Full wwPDB EM Validation Report (i)

Mar 19, 2025 – 04:22 PM EDT

PDB ID	:	9E2W
EMDB ID	:	EMD-47470
Title	:	Cryo-EM structure of yeast CMG helicase stalled at G4-containing DNA template, state 1
Authors	:	Allwein, B.; Batra, S.; Remus, D.; Hite, R.
Deposited on	:	2024-10-23
Resolution	:	3.30 Å(reported)
Based on initial model	:	.

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 (i) 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 (1)) were used in the production of this report:

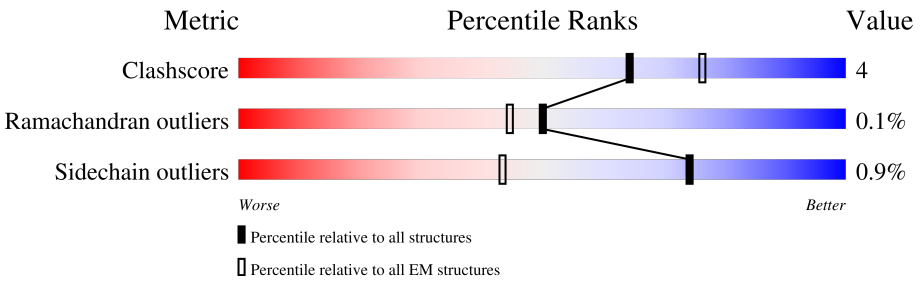
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	2	868	65% 11% 24%
2	3	971	56% 7% 36%
3	4	933	56% 9% • 34%
4	5	775	67% 9% 23%
5	6	1017	53% 9% • 38%
6	7	845	62% 11% 27%
7	A	208	81% 13% 6%
8	B	213	77% 11% 11%
9	C	217	73% 6% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	D	294	66% 10% 24%
11	E	650	78% 9% 13%
12	F	48	21% 60% 19%
13	G	21	76% 19% 5%
14	X	1238	46% 10% 43%
15	Y	92	71% 26%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 96909 atoms, of which 48318 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	2	664	10576	3305	5309	944	999	19	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	3	618	9718	3044	4893	860	908	13	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4	614	9812	3077	4933	840	934	28	0	0

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	594	9417	2945	4746	798	905	23	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	6	634	10040	3159	5035	873	948	25	0	0

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	7	615	9786	3075	4921	847	917	26	0	0

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	A	196	3202	1005	1602	276	310	9	0	0

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	B	189	3195	1014	1618	276	282	5	0	0

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	C	173	2805	910	1409	224	256	6	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	SER	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146
C	-18	HIS	-	expression tag	UNP Q12146
C	-17	HIS	-	expression tag	UNP Q12146
C	-16	HIS	-	expression tag	UNP Q12146
C	-15	HIS	-	expression tag	UNP Q12146
C	-14	HIS	-	expression tag	UNP Q12146
C	-13	HIS	-	expression tag	UNP Q12146
C	-12	SER	-	expression tag	UNP Q12146
C	-11	SER	-	expression tag	UNP Q12146
C	-10	GLY	-	expression tag	UNP Q12146
C	-9	LEU	-	expression tag	UNP Q12146
C	-8	VAL	-	expression tag	UNP Q12146
C	-7	PRO	-	expression tag	UNP Q12146
C	-6	ARG	-	expression tag	UNP Q12146
C	-5	GLY	-	expression tag	UNP Q12146
C	-4	SER	-	expression tag	UNP Q12146
C	-3	HIS	-	expression tag	UNP Q12146
C	-2	MET	-	expression tag	UNP Q12146
C	-1	ALA	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	D	222	3671	1170	1843	299	347	12	0	0

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	E	566	9129	2922	4560	770	863	14	0	0

- Molecule 12 is a DNA chain called Leading strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
12	F	48	1547	475	544	182	298	48	0	0

- Molecule 13 is a DNA chain called Lagging strand DNA template.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
13	G	21	664	204	234	84	121	21	0	0

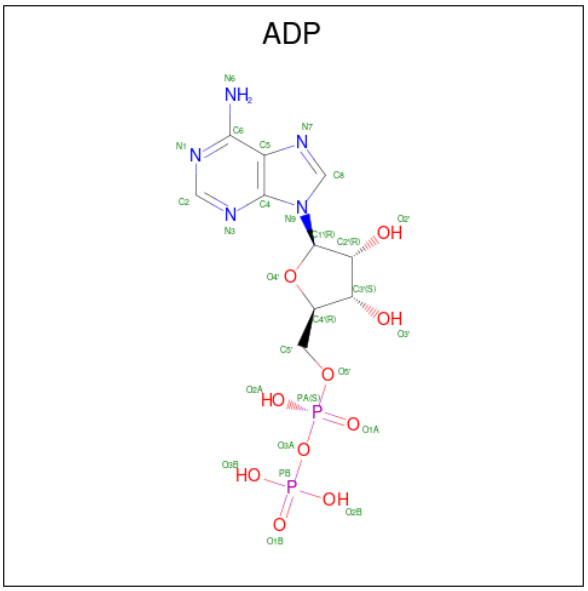
- Molecule 14 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	X	705	11543	3691	5828	962	1043	19	0	0

- Molecule 15 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	Y	92	1539	495	771	138	131	4	0	0

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
16	2	1	39	10	12	5	10	2	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
17	2	1	1	1	0
17	3	1	1	1	0
17	4	1	1	1	0
17	5	1	1	1	0
17	6	1	1	1	0
17	7	1	1	1	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

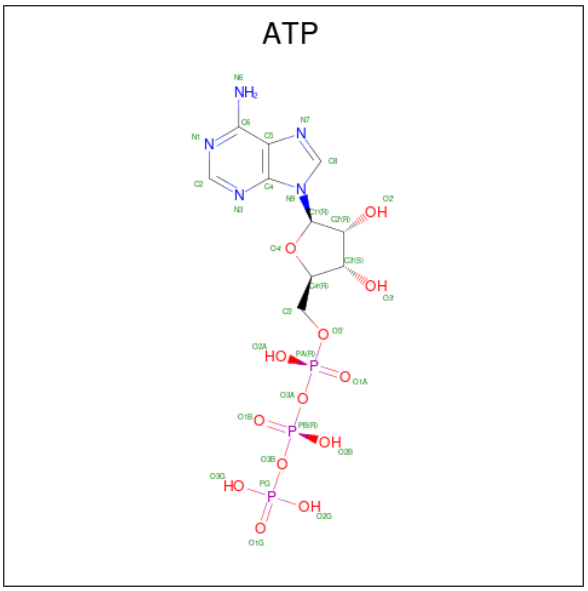
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	2	1	1	1	0
18	4	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	5	1	1	1	0
			Total	Zn	
18	6	1	1	1	0
			Total	Zn	
18	7	1	1	1	0

