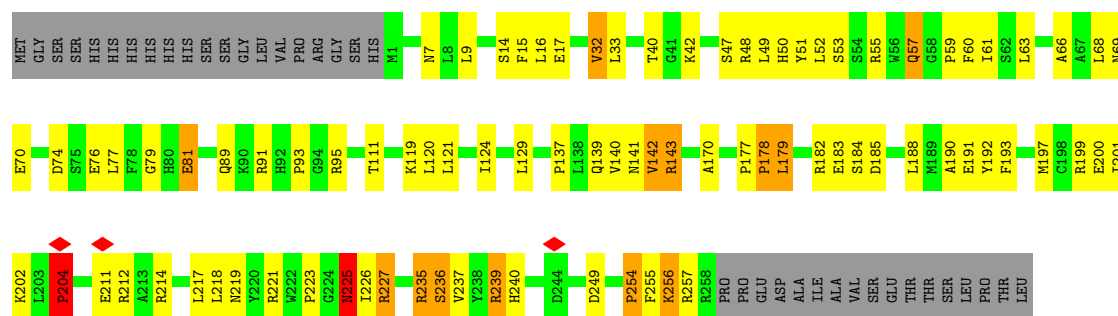


- Molecule 7: Transcription activator PspF



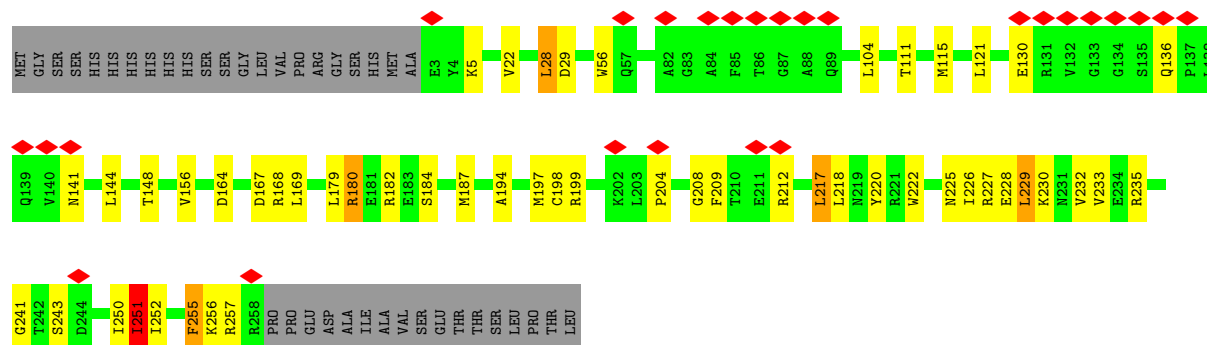
- Molecule 7: Transcription activator PspF

Chain b: 



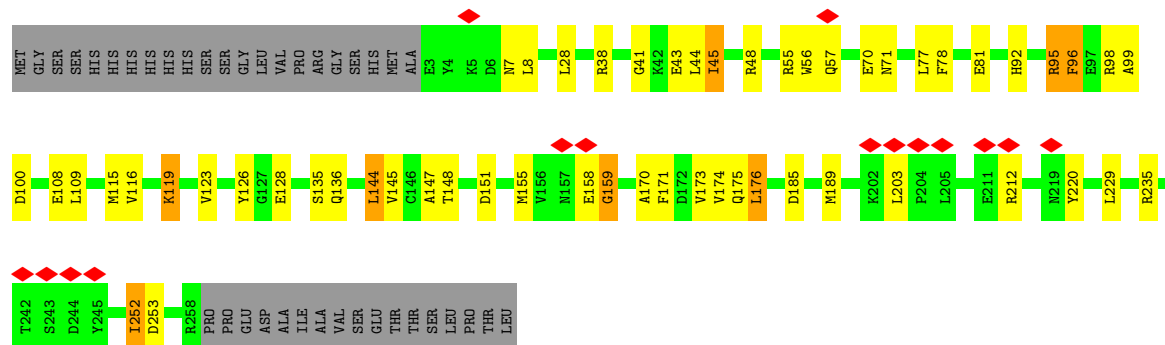
• Molecule 7: Transcription activator PspF

Chain c: 



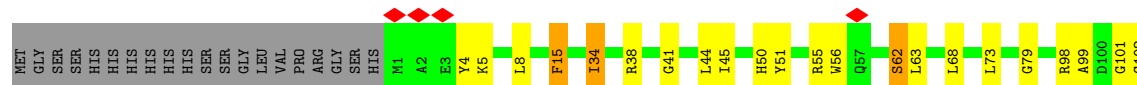
• Molecule 7: Transcription activator PspF

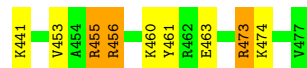
Chain d: 



• Molecule 7: Transcription activator PspF

Chain f: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33285	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.302	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AF3

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	0.23	0/2351	0.44	0/3202
1	B	0.22	0/1693	0.43	0/2300
2	C	0.23	0/10283	0.40	0/13940
3	D	0.23	0/9768	0.41	1/13270 (0.0%)
4	E	0.21	0/547	0.36	0/740
5	N	0.90	5/827 (0.6%)	1.32	12/1274 (0.9%)
6	T	1.28	9/827 (1.1%)	1.43	18/1274 (1.4%)
7	a	1.89	61/2093 (2.9%)	2.03	83/2833 (2.9%)
7	b	1.87	69/2093 (3.3%)	2.04	78/2832 (2.8%)
7	c	1.21	27/2038 (1.3%)	1.49	37/2762 (1.3%)
7	d	1.17	14/2082 (0.7%)	1.54	42/2817 (1.5%)
7	e	1.52	44/2104 (2.1%)	1.73	66/2848 (2.3%)
7	f	1.74	52/2095 (2.5%)	1.74	70/2837 (2.5%)
8	M	1.80	84/3348 (2.5%)	1.95	145/4533 (3.2%)
All	All	1.04	365/42149 (0.9%)	1.19	552/57462 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	a	0	1
7	b	0	1
7	d	0	1
All	All	0	3

All (365) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	98	ARG	CZ-NH2	28.28	1.69	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	143	ARG	CZ-NH1	24.18	1.64	1.33
7	f	128	GLU	CD-OE1	21.25	1.49	1.25
7	a	48	ARG	CZ-NH1	20.99	1.60	1.33
7	f	193	PHE	CG-CD2	19.56	1.68	1.38
7	a	98	ARG	CZ-NH1	19.53	1.58	1.33
7	a	185	ASP	C-O	17.43	1.56	1.23
7	b	192	TYR	CG-CD2	17.16	1.61	1.39
7	f	193	PHE	CG-CD1	15.35	1.61	1.38
7	f	149	ASN	CG-OD1	15.33	1.57	1.24
7	a	65	CYS	CB-SG	15.13	2.08	1.82
7	e	62	SER	C-O	14.46	1.50	1.23
6	T	9	DT	C4'-O4'	-13.95	1.31	1.45
7	e	23	SER	C-O	13.18	1.48	1.23
7	b	193	PHE	CG-CD1	13.00	1.58	1.38
7	b	143	ARG	CZ-NH2	12.84	1.49	1.33
7	a	184	SER	C-O	12.73	1.47	1.23
7	a	182	ARG	CZ-NH1	12.69	1.49	1.33
7	a	79	GLY	C-O	12.62	1.43	1.23
8	M	126	TRP	CE2-CZ2	12.24	1.60	1.39
7	d	100	ASP	CG-OD1	12.11	1.53	1.25
7	f	214	ARG	CZ-NH1	12.00	1.48	1.33
8	M	203	LEU	C-O	11.73	1.45	1.23
7	b	178	PRO	N-CA	11.34	1.66	1.47
6	T	6	DT	C4'-O4'	-11.29	1.33	1.45
8	M	130	LEU	C-O	11.24	1.44	1.23
7	e	62	SER	N-CA	11.20	1.68	1.46
7	b	239	ARG	C-O	11.15	1.44	1.23
8	M	198	CYS	CB-SG	11.12	2.01	1.82
8	M	456	ARG	CZ-NH1	10.64	1.46	1.33
7	c	197	MET	CG-SD	10.51	2.08	1.81
8	M	271	TYR	CE2-CZ	10.49	1.52	1.38
7	f	163	ALA	C-O	10.47	1.43	1.23
7	b	32	VAL	C-O	10.42	1.43	1.23
8	M	126	TRP	CB-CG	10.33	1.68	1.50
8	M	28	LEU	C-O	10.29	1.43	1.23
7	b	192	TYR	CG-CD1	10.28	1.52	1.39
7	f	193	PHE	CE2-CZ	10.21	1.56	1.37
6	T	9	DT	O3'-P	-10.08	1.49	1.61
7	f	141	ASN	CG-OD1	10.07	1.46	1.24
7	d	100	ASP	CG-OD2	10.07	1.48	1.25
7	e	47	SER	CA-CB	10.02	1.68	1.52
7	e	222	TRP	CE3-CZ3	10.01	1.55	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	389	TYR	CG-CD1	10.00	1.52	1.39
7	e	173	VAL	N-CA	9.99	1.66	1.46
7	a	223	PRO	C-O	9.97	1.43	1.23
7	b	141	ASN	C-O	9.88	1.42	1.23
8	M	120	LEU	C-O	9.87	1.42	1.23
7	a	48	ARG	NE-CZ	9.85	1.45	1.33
7	f	197	MET	C-O	9.83	1.42	1.23
7	e	32	VAL	C-O	9.83	1.42	1.23
6	T	7	DG	C4'-O4'	-9.81	1.35	1.45
7	a	221	ARG	C-O	9.78	1.42	1.23
7	b	50	HIS	CA-CB	-9.75	1.32	1.53
7	d	159	GLY	N-CA	9.63	1.60	1.46
7	e	189	MET	CG-SD	9.58	2.06	1.81
7	f	222	TRP	C-O	9.55	1.41	1.23
7	f	179	LEU	C-O	9.49	1.41	1.23
7	e	39	GLY	C-O	9.44	1.38	1.23
7	a	141	ASN	CG-ND2	9.43	1.56	1.32
7	b	193	PHE	CE2-CZ	9.40	1.55	1.37
7	b	49	LEU	CA-CB	9.33	1.75	1.53
8	M	456	ARG	CZ-NH2	9.32	1.45	1.33
7	b	60	PHE	CG-CD1	-9.26	1.24	1.38
7	b	193	PHE	CG-CD2	9.22	1.52	1.38
7	c	255	PHE	CG-CD2	9.11	1.52	1.38
7	a	184	SER	CB-OG	8.93	1.53	1.42
7	b	192	TYR	CE1-CZ	8.74	1.50	1.38
8	M	271	TYR	CB-CG	8.65	1.64	1.51
7	a	141	ASN	CG-OD1	8.64	1.43	1.24
6	T	8	DA	C4'-O4'	-8.64	1.36	1.45
8	M	143	SER	CB-OG	8.62	1.53	1.42
7	c	167	ASP	CB-CG	8.61	1.69	1.51
7	b	143	ARG	C-O	8.57	1.39	1.23
7	b	236	SER	C-O	8.45	1.39	1.23
7	f	214	ARG	CD-NE	8.45	1.60	1.46
7	b	190	ALA	C-O	8.44	1.39	1.23
7	a	221	ARG	CA-C	8.43	1.74	1.52
7	b	51	TYR	CG-CD1	8.42	1.50	1.39
7	e	62	SER	CB-OG	-8.41	1.31	1.42
7	b	69	ASN	CG-ND2	8.41	1.53	1.32
7	f	255	PHE	CG-CD1	8.32	1.51	1.38
7	f	176	LEU	CA-CB	-8.29	1.34	1.53
7	f	56	TRP	CD2-CE3	8.26	1.52	1.40
7	f	101	GLY	C-O	8.24	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	f	146	CYS	C-O	8.24	1.39	1.23
8	M	126	TRP	CE3-CZ3	8.22	1.52	1.38
8	M	271	TYR	CG-CD2	8.20	1.49	1.39
8	M	126	TRP	CG-CD1	8.20	1.48	1.36
7	a	193	PHE	CG-CD1	8.18	1.51	1.38
7	f	141	ASN	N-CA	8.18	1.62	1.46
7	a	173	VAL	CB-CG1	8.15	1.70	1.52
7	e	172	ASP	C-O	8.15	1.38	1.23
7	a	220	TYR	CG-CD1	8.14	1.49	1.39
7	e	22	VAL	C-O	8.12	1.38	1.23
7	f	56	TRP	CZ3-CH2	8.11	1.53	1.40
8	M	189	GLY	C-O	8.10	1.36	1.23
7	b	32	VAL	CB-CG2	8.08	1.69	1.52
7	d	96	PHE	CB-CG	-8.06	1.37	1.51
8	M	263	SER	CB-OG	-7.98	1.31	1.42
8	M	318	PHE	CG-CD1	7.92	1.50	1.38
7	e	161	PHE	CE2-CZ	7.89	1.52	1.37
7	a	79	GLY	CA-C	7.88	1.64	1.51
8	M	190	VAL	C-O	7.84	1.38	1.23
7	a	79	GLY	N-CA	7.82	1.57	1.46
7	e	224	GLY	N-CA	7.81	1.57	1.46
7	f	99	ALA	CA-CB	7.79	1.68	1.52
8	M	120	LEU	CA-C	-7.79	1.32	1.52
7	b	49	LEU	N-CA	7.74	1.61	1.46
8	M	125	MET	CA-CB	-7.72	1.36	1.53
8	M	382	SER	CA-CB	-7.71	1.41	1.52
7	b	51	TYR	CG-CD2	-7.68	1.29	1.39
7	a	224	GLY	N-CA	7.67	1.57	1.46
7	f	231	ASN	CG-OD1	7.61	1.40	1.24
7	f	127	GLY	C-O	7.61	1.35	1.23
7	d	158	GLU	C-O	7.60	1.37	1.23
7	e	142	VAL	CB-CG1	7.59	1.68	1.52
7	e	201	ILE	C-O	7.55	1.37	1.23
8	M	389	TYR	CD1-CE1	7.53	1.50	1.39
7	b	32	VAL	CA-CB	7.53	1.70	1.54
5	N	-27	DT	C4'-O4'	-7.50	1.37	1.45
7	b	15	PHE	CG-CD2	7.50	1.50	1.38
7	c	241	GLY	CA-C	7.47	1.63	1.51
7	a	172	ASP	C-O	-7.47	1.09	1.23
7	a	224	GLY	C-O	7.44	1.35	1.23
7	b	121	LEU	N-CA	-7.43	1.31	1.46
8	M	133	PHE	CA-CB	7.39	1.70	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	190	VAL	CB-CG2	-7.34	1.37	1.52
7	b	190	ALA	CA-C	7.33	1.72	1.52
7	d	123	VAL	C-O	-7.32	1.09	1.23
7	e	187	MET	C-O	7.31	1.37	1.23
7	b	51	TYR	C-O	7.30	1.37	1.23
7	f	127	GLY	N-CA	7.30	1.56	1.46
7	a	222	TRP	CD2-CE2	-7.30	1.32	1.41
7	a	173	VAL	C-O	7.28	1.37	1.23
5	N	-12	DC	C4'-O4'	-7.26	1.37	1.45
8	M	126	TRP	CD2-CE2	-7.25	1.32	1.41
7	f	255	PHE	CG-CD2	-7.22	1.27	1.38
7	c	230	LYS	C-O	7.18	1.36	1.23
7	f	222	TRP	N-CA	7.17	1.60	1.46
7	f	98	ARG	CZ-NH2	-7.08	1.23	1.33
7	b	235	ARG	CB-CG	7.05	1.71	1.52
7	b	235	ARG	CG-CD	7.05	1.69	1.51
8	M	133	PHE	CE2-CZ	7.04	1.50	1.37
7	b	235	ARG	CZ-NH2	7.04	1.42	1.33
8	M	129	GLU	CA-CB	-7.03	1.38	1.53
7	f	127	GLY	CA-C	7.02	1.63	1.51
7	b	69	ASN	CB-CG	6.98	1.67	1.51
7	c	255	PHE	CG-CD1	6.96	1.49	1.38
8	M	127	GLN	C-O	6.96	1.36	1.23
7	b	184	SER	CB-OG	6.94	1.51	1.42
7	b	70	GLU	CA-CB	6.94	1.69	1.53
7	c	220	TYR	CG-CD1	6.93	1.48	1.39
8	M	262	GLN	C-O	6.93	1.36	1.23
8	M	461	TYR	CB-CG	-6.92	1.41	1.51
8	M	147	ALA	N-CA	-6.89	1.32	1.46
7	b	255	PHE	C-O	6.83	1.36	1.23
7	f	255	PHE	CA-C	6.82	1.70	1.52
7	a	200	GLU	CD-OE2	6.81	1.33	1.25
7	b	239	ARG	CZ-NH2	6.80	1.41	1.33
7	b	193	PHE	CE1-CZ	6.79	1.50	1.37
7	e	34	ILE	C-O	6.78	1.36	1.23
7	b	32	VAL	CA-C	-6.77	1.35	1.52
7	f	255	PHE	CD1-CE1	6.76	1.52	1.39
8	M	328	TRP	CE3-CZ3	6.76	1.50	1.38
7	f	214	ARG	NE-CZ	6.74	1.41	1.33
7	f	193	PHE	CE1-CZ	6.74	1.50	1.37
7	a	209	PHE	CE1-CZ	6.73	1.50	1.37
7	a	222	TRP	CZ3-CH2	-6.73	1.29	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	193	PHE	CG-CD1	6.70	1.48	1.38
7	b	256	LYS	CA-C	6.70	1.70	1.52
7	c	241	GLY	C-O	6.68	1.34	1.23
7	d	99	ALA	CA-C	6.66	1.70	1.52
7	e	161	PHE	CG-CD1	6.65	1.48	1.38
7	e	234	GLU	CG-CD	6.64	1.61	1.51
7	b	237	VAL	CA-CB	6.62	1.68	1.54
8	M	184	ARG	C-O	6.62	1.35	1.23
7	a	220	TYR	CG-CD2	6.62	1.47	1.39
8	M	276	VAL	CA-CB	-6.62	1.40	1.54
7	a	170	ALA	CA-C	-6.58	1.35	1.52
8	M	285	TRP	CB-CG	-6.56	1.38	1.50
8	M	379	SER	CB-OG	6.56	1.50	1.42
7	a	186	ILE	C-O	6.55	1.35	1.23
7	c	194	ALA	C-O	6.55	1.35	1.23
7	b	182	ARG	CZ-NH1	6.54	1.41	1.33
6	T	7	DG	O3'-P	6.53	1.69	1.61
7	e	194	ALA	C-O	6.50	1.35	1.23
7	e	46	ALA	CA-C	6.50	1.69	1.52
7	a	193	PHE	CE2-CZ	6.47	1.49	1.37
8	M	389	TYR	C-O	6.45	1.35	1.23
8	M	260	PRO	CA-C	6.44	1.65	1.52
8	M	326	ALA	N-CA	-6.44	1.33	1.46
7	b	221	ARG	N-CA	6.43	1.59	1.46
7	e	55	ARG	CA-C	6.43	1.69	1.52
7	b	177	PRO	N-CD	6.41	1.56	1.47
7	f	222	TRP	CG-CD1	-6.39	1.27	1.36
7	c	220	TYR	CG-CD2	6.38	1.47	1.39
7	a	220	TYR	CE2-CZ	6.36	1.46	1.38
7	f	141	ASN	CB-CG	6.36	1.65	1.51
8	M	27	GLN	CG-CD	6.34	1.65	1.51
8	M	153	TYR	CA-C	-6.33	1.36	1.52
7	c	222	TRP	N-CA	6.33	1.59	1.46
7	d	96	PHE	CG-CD2	6.33	1.48	1.38
7	b	57	GLN	CG-CD	6.32	1.65	1.51
7	a	173	VAL	CB-CG2	6.32	1.66	1.52
7	b	183	GLU	C-O	6.31	1.35	1.23
7	c	184	SER	C-O	6.31	1.35	1.23
7	b	59	PRO	C-O	6.30	1.35	1.23
7	e	230	LYS	CE-NZ	6.29	1.64	1.49
7	c	255	PHE	CE1-CZ	6.28	1.49	1.37
8	M	389	TYR	CD2-CE2	6.26	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	204	PRO	CA-C	6.24	1.65	1.52
7	e	46	ALA	N-CA	6.24	1.58	1.46
7	e	39	GLY	N-CA	-6.23	1.36	1.46
7	f	15	PHE	CD1-CE1	6.20	1.51	1.39
7	e	142	VAL	C-O	6.20	1.35	1.23
8	M	278	VAL	C-O	6.20	1.35	1.23
7	b	236	SER	CA-CB	-6.20	1.43	1.52
7	c	229	LEU	C-O	6.19	1.35	1.23
8	M	419	ALA	N-CA	-6.16	1.34	1.46
7	e	32	VAL	CA-C	-6.15	1.36	1.52
7	d	171	PHE	C-O	6.12	1.34	1.23
7	b	70	GLU	CA-C	6.11	1.68	1.52
8	M	120	LEU	CB-CG	6.09	1.70	1.52
8	M	415	ALA	C-O	6.09	1.34	1.23
8	M	389	TYR	CE2-CZ	6.09	1.46	1.38
7	c	197	MET	SD-CE	6.07	2.11	1.77
7	f	128	GLU	CG-CD	6.05	1.61	1.51
7	b	184	SER	C-O	6.04	1.34	1.23
7	b	227	ARG	CA-CB	6.04	1.67	1.53
7	b	15	PHE	CD1-CE1	6.04	1.51	1.39
7	c	255	PHE	N-CA	6.04	1.58	1.46
7	d	119	LYS	CD-CE	6.02	1.66	1.51
6	T	1	DA	O3'-P	-6.01	1.53	1.61
7	f	102	GLY	C-O	6.00	1.33	1.23
7	b	182	ARG	CZ-NH2	6.00	1.40	1.33
7	a	100	ASP	C-O	5.99	1.34	1.23
7	b	142	VAL	C-O	5.99	1.34	1.23
8	M	276	VAL	C-O	5.99	1.34	1.23
7	a	100	ASP	CA-CB	-5.97	1.40	1.53
8	M	127	GLN	CB-CG	-5.96	1.36	1.52
7	c	255	PHE	CB-CG	5.96	1.61	1.51
8	M	35	GLN	CG-CD	5.92	1.64	1.51
7	a	182	ARG	NE-CZ	5.92	1.40	1.33
7	a	209	PHE	CG-CD2	5.91	1.47	1.38
7	e	189	MET	CB-CG	5.88	1.70	1.51
7	e	255	PHE	N-CA	5.88	1.58	1.46
5	N	-22	DC	O3'-P	-5.85	1.54	1.61
7	b	182	ARG	C-O	5.85	1.34	1.23
7	c	187	MET	C-O	5.84	1.34	1.23
7	a	187	MET	N-CA	-5.84	1.34	1.46
7	e	44	LEU	CB-CG	5.84	1.69	1.52
8	M	403	PHE	CG-CD1	5.82	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	200	GLU	CD-OE1	5.80	1.32	1.25
7	e	48	ARG	C-O	5.78	1.34	1.23
7	a	100	ASP	N-CA	-5.77	1.34	1.46
7	d	45	ILE	N-CA	-5.77	1.34	1.46
7	c	255	PHE	CD1-CE1	5.76	1.50	1.39
8	M	27	GLN	C-O	5.75	1.34	1.23
8	M	183	GLN	CA-C	-5.75	1.38	1.52
7	e	161	PHE	CA-CB	5.73	1.66	1.53
7	a	220	TYR	CD1-CE1	-5.72	1.30	1.39
8	M	258	PRO	N-CD	5.70	1.55	1.47
8	M	386	THR	CB-CG2	5.70	1.71	1.52
7	b	178	PRO	CG-CD	5.68	1.69	1.50
7	f	230	LYS	CA-CB	-5.68	1.41	1.53
7	b	183	GLU	CD-OE1	5.68	1.31	1.25
8	M	403	PHE	CB-CG	5.68	1.61	1.51
7	a	199	ARG	CZ-NH2	5.67	1.40	1.33
8	M	260	PRO	C-O	5.67	1.34	1.23
7	a	209	PHE	CG-CD1	5.67	1.47	1.38
7	b	193	PHE	CD2-CE2	5.66	1.50	1.39
7	b	177	PRO	C-O	5.65	1.34	1.23
8	M	399	LEU	CA-CB	-5.64	1.40	1.53
7	e	192	TYR	C-O	5.62	1.34	1.23
7	b	254	PRO	N-CA	5.62	1.56	1.47
8	M	418	THR	CB-CG2	5.61	1.70	1.52
7	e	223	PRO	N-CD	5.59	1.55	1.47
7	b	60	PHE	N-CA	5.58	1.57	1.46
7	f	222	TRP	CD2-CE2	-5.56	1.34	1.41
8	M	356	GLU	C-O	5.55	1.33	1.23
7	a	222	TRP	N-CA	5.53	1.57	1.46
7	f	62	SER	CB-OG	5.53	1.49	1.42
7	a	226	ILE	C-O	5.51	1.33	1.23
7	b	239	ARG	CD-NE	5.51	1.55	1.46
8	M	271	TYR	CZ-OH	5.50	1.47	1.37
7	b	188	LEU	CA-C	5.49	1.67	1.52
7	f	255	PHE	CD2-CE2	5.48	1.50	1.39
7	b	60	PHE	CD2-CE2	-5.46	1.28	1.39
7	c	255	PHE	CA-CB	-5.44	1.42	1.53
7	a	193	PHE	CD1-CE1	5.43	1.50	1.39
8	M	128	VAL	CA-CB	-5.41	1.43	1.54
8	M	354	PHE	CE1-CZ	5.40	1.47	1.37
7	c	255	PHE	CD2-CE2	5.39	1.50	1.39
7	e	254	PRO	CA-C	5.39	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	171	PHE	CG-CD1	5.39	1.46	1.38
7	b	235	ARG	NE-CZ	5.37	1.40	1.33
7	f	44	LEU	N-CA	-5.37	1.35	1.46
7	b	227	ARG	C-O	5.37	1.33	1.23
8	M	343	VAL	CB-CG2	5.36	1.64	1.52
7	a	174	VAL	CA-C	-5.36	1.39	1.52
8	M	344	SER	C-O	5.36	1.33	1.23
8	M	147	ALA	CA-CB	-5.35	1.41	1.52
7	e	43	GLU	CD-OE1	5.34	1.31	1.25
8	M	354	PHE	CA-C	-5.34	1.39	1.52
7	a	220	TYR	CB-CG	-5.33	1.43	1.51
7	c	199	ARG	CG-CD	5.33	1.65	1.51
7	e	192	TYR	CE1-CZ	5.33	1.45	1.38
7	c	252	ILE	N-CA	-5.32	1.35	1.46
7	f	79	GLY	C-O	-5.32	1.15	1.23
7	a	183	GLU	C-O	5.31	1.33	1.23
7	f	212	ARG	CZ-NH2	5.31	1.40	1.33
8	M	386	THR	N-CA	5.30	1.56	1.46
7	a	98	ARG	CB-CG	5.30	1.66	1.52
7	e	147	ALA	CA-CB	5.30	1.63	1.52
7	a	184	SER	CA-CB	5.30	1.60	1.52
6	T	10	DC	C4'-O4'	-5.29	1.39	1.45
7	a	215	GLU	CD-OE1	5.28	1.31	1.25
7	e	198	CYS	C-O	5.27	1.33	1.23
8	M	389	TYR	CA-CB	-5.27	1.42	1.53
7	d	96	PHE	CD2-CE2	5.26	1.49	1.39
7	e	21	GLN	N-CA	-5.26	1.35	1.46
7	f	146	CYS	CB-SG	5.25	1.91	1.82
7	f	177	PRO	C-N	-5.25	1.24	1.34
8	M	117	THR	N-CA	5.24	1.56	1.46
8	M	285	TRP	CA-CB	-5.24	1.42	1.53
7	c	228	GLU	CB-CG	5.23	1.62	1.52
7	f	56	TRP	CZ2-CH2	5.23	1.47	1.37
7	a	80	HIS	CA-C	-5.22	1.39	1.52
7	f	176	LEU	N-CA	5.21	1.56	1.46
8	M	380	THR	CA-CB	-5.21	1.39	1.53
8	M	363	LYS	N-CA	5.19	1.56	1.46
7	a	190	ALA	N-CA	5.18	1.56	1.46
7	a	180	ARG	CZ-NH1	5.18	1.39	1.33
7	e	230	LYS	CD-CE	5.17	1.64	1.51
6	T	16	DA	O3'-P	-5.16	1.54	1.61
7	b	143	ARG	N-CA	5.16	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	182	ARG	CA-CB	-5.16	1.42	1.53
8	M	146	ASP	CB-CG	-5.16	1.41	1.51
7	a	213	ALA	C-O	5.14	1.33	1.23
8	M	278	VAL	N-CA	5.14	1.56	1.46
7	c	232	VAL	CB-CG1	5.12	1.63	1.52
8	M	329	LEU	CA-C	-5.12	1.39	1.52
7	c	208	GLY	C-O	5.12	1.31	1.23
7	a	222	TRP	CA-C	5.12	1.66	1.52
7	f	55	ARG	CG-CD	5.11	1.64	1.51
5	N	-17	DT	C4'-O4'	5.11	1.50	1.45
8	M	262	GLN	CA-C	-5.10	1.39	1.52
7	f	255	PHE	C-O	5.10	1.33	1.23
7	c	197	MET	CB-CG	5.10	1.67	1.51
8	M	195	LEU	CA-C	-5.09	1.39	1.52
8	M	461	TYR	CZ-OH	-5.09	1.29	1.37
7	a	200	GLU	CG-CD	5.08	1.59	1.51
7	a	196	GLN	C-O	5.07	1.32	1.23
7	f	259	PRO	C-O	5.07	1.33	1.23
7	f	169	LEU	N-CA	5.07	1.56	1.46
8	M	387	GLN	CG-CD	5.07	1.62	1.51
7	d	175	GLN	CD-OE1	5.06	1.35	1.24
5	N	-28	DC	C4'-O4'	-5.05	1.40	1.45
8	M	205	GLN	CG-CD	5.04	1.62	1.51
8	M	461	TYR	CG-CD1	-5.04	1.32	1.39
7	b	184	SER	CA-C	-5.02	1.40	1.52
7	b	237	VAL	CB-CG1	5.01	1.63	1.52
7	f	197	MET	CB-CG	5.01	1.67	1.51
7	e	49	LEU	CG-CD2	5.00	1.70	1.51