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



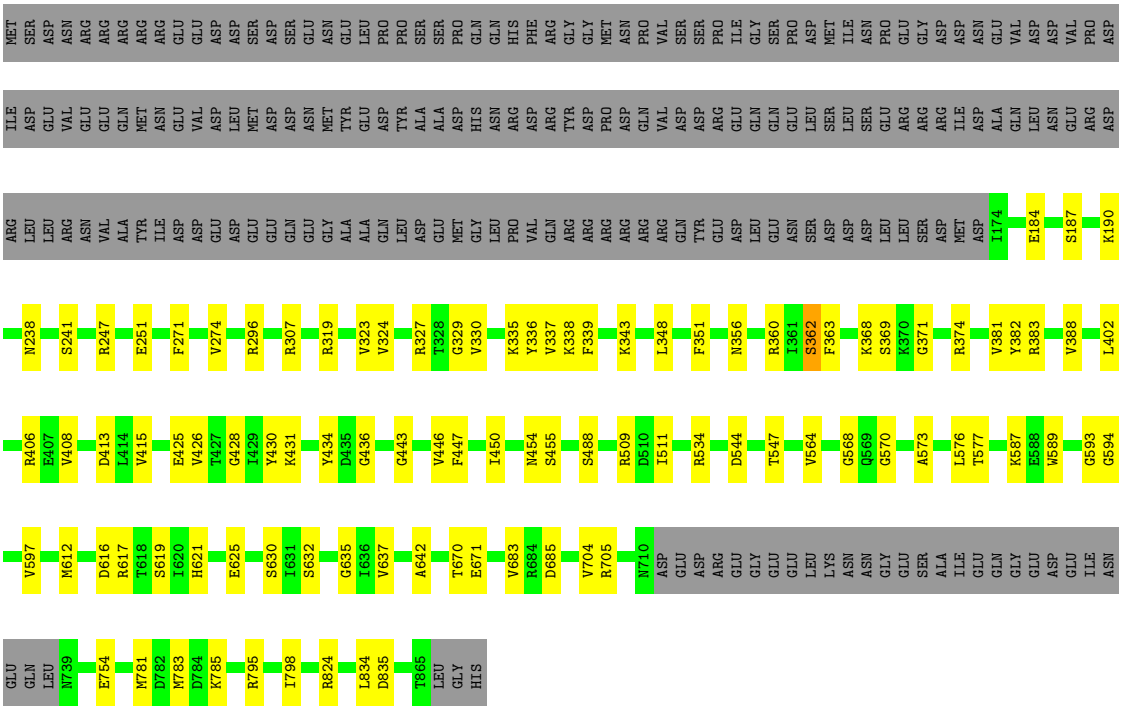
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
19	3	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
19	4	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
19	5	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
19	6	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
19	7	1	43	10	12	5	13	3	0

3 Residue-property plots (i)

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

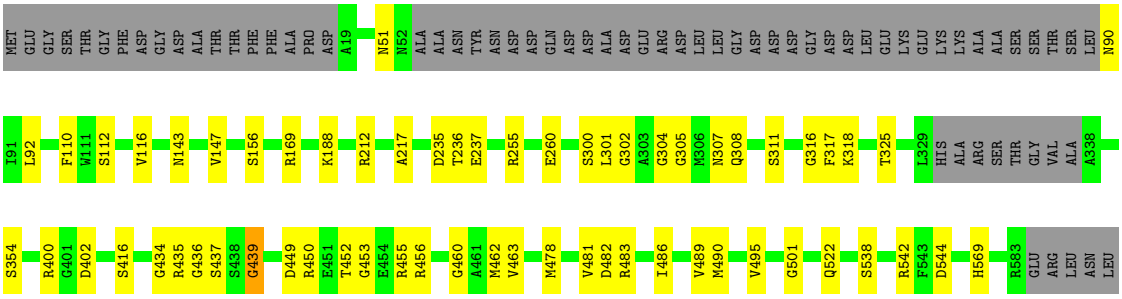
• Molecule 1: DNA replication licensing factor MCM2

Chain 2: 65% 11% 24%



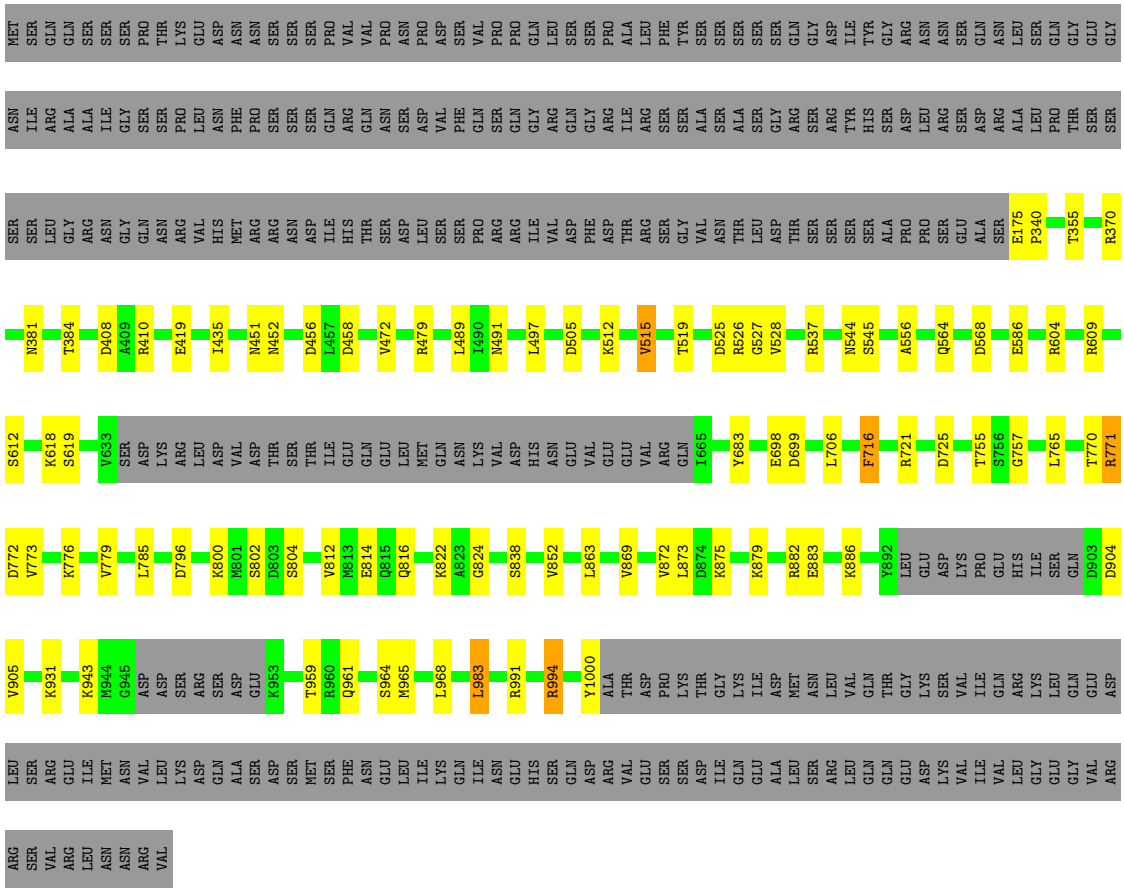
• Molecule 2: DNA replication licensing factor MCM3

Chain 3: 56% 7% 36%



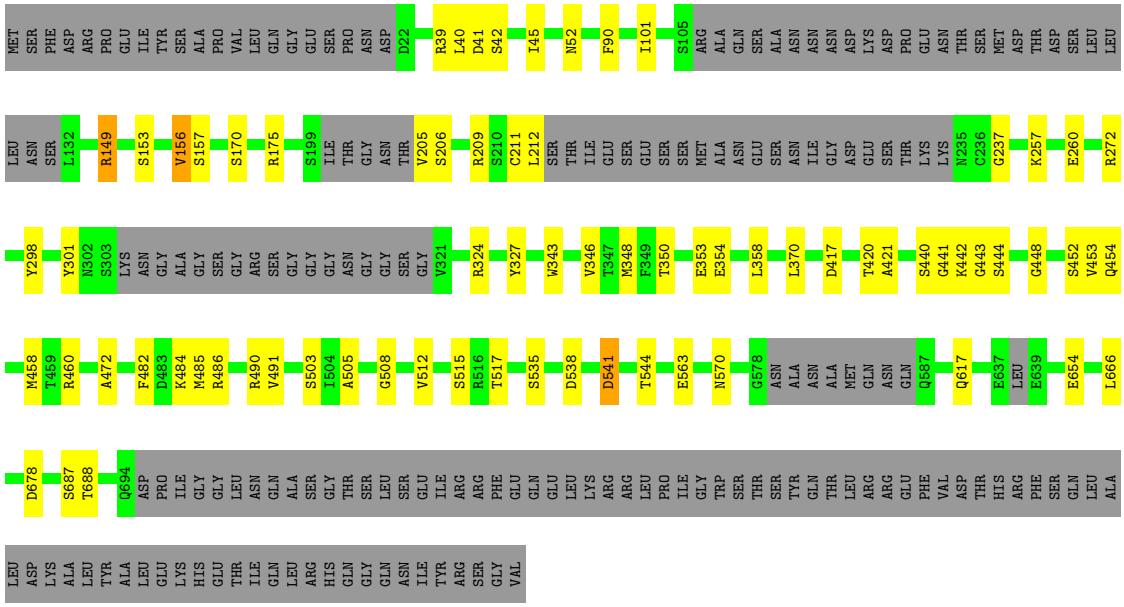
- Molecule 3: DNA replication licensing factor MCM4