All (552) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	48	ARG	NE-CZ-NH1	38.39	139.50	120.30
7	b	143	ARG	NE-CZ-NH2	-38.03	101.29	120.30
7	a	98	ARG	NE-CZ-NH1	-34.60	103.00	120.30
7	d	100	ASP	CB-CG-OD2	-30.82	90.56	118.30
7	a	48	ARG	NE-CZ-NH2	-22.94	108.83	120.30
7	c	197	MET	CG-SD-CE	22.69	136.50	100.20
7	b	235	ARG	NE-CZ-NH1	-22.35	109.12	120.30
7	e	182	ARG	NE-CZ-NH2	-19.27	110.67	120.30
7	d	176	LEU	CB-CG-CD1	-19.25	78.27	111.00
7	e	49	LEU	CB-CG-CD1	-18.63	79.33	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	235	ARG	NE-CZ-NH2	18.37	129.48	120.30
7	b	182	ARG	NE-CZ-NH2	-18.08	111.26	120.30
7	e	182	ARG	NE-CZ-NH1	17.87	129.24	120.30
7	a	182	ARG	NE-CZ-NH1	17.64	129.12	120.30
7	f	212	ARG	NE-CZ-NH2	17.15	128.87	120.30
6	T	13	DG	O5'-P-OP1	-17.06	90.23	110.70
7	f	203	LEU	CB-CG-CD1	-16.99	82.12	111.00
7	f	169	LEU	CB-CG-CD2	-16.77	82.49	111.00
7	b	227	ARG	NE-CZ-NH1	16.36	128.48	120.30
7	b	143	ARG	NH1-CZ-NH2	16.24	137.26	119.40
7	a	98	ARG	NH1-CZ-NH2	16.12	137.13	119.40
7	c	229	LEU	CB-CG-CD1	-15.96	83.88	111.00
8	M	329	LEU	CB-CG-CD2	15.72	137.73	111.00
7	c	229	LEU	CB-CG-CD2	15.57	137.48	111.00
7	f	98	ARG	NE-CZ-NH1	15.46	128.03	120.30
7	f	193	PHE	CG-CD2-CE2	-15.26	104.01	120.80
7	f	193	PHE	CB-CG-CD1	-15.24	110.13	120.80
8	M	456	ARG	NE-CZ-NH1	-15.14	112.73	120.30
7	a	217	LEU	CB-CG-CD2	-15.07	85.38	111.00
7	b	227	ARG	CG-CD-NE	-14.15	82.08	111.80
7	a	173	VAL	CG1-CB-CG2	14.04	133.36	110.90
6	T	13	DG	O5'-P-OP2	13.90	127.38	110.70
8	M	128	VAL	CA-CB-CG2	-13.78	90.24	110.90
8	M	184	ARG	NE-CZ-NH1	-13.77	113.41	120.30
7	a	220	TYR	CG-CD2-CE2	-13.46	110.53	121.30
7	f	140	VAL	CG1-CB-CG2	-13.36	89.53	110.90
7	a	65	CYS	CA-CB-SG	-13.13	90.36	114.00
7	b	49	LEU	CB-CG-CD1	-13.02	88.86	111.00
5	N	-11	DA	O3'-P-O5'	-12.84	79.61	104.00
7	c	182	ARG	NE-CZ-NH1	12.82	126.71	120.30
5	N	-11	DA	P-O3'-C3'	-12.63	104.54	119.70
7	d	100	ASP	OD1-CG-OD2	12.63	147.29	123.30
8	M	384	VAL	CG1-CB-CG2	-12.61	90.73	110.90
7	f	214	ARG	NE-CZ-NH1	12.56	126.58	120.30
7	a	48	ARG	CG-CD-NE	12.52	138.09	111.80
5	N	-27	DT	O5'-P-OP1	12.44	125.63	110.70
7	b	49	LEU	CA-CB-CG	-12.37	86.84	115.30
7	b	68	LEU	CB-CG-CD2	-12.22	90.22	111.00
7	b	33	LEU	CB-CG-CD2	-11.92	90.73	111.00
8	M	258	PRO	CB-CA-C	-11.87	82.32	112.00
5	N	-28	DC	O5'-P-OP2	-11.86	95.03	105.70
7	a	203	LEU	CB-CG-CD1	-11.74	91.05	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	144	LEU	CB-CG-CD2	-11.54	91.38	111.00
7	e	189	MET	CB-CG-SD	11.53	147.00	112.40
7	e	45	ILE	CB-CA-C	-11.50	88.60	111.60
8	M	345	ARG	NE-CZ-NH2	-11.48	114.56	120.30
7	a	187	MET	CG-SD-CE	11.47	118.55	100.20
8	M	37	LEU	CB-CG-CD2	-11.31	91.77	111.00
8	M	120	LEU	CD1-CG-CD2	-11.25	76.75	110.50
7	c	182	ARG	NE-CZ-NH2	-11.21	114.69	120.30
7	b	16	LEU	CB-CG-CD1	11.20	130.04	111.00
7	f	199	ARG	NE-CZ-NH2	-11.18	114.71	120.30
7	a	220	TYR	CB-CG-CD1	-10.92	114.45	121.00
7	b	235	ARG	CB-CA-C	-10.92	88.56	110.40
8	M	297	LEU	CB-CG-CD1	-10.81	92.62	111.00
7	f	140	VAL	CB-CA-C	-10.81	90.87	111.40
7	d	96	PHE	N-CA-CB	10.79	130.02	110.60
8	M	333	LEU	CB-CG-CD1	-10.79	92.66	111.00
7	f	15	PHE	CD1-CE1-CZ	10.76	133.01	120.10
7	e	34	ILE	CG1-CB-CG2	10.63	134.78	111.40
8	M	323	LEU	CB-CG-CD1	-10.62	92.94	111.00
7	a	188	LEU	CB-CG-CD2	10.60	129.03	111.00
7	b	218	LEU	CB-CG-CD2	10.60	129.02	111.00
8	M	125	MET	CA-CB-CG	-10.58	95.32	113.30
7	b	188	LEU	CB-CG-CD1	-10.57	93.03	111.00
8	M	348	VAL	CG1-CB-CG2	-10.56	94.00	110.90
8	M	396	ILE	CG1-CB-CG2	-10.54	88.21	111.40
7	b	239	ARG	NE-CZ-NH1	-10.54	115.03	120.30
8	M	158	ILE	CG1-CB-CG2	10.48	134.46	111.40
7	d	96	PHE	CB-CG-CD2	-10.41	113.51	120.80
7	e	44	LEU	CB-CG-CD2	10.40	128.69	111.00
7	a	180	ARG	NE-CZ-NH2	-10.28	115.16	120.30
7	f	255	PHE	CB-CG-CD1	10.12	127.88	120.80
7	b	49	LEU	N-CA-CB	10.07	130.53	110.40
7	e	33	LEU	CB-CG-CD1	-10.05	93.92	111.00
7	c	169	LEU	CB-CG-CD1	10.02	128.04	111.00
7	e	229	LEU	CB-CG-CD2	9.97	127.95	111.00
7	b	235	ARG	CD-NE-CZ	9.85	137.40	123.60
7	e	251	ILE	CG1-CB-CG2	-9.62	90.25	111.40
8	M	259	ARG	CB-CG-CD	-9.62	86.60	111.60
8	M	195	LEU	CB-CA-C	-9.51	92.13	110.20
8	M	456	ARG	NH1-CZ-NH2	9.50	129.85	119.40
5	N	-11	DA	OP2-P-O3'	9.48	126.06	105.20
7	d	252	ILE	CG1-CB-CG2	9.44	132.16	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	109	LEU	CB-CG-CD1	9.43	127.03	111.00
8	M	329	LEU	CB-CG-CD1	-9.41	95.00	111.00
8	M	190	VAL	CA-CB-CG1	-9.35	96.88	110.90
8	M	262	GLN	O-C-N	9.34	137.64	122.70
7	f	233	VAL	CG1-CB-CG2	-9.30	96.02	110.90
7	b	33	LEU	CB-CG-CD1	-9.30	95.20	111.00
8	M	133	PHE	CB-CA-C	-9.23	91.94	110.40
7	f	44	LEU	CB-CG-CD1	9.23	126.69	111.00
7	a	185	ASP	O-C-N	9.22	137.45	122.70
7	f	214	ARG	NE-CZ-NH2	-9.16	115.72	120.30
7	c	167	ASP	CB-CG-OD1	9.14	126.53	118.30
7	e	172	ASP	N-CA-CB	-9.14	94.15	110.60
7	b	182	ARG	NH1-CZ-NH2	9.14	129.45	119.40
7	c	28	LEU	CB-CG-CD2	9.11	126.49	111.00
7	e	45	ILE	CG1-CB-CG2	-9.08	91.42	111.40
7	b	239	ARG	NE-CZ-NH2	9.05	124.83	120.30
8	M	28	LEU	CB-CG-CD1	9.02	126.34	111.00
7	d	96	PHE	CG-CD1-CE1	-9.01	110.89	120.80
6	T	14	DC	O5'-P-OP1	8.97	121.47	110.70
6	T	14	DC	P-O5'-C5'	-8.86	106.72	120.90
7	a	226	ILE	CG1-CB-CG2	-8.83	91.97	111.40
7	e	18	VAL	CG1-CB-CG2	8.83	125.03	110.90
7	b	120	LEU	CB-CG-CD1	8.80	125.95	111.00
7	b	214	ARG	CB-CG-CD	-8.73	88.91	111.60
7	a	183	GLU	OE1-CD-OE2	8.70	133.73	123.30
7	d	185	ASP	CB-CG-OD1	8.67	126.11	118.30
7	a	185	ASP	CA-C-N	-8.64	98.20	117.20
7	e	189	MET	CG-SD-CE	-8.61	86.42	100.20
8	M	271	TYR	CB-CA-C	-8.60	93.21	110.40
7	e	32	VAL	CB-CA-C	-8.57	95.11	111.40
7	e	55	ARG	CB-CG-CD	8.45	133.56	111.60
8	M	197	ASP	CB-CG-OD2	-8.44	110.70	118.30
7	a	193	PHE	CD1-CE1-CZ	-8.43	109.99	120.10
7	e	33	LEU	CA-CB-CG	-8.40	95.99	115.30
7	d	48	ARG	NE-CZ-NH2	8.39	124.50	120.30
7	e	8	LEU	CB-CG-CD2	-8.39	96.74	111.00
8	M	343	VAL	CG1-CB-CG2	8.39	124.32	110.90
7	e	203	LEU	CB-CG-CD2	-8.31	96.87	111.00
7	b	239	ARG	O-C-N	8.25	135.90	122.70
7	b	193	PHE	CG-CD2-CE2	-8.24	111.74	120.80
8	M	389	TYR	N-CA-CB	-8.23	95.78	110.60
7	f	255	PHE	CB-CG-CD2	-8.23	115.04	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	256	LEU	CA-CB-CG	8.20	134.15	115.30
8	M	329	LEU	CB-CA-C	-8.20	94.63	110.20
7	d	144	LEU	CB-CG-CD1	8.19	124.92	111.00
7	b	59	PRO	N-CA-C	-8.17	90.86	112.10
7	a	188	LEU	CA-CB-CG	-8.15	96.56	115.30
7	b	120	LEU	CA-CB-CG	-8.11	96.66	115.30
8	M	179	LEU	CB-CG-CD2	8.08	124.73	111.00
7	b	51	TYR	CB-CA-C	8.07	126.54	110.40
8	M	126	TRP	CG-CD1-NE1	-8.05	102.05	110.10
8	M	407	VAL	CG1-CB-CG2	8.05	123.78	110.90
8	M	196	ARG	N-CA-C	-8.04	89.29	111.00
8	M	120	LEU	N-CA-CB	8.04	126.48	110.40
7	c	217	LEU	CB-CG-CD2	8.03	124.66	111.00
7	a	174	VAL	CA-CB-CG1	8.00	122.90	110.90
7	a	203	LEU	CB-CG-CD2	7.98	124.56	111.00
7	d	96	PHE	CZ-CE2-CD2	-7.98	110.53	120.10
7	b	68	LEU	CA-CB-CG	-7.96	97.00	115.30
7	d	212	ARG	NE-CZ-NH2	7.92	124.26	120.30
7	b	192	TYR	CG-CD2-CE2	-7.88	114.99	121.30
7	f	255	PHE	N-CA-CB	-7.87	96.44	110.60
7	b	79	GLY	O-C-N	-7.86	110.13	122.70
7	e	230	LYS	CD-CE-NZ	7.83	129.70	111.70
8	M	142	THR	CA-CB-CG2	-7.81	101.46	112.40
7	f	212	ARG	NE-CZ-NH1	-7.81	116.39	120.30
7	f	255	PHE	N-CA-C	7.80	132.07	111.00
7	b	193	PHE	CB-CG-CD1	-7.78	115.36	120.80
7	b	32	VAL	CA-CB-CG2	7.76	122.53	110.90
7	e	173	VAL	CA-CB-CG2	-7.76	99.26	110.90
7	b	51	TYR	CB-CG-CD1	7.74	125.65	121.00
8	M	271	TYR	N-CA-CB	-7.72	96.71	110.60
7	e	33	LEU	CB-CA-C	7.71	124.86	110.20
8	M	354	PHE	CZ-CE2-CD2	-7.68	110.89	120.10
6	T	6	DT	C5'-C4'-O4'	7.65	123.84	109.30
7	f	193	PHE	CD1-CG-CD2	7.64	128.23	118.30
7	b	51	TYR	CA-CB-CG	-7.63	98.91	113.40
7	e	182	ARG	CA-CB-CG	-7.60	96.68	113.40
7	a	183	GLU	CB-CA-C	-7.59	95.22	110.40
7	e	235	ARG	NE-CZ-NH1	-7.58	116.51	120.30
7	c	212	ARG	NE-CZ-NH2	-7.57	116.52	120.30
7	a	223	PRO	CB-CA-C	-7.55	93.12	112.00
7	a	169	LEU	CA-CB-CG	-7.53	97.98	115.30
7	a	185	ASP	C-N-CA	-7.51	102.92	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	188	LEU	CA-CB-CG	7.46	132.45	115.30
8	M	184	ARG	NH1-CZ-NH2	7.45	127.59	119.40
7	a	98	ARG	CA-C-N	-7.45	100.82	117.20
7	d	44	LEU	CB-CG-CD2	7.43	123.64	111.00
7	f	15	PHE	CG-CD1-CE1	-7.43	112.63	120.80
7	c	28	LEU	CA-CB-CG	7.41	132.34	115.30
7	b	60	PHE	CB-CG-CD2	-7.40	115.62	120.80
7	e	255	PHE	CB-CG-CD2	-7.40	115.62	120.80
7	c	187	MET	CG-SD-CE	7.39	112.03	100.20
7	f	233	VAL	CA-CB-CG2	7.37	121.95	110.90
6	T	9	DT	P-O3'-C3'	-7.36	110.86	119.70
8	M	158	ILE	CB-CA-C	-7.36	96.87	111.60
7	e	33	LEU	CB-CG-CD2	7.35	123.49	111.00
8	M	203	LEU	O-C-N	7.34	134.45	122.70
8	M	37	LEU	CA-CB-CG	7.28	132.05	115.30
7	e	173	VAL	CG1-CB-CG2	-7.27	99.27	110.90
7	d	99	ALA	CB-CA-C	7.26	120.99	110.10
7	b	179	LEU	CB-CG-CD1	7.24	123.31	111.00
7	f	193	PHE	CD1-CE1-CZ	-7.24	111.41	120.10
7	f	140	VAL	CA-CB-CG2	7.23	121.75	110.90
8	M	384	VAL	CB-CA-C	-7.19	97.73	111.40
8	M	120	LEU	CB-CG-CD2	7.17	123.19	111.00
7	d	99	ALA	C-N-CA	-7.16	103.79	121.70
8	M	340	LEU	CB-CG-CD2	7.16	123.17	111.00
8	M	189	GLY	CA-C-N	-7.14	101.48	117.20
7	e	253	ASP	CB-CG-OD2	7.14	124.72	118.30
7	f	55	ARG	NE-CZ-NH1	7.13	123.87	120.30
7	d	144	LEU	CA-CB-CG	-7.11	98.96	115.30
7	e	62	SER	CA-C-O	-7.10	105.19	120.10
7	a	185	ASP	CB-CG-OD1	-7.08	111.92	118.30
7	e	32	VAL	O-C-N	7.08	134.03	122.70
7	b	235	ARG	CB-CG-CD	7.08	130.00	111.60
7	a	48	ARG	CB-CG-CD	-7.08	93.20	111.60
7	a	217	LEU	CB-CA-C	-7.06	96.78	110.20
7	a	48	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
7	f	34	ILE	CG1-CB-CG2	7.02	126.85	111.40
8	M	119	THR	N-CA-C	7.02	129.94	111.00
8	M	279	ARG	N-CA-C	7.01	129.93	111.00
7	f	99	ALA	CB-CA-C	7.01	120.61	110.10
7	b	212	ARG	NE-CZ-NH1	-7.00	116.80	120.30
8	M	195	LEU	CD1-CG-CD2	-6.98	89.56	110.50
7	b	212	ARG	NE-CZ-NH2	6.97	123.78	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	55	ARG	CA-CB-CG	-6.96	98.09	113.40
7	b	32	VAL	C-N-CA	-6.96	104.31	121.70
7	c	197	MET	CB-CG-SD	6.95	133.26	112.40
8	M	256	LEU	CB-CG-CD2	-6.94	99.21	111.00
7	b	256	LYS	N-CA-CB	-6.93	98.12	110.60
7	a	182	ARG	NE-CZ-NH2	-6.92	116.84	120.30
7	f	98	ARG	NH1-CZ-NH2	-6.92	111.78	119.40
8	M	389	TYR	CB-CG-CD1	6.92	125.15	121.00
7	a	199	ARG	CA-CB-CG	6.90	128.57	113.40
7	d	147	ALA	CB-CA-C	6.87	120.41	110.10
7	f	197	MET	CA-CB-CG	6.87	124.98	113.30
7	a	220	TYR	CD1-CE1-CZ	-6.85	113.63	119.80
8	M	380	THR	CA-CB-OG1	-6.85	94.62	109.00
8	M	386	THR	CA-CB-CG2	-6.84	102.82	112.40
7	a	209	PHE	CG-CD1-CE1	-6.84	113.28	120.80
7	b	70	GLU	CB-CA-C	6.84	124.07	110.40
7	c	220	TYR	CG-CD2-CE2	-6.82	115.84	121.30
7	e	239	ARG	NE-CZ-NH2	-6.82	116.89	120.30
8	M	195	LEU	CB-CG-CD2	-6.81	99.42	111.00
7	f	169	LEU	CA-C-O	6.81	134.40	120.10
7	f	15	PHE	CB-CG-CD2	-6.78	116.06	120.80
8	M	197	ASP	OD1-CG-OD2	6.77	136.16	123.30
7	f	167	ASP	CB-CG-OD1	-6.75	112.23	118.30
7	d	189	MET	CG-SD-CE	6.74	110.98	100.20
8	M	260	PRO	C-N-CA	-6.71	108.20	122.30
8	M	354	PHE	CB-CG-CD2	-6.71	116.11	120.80
7	c	229	LEU	O-C-N	6.69	133.40	122.70
8	M	394	ARG	CA-CB-CG	-6.68	98.70	113.40
5	N	-15	DT	O5'-P-OP2	-6.67	99.69	105.70
8	M	147	ALA	N-CA-CB	-6.64	100.80	110.10
7	e	188	LEU	CB-CG-CD1	6.64	122.29	111.00
8	M	258	PRO	N-CD-CG	6.62	113.14	103.20
7	b	225	ASN	N-CA-C	6.62	128.88	111.00
7	a	80	HIS	N-CA-C	6.61	128.84	111.00
8	M	235	LEU	CA-CB-CG	6.60	130.48	115.30
7	a	183	GLU	CG-CD-OE1	-6.60	105.10	118.30
7	e	44	LEU	CB-CA-C	6.59	122.72	110.20
7	d	173	VAL	CB-CA-C	-6.58	98.90	111.40
7	f	229	LEU	CB-CG-CD1	-6.58	99.82	111.00
7	e	32	VAL	CA-C-N	-6.57	102.74	117.20
7	f	15	PHE	CE1-CZ-CE2	-6.55	108.21	120.00
6	T	8	DA	C5'-C4'-O4'	6.54	121.72	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	396	ILE	CB-CG1-CD1	-6.54	95.59	113.90
7	d	145	VAL	N-CA-CB	6.53	125.87	111.50
7	d	45	ILE	CB-CG1-CD1	-6.52	95.65	113.90
7	e	193	PHE	CZ-CE2-CD2	6.52	127.92	120.10
7	a	98	ARG	CA-C-O	6.49	133.72	120.10
5	N	-27	DT	O5'-P-OP2	-6.46	99.88	105.70
7	c	256	LYS	N-CA-CB	-6.45	99.00	110.60
7	a	98	ARG	CB-CG-CD	-6.42	94.92	111.60
7	f	224	GLY	N-CA-C	-6.42	97.06	113.10
7	b	217	LEU	CB-CG-CD1	-6.41	100.11	111.00
7	e	44	LEU	CD1-CG-CD2	-6.40	91.30	110.50
7	a	99	ALA	CB-CA-C	6.39	119.68	110.10
8	M	47	LEU	N-CA-CB	-6.38	97.63	110.40
7	e	172	ASP	C-N-CA	-6.36	105.79	121.70
7	f	149	ASN	CB-CG-ND2	-6.36	101.44	116.70
8	M	456	ARG	CG-CD-NE	6.35	125.14	111.80
7	b	256	LYS	CB-CA-C	6.34	123.09	110.40
8	M	252	LEU	CA-CB-CG	6.33	129.85	115.30
5	N	-18	DT	C5'-C4'-O4'	6.33	121.32	109.30
7	e	46	ALA	CA-C-O	6.33	133.39	120.10
7	f	232	VAL	CG1-CB-CG2	-6.32	100.79	110.90
8	M	128	VAL	CG1-CB-CG2	-6.32	100.80	110.90
7	f	232	VAL	CB-CA-C	-6.31	99.41	111.40
7	c	198	CYS	CA-CB-SG	-6.30	102.66	114.00
7	c	179	LEU	CB-CG-CD2	-6.29	100.31	111.00
7	c	235	ARG	NE-CZ-NH1	-6.29	117.15	120.30
7	d	119	LYS	CD-CE-NZ	-6.29	97.23	111.70
7	a	199	ARG	NE-CZ-NH1	-6.29	117.16	120.30
7	f	257	ARG	CB-CG-CD	-6.28	95.28	111.60
8	M	390	LEU	CA-CB-CG	-6.27	100.88	115.30
7	e	193	PHE	CG-CD1-CE1	6.25	127.67	120.80
7	e	235	ARG	NE-CZ-NH2	6.24	123.42	120.30
8	M	143	SER	CA-CB-OG	-6.24	94.35	111.20
8	M	345	ARG	CB-CA-C	6.24	122.88	110.40
7	e	46	ALA	N-CA-C	6.24	127.84	111.00
7	a	187	MET	N-CA-CB	-6.23	99.39	110.60
7	e	255	PHE	CB-CG-CD1	6.22	125.15	120.80
8	M	420	ILE	CA-CB-CG1	-6.21	99.19	111.00
7	a	222	TRP	CE3-CZ3-CH2	-6.20	114.38	121.20
7	d	203	LEU	CB-CG-CD1	-6.18	100.49	111.00
7	f	127	GLY	N-CA-C	-6.18	97.65	113.10
7	f	45	ILE	CB-CA-C	-6.17	99.26	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	26	LEU	CB-CA-C	-6.16	98.50	110.20
7	a	186	ILE	CA-C-N	-6.16	103.66	117.20
8	M	179	LEU	CA-CB-CG	6.15	129.45	115.30
7	b	179	LEU	CB-CG-CD2	-6.13	100.58	111.00
7	e	49	LEU	CB-CG-CD2	6.12	121.40	111.00
8	M	276	VAL	CG1-CB-CG2	-6.11	101.12	110.90
8	M	347	ILE	CB-CG1-CD1	-6.11	96.78	113.90
8	M	145	VAL	CA-CB-CG1	-6.11	101.74	110.90
7	e	46	ALA	O-C-N	-6.09	112.96	122.70
7	e	205	LEU	CB-CG-CD1	6.09	121.35	111.00
7	d	175	GLN	CB-CA-C	6.04	122.48	110.40
8	M	200	LEU	CB-CG-CD2	6.04	121.27	111.00
8	M	130	LEU	C-N-CA	-6.03	106.62	121.70
7	f	193	PHE	CE1-CZ-CE2	6.02	130.83	120.00
7	b	120	LEU	CA-C-O	6.01	132.73	120.10
8	M	126	TRP	CD1-NE1-CE2	6.01	114.41	109.00
7	a	174	VAL	CG1-CB-CG2	-5.99	101.31	110.90
7	c	179	LEU	CA-CB-CG	5.99	129.07	115.30
7	f	197	MET	O-C-N	5.99	132.28	122.70
7	e	179	LEU	CA-CB-CG	5.99	129.07	115.30
7	e	255	PHE	CB-CA-C	-5.99	98.42	110.40
7	d	128	GLU	O-C-N	-5.97	113.15	122.70
7	b	120	LEU	CA-C-N	-5.96	104.09	117.20
7	c	22	VAL	CG1-CB-CG2	-5.95	101.37	110.90
7	c	217	LEU	CA-CB-CG	-5.95	101.61	115.30
7	b	33	LEU	N-CA-C	5.94	127.04	111.00
8	M	153	TYR	CB-CG-CD1	-5.94	117.44	121.00
8	M	190	VAL	N-CA-C	-5.94	94.96	111.00
7	f	253	ASP	CB-CG-OD1	5.94	123.65	118.30
7	a	221	ARG	CB-CA-C	5.93	122.27	110.40
8	M	146	ASP	CB-CG-OD1	-5.93	112.96	118.30
7	a	13	ASN	CB-CG-OD1	5.92	133.44	121.60
8	M	41	LEU	CB-CG-CD2	-5.92	100.93	111.00
7	b	140	VAL	N-CA-CB	-5.92	98.48	111.50
7	a	220	TYR	C-N-CA	-5.92	106.91	121.70
8	M	333	LEU	CB-CA-C	-5.91	98.97	110.20
8	M	215	GLU	OE1-CD-OE2	-5.91	116.21	123.30
7	a	48	ARG	CA-CB-CG	-5.91	100.41	113.40
7	b	237	VAL	CB-CA-C	-5.91	100.18	111.40
8	M	456	ARG	NE-CZ-NH2	-5.90	117.35	120.30
8	M	189	GLY	CA-C-O	5.90	131.22	120.60
7	f	257	ARG	NE-CZ-NH2	5.90	123.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	255	PHE	N-CA-CB	5.89	121.20	110.60
7	a	247	LEU	CB-CG-CD2	5.88	121.00	111.00
8	M	263	SER	N-CA-CB	5.88	119.33	110.50
7	e	49	LEU	CD1-CG-CD2	5.88	128.15	110.50
7	e	194	ALA	CA-C-N	-5.87	104.28	117.20
7	b	227	ARG	NE-CZ-NH2	-5.87	117.37	120.30
7	f	230	LYS	CB-CG-CD	5.87	126.85	111.60
7	d	155	MET	CG-SD-CE	5.86	109.57	100.20
7	a	212	ARG	CA-CB-CG	5.86	126.28	113.40
7	f	149	ASN	CB-CG-OD1	5.86	133.31	121.60
7	b	177	PRO	CA-N-CD	5.85	119.89	111.70
7	b	188	LEU	CB-CG-CD2	5.85	120.95	111.00
7	e	22	VAL	O-C-N	5.85	132.06	122.70
5	N	-27	DT	P-O5'-C5'	-5.85	111.55	120.90
6	T	9	DT	C1'-O4'-C4'	5.85	115.95	110.10
7	b	249	ASP	CB-CG-OD2	-5.85	113.04	118.30
8	M	473	ARG	CD-NE-CZ	-5.84	115.43	123.60
7	f	146	CYS	N-CA-C	-5.83	95.25	111.00
7	a	79	GLY	N-CA-C	-5.83	98.52	113.10
7	a	173	VAL	CB-CA-C	-5.83	100.32	111.40
7	e	187	MET	C-N-CA	-5.82	107.15	121.70
8	M	376	MET	CA-CB-CG	5.82	123.20	113.30
7	b	52	LEU	CB-CG-CD2	5.81	120.87	111.00
7	c	232	VAL	CB-CA-C	-5.80	100.37	111.40
7	b	236	SER	N-CA-CB	-5.80	101.80	110.50
8	M	147	ALA	CB-CA-C	5.80	118.80	110.10
7	a	193	PHE	CB-CG-CD2	-5.79	116.75	120.80
7	f	255	PHE	CZ-CE2-CD2	5.79	127.05	120.10
7	c	255	PHE	CG-CD2-CE2	5.79	127.17	120.80
8	M	259	ARG	NE-CZ-NH1	5.78	123.19	120.30
7	f	197	MET	CG-SD-CE	5.78	109.45	100.20
8	M	127	GLN	C-N-CA	-5.77	107.28	121.70
8	M	197	ASP	CB-CG-OD1	-5.75	113.12	118.30
8	M	142	THR	OG1-CB-CG2	-5.75	96.77	110.00
6	T	7	DG	P-O3'-C3'	5.75	126.60	119.70
7	b	178	PRO	N-CA-CB	5.75	110.20	103.30
7	f	79	GLY	CA-C-O	-5.75	110.25	120.60
7	a	80	HIS	CB-CA-C	-5.75	98.90	110.40
8	M	253	ILE	CG1-CB-CG2	5.74	124.03	111.40
8	M	179	LEU	CD1-CG-CD2	-5.74	93.28	110.50
7	e	147	ALA	CB-CA-C	5.74	118.70	110.10
7	c	243	SER	N-CA-C	5.73	126.47	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	167	ASP	CA-C-N	5.72	129.78	117.20
7	f	214	ARG	CB-CG-CD	5.71	126.43	111.60
7	a	169	LEU	CD1-CG-CD2	-5.70	93.41	110.50
7	c	230	LYS	CD-CE-NZ	-5.70	98.59	111.70
8	M	461	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
7	c	169	LEU	CB-CG-CD2	-5.68	101.34	111.00
7	a	34	ILE	CB-CG1-CD1	-5.68	98.00	113.90
8	M	348	VAL	CB-CA-C	-5.66	100.64	111.40
7	a	65	CYS	CB-CA-C	5.65	121.71	110.40
7	e	235	ARG	CB-CA-C	5.65	121.70	110.40
8	M	420	ILE	CB-CA-C	-5.64	100.31	111.60
7	f	45	ILE	CG1-CB-CG2	5.64	123.80	111.40
8	M	463	GLU	OE1-CD-OE2	5.63	130.06	123.30
7	b	142	VAL	CA-CB-CG1	5.63	119.34	110.90
5	N	-26	DG	C1'-O4'-C4'	-5.62	104.48	110.10
8	M	343	VAL	CA-CB-CG1	-5.62	102.47	110.90
5	N	-26	DG	P-O5'-C5'	-5.62	111.91	120.90
7	a	223	PRO	O-C-N	5.62	132.75	123.20
8	M	125	MET	CB-CA-C	-5.62	99.17	110.40
7	e	147	ALA	N-CA-CB	5.60	117.94	110.10
7	f	247	LEU	CB-CG-CD1	5.59	120.51	111.00
7	b	199	ARG	CA-CB-CG	5.59	125.70	113.40
7	a	224	GLY	O-C-N	5.58	131.63	122.70
8	M	127	GLN	CA-CB-CG	-5.58	101.13	113.40
7	b	14	SER	C-N-CA	-5.57	107.77	121.70
8	M	118	GLN	O-C-N	-5.57	113.79	122.70
6	T	8	DA	O3'-P-O5'	5.57	114.57	104.00
7	b	143	ARG	N-CA-CB	-5.57	100.58	110.60
7	b	184	SER	CA-C-O	-5.57	108.41	120.10
7	d	212	ARG	NE-CZ-NH1	-5.56	117.52	120.30
7	a	200	GLU	CA-CB-CG	-5.56	101.18	113.40
8	M	357	GLN	C-N-CA	-5.56	110.63	122.30
7	c	180	ARG	NE-CZ-NH2	5.55	123.08	120.30
7	f	167	ASP	CB-CG-OD2	5.55	123.30	118.30
7	b	79	GLY	CA-C-N	5.55	129.40	117.20
7	b	193	PHE	CD1-CG-CD2	5.54	125.50	118.30
8	M	37	LEU	CB-CG-CD1	-5.53	101.60	111.00
7	f	34	ILE	CA-C-O	5.53	131.70	120.10
7	a	220	TYR	CD1-CG-CD2	5.52	123.97	117.90
7	c	255	PHE	N-CA-C	5.52	125.90	111.00
7	b	40	THR	N-CA-C	5.51	125.88	111.00
7	a	180	ARG	NE-CZ-NH1	5.50	123.05	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	169	LEU	CA-C-N	-5.50	105.11	117.20
7	e	234	GLU	OE1-CD-OE2	-5.50	116.70	123.30
8	M	257	ASP	C-N-CD	-5.49	108.52	120.60
7	a	220	TYR	CE1-CZ-OH	-5.48	105.30	120.10
8	M	183	GLN	O-C-N	5.48	131.47	122.70
8	M	129	GLU	CB-CA-C	-5.47	99.46	110.40
7	a	48	ARG	N-CA-CB	5.46	120.43	110.60
7	a	100	ASP	CB-CG-OD1	-5.46	113.39	118.30
7	b	61	ILE	CG1-CB-CG2	5.46	123.41	111.40
8	M	202	GLN	N-CA-CB	5.45	120.42	110.60
7	d	158	GLU	C-N-CA	5.45	133.75	122.30
7	a	183	GLU	CA-CB-CG	5.45	125.39	113.40
6	T	9	DT	C5'-C4'-O4'	5.45	119.65	109.30
7	d	174	VAL	CA-C-N	-5.45	105.22	117.20
8	M	320	ARG	NE-CZ-NH2	-5.44	117.58	120.30
7	f	251	ILE	CB-CG1-CD1	5.44	129.13	113.90
7	a	94	GLY	CA-C-O	5.43	130.38	120.60
7	e	199	ARG	NE-CZ-NH2	5.43	123.01	120.30
8	M	199	LEU	CA-CB-CG	-5.42	102.83	115.30
7	b	191	GLU	CA-CB-CG	-5.42	101.48	113.40
7	f	201	ILE	CG1-CB-CG2	5.42	123.32	111.40
7	b	59	PRO	N-CD-CG	5.42	111.33	103.20
8	M	339	THR	CA-CB-CG2	-5.42	104.82	112.40
8	M	329	LEU	CA-CB-CG	5.41	127.75	115.30
8	M	354	PHE	CG-CD2-CE2	5.41	126.75	120.80
8	M	41	LEU	CD1-CG-CD2	5.41	126.73	110.50
8	M	461	TYR	CG-CD1-CE1	-5.40	116.98	121.30
8	M	330	ILE	CA-CB-CG2	-5.40	100.11	110.90
7	c	167	ASP	OD1-CG-OD2	-5.39	113.05	123.30
7	f	128	GLU	CA-CB-CG	5.39	125.26	113.40
7	c	252	ILE	N-CA-CB	-5.39	98.40	110.80
7	d	252	ILE	CB-CG1-CD1	5.39	128.98	113.90
6	T	7	DG	OP1-P-O3'	5.37	117.02	105.20
7	b	16	LEU	CA-CB-CG	-5.37	102.95	115.30
8	M	198	CYS	CA-CB-SG	5.36	123.65	114.00
7	e	199	ARG	NE-CZ-NH1	-5.34	117.63	120.30
8	M	390	LEU	CB-CG-CD2	5.34	120.08	111.00
7	f	256	LYS	CB-CG-CD	5.34	125.48	111.60
8	M	262	GLN	N-CA-C	-5.34	96.59	111.00
7	e	180	ARG	CB-CG-CD	5.32	125.42	111.60
7	d	48	ARG	CG-CD-NE	5.31	122.95	111.80
7	d	170	ALA	N-CA-C	-5.31	96.67	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	153	TYR	CB-CA-C	-5.30	99.79	110.40
7	a	218	LEU	CB-CG-CD1	-5.30	101.99	111.00
7	d	109	LEU	CB-CG-CD2	-5.29	102.00	111.00
8	M	428	ILE	CG1-CB-CG2	-5.29	99.75	111.40
7	f	212	ARG	CG-CD-NE	5.29	122.91	111.80
7	a	258	ARG	CB-CA-C	5.28	120.97	110.40
8	M	259	ARG	NE-CZ-NH2	-5.28	117.66	120.30
7	c	209	PHE	CB-CG-CD1	-5.28	117.11	120.80
7	b	236	SER	O-C-N	5.27	131.13	122.70
8	M	380	THR	C-N-CA	-5.27	108.53	121.70
7	c	251	ILE	CA-C-O	5.26	131.15	120.10
8	M	46	LEU	CA-CB-CG	-5.26	103.20	115.30
7	e	62	SER	N-CA-CB	5.25	118.37	110.50
7	b	255	PHE	O-C-N	5.25	131.09	122.70
8	M	399	LEU	CB-CA-C	-5.25	100.23	110.20
8	M	28	LEU	N-CA-C	-5.24	96.86	111.00
8	M	249	ALA	CB-CA-C	-5.24	102.24	110.10
8	M	38	GLN	CB-CA-C	-5.24	99.93	110.40
7	c	212	ARG	CG-CD-NE	-5.23	100.81	111.80
7	b	190	ALA	CA-C-O	5.23	131.08	120.10
7	d	108	GLU	OE1-CD-OE2	-5.23	117.02	123.30
8	M	210	THR	N-CA-CB	5.23	120.24	110.30
7	f	217	LEU	CB-CG-CD1	5.23	119.89	111.00
7	a	226	ILE	CA-CB-CG2	5.23	121.36	110.90
7	d	96	PHE	CD1-CE1-CZ	5.23	126.37	120.10
8	M	354	PHE	C-N-CA	-5.22	108.64	121.70
6	T	9	DT	OP1-P-O3'	-5.22	93.72	105.20
7	b	32	VAL	O-C-N	5.22	131.05	122.70
6	T	20	DT	C1'-O4'-C4'	-5.22	104.88	110.10
6	T	7	DG	C1'-O4'-C4'	5.21	115.31	110.10
7	d	95	ARG	C-N-CA	-5.21	108.67	121.70
7	a	222	TRP	CD2-CE3-CZ3	5.20	125.56	118.80
8	M	455	ARG	N-CA-CB	5.20	119.96	110.60
7	a	174	VAL	N-CA-C	-5.19	96.98	111.00
7	b	197	MET	CB-CG-SD	-5.19	96.83	112.40
7	a	188	LEU	CB-CA-C	5.19	120.06	110.20
8	M	258	PRO	CB-CG-CD	-5.19	86.27	106.50
7	a	220	TYR	CE1-CZ-CE2	5.18	128.10	119.80
3	D	870	ASP	CB-CG-OD2	5.17	122.96	118.30
7	a	219	ASN	CB-CA-C	5.17	120.74	110.40
7	b	32	VAL	CA-C-N	-5.17	105.84	117.20
7	a	48	ARG	CB-CA-C	5.16	120.72	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	65	CYS	CA-C-O	5.16	130.93	120.10
7	c	218	LEU	CB-CA-C	5.15	119.98	110.20
7	e	185	ASP	CB-CG-OD1	-5.14	113.67	118.30
7	a	184	SER	C-N-CA	-5.14	108.84	121.70
8	M	190	VAL	N-CA-CB	-5.14	100.19	111.50
8	M	199	LEU	CB-CG-CD1	5.14	119.74	111.00
7	a	205	LEU	CB-CG-CD2	5.14	119.73	111.00
7	f	79	GLY	N-CA-C	5.13	125.93	113.10
7	d	176	LEU	CB-CG-CD2	5.12	119.71	111.00
7	f	247	LEU	CA-CB-CG	-5.12	103.52	115.30
7	e	62	SER	CA-CB-OG	-5.12	97.37	111.20
8	M	372	GLN	CB-CA-C	5.12	120.64	110.40
7	c	222	TRP	CB-CA-C	-5.12	100.16	110.40
6	T	22	DG	OP1-P-OP2	-5.12	111.93	119.60
8	M	376	MET	CB-CG-SD	-5.12	97.06	112.40
7	f	214	ARG	CD-NE-CZ	5.11	130.76	123.60
7	e	210	THR	CA-CB-CG2	-5.11	105.24	112.40
7	a	217	LEU	CB-CG-CD1	-5.11	102.31	111.00
6	T	23	DT	O5'-P-OP1	5.11	116.83	110.70
8	M	158	ILE	CA-CB-CG2	-5.11	100.69	110.90
8	M	453	VAL	CG1-CB-CG2	-5.11	102.73	110.90
7	e	180	ARG	N-CA-C	-5.10	97.23	111.00
6	T	9	DT	OP2-P-O3'	5.10	116.42	105.20
7	f	44	LEU	CB-CA-C	5.08	119.85	110.20
7	c	220	TYR	CB-CG-CD1	-5.06	117.96	121.00
7	d	151	ASP	CB-CG-OD1	5.06	122.86	118.30
8	M	289	LEU	N-CA-CB	-5.05	100.29	110.40
7	f	44	LEU	CA-CB-CG	-5.05	103.68	115.30
5	N	-21	DG	O5'-P-OP1	5.05	116.76	110.70
7	f	169	LEU	CB-CG-CD1	5.05	119.58	111.00
7	b	179	LEU	CB-CA-C	-5.04	100.62	110.20
8	M	345	ARG	NE-CZ-NH1	5.04	122.82	120.30
8	M	46	LEU	CB-CG-CD2	-5.03	102.44	111.00
8	M	140	ILE	CG1-CB-CG2	5.03	122.47	111.40
7	a	184	SER	N-CA-C	-5.03	97.43	111.00
7	d	96	PHE	CB-CG-CD1	5.03	124.32	120.80
8	M	473	ARG	N-CA-CB	5.02	119.64	110.60
7	d	253	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	a	162	ARG	Mainchain
7	b	219	ASN	Mainchain
7	d	92	HIS	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	305/329 (93%)	282 (92%)	22 (7%)	1 (0%)	41	75
1	B	219/329 (67%)	203 (93%)	16 (7%)	0	100	100
2	C	1339/1342 (100%)	1264 (94%)	75 (6%)	0	100	100
3	D	1322/1407 (94%)	1226 (93%)	93 (7%)	3 (0%)	47	81
4	E	72/91 (79%)	70 (97%)	2 (3%)	0	100	100
7	a	257/295 (87%)	200 (78%)	43 (17%)	14 (5%)	2	17
7	b	256/295 (87%)	216 (84%)	27 (10%)	13 (5%)	2	19
7	c	254/295 (86%)	221 (87%)	31 (12%)	2 (1%)	19	58
7	d	254/295 (86%)	226 (89%)	23 (9%)	5 (2%)	7	39
7	e	257/295 (87%)	217 (84%)	30 (12%)	10 (4%)	3	25
7	f	257/295 (87%)	225 (88%)	22 (9%)	10 (4%)	3	25
8	M	413/477 (87%)	360 (87%)	42 (10%)	11 (3%)	5	33
All	All	5205/5745 (91%)	4710 (90%)	426 (8%)	69 (1%)	16	48