Chain 4:



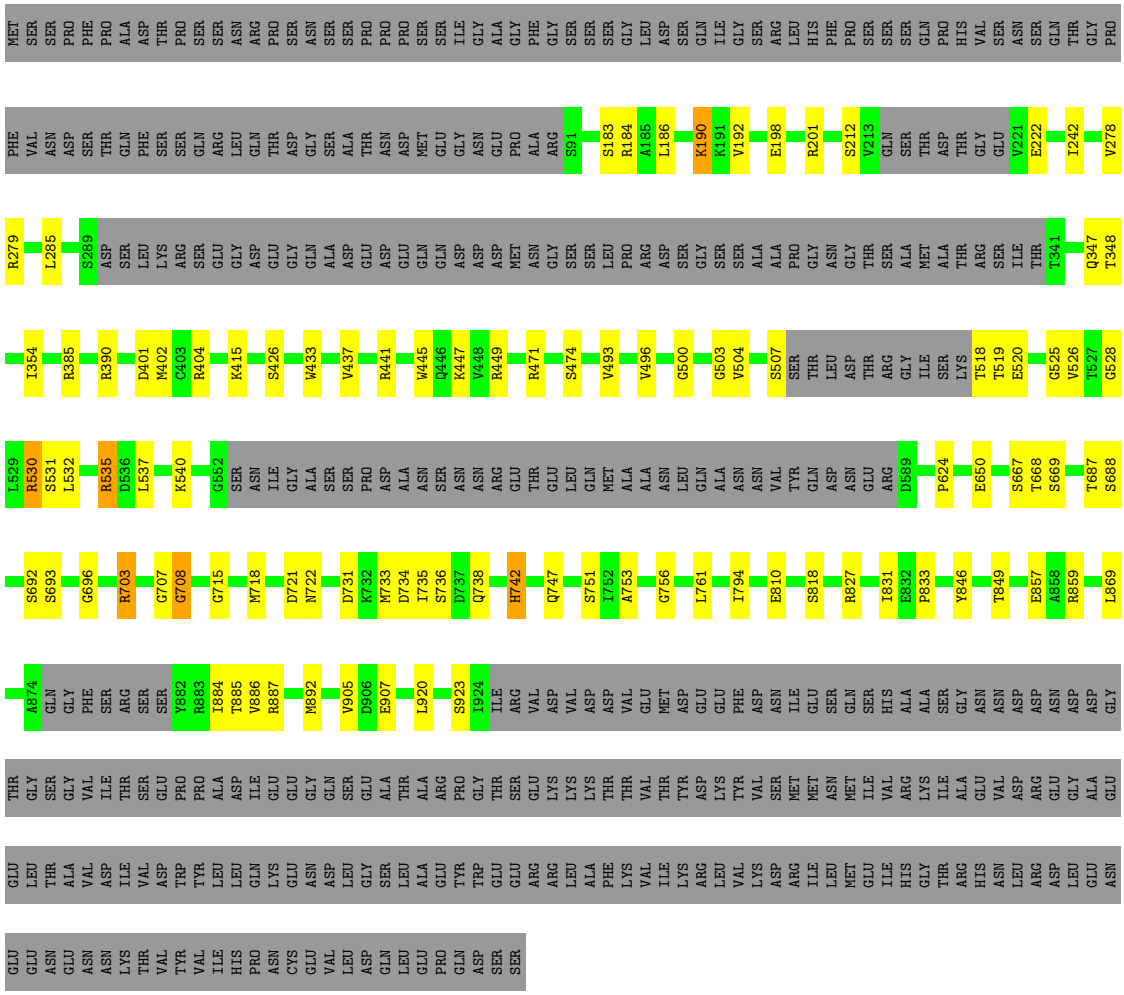
- Molecule 4: Minichromosome maintenance protein 5

Chain 5:



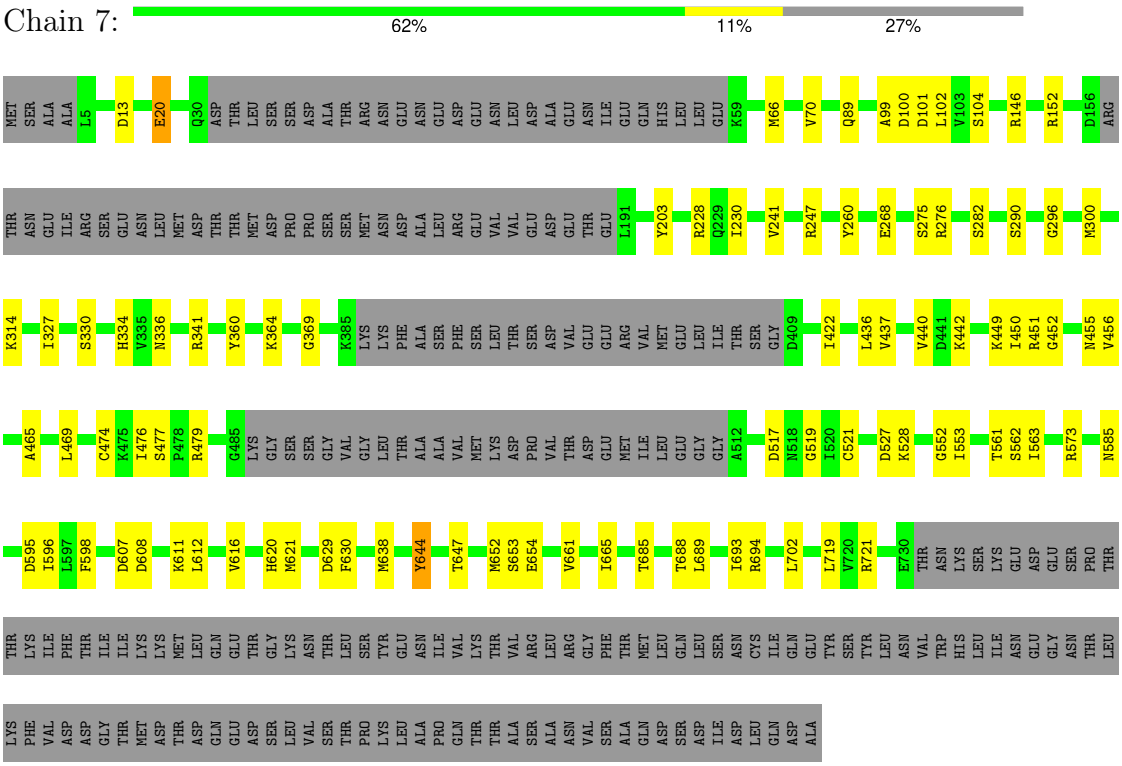
• Molecule 5: DNA replication licensing factor MCM6

Chain 6: 53% 9% • 38%



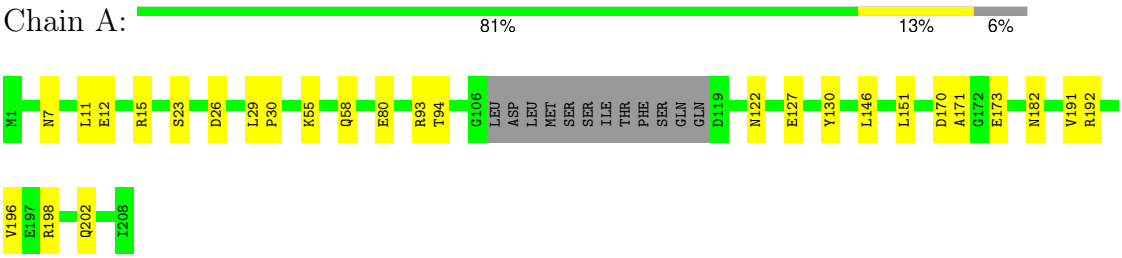
• Molecule 6: DNA replication licensing factor MCM7

Chain 7:



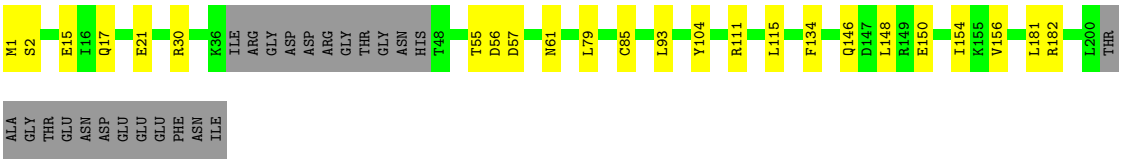
• Molecule 7: DNA replication complex GINS protein PSF1

Chain A:



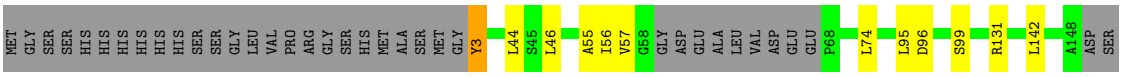
• Molecule 8: DNA replication complex GINS protein PSF2

Chain B:



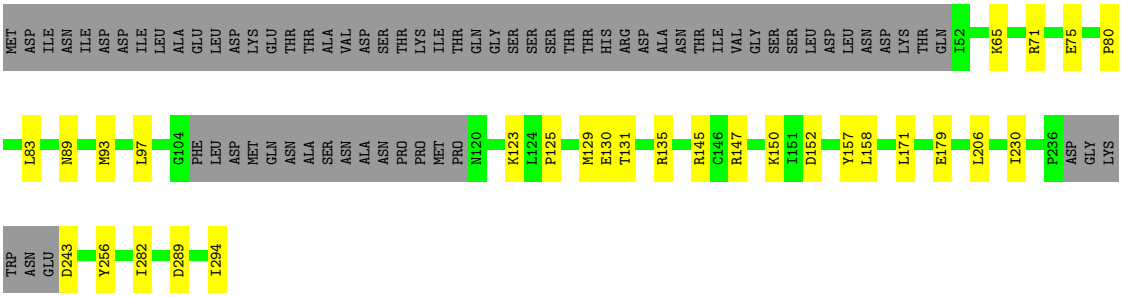
• Molecule 9: DNA replication complex GINS protein PSF3

Chain C:



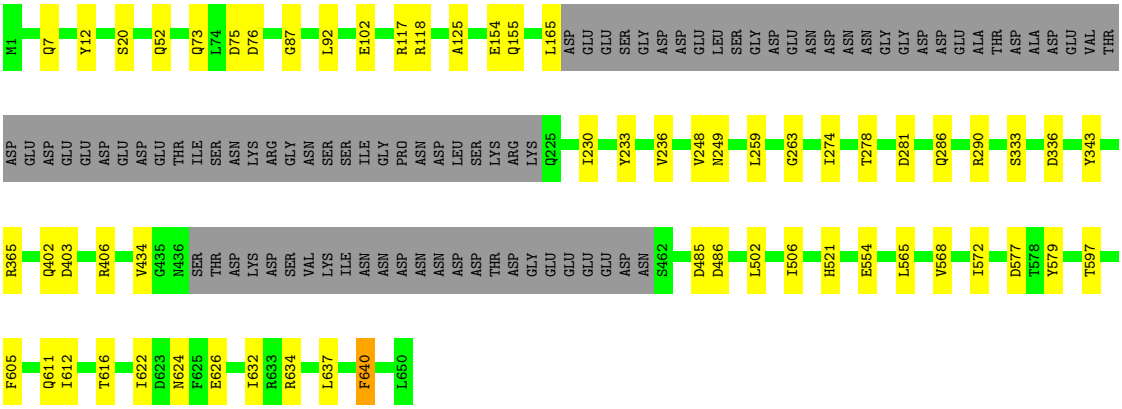
• Molecule 10: DNA replication complex GINS protein SLD5

Chain D:



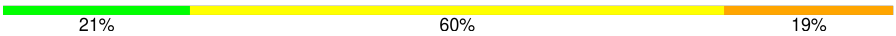
• Molecule 11: Cell division control protein 45

Chain E:



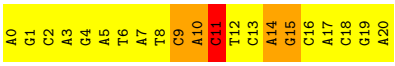
• Molecule 12: Leading strand DNA template

Chain F:



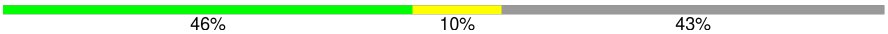
• Molecule 13: Lagging strand DNA template

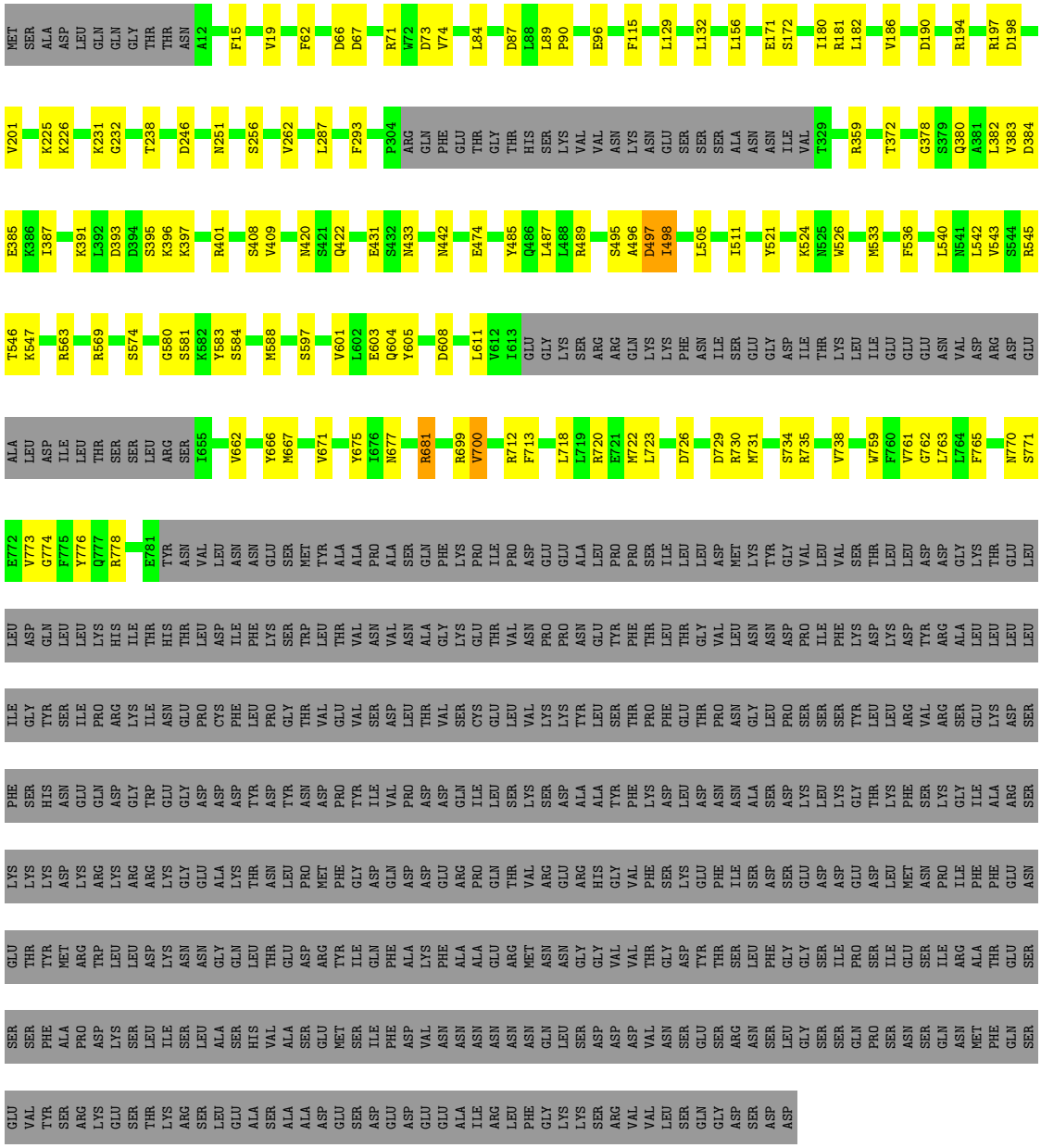
Chain G:



• Molecule 14: Topoisomerase 1-associated factor 1

Chain X:





• Molecule 15: Chromosome segregation in meiosis protein 3

Chain Y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66410	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	1.16	67/5356 (1.3%)	1.03	12/7233 (0.2%)
2	3	0.93	34/4909 (0.7%)	0.84	7/6657 (0.1%)
3	4	0.74	23/4952 (0.5%)	0.72	3/6693 (0.0%)
4	5	1.00	43/4737 (0.9%)	0.89	11/6403 (0.2%)
5	6	1.02	44/5086 (0.9%)	0.89	8/6860 (0.1%)
6	7	0.73	17/4943 (0.3%)	0.72	3/6682 (0.0%)
7	A	0.25	0/1620	0.46	0/2179
8	B	0.24	0/1609	0.48	0/2177
9	C	0.33	0/1429	0.51	2/1932 (0.1%)
10	D	0.25	0/1861	0.45	0/2512
11	E	0.25	0/4656	0.48	0/6306
12	F	1.55	0/1125	2.37	73/1741 (4.2%)
13	G	1.52	0/483	2.44	44/742 (5.9%)
14	X	0.97	45/5828 (0.8%)	0.88	15/7868 (0.2%)
15	Y	1.71	18/784 (2.3%)	1.45	6/1049 (0.6%)
All	All	0.89	291/49378 (0.6%)	0.91	184/67034 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	3
2	3	0	1
3	4	0	4
4	5	0	2
8	B	0	1
11	E	0	1
12	F	0	11
13	G	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	Y	0	2
All	All	0	30