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	a	12	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	56	TRP
7	a	121	LEU
7	b	81	GLU
7	b	93	PRO
7	b	225	ASN
7	b	226	ILE
7	f	183	GLU
7	e	72	LEU
7	e	211	GLU
8	M	194	ASP
8	M	196	ARG
8	M	353	ALA
7	a	5	LYS
7	a	7	ASN
7	a	74	ASP
7	a	184	SER
7	b	223	PRO
7	d	41	GLY
7	f	110	ALA
7	f	255	PHE
8	M	189	GLY
7	a	2	ALA
7	a	51	TYR
7	a	126	TYR
7	b	66	ALA
7	b	170	ALA
7	d	43	GLU
7	d	135	SER
7	f	223	PRO
7	e	54	SER
7	e	71	ASN
8	M	112	TYR
8	M	120	LEU
8	M	309	SER
3	D	886	VAL
7	a	166	LEU
7	b	55	ARG
7	b	137	PRO
7	d	77	LEU
7	d	159	GLY
7	f	132	VAL
7	e	112	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	e	125	GLU
3	D	340	GLN
7	b	178	PRO
7	b	254	PRO
7	f	73	LEU
7	e	69	ASN
7	e	182	ARG
8	M	10	SER
8	M	110	PRO
1	A	194	GLN
7	a	127	GLY
7	b	9	LEU
7	c	251	ILE
7	f	254	PRO
7	e	14	SER
7	e	111	THR
8	M	264	ILE
7	a	145	VAL
7	b	204	PRO
7	f	204	PRO
7	a	204	PRO
7	c	204	PRO
7	f	252	ILE
8	M	272	VAL
3	D	750	PRO
7	f	41	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/286 (87%)	240 (96%)	9 (4%)	35	66
1	B	180/286 (63%)	171 (95%)	9 (5%)	24	58
2	C	1047/1157 (90%)	1010 (96%)	37 (4%)	36	67
3	D	913/1168 (78%)	872 (96%)	41 (4%)	27	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	53/75 (71%)	53 (100%)	0	100	100
7	a	219/252 (87%)	156 (71%)	63 (29%)	0	2
7	b	219/252 (87%)	181 (83%)	38 (17%)	2	11
7	c	208/252 (82%)	181 (87%)	27 (13%)	4	21
7	d	218/252 (86%)	191 (88%)	27 (12%)	4	23
7	e	220/252 (87%)	192 (87%)	28 (13%)	4	22
7	f	219/252 (87%)	192 (88%)	27 (12%)	4	23
8	M	367/423 (87%)	286 (78%)	81 (22%)	1	5
All	All	4112/4907 (84%)	3725 (91%)	387 (9%)	12	35