All (291) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	406	ARG	CZ-NH2	-8.04	1.22	1.33
1	2	383	ARG	CZ-NH2	-8.02	1.22	1.33
4	5	272	ARG	CZ-NH2	-8.02	1.22	1.33
3	4	609	ARG	CZ-NH2	-8.01	1.22	1.33
5	6	184	ARG	CZ-NH2	-7.99	1.22	1.33
14	X	712	ARG	CZ-NH2	-7.99	1.22	1.33
4	5	324	ARG	CZ-NH2	-7.98	1.22	1.33
3	4	537	ARG	CZ-NH2	-7.98	1.22	1.33
4	5	149	ARG	CZ-NH2	-7.98	1.22	1.33
14	X	681	ARG	CZ-NH2	-7.97	1.22	1.33
1	2	360	ARG	CZ-NH2	-7.97	1.22	1.33
4	5	175	ARG	CZ-NH2	-7.96	1.22	1.33
2	3	255	ARG	CZ-NH2	-7.96	1.22	1.33
4	5	490	ARG	CZ-NH2	-7.95	1.22	1.33
1	2	617	ARG	CZ-NH2	-7.95	1.22	1.33
15	Y	129	ARG	CZ-NH2	-7.95	1.22	1.33
3	4	771	ARG	CZ-NH2	-7.95	1.22	1.33
5	6	530	ARG	CZ-NH2	-7.95	1.22	1.33
15	Y	134	ARG	CZ-NH2	-7.94	1.22	1.33
2	3	450	ARG	CZ-NH2	-7.93	1.22	1.33
5	6	385	ARG	CZ-NH2	-7.93	1.22	1.33
5	6	390	ARG	CZ-NH2	-7.92	1.22	1.33
5	6	703	ARG	CZ-NH2	-7.92	1.22	1.33
2	3	435	ARG	CZ-NH2	-7.91	1.22	1.33
4	5	209	ARG	CZ-NH2	-7.91	1.22	1.33
1	2	327	ARG	CZ-NH2	-7.91	1.22	1.33
6	7	247	ARG	CZ-NH2	-7.91	1.22	1.33
6	7	276	ARG	CZ-NH2	-7.91	1.22	1.33
14	X	778	ARG	CZ-NH2	-7.91	1.22	1.33
2	3	483	ARG	CZ-NH2	-7.89	1.22	1.33
2	3	456	ARG	CZ-NH2	-7.87	1.22	1.33
5	6	449	ARG	CZ-NH2	-7.87	1.22	1.33
1	2	406	ARG	CZ-NH1	-7.51	1.23	1.33
14	X	712	ARG	CZ-NH1	-7.51	1.23	1.33
1	2	383	ARG	CZ-NH1	-7.50	1.23	1.33
4	5	324	ARG	CZ-NH1	-7.50	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	129	ARG	CZ-NH1	-7.50	1.23	1.33
5	6	385	ARG	CZ-NH1	-7.48	1.23	1.33
1	2	360	ARG	CZ-NH1	-7.48	1.23	1.33
1	2	617	ARG	CZ-NH1	-7.47	1.23	1.33
6	7	247	ARG	CZ-NH1	-7.47	1.23	1.33
3	4	537	ARG	CZ-NH1	-7.47	1.23	1.33
14	X	681	ARG	CZ-NH1	-7.47	1.23	1.33
4	5	149	ARG	CZ-NH1	-7.46	1.23	1.33
5	6	390	ARG	CZ-NH1	-7.45	1.23	1.33
5	6	184	ARG	CZ-NH1	-7.45	1.23	1.33
2	3	483	ARG	CZ-NH1	-7.45	1.23	1.33
15	Y	134	ARG	CZ-NH1	-7.43	1.23	1.33
2	3	435	ARG	CZ-NH1	-7.43	1.23	1.33
4	5	272	ARG	CZ-NH1	-7.42	1.23	1.33
6	7	276	ARG	CZ-NH1	-7.42	1.23	1.33
2	3	456	ARG	CZ-NH1	-7.42	1.23	1.33
4	5	175	ARG	CZ-NH1	-7.41	1.23	1.33
4	5	209	ARG	CZ-NH1	-7.40	1.23	1.33
4	5	490	ARG	CZ-NH1	-7.40	1.23	1.33
2	3	255	ARG	CZ-NH1	-7.40	1.23	1.33
1	2	327	ARG	CZ-NH1	-7.39	1.23	1.33
14	X	778	ARG	CZ-NH1	-7.39	1.23	1.33
3	4	609	ARG	CZ-NH1	-7.38	1.23	1.33
5	6	449	ARG	CZ-NH1	-7.37	1.23	1.33
5	6	530	ARG	CZ-NH1	-7.37	1.23	1.33
2	3	450	ARG	CZ-NH1	-7.37	1.23	1.33
5	6	703	ARG	CZ-NH1	-7.35	1.23	1.33
3	4	771	ARG	CZ-NH1	-7.33	1.23	1.33
4	5	452	SER	CA-CB	-6.31	1.43	1.52
4	5	237	GLY	N-CA	-5.87	1.37	1.46
1	2	371	GLY	N-CA	-5.85	1.37	1.46
14	X	675	TYR	CD2-CE2	-5.77	1.30	1.39
1	2	593	GLY	N-CA	-5.76	1.37	1.46
15	Y	128	TYR	CD1-CE1	-5.72	1.30	1.39
14	X	666	TYR	CD1-CE1	-5.71	1.30	1.39
5	6	525	GLY	N-CA	-5.70	1.37	1.46
5	6	696	GLY	N-CA	-5.68	1.37	1.46
1	2	430	TYR	CD2-CE2	-5.67	1.30	1.39
5	6	715	GLY	N-CA	-5.66	1.37	1.46
1	2	430	TYR	CD1-CE1	-5.65	1.30	1.39
14	X	700	VAL	CB-CG2	-5.65	1.41	1.52
14	X	521	TYR	CD1-CE1	-5.63	1.30	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	776	TYR	CD1-CE1	-5.63	1.30	1.39
1	2	329	GLY	N-CA	-5.62	1.37	1.46
14	X	675	TYR	CD1-CE1	-5.62	1.30	1.39
1	2	434	TYR	CD1-CE1	-5.61	1.30	1.39
2	3	460	GLY	N-CA	-5.61	1.37	1.46
14	X	583	TYR	CD1-CE1	-5.61	1.30	1.39
1	2	382	TYR	CD2-CE2	-5.59	1.30	1.39
2	3	436	GLY	N-CA	-5.59	1.37	1.46
14	X	761	VAL	CB-CG2	-5.59	1.41	1.52
15	Y	128	TYR	CD2-CE2	-5.59	1.30	1.39
4	5	327	TYR	CD1-CE1	-5.58	1.30	1.39
14	X	666	TYR	CD2-CE2	-5.58	1.30	1.39
5	6	503	GLY	N-CA	-5.58	1.37	1.46
1	2	382	TYR	CD1-CE1	-5.57	1.30	1.39
4	5	298	TYR	CD1-CE1	-5.57	1.30	1.39
2	3	302	GLY	N-CA	-5.56	1.37	1.46
1	2	408	VAL	CB-CG1	-5.56	1.41	1.52
4	5	156	VAL	CB-CG2	-5.55	1.41	1.52
1	2	434	TYR	CD2-CE2	-5.55	1.31	1.39
4	5	298	TYR	CD2-CE2	-5.55	1.31	1.39
4	5	301	TYR	CD1-CE1	-5.55	1.31	1.39
6	7	360	TYR	CD2-CE2	-5.55	1.31	1.39
1	2	564	VAL	CB-CG2	-5.55	1.41	1.52
1	2	597	VAL	CB-CG1	-5.54	1.41	1.52
2	3	305	GLY	N-CA	-5.54	1.37	1.46
14	X	776	TYR	CD2-CE2	-5.54	1.31	1.39
15	Y	118	VAL	CB-CG1	-5.54	1.41	1.52
4	5	327	TYR	CD2-CE2	-5.54	1.31	1.39
14	X	521	TYR	CD2-CE2	-5.54	1.31	1.39
2	3	316	GLY	N-CA	-5.54	1.37	1.46
1	2	388	VAL	CB-CG2	-5.53	1.41	1.52
1	2	570	GLY	N-CA	-5.53	1.37	1.46
6	7	360	TYR	CD1-CE1	-5.53	1.31	1.39
4	5	508	GLY	N-CA	-5.52	1.37	1.46
6	7	260	TYR	CD2-CE2	-5.52	1.31	1.39
5	6	493	VAL	CB-CG2	-5.52	1.41	1.52
14	X	583	TYR	CD2-CE2	-5.52	1.31	1.39
6	7	260	TYR	CD1-CE1	-5.51	1.31	1.39
5	6	526	VAL	CB-CG2	-5.51	1.41	1.52
1	2	323	VAL	CB-CG2	-5.50	1.41	1.52
14	X	773	VAL	CB-CG1	-5.49	1.41	1.52
1	2	446	VAL	CB-CG1	-5.49	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	388	VAL	CB-CG1	-5.49	1.41	1.52
14	X	671	VAL	CB-CG2	-5.49	1.41	1.52
1	2	635	GLY	N-CA	-5.48	1.37	1.46
14	X	671	VAL	CB-CG1	-5.48	1.41	1.52
14	X	662	VAL	CB-CG1	-5.47	1.41	1.52
1	2	426	VAL	CB-CG1	-5.47	1.41	1.52
1	2	564	VAL	CB-CG1	-5.47	1.41	1.52
14	X	761	VAL	CB-CG1	-5.47	1.41	1.52
1	2	408	VAL	CB-CG2	-5.46	1.41	1.52
14	X	232	GLY	N-CA	-5.46	1.37	1.46
3	4	824	GLY	N-CA	-5.46	1.37	1.46
4	5	301	TYR	CD2-CE2	-5.46	1.31	1.39
1	2	330	VAL	CB-CG2	-5.46	1.41	1.52
14	X	396	LYS	CE-NZ	-5.45	1.35	1.49
1	2	637	VAL	CB-CG2	-5.45	1.41	1.52
1	2	431	LYS	CE-NZ	-5.44	1.35	1.49
2	3	495	VAL	CB-CG2	-5.44	1.41	1.52
1	2	415	VAL	CB-CG1	-5.43	1.41	1.52
1	2	426	VAL	CB-CG2	-5.43	1.41	1.52
3	4	515	VAL	CB-CG2	-5.43	1.41	1.52
1	2	446	VAL	CB-CG2	-5.43	1.41	1.52
5	6	504	VAL	CB-CG2	-5.43	1.41	1.52
5	6	756	GLY	N-CA	-5.43	1.38	1.46
1	2	455	SER	CB-OG	-5.43	1.35	1.42
2	3	495	VAL	CB-CG1	-5.42	1.41	1.52
14	X	581	SER	CB-OG	-5.42	1.35	1.42
15	Y	118	VAL	CB-CG2	-5.42	1.41	1.52
1	2	330	VAL	CB-CG1	-5.42	1.41	1.52
1	2	336	TYR	CD2-CE2	-5.42	1.31	1.39
15	Y	113	LYS	CE-NZ	-5.41	1.35	1.49
3	4	822	LYS	CE-NZ	-5.41	1.35	1.49
4	5	156	VAL	CB-CG1	-5.41	1.41	1.52
3	4	515	VAL	CB-CG1	-5.41	1.41	1.52
4	5	484	LYS	CE-NZ	-5.41	1.35	1.49
5	6	493	VAL	CB-CG1	-5.41	1.41	1.52
1	2	637	VAL	CB-CG1	-5.41	1.41	1.52
5	6	500	GLY	N-CA	-5.41	1.38	1.46
5	6	528	GLY	N-CA	-5.41	1.38	1.46
2	3	489	VAL	CB-CG2	-5.41	1.41	1.52
15	Y	107	LYS	CE-NZ	-5.41	1.35	1.49
1	2	323	VAL	CB-CG1	-5.40	1.41	1.52
5	6	437	VAL	CB-CG1	-5.40	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	119	GLY	N-CA	-5.40	1.38	1.46
15	Y	130	VAL	CB-CG1	-5.40	1.41	1.52
1	2	381	VAL	CB-CG2	-5.40	1.41	1.52
1	2	443	GLY	N-CA	-5.40	1.38	1.46
2	3	463	VAL	CB-CG2	-5.40	1.41	1.52
5	6	708	GLY	N-CA	-5.40	1.38	1.46
3	4	779	VAL	CB-CG1	-5.40	1.41	1.52
4	5	512	VAL	CB-CG2	-5.39	1.41	1.52
1	2	324	VAL	CB-CG2	-5.39	1.41	1.52
3	4	527	GLY	N-CA	-5.39	1.38	1.46
1	2	324	VAL	CB-CG1	-5.39	1.41	1.52
4	5	42	SER	CA-CB	-5.39	1.44	1.52
14	X	397	LYS	CE-NZ	-5.39	1.35	1.49
1	2	337	VAL	CB-CG2	-5.38	1.41	1.52
15	Y	130	VAL	CB-CG2	-5.38	1.41	1.52
1	2	336	TYR	CD1-CE1	-5.38	1.31	1.39
14	X	226	LYS	CE-NZ	-5.38	1.35	1.49
15	Y	109	LYS	CE-NZ	-5.38	1.35	1.49
1	2	597	VAL	CB-CG2	-5.37	1.41	1.52
1	2	619	SER	CB-OG	-5.37	1.35	1.42
5	6	496	VAL	CB-CG1	-5.37	1.41	1.52
4	5	440	SER	CB-OG	-5.36	1.35	1.42
4	5	442	LYS	CE-NZ	-5.36	1.35	1.49
1	2	343	LYS	CE-NZ	-5.36	1.35	1.49
1	2	381	VAL	CB-CG1	-5.36	1.41	1.52
15	Y	58	LYS	CE-NZ	-5.36	1.35	1.49
5	6	447	LYS	CE-NZ	-5.35	1.35	1.49
1	2	335	LYS	CE-NZ	-5.35	1.35	1.49
1	2	630	SER	CB-OG	-5.35	1.35	1.42
4	5	491	VAL	CB-CG1	-5.35	1.41	1.52
4	5	515	SER	CB-OG	-5.35	1.35	1.42
2	3	501	GLY	N-CA	-5.35	1.38	1.46
4	5	441	GLY	N-CA	-5.34	1.38	1.46
5	6	426	SER	CB-OG	-5.34	1.35	1.42
14	X	225	LYS	CE-NZ	-5.34	1.35	1.49
14	X	524	LYS	CE-NZ	-5.34	1.35	1.49
1	2	568	GLY	N-CA	-5.34	1.38	1.46
4	5	206	SER	CB-OG	-5.34	1.35	1.42
4	5	205	VAL	CB-CG1	-5.34	1.41	1.52
4	5	443	GLY	N-CA	-5.34	1.38	1.46
1	2	594	GLY	N-CA	-5.34	1.38	1.46
2	3	188	LYS	CE-NZ	-5.34	1.35	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	6	415	LYS	CE-NZ	-5.34	1.35	1.49
14	X	773	VAL	CB-CG2	-5.34	1.41	1.52
1	2	587	LYS	CE-NZ	-5.33	1.35	1.49
5	6	526	VAL	CB-CG1	-5.33	1.41	1.52
6	7	364	LYS	CE-NZ	-5.33	1.35	1.49
2	3	437	SER	CB-OG	-5.33	1.35	1.42
3	4	528	VAL	CB-CG2	-5.33	1.41	1.52
4	5	444	SER	CB-OG	-5.33	1.35	1.42
6	7	330	SER	CB-OG	-5.33	1.35	1.42
6	7	369	GLY	N-CA	-5.33	1.38	1.46
1	2	338	LYS	CE-NZ	-5.33	1.35	1.49
1	2	368	LYS	CE-NZ	-5.33	1.35	1.49
2	3	489	VAL	CB-CG1	-5.33	1.41	1.52
5	6	190	LYS	CE-NZ	-5.33	1.35	1.49
4	5	257	LYS	CE-NZ	-5.32	1.35	1.49
3	4	612	SER	CB-OG	-5.32	1.35	1.42
14	X	584	SER	CB-OG	-5.32	1.35	1.42
2	3	481	VAL	CB-CG1	-5.32	1.41	1.52
3	4	528	VAL	CB-CG1	-5.32	1.41	1.52
5	6	504	VAL	CB-CG1	-5.32	1.41	1.52
2	3	434	GLY	N-CA	-5.32	1.38	1.46
14	X	231	LYS	CE-NZ	-5.32	1.35	1.49
15	Y	131	SER	CB-OG	-5.32	1.35	1.42
14	X	408	SER	CB-OG	-5.31	1.35	1.42
15	Y	124	VAL	CB-CG2	-5.31	1.41	1.52
2	3	463	VAL	CB-CG1	-5.31	1.41	1.52
4	5	512	VAL	CB-CG1	-5.30	1.41	1.52
4	5	153	SER	CB-OG	-5.30	1.35	1.42
3	4	618	LYS	CE-NZ	-5.29	1.35	1.49
1	2	337	VAL	CB-CG1	-5.29	1.41	1.52
1	2	362	SER	CB-OG	-5.29	1.35	1.42
4	5	491	VAL	CB-CG2	-5.29	1.41	1.52
14	X	569	ARG	CZ-NH2	-5.29	1.26	1.33
14	X	700	VAL	CB-CG1	-5.29	1.41	1.52
5	6	496	VAL	CB-CG2	-5.29	1.41	1.52
1	2	632	SER	CB-OG	-5.29	1.35	1.42
4	5	205	VAL	CB-CG2	-5.28	1.41	1.52
6	7	282	SER	CB-OG	-5.28	1.35	1.42
6	7	314	LYS	CE-NZ	-5.28	1.35	1.49
14	X	662	VAL	CB-CG2	-5.28	1.41	1.52
1	2	415	VAL	CB-CG2	-5.28	1.41	1.52
4	5	503	SER	CB-OG	-5.28	1.35	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	428	GLY	N-CA	-5.27	1.38	1.46
4	5	448	GLY	N-CA	-5.27	1.38	1.46
5	6	736	SER	CB-OG	-5.27	1.35	1.42
1	2	369	SER	CB-OG	-5.27	1.35	1.42
2	3	300	SER	CB-OG	-5.27	1.35	1.42
5	6	531	SER	CB-OG	-5.27	1.35	1.42
5	6	540	LYS	CE-NZ	-5.27	1.35	1.49
14	X	574	SER	CB-OG	-5.27	1.35	1.42
1	2	436	GLY	N-CA	-5.26	1.38	1.46
2	3	212	ARG	CZ-NH2	-5.26	1.26	1.33
6	7	275	SER	CB-OG	-5.26	1.35	1.42
6	7	552	GLY	N-CA	-5.25	1.38	1.46
3	4	619	SER	CB-OG	-5.25	1.35	1.42
5	6	507	SER	CB-OG	-5.25	1.35	1.42
14	X	395	SER	CB-OG	-5.25	1.35	1.42
14	X	771	SER	CB-OG	-5.25	1.35	1.42
14	X	762	GLY	N-CA	-5.25	1.38	1.46
5	6	751	SER	CB-OG	-5.24	1.35	1.42
3	4	779	VAL	CB-CG2	-5.24	1.41	1.52
3	4	773	VAL	CB-CG2	-5.24	1.41	1.52
14	X	580	GLY	N-CA	-5.23	1.38	1.46
2	3	311	SER	CB-OG	-5.23	1.35	1.42
5	6	693	SER	CB-OG	-5.23	1.35	1.42
2	3	318	LYS	CE-NZ	-5.22	1.35	1.49
3	4	545	SER	CB-OG	-5.22	1.35	1.42
6	7	290	SER	CB-OG	-5.22	1.35	1.42
3	4	773	VAL	CB-CG1	-5.22	1.41	1.52
5	6	692	SER	CB-OG	-5.21	1.35	1.42
14	X	526	TRP	CD1-NE1	-5.21	1.29	1.38
5	6	445	TRP	CD1-NE1	-5.20	1.29	1.38
14	X	774	GLY	N-CA	-5.20	1.38	1.46
14	X	759	TRP	CD1-NE1	-5.19	1.29	1.38
3	4	802	SER	CB-OG	-5.19	1.35	1.42
5	6	433	TRP	CD1-NE1	-5.18	1.29	1.38
2	3	481	VAL	CB-CG2	-5.18	1.42	1.52
3	4	804	SER	CB-OG	-5.18	1.35	1.42
2	3	439	GLY	N-CA	-5.17	1.38	1.46
2	3	304	GLY	N-CA	-5.15	1.38	1.46
6	7	296	GLY	N-CA	-5.15	1.38	1.46
5	6	437	VAL	CB-CG2	-5.15	1.42	1.52
2	3	453	GLY	N-CA	-5.15	1.38	1.46
15	Y	124	VAL	CB-CG1	-5.11	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	505	ALA	CA-CB	-5.10	1.41	1.52
5	6	753	ALA	CA-CB	-5.10	1.41	1.52
1	2	642	ALA	CA-CB	-5.08	1.41	1.52