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	8	PHE
1	A	31	LEU
1	A	92	VAL
1	A	100	LEU
1	A	195	ARG
1	A	201	LEU
1	A	278	ILE
1	A	321	TRP
1	B	16	ILE
1	B	72	GLU
1	B	145	LYS
1	B	150	ARG
1	B	174	ASP
1	B	182	ARG
1	B	224	LEU
1	B	228	LEU
1	B	229	GLU
2	C	37	LYS
2	C	91	THR
2	C	150	HIS
2	C	189	ASP
2	C	200	ARG
2	C	208	ILE
2	C	209	ILE
2	C	221	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	237	LEU
2	C	246	LEU
2	C	324	LYS
2	C	397	LEU
2	C	405	PHE
2	C	484	LEU
2	C	487	LEU
2	C	496	LYS
2	C	540	ARG
2	C	589	THR
2	C	697	LYS
2	C	755	LYS
2	C	796	LEU
2	C	817	LEU
2	C	841	ARG
2	C	873	ILE
2	C	918	LEU
2	C	927	THR
2	C	1014	LEU
2	C	1026	GLU
2	C	1027	LYS
2	C	1029	LEU
2	C	1060	ILE
2	C	1069	ARG
2	C	1073	LYS
2	C	1161	LEU
2	C	1176	LEU
2	C	1233	LEU
2	C	1268	GLN
3	D	5	LEU
3	D	44	ILE
3	D	50	LYS
3	D	53	ARG
3	D	74	LYS
3	D	92	VAL
3	D	113	HIS
3	D	117	LEU
3	D	142	GLU
3	D	161	THR
3	D	166	LEU
3	D	171	GLU
3	D	223	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	265	LEU
3	D	295	GLU
3	D	316	ILE
3	D	321	LYS
3	D	324	LEU
3	D	325	LYS
3	D	340	GLN
3	D	422	LEU
3	D	428	THR
3	D	430	HIS
3	D	445	LYS
3	D	460	ASP
3	D	505	ASP
3	D	517	CYS
3	D	518	VAL
3	D	563	LEU
3	D	570	LYS
3	D	695	LYS
3	D	703	THR
3	D	747	MET
3	D	802	ASP
3	D	825	VAL
3	D	827	GLU
3	D	885	VAL
3	D	901	ARG
3	D	911	LYS
3	D	960	LEU
3	D	1266	ILE
7	a	1	MET
7	a	3	GLU
7	a	4	TYR
7	a	5	LYS
7	a	9	LEU
7	a	11	GLU
7	a	22	VAL
7	a	30	LYS
7	a	32	VAL
7	a	33	LEU
7	a	38	ARG
7	a	42	LYS
7	a	44	LEU
7	a	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	54	SER
7	a	55	ARG
7	a	56	TRP
7	a	63	LEU
7	a	70	GLU
7	a	86	THR
7	a	89	GLN
7	a	91	ARG
7	a	95	ARG
7	a	98	ARG
7	a	103	THR
7	a	104	LEU
7	a	106	LEU
7	a	107	ASP
7	a	114	MET
7	a	115	MET
7	a	117	GLN
7	a	118	GLU
7	a	119	LYS
7	a	126	TYR
7	a	128	GLU
7	a	129	LEU
7	a	138	LEU
7	a	140	VAL
7	a	143	ARG
7	a	144	LEU
7	a	149	ASN
7	a	155	MET
7	a	161	PHE
7	a	166	LEU
7	a	171	PHE
7	a	173	VAL
7	a	175	GLN
7	a	176	LEU
7	a	179	LEU
7	a	180	ARG
7	a	185	ASP
7	a	188	LEU
7	a	196	GLN
7	a	197	MET
7	a	199	ARG
7	a	211	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	a	225	ASN
7	a	226	ILE
7	a	234	GLU
7	a	239	ARG
7	a	250	ILE
7	a	251	ILE
7	a	253	ASP
7	b	7	ASN
7	b	17	GLU
7	b	32	VAL
7	b	42	LYS
7	b	47	SER
7	b	48	ARG
7	b	53	SER
7	b	57	GLN
7	b	63	LEU
7	b	74	ASP
7	b	76	GLU
7	b	77	LEU
7	b	81	GLU
7	b	89	GLN
7	b	91	ARG
7	b	95	ARG
7	b	111	THR
7	b	119	LYS
7	b	124	ILE
7	b	129	LEU
7	b	139	GLN
7	b	142	VAL
7	b	143	ARG
7	b	179	LEU
7	b	185	ASP
7	b	200	GLU
7	b	201	ILE
7	b	202	LYS
7	b	204	PRO
7	b	211	GLU
7	b	225	ASN
7	b	227	ARG
7	b	235	ARG
7	b	236	SER
7	b	239	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	b	240	HIS
7	b	256	LYS
7	b	257	ARG
7	c	5	LYS
7	c	28	LEU
7	c	29	ASP
7	c	56	TRP
7	c	104	LEU
7	c	111	THR
7	c	115	MET
7	c	121	LEU
7	c	130	GLU
7	c	136	GLN
7	c	141	ASN
7	c	144	LEU
7	c	148	THR
7	c	156	VAL
7	c	164	ASP
7	c	168	ARG
7	c	180	ARG
7	c	217	LEU
7	c	225	ASN
7	c	226	ILE
7	c	227	ARG
7	c	229	LEU
7	c	233	VAL
7	c	250	ILE
7	c	251	ILE
7	c	255	PHE
7	c	257	ARG
7	d	7	ASN
7	d	8	LEU
7	d	28	LEU
7	d	38	ARG
7	d	45	ILE
7	d	55	ARG
7	d	56	TRP
7	d	57	GLN
7	d	70	GLU
7	d	71	ASN
7	d	78	PHE
7	d	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	d	95	ARG
7	d	96	PHE
7	d	98	ARG
7	d	115	MET
7	d	116	VAL
7	d	119	LYS
7	d	126	TYR
7	d	136	GLN
7	d	144	LEU
7	d	148	THR
7	d	176	LEU
7	d	220	TYR
7	d	229	LEU
7	d	235	ARG
7	d	252	ILE
7	f	4	TYR
7	f	5	LYS
7	f	8	LEU
7	f	15	PHE
7	f	34	ILE
7	f	38	ARG
7	f	50	HIS
7	f	51	TYR
7	f	62	SER
7	f	63	LEU
7	f	68	LEU
7	f	122	ARG
7	f	128	GLU
7	f	129	LEU
7	f	136	GLN
7	f	138	LEU
7	f	141	ASN
7	f	166	LEU
7	f	172	ASP
7	f	202	LYS
7	f	205	LEU
7	f	214	ARG
7	f	242	THR
7	f	247	LEU
7	f	252	ILE
7	f	256	LYS
7	f	257	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	e	7	ASN
7	e	13	ASN
7	e	15	PHE
7	e	16	LEU
7	e	22	VAL
7	e	33	LEU
7	e	38	ARG
7	e	42	LYS
7	e	49	LEU
7	e	57	GLN
7	e	69	ASN
7	e	90	LYS
7	e	91	ARG
7	e	97	GLU
7	e	104	LEU
7	e	109	LEU
7	e	122	ARG
7	e	129	LEU
7	e	139	GLN
7	e	142	VAL
7	e	158	GLU
7	e	164	ASP
7	e	179	LEU
7	e	199	ARG
7	e	225	ASN
7	e	251	ILE
7	e	255	PHE
7	e	257	ARG
8	M	7	LEU
8	M	8	ARG
8	M	9	LEU
8	M	11	GLN
8	M	13	LEU
8	M	15	MET
8	M	16	THR
8	M	18	GLN
8	M	23	ILE
8	M	24	ARG
8	M	26	LEU
8	M	27	GLN
8	M	32	GLU
8	M	41	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	M	46	LEU
8	M	109	LEU
8	M	118	GLN
8	M	119	THR
8	M	131	THR
8	M	143	SER
8	M	154	LEU
8	M	156	ILE
8	M	159	GLU
8	M	163	ASP
8	M	182	ILE
8	M	184	ARG
8	M	185	PHE
8	M	186	ASP
8	M	188	VAL
8	M	195	LEU
8	M	196	ARG
8	M	200	LEU
8	M	201	ILE
8	M	205	GLN
8	M	213	LEU
8	M	217	ARG
8	M	218	LEU
8	M	224	LEU
8	M	225	ASP
8	M	227	LEU
8	M	229	ASN
8	M	231	ASP
8	M	233	ARG
8	M	240	ARG
8	M	246	LEU
8	M	252	LEU
8	M	254	GLN
8	M	256	LEU
8	M	259	ARG
8	M	271	TYR
8	M	272	VAL
8	M	279	ARG
8	M	285	TRP
8	M	292	ASP
8	M	306	MET
8	M	308	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	M	329	LEU
8	M	331	LYS
8	M	340	LEU
8	M	341	LEU
8	M	342	ARG
8	M	347	ILE
8	M	350	GLN
8	M	355	PHE
8	M	363	LYS
8	M	370	ILE
8	M	372	GLN
8	M	375	GLU
8	M	381	ILE
8	M	386	THR
8	M	387	GLN
8	M	403	PHE
8	M	416	SER
8	M	425	LYS
8	M	431	GLU
8	M	441	LYS
8	M	455	ARG
8	M	456	ARG
8	M	460	LYS
8	M	473	ARG
8	M	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	GLN
2	C	513	GLN
2	C	1013	GLN
2	C	1061	GLN
3	D	200	GLN
3	D	448	GLN
7	a	21	GLN
7	a	24	HIS
7	a	92	HIS
7	a	117	GLN
7	a	225	ASN
7	a	231	ASN
7	b	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	b	92	HIS
7	b	139	GLN
7	b	157	ASN
7	b	225	ASN
7	c	21	GLN
7	c	50	HIS
7	c	64	ASN
7	c	136	GLN
7	c	141	ASN
7	c	157	ASN
7	d	7	ASN
7	d	92	HIS
7	f	7	ASN
7	f	13	ASN
7	f	24	HIS
7	f	80	HIS
7	f	117	GLN
7	f	136	GLN
7	f	157	ASN
7	e	7	ASN
7	e	13	ASN
7	e	89	GLN
7	e	139	GLN
7	e	149	ASN
8	M	3	GLN
8	M	11	GLN
8	M	20	GLN
8	M	118	GLN
8	M	127	GLN
8	M	262	GLN
8	M	265	GLN
8	M	324	GLN
8	M	351	GLN
8	M	377	HIS
8	M	432	ASN
8	M	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands 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
9	ADP	a	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
9	ADP	f	601	-	24,29,29	3.84	12 (50%)	29,45,45	4.30	24 (82%)
10	AF3	e	602	-	0,3,3	-	-	-	-	-
9	ADP	c	400	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
10	AF3	a	602	-	0,3,3	-	-	-	-	-
10	AF3	b	602	-	0,3,3	-	-	-	-	-
9	ADP	b	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
9	ADP	e	601	-	24,29,29	2.14	7 (29%)	29,45,45	3.31	19 (65%)
10	AF3	f	602	-	0,3,3	-	-	-	-	-

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
9	ADP	a	601	-	-	3/12/32/32	0/3/3/3
9	ADP	f	601	-	-	5/12/32/32	0/3/3/3
9	ADP	c	400	-	-	2/12/32/32	0/3/3/3
9	ADP	b	601	-	-	5/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	e	601	-	-	1/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	601	ADP	O4'-C1'	9.06	1.53	1.41
9	f	601	ADP	C2'-C1'	-9.05	1.40	1.53
9	f	601	ADP	O2'-C2'	7.49	1.60	1.43
9	f	601	ADP	PA-O1A	5.67	1.71	1.50
9	e	601	ADP	PA-O1A	-4.86	1.33	1.50
9	e	601	ADP	C2-N3	4.59	1.39	1.32
9	e	601	ADP	C5-C4	4.41	1.52	1.40
9	f	601	ADP	C2'-C3'	4.39	1.65	1.53
9	f	601	ADP	C5'-C4'	4.29	1.65	1.51
9	e	601	ADP	C2'-C1'	-4.14	1.47	1.53
9	f	601	ADP	PB-O2B	3.26	1.67	1.54
9	f	601	ADP	O4'-C4'	3.01	1.51	1.45
9	f	601	ADP	PA-O2A	2.92	1.69	1.55
9	f	601	ADP	C3'-C4'	-2.68	1.46	1.53
9	e	601	ADP	O4'-C1'	2.55	1.44	1.41
9	f	601	ADP	C4-N3	2.54	1.39	1.35
9	b	601	ADP	C5-C4	2.52	1.47	1.40
9	c	400	ADP	C5-C4	2.52	1.47	1.40
9	a	601	ADP	C5-C4	2.41	1.47	1.40
9	e	601	ADP	C6-C5	2.40	1.52	1.43
9	f	601	ADP	C5-N7	-2.14	1.32	1.39
9	e	601	ADP	O4'-C4'	-2.11	1.40	1.45

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	601	ADP	PA-O3A-PB	-8.19	104.71	132.83
9	e	601	ADP	PA-O3A-PB	-6.94	109.00	132.83
9	f	601	ADP	O4'-C4'-C5'	6.52	130.81	109.37
9	f	601	ADP	C5'-C4'-C3'	-6.47	90.95	115.18
9	f	601	ADP	O2A-PA-O1A	6.24	143.08	112.24
9	f	601	ADP	O3B-PB-O2B	6.20	131.34	107.64
9	e	601	ADP	O5'-PA-O1A	5.58	130.86	109.07
9	f	601	ADP	O5'-PA-O1A	5.51	130.58	109.07
9	f	601	ADP	O3'-C3'-C2'	5.48	129.55	111.82
9	e	601	ADP	C5-C6-N6	5.07	128.06	120.35
9	e	601	ADP	C3'-C2'-C1'	5.01	108.52	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	f	601	ADP	O3B-PB-O3A	-4.99	87.92	104.64
9	f	601	ADP	O4'-C1'-C2'	4.86	114.03	106.93
9	f	601	ADP	N6-C6-N1	-4.79	108.63	118.57
9	f	601	ADP	O4'-C4'-C3'	-4.73	95.75	105.11
9	f	601	ADP	C5-C6-N6	4.68	127.46	120.35
9	f	601	ADP	O2A-PA-O5'	-4.64	86.18	107.75
9	e	601	ADP	O5'-C5'-C4'	4.34	123.92	108.99
9	f	601	ADP	C4-C5-N7	4.25	113.83	109.40
9	f	601	ADP	O2'-C2'-C1'	-4.22	95.27	110.85
9	e	601	ADP	O2B-PB-O3A	-4.07	90.98	104.64
9	e	601	ADP	C4-C5-N7	-4.01	105.22	109.40
9	e	601	ADP	C5'-C4'-C3'	-3.94	100.40	115.18
9	e	601	ADP	O3B-PB-O1B	3.85	125.75	110.68
9	e	601	ADP	O4'-C4'-C5'	-3.77	96.97	109.37
9	e	601	ADP	O4'-C1'-C2'	-3.63	101.62	106.93
9	b	601	ADP	PA-O3A-PB	-3.61	120.43	132.83
9	c	400	ADP	PA-O3A-PB	-3.60	120.47	132.83
9	a	601	ADP	PA-O3A-PB	-3.59	120.50	132.83
9	e	601	ADP	O2A-PA-O5'	-3.55	91.26	107.75
9	e	601	ADP	O3'-C3'-C2'	3.52	123.21	111.82
9	f	601	ADP	C3'-C2'-C1'	-3.45	95.78	100.98
9	a	601	ADP	C3'-C2'-C1'	3.44	106.16	100.98
9	e	601	ADP	O3B-PB-O2B	-3.44	94.49	107.64
9	f	601	ADP	PA-O5'-C5'	-3.41	101.66	121.68
9	b	601	ADP	C3'-C2'-C1'	3.34	106.01	100.98
9	c	400	ADP	C3'-C2'-C1'	3.28	105.92	100.98
9	b	601	ADP	N3-C2-N1	-3.18	123.70	128.68
9	c	400	ADP	N3-C2-N1	-3.17	123.72	128.68
9	a	601	ADP	N3-C2-N1	-3.11	123.81	128.68
9	f	601	ADP	C2'-C3'-C4'	2.97	108.42	102.64
9	f	601	ADP	N3-C2-N1	-2.71	124.44	128.68
9	b	601	ADP	C4-C5-N7	-2.70	106.59	109.40
9	a	601	ADP	C4-C5-N7	-2.69	106.60	109.40
9	c	400	ADP	C4-C5-N7	-2.68	106.61	109.40
9	e	601	ADP	O3'-C3'-C4'	2.64	118.69	111.05
9	e	601	ADP	N6-C6-N1	-2.64	113.10	118.57
9	f	601	ADP	O2B-PB-O1B	2.59	120.81	110.68
9	f	601	ADP	O2B-PB-O3A	-2.55	96.09	104.64
9	f	601	ADP	C1'-N9-C4	-2.49	122.27	126.64
9	f	601	ADP	O3'-C3'-C4'	-2.35	104.25	111.05
9	e	601	ADP	O2B-PB-O1B	2.35	119.86	110.68
9	f	601	ADP	O3B-PB-O1B	-2.31	101.62	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	e	601	ADP	C2-N1-C6	2.25	122.60	118.75
9	e	601	ADP	O2'-C2'-C1'	2.23	119.10	110.85

There are no chirality outliers.

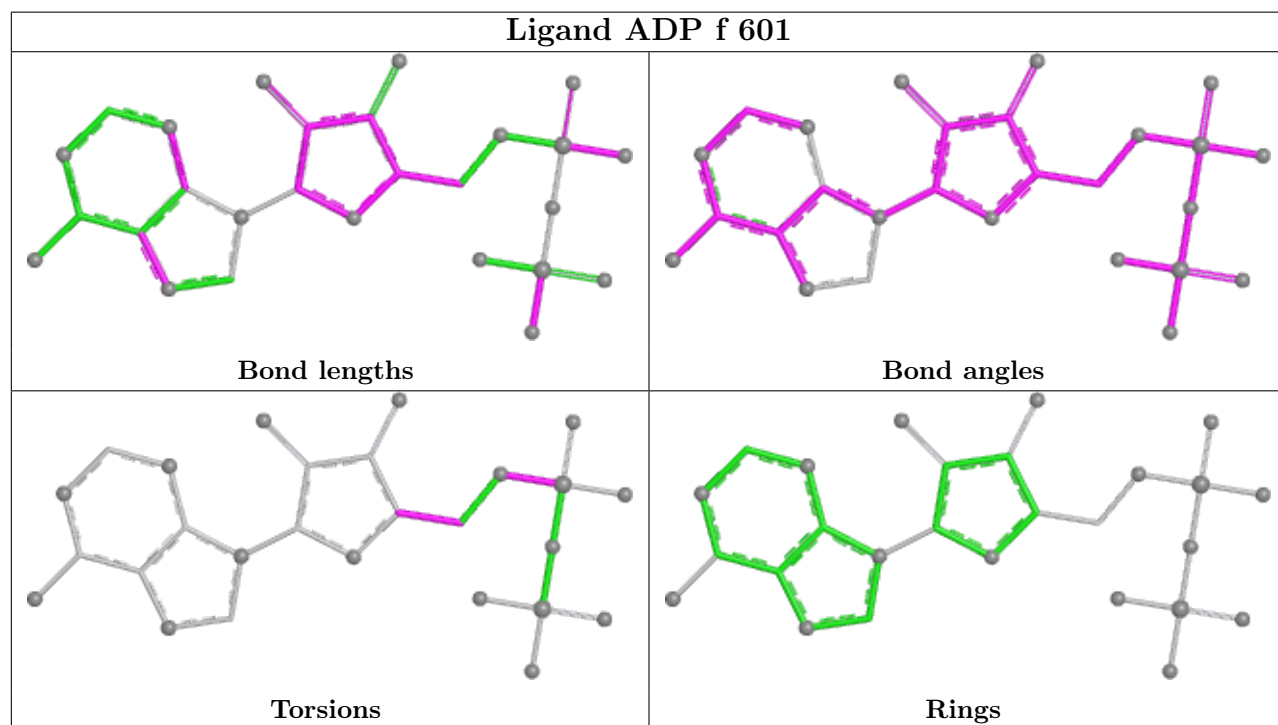
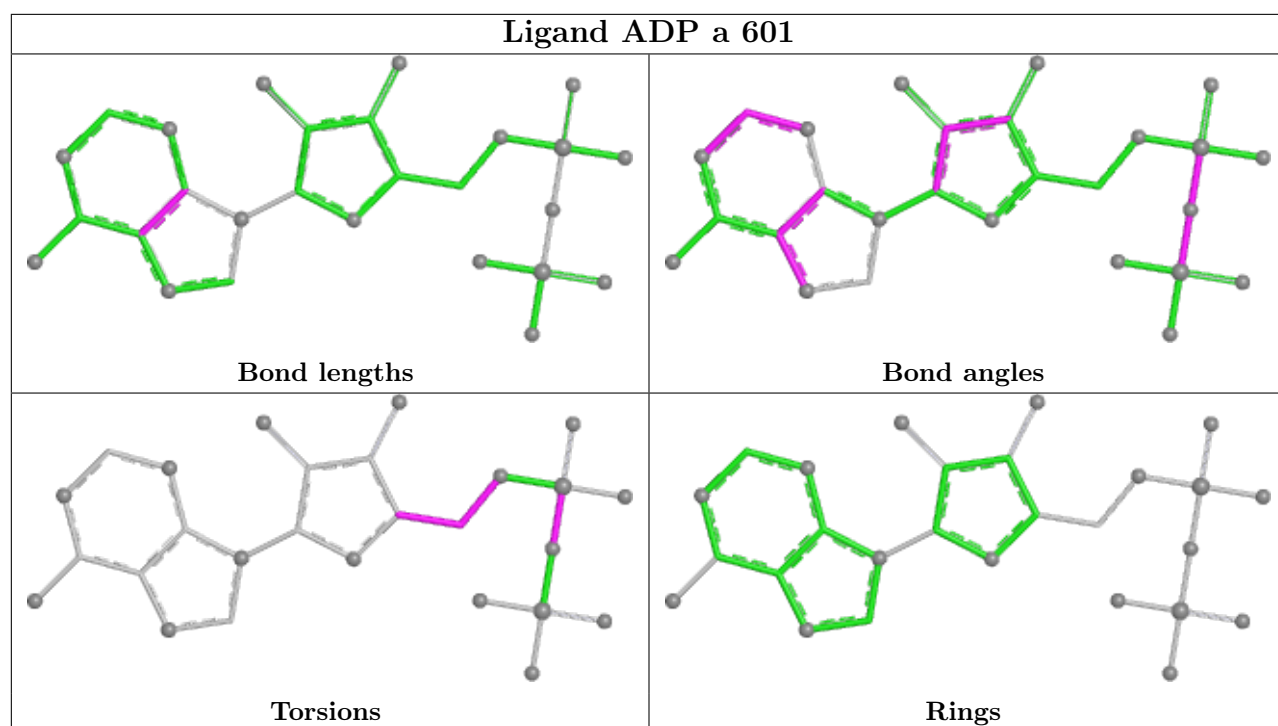
All (16) torsion outliers are listed below:

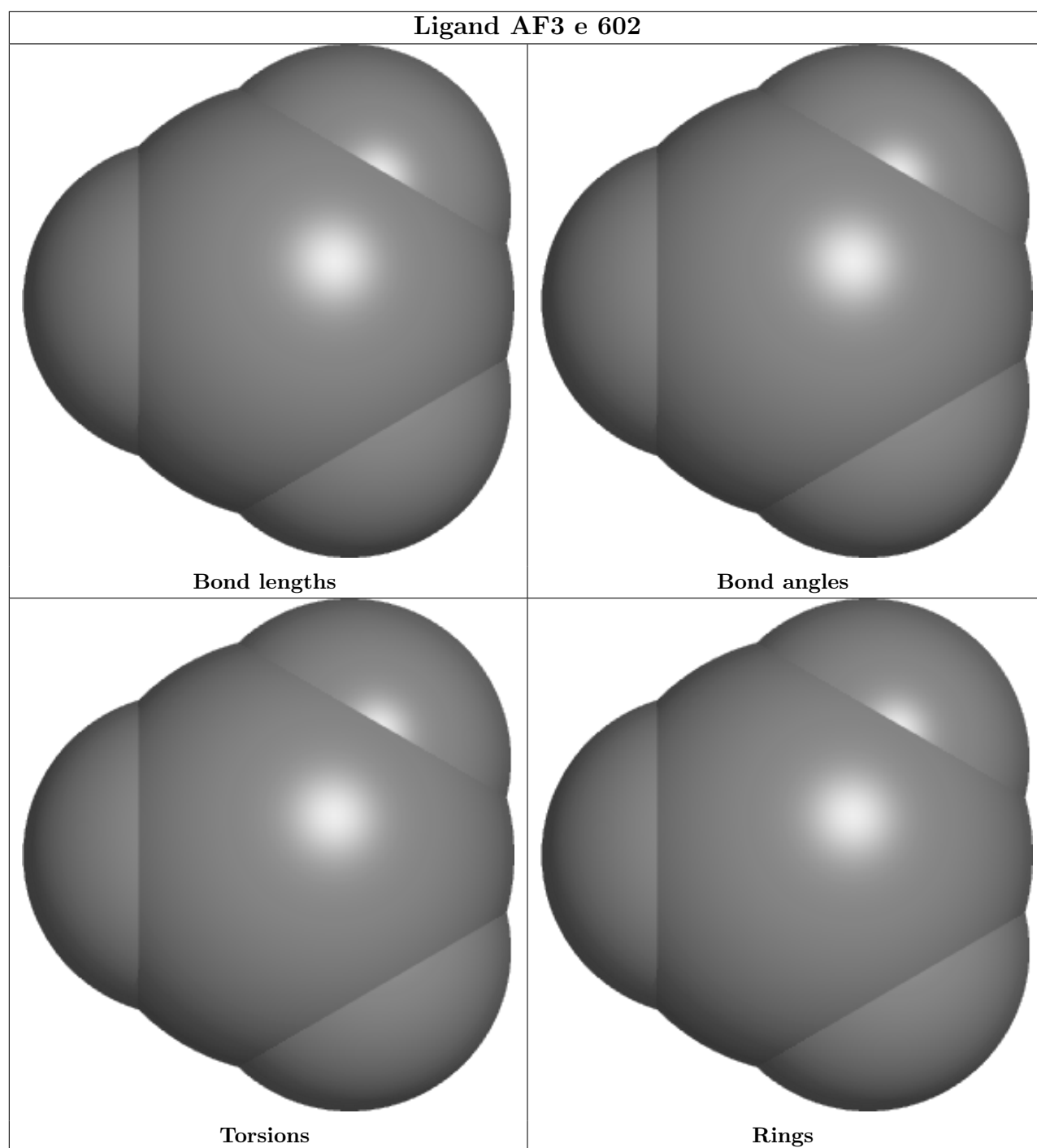
Mol	Chain	Res	Type	Atoms
9	b	601	ADP	C5'-O5'-PA-O2A
9	c	400	ADP	C5'-O5'-PA-O1A
9	f	601	ADP	C5'-O5'-PA-O2A
9	f	601	ADP	C3'-C4'-C5'-O5'
9	f	601	ADP	O4'-C4'-C5'-O5'
9	e	601	ADP	O4'-C4'-C5'-O5'
9	b	601	ADP	O4'-C4'-C5'-O5'
9	a	601	ADP	O4'-C4'-C5'-O5'
9	b	601	ADP	C5'-O5'-PA-O3A
9	f	601	ADP	C5'-O5'-PA-O3A
9	b	601	ADP	C5'-O5'-PA-O1A
9	b	601	ADP	C3'-C4'-C5'-O5'
9	a	601	ADP	C4'-C5'-O5'-PA
9	a	601	ADP	PB-O3A-PA-O2A
9	f	601	ADP	C5'-O5'-PA-O1A
9	c	400	ADP	O4'-C4'-C5'-O5'

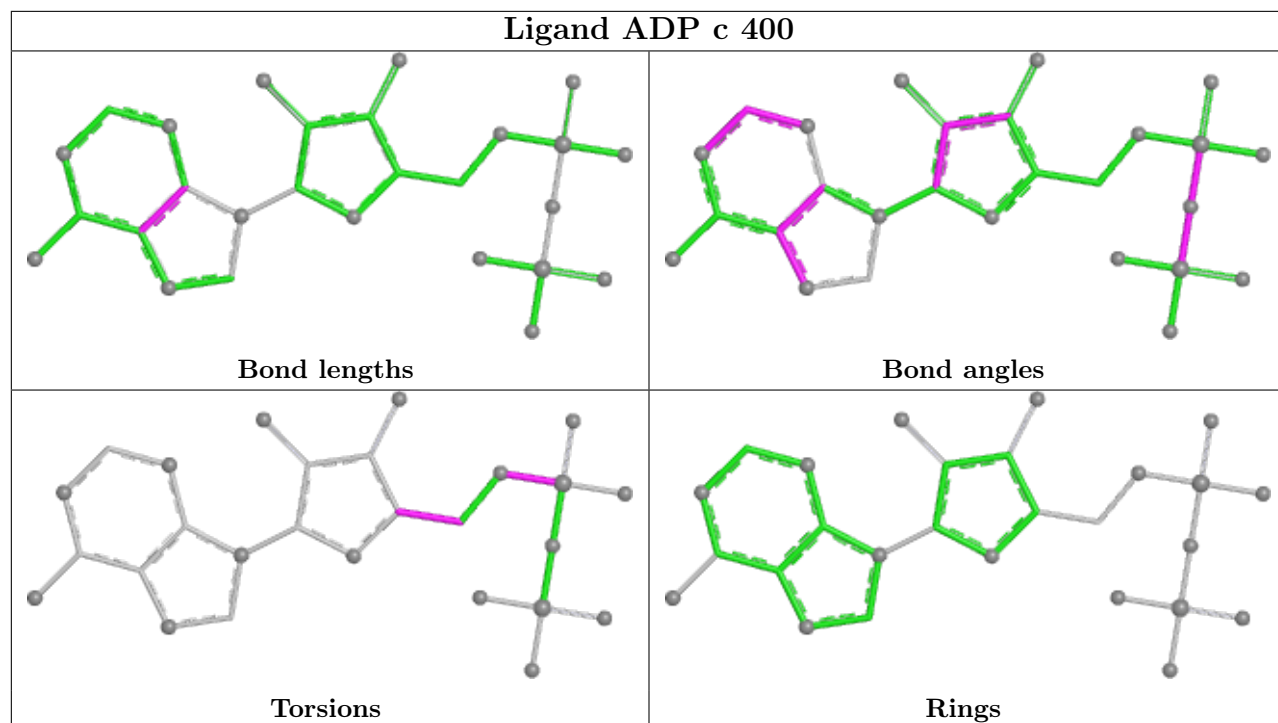
There are no ring outliers.

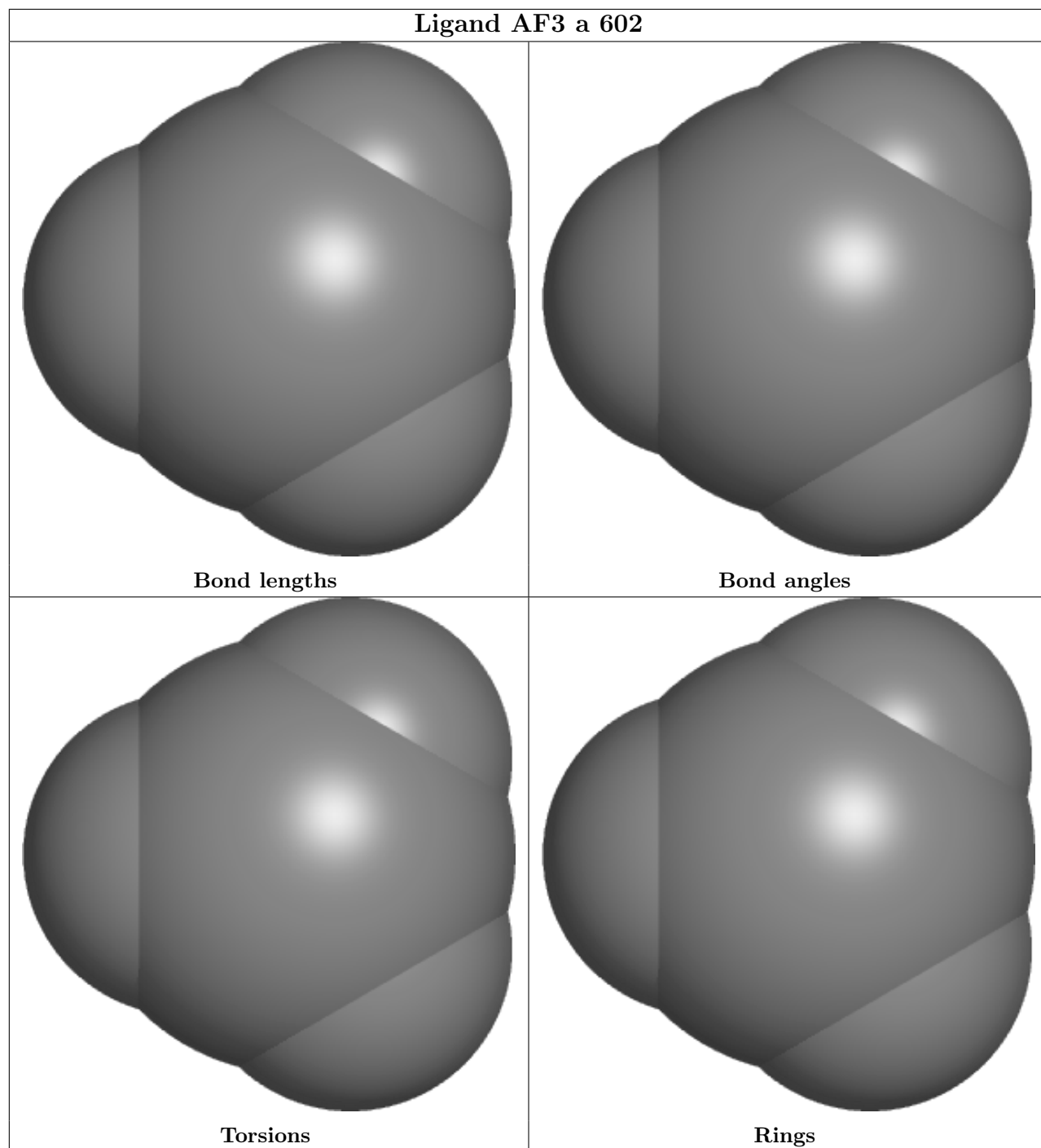
No monomer is involved in short contacts.

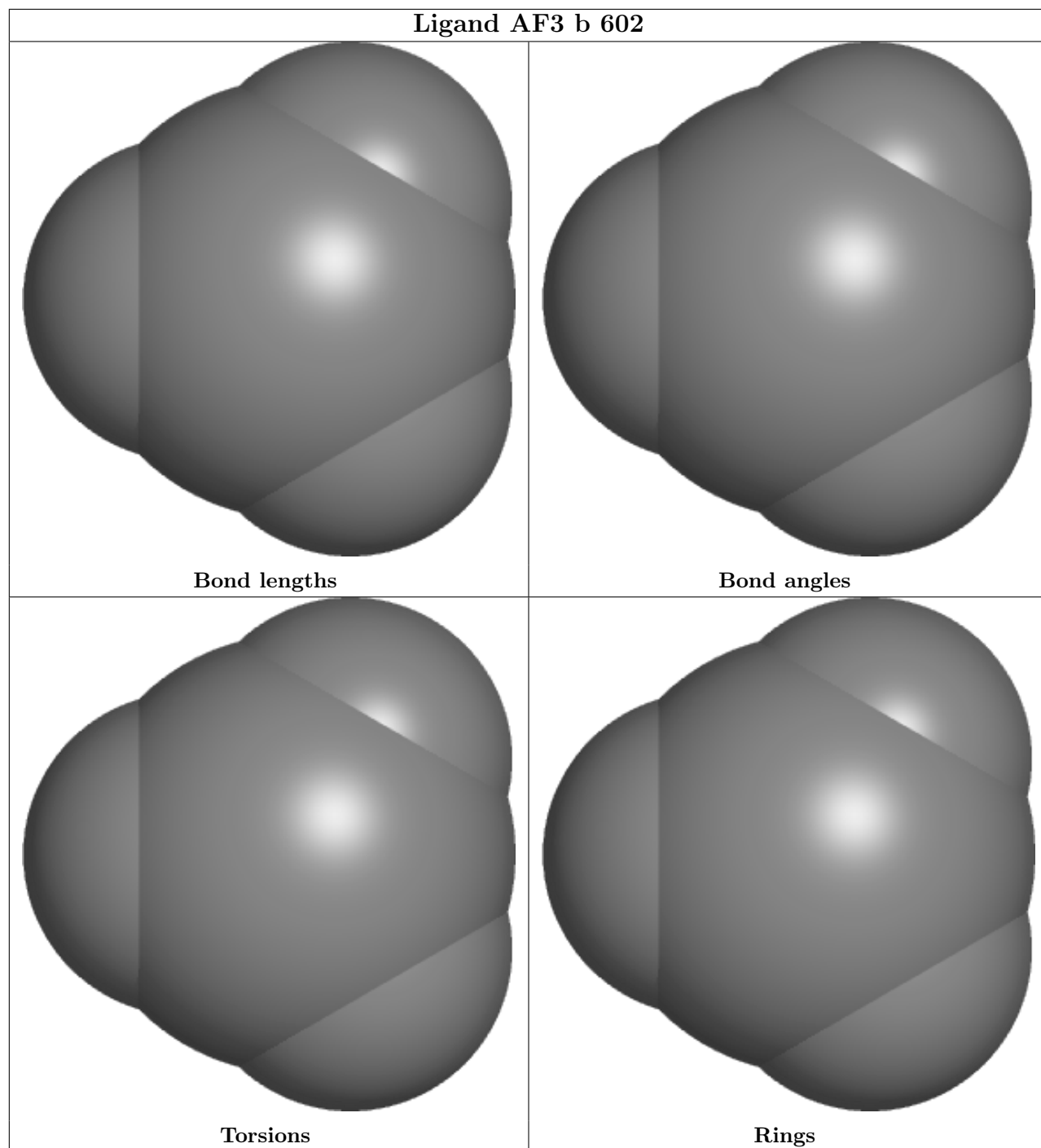
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

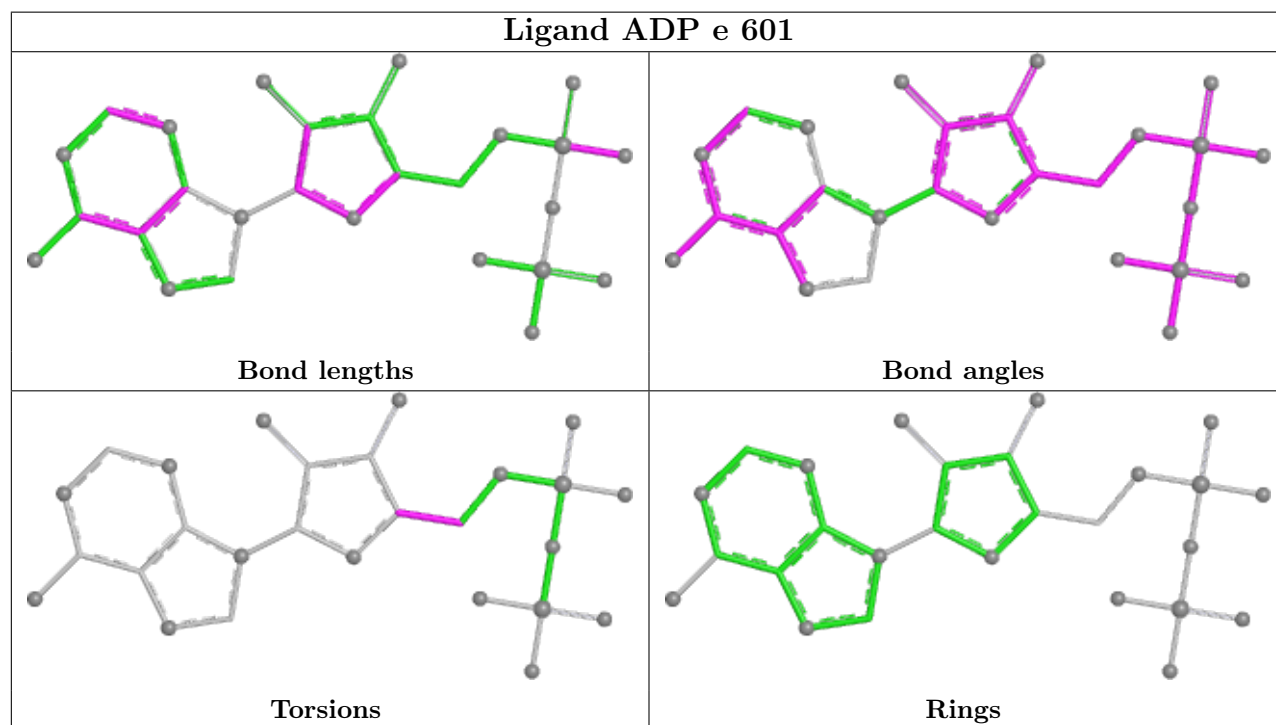
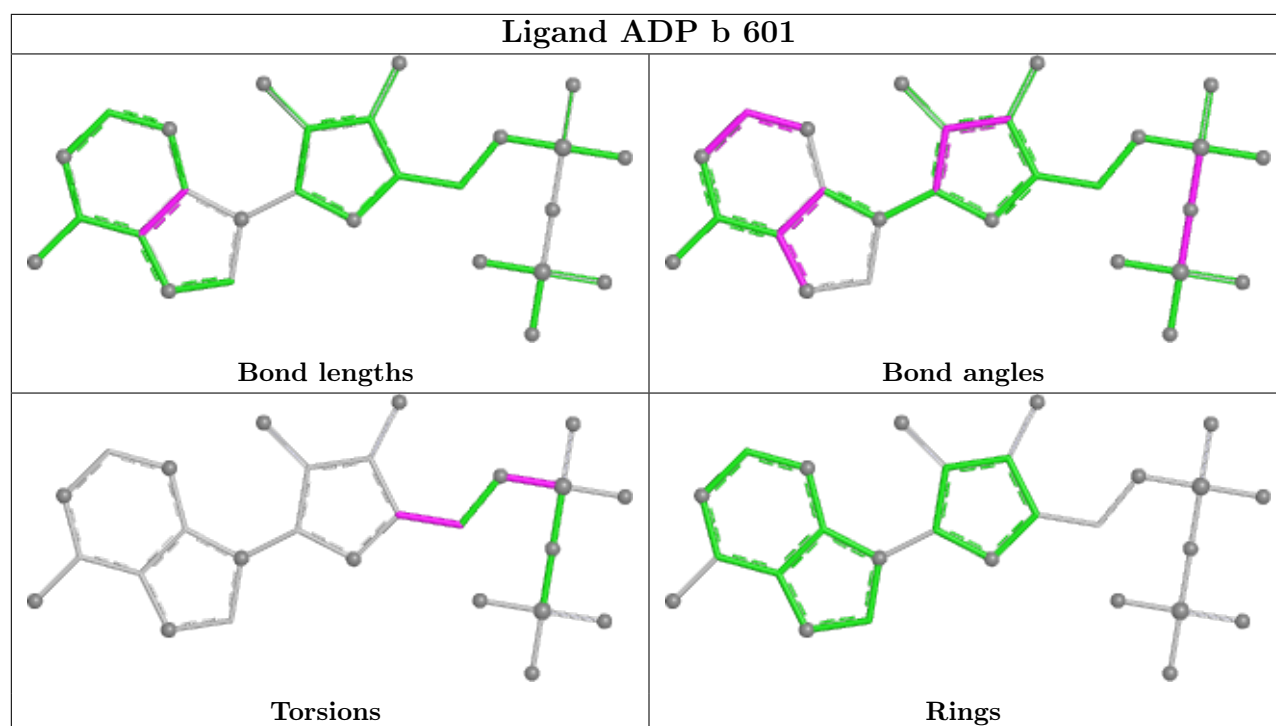


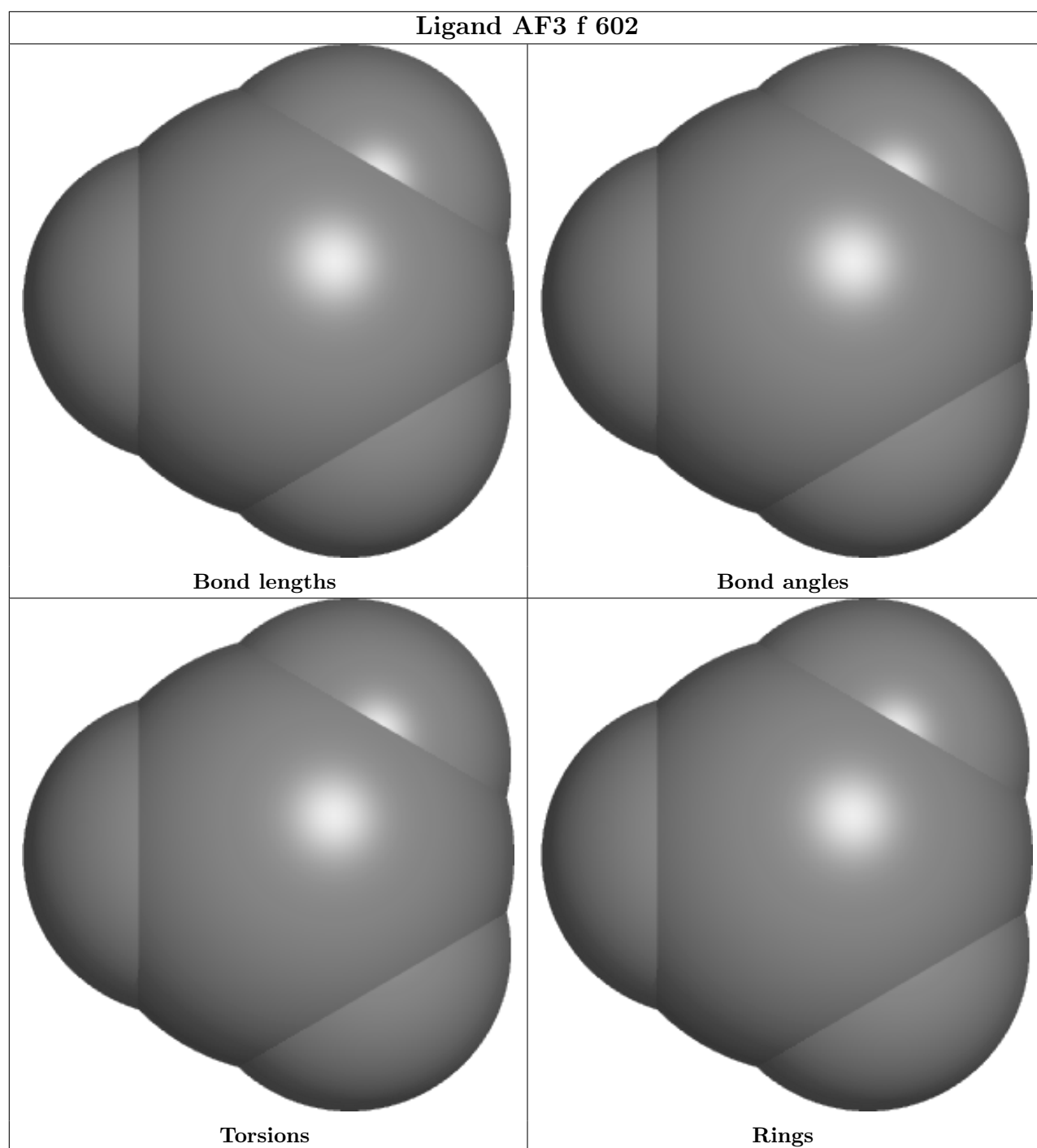












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

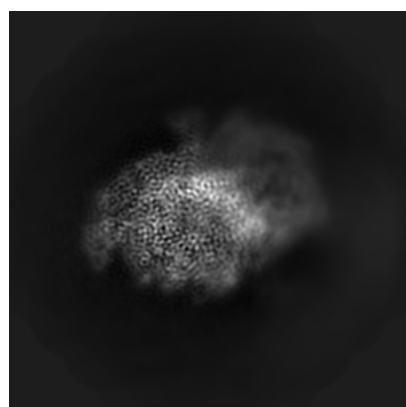
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14171. These allow visual inspection of the internal detail of the map and identification of artifacts.

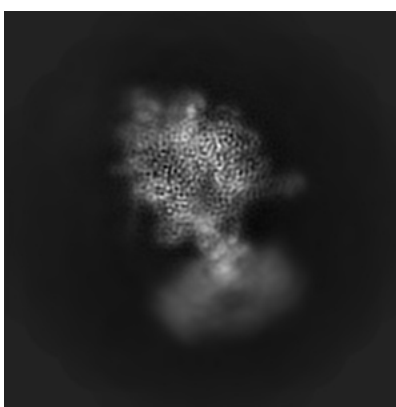
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

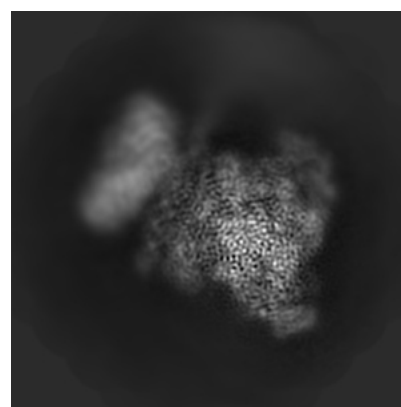
6.1.1 Primary map



X



Y

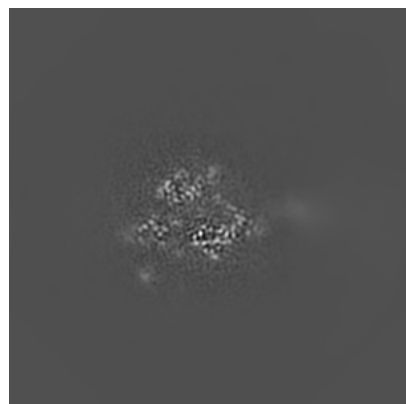


Z

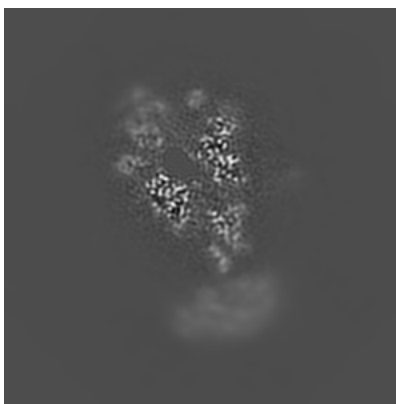
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

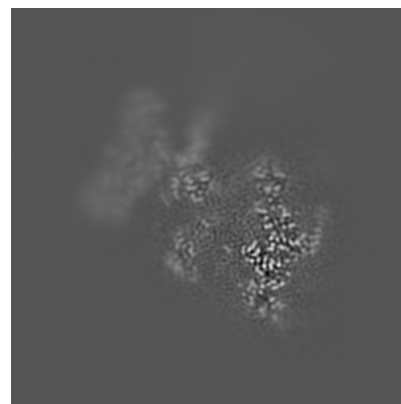
6.2.1 Primary map



X Index: 140



Y Index: 140

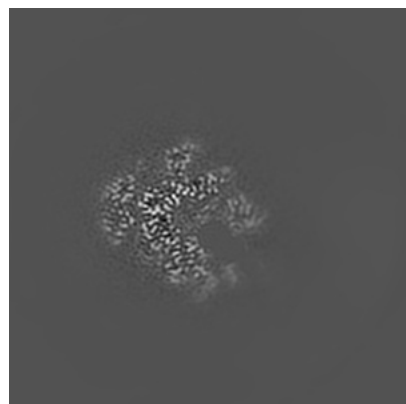


Z Index: 140

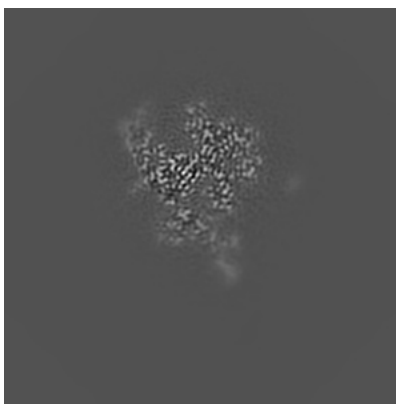
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

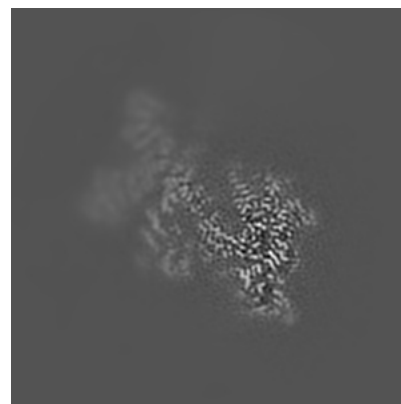
6.3.1 Primary map



X Index: 173



Y Index: 111



Z Index: 149

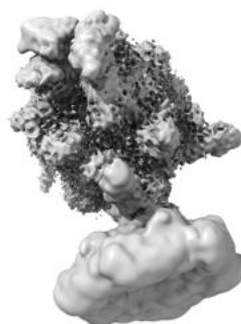
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

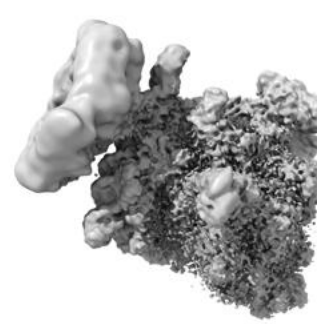
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

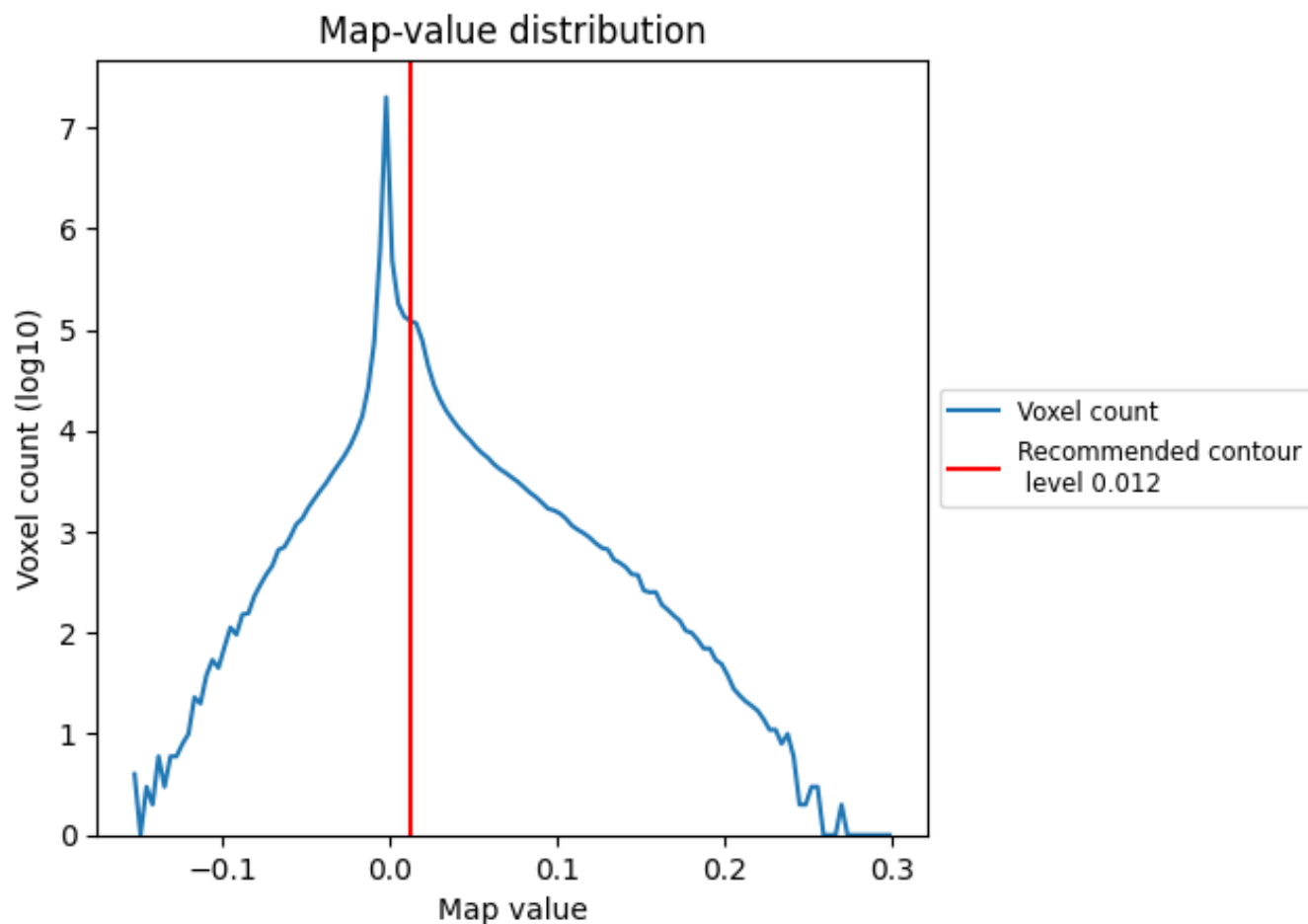
6.5 Mask visualisation

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

7 Map analysis [i](#)

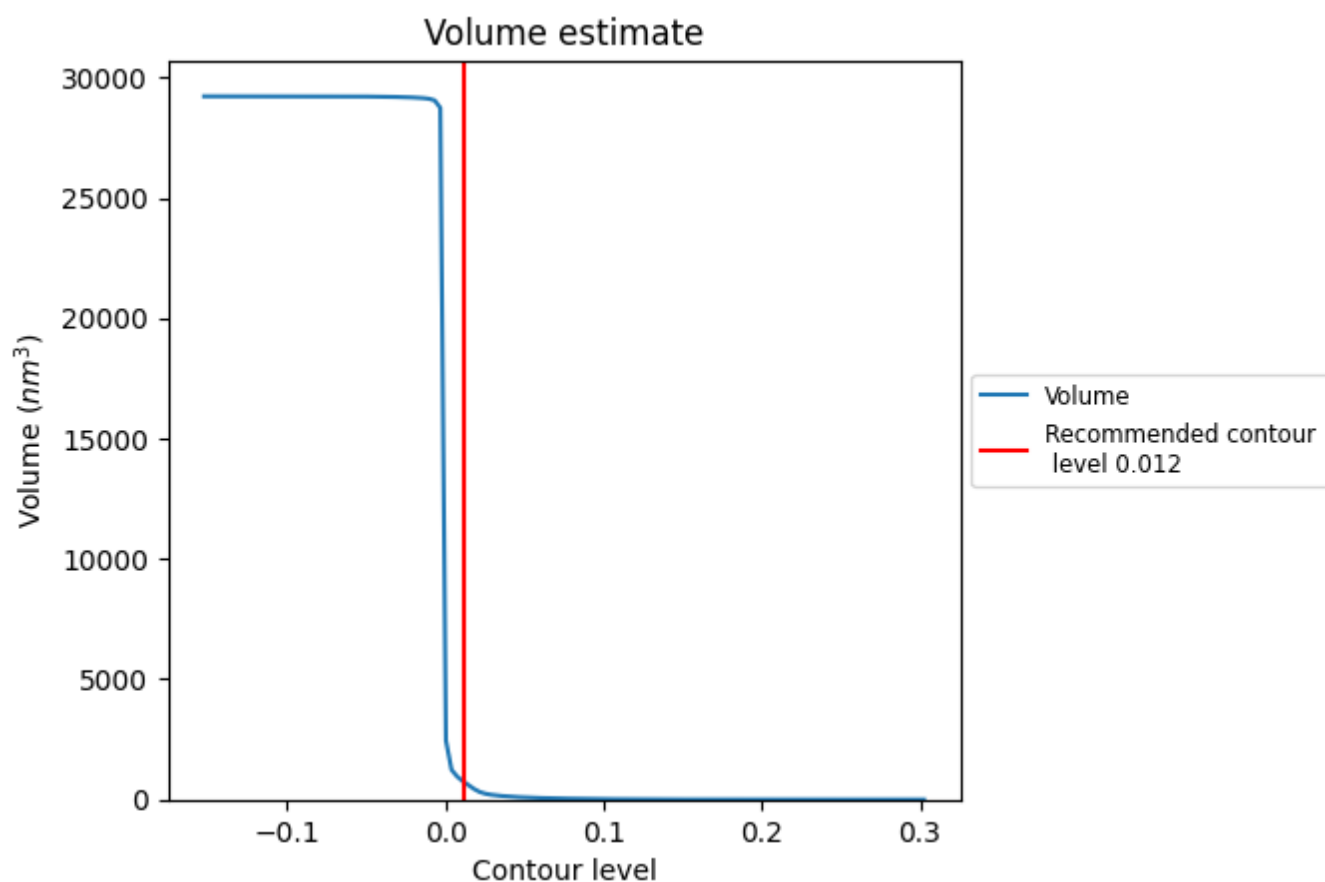
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

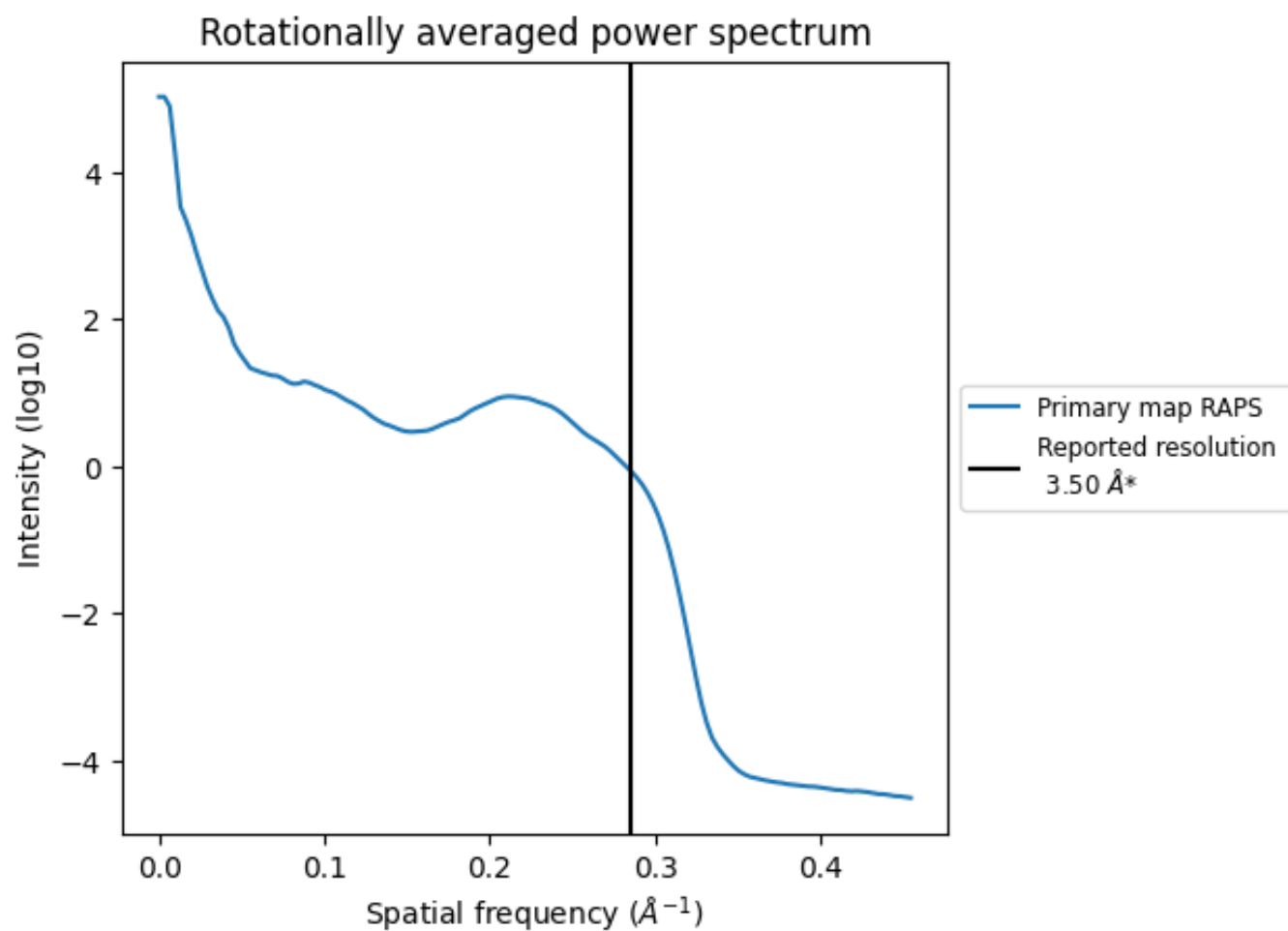
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm³; this corresponds to an approximate mass of 653 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 0.286 Å⁻¹

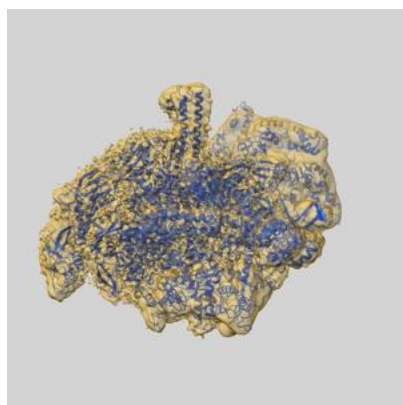
8 Fourier-Shell correlation

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

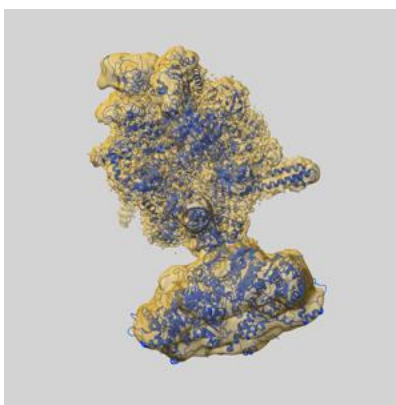
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14171 and PDB model 7QV9. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

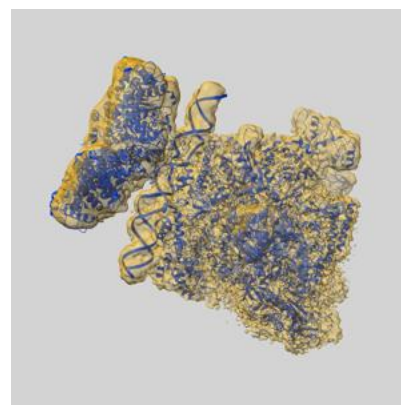
9.1 Map-model overlay [i](#)



X



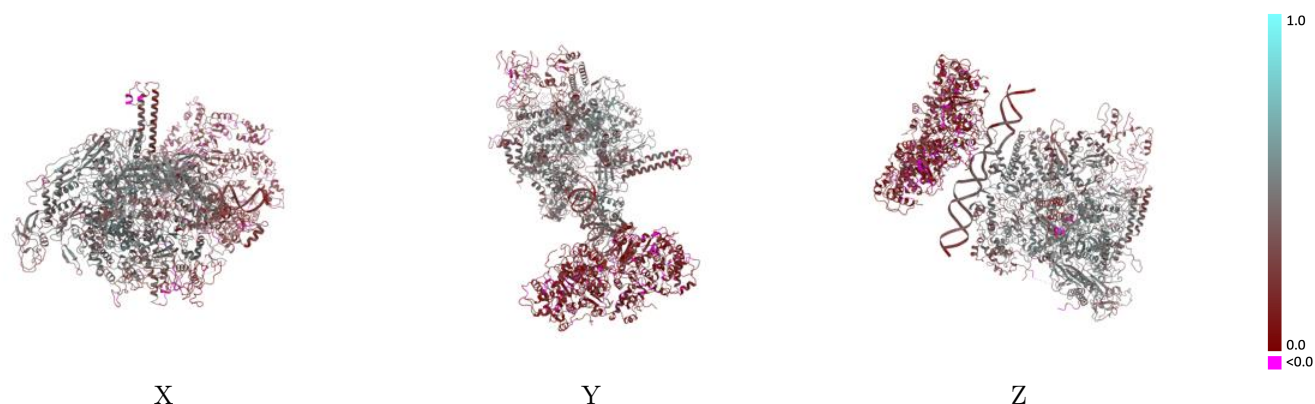
Y



Z

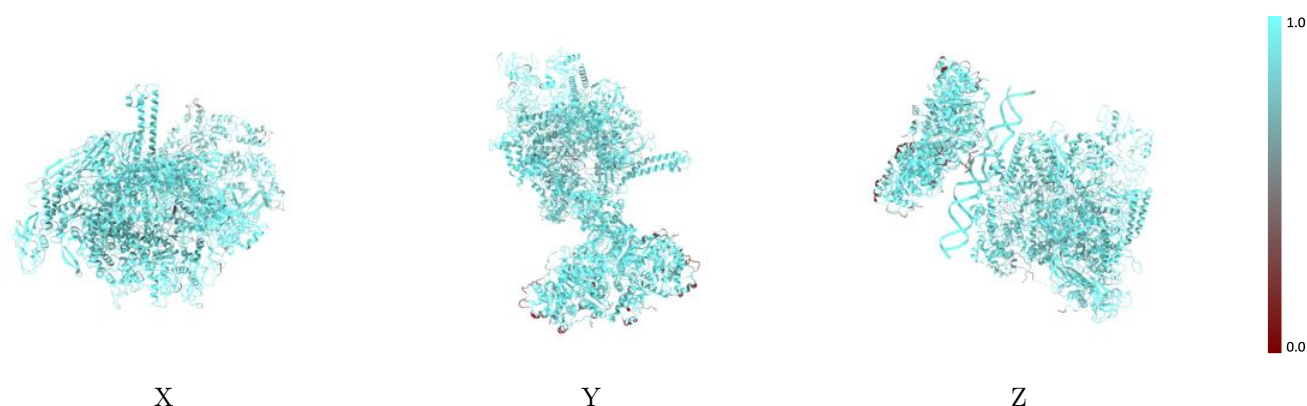
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



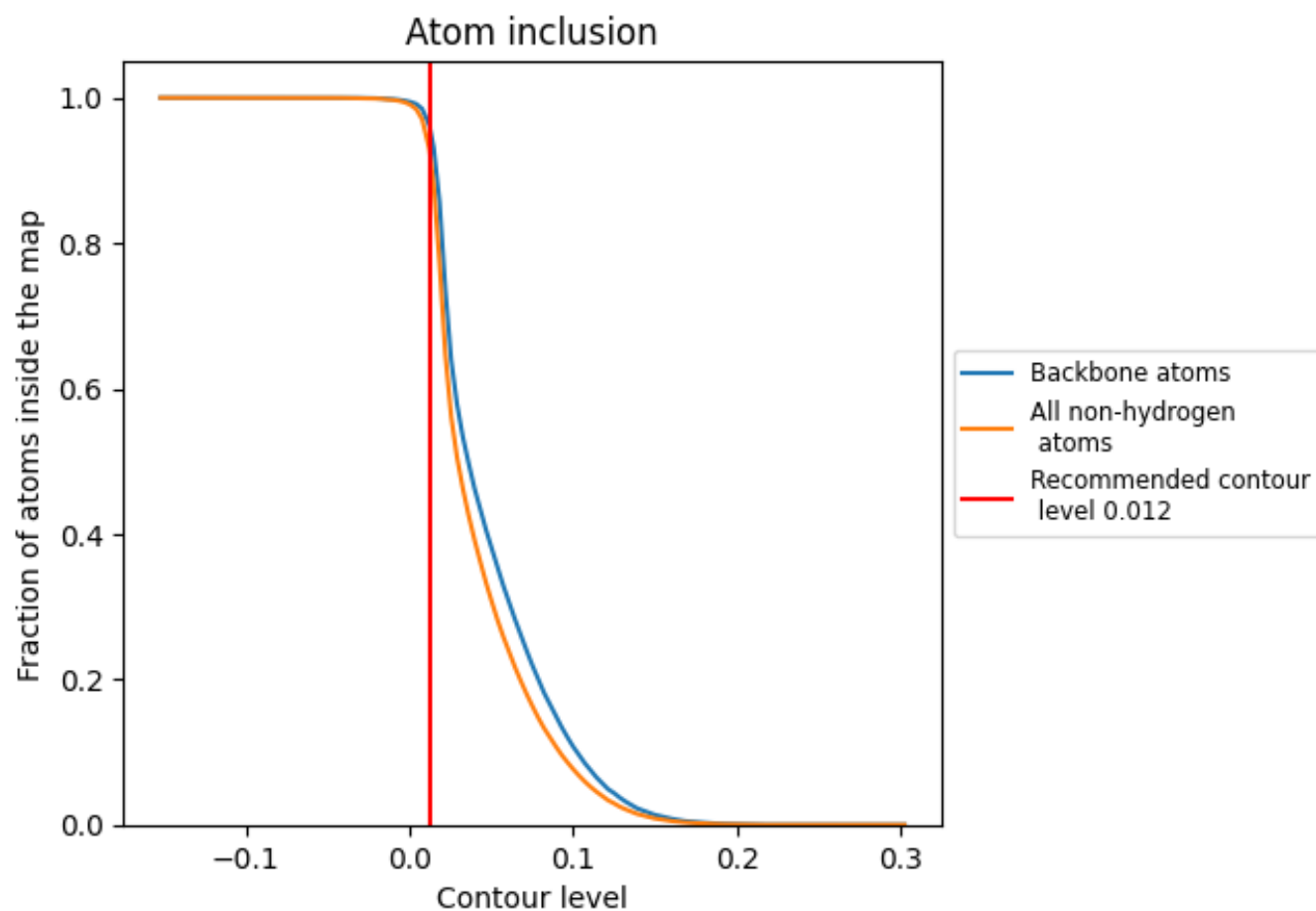
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9293	<div></div> 0.3230
A	<div></div> 0.8955	<div></div> 0.3980
B	<div></div> 0.9264	<div></div> 0.3830
C	<div></div> 0.9414	<div></div> 0.4200
D	<div></div> 0.9287	<div></div> 0.3910
E	<div></div> 0.9491	<div></div> 0.4320
M	<div></div> 0.9586	<div></div> 0.4280
N	<div></div> 0.9864	<div></div> 0.3110
T	<div></div> 0.9770	<div></div> 0.3090
a	<div></div> 0.9169	<div></div> 0.1500
b	<div></div> 0.9390	<div></div> 0.1620
c	<div></div> 0.8731	<div></div> 0.1240
d	<div></div> 0.9079	<div></div> 0.1270
e	<div></div> 0.9294	<div></div> 0.1350
f	<div></div> 0.9017	<div></div> 0.1310