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	45	DT	O4'-C1'-N1	12.83	116.98	108.00
12	F	53	DT	N3-C2-O2	-9.48	116.61	122.30
13	G	20	DA	N1-C6-N6	-9.35	112.99	118.60
12	F	60	DA	N1-C6-N6	-9.27	113.04	118.60
12	F	29	DA	N1-C6-N6	-9.18	113.09	118.60
13	G	14	DA	N1-C6-N6	-9.04	113.18	118.60
12	F	61	DA	N1-C6-N6	-8.84	113.30	118.60
12	F	53	DT	O4'-C1'-N1	8.71	114.10	108.00
13	G	7	DA	N1-C6-N6	-8.32	113.61	118.60
12	F	45	DT	N3-C2-O2	-8.20	117.38	122.30
12	F	23	DA	N1-C6-N6	-8.18	113.69	118.60
13	G	10	DA	N1-C6-N6	-8.06	113.76	118.60
13	G	5	DA	N1-C6-N6	-7.98	113.81	118.60
12	F	52	DG	O4'-C1'-N9	7.96	113.57	108.00
13	G	17	DA	N1-C6-N6	-7.88	113.87	118.60
12	F	56	DA	C5-C6-N1	7.77	121.58	117.70
1	2	430	TYR	CB-CG-CD2	7.71	125.62	121.00
13	G	0	DA	C5-C6-N1	7.60	121.50	117.70
13	G	15	DG	O4'-C1'-N9	7.60	113.32	108.00
12	F	60	DA	C5-C6-N1	7.59	121.50	117.70
13	G	10	DA	C5-C6-N1	7.50	121.45	117.70
12	F	23	DA	C5-C6-N1	7.49	121.45	117.70
12	F	37	DT	O4'-C1'-N1	7.48	113.24	108.00
13	G	0	DA	N1-C6-N6	-7.45	114.13	118.60
12	F	27	DA	C5-C6-N1	7.42	121.41	117.70
13	G	13	DC	N3-C2-O2	-7.39	116.73	121.90
13	G	14	DA	C4-C5-C6	-7.37	113.31	117.00
12	F	56	DA	N1-C6-N6	-7.31	114.21	118.60
12	F	29	DA	C5-C6-N1	7.26	121.33	117.70
12	F	56	DA	C4-C5-C6	-7.24	113.38	117.00
12	F	31	DC	N3-C2-O2	-7.17	116.88	121.90
12	F	16	DC	N3-C2-O2	-7.13	116.91	121.90
12	F	61	DA	C5-C6-N1	7.12	121.26	117.70
13	G	9	DC	N3-C2-O2	-7.11	116.92	121.90
12	F	20	DC	N3-C2-O2	-7.10	116.93	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	X	583	TYR	CB-CG-CD2	7.10	125.26	121.00
13	G	5	DA	C4-C5-C6	-7.09	113.45	117.00
13	G	3	DA	C5-C6-N1	7.05	121.23	117.70
1	2	447	PHE	CB-CG-CD2	7.03	125.72	120.80
13	G	7	DA	C5-C6-N1	7.00	121.20	117.70
13	G	2	DC	N3-C2-O2	-7.00	117.00	121.90
13	G	20	DA	C5-C6-N1	6.95	121.18	117.70
13	G	11	DC	N3-C2-O2	-6.89	117.07	121.90
12	F	22	DG	O4'-C1'-N9	6.89	112.82	108.00
14	X	675	TYR	CB-CG-CD2	6.87	125.12	121.00
13	G	16	DC	N3-C2-O2	-6.86	117.10	121.90
12	F	60	DA	C4-C5-C6	-6.82	113.59	117.00
12	F	30	DT	O4'-C1'-N1	6.80	112.76	108.00
1	2	612	MET	CA-CB-CG	6.80	124.85	113.30
12	F	59	DC	N3-C2-O2	-6.79	117.15	121.90
12	F	23	DA	O4'-C1'-N9	6.76	112.73	108.00
13	G	18	DC	N3-C2-O2	-6.75	117.17	121.90
12	F	29	DA	C4-C5-C6	-6.73	113.63	117.00
3	4	609	ARG	CD-NE-CZ	6.72	133.01	123.60
14	X	778	ARG	CD-NE-CZ	6.72	133.01	123.60
13	G	20	DA	C4-C5-C6	-6.72	113.64	117.00
12	F	23	DA	C4-C5-C6	-6.71	113.65	117.00
1	2	360	ARG	CD-NE-CZ	6.71	132.99	123.60
1	2	383	ARG	CD-NE-CZ	6.71	132.99	123.60
13	G	3	DA	N1-C6-N6	-6.70	114.58	118.60
2	3	435	ARG	CD-NE-CZ	6.69	132.97	123.60
6	7	276	ARG	CD-NE-CZ	6.68	132.95	123.60
14	X	712	ARG	CD-NE-CZ	6.68	132.95	123.60
4	5	175	ARG	CD-NE-CZ	6.67	132.94	123.60
5	6	449	ARG	CD-NE-CZ	6.66	132.92	123.60
4	5	272	ARG	CD-NE-CZ	6.64	132.90	123.60
4	5	490	ARG	CD-NE-CZ	6.64	132.90	123.60
13	G	5	DA	C5-C6-N1	6.64	121.02	117.70
15	Y	129	ARG	CD-NE-CZ	6.63	132.88	123.60
1	2	327	ARG	CD-NE-CZ	6.63	132.88	123.60
15	Y	134	ARG	CD-NE-CZ	6.63	132.88	123.60
5	6	703	ARG	CD-NE-CZ	6.62	132.87	123.60
12	F	41	DT	C6-C5-C7	-6.60	118.94	122.90
2	3	255	ARG	CD-NE-CZ	6.58	132.81	123.60
3	4	537	ARG	CD-NE-CZ	6.58	132.81	123.60
13	G	17	DA	C5-C6-N1	6.54	120.97	117.70
12	F	34	DC	N3-C2-O2	-6.54	117.33	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	49	DT	C6-C5-C7	-6.51	118.99	122.90
5	6	385	ARG	CD-NE-CZ	6.49	132.68	123.60
12	F	25	DT	N3-C2-O2	-6.48	118.41	122.30
13	G	7	DA	C4-C5-C6	-6.47	113.76	117.00
12	F	37	DT	C6-C5-C7	-6.45	119.03	122.90
14	X	588	MET	CA-CB-CG	6.45	124.26	113.30
2	3	478	MET	CA-CB-CG	6.41	124.20	113.30
5	6	718	MET	CA-CB-CG	6.40	124.18	113.30
12	F	27	DA	N1-C6-N6	-6.40	114.76	118.60
13	G	10	DA	C4-C5-C6	-6.39	113.80	117.00
13	G	12	DT	C6-C5-C7	-6.32	119.11	122.90
14	X	776	TYR	CB-CG-CD2	6.31	124.78	121.00
9	C	3	TYR	CB-CA-C	-6.28	97.84	110.40
12	F	61	DA	C4-C5-C6	-6.27	113.86	117.00
12	F	18	DT	C6-C5-C7	-6.26	119.15	122.90
12	F	62	DT	C6-C5-C7	-6.25	119.15	122.90
3	4	771	ARG	CD-NE-CZ	6.24	132.34	123.60
12	F	28	DT	C6-C5-C7	-6.23	119.16	122.90
2	3	455	ARG	NE-CZ-NH2	6.21	123.41	120.30
13	G	17	DA	C4-C5-C6	-6.19	113.91	117.00
12	F	51	DG	N3-C2-N2	-6.16	115.59	119.90
12	F	21	DT	C6-C5-C7	-6.16	119.21	122.90
12	F	27	DA	C4-C5-C6	-6.13	113.94	117.00
12	F	35	DT	C6-C5-C7	-6.12	119.23	122.90
15	Y	103	PHE	CB-CG-CD2	6.11	125.08	120.80
4	5	486	ARG	NE-CZ-NH2	6.11	123.35	120.30
13	G	14	DA	C5-C6-N1	6.10	120.75	117.70
6	7	300	MET	CA-CB-CG	6.07	123.63	113.30
13	G	3	DA	C4-C5-C6	-6.07	113.97	117.00
12	F	35	DT	P-O3'-C3'	6.03	126.93	119.70
14	X	666	TYR	CB-CG-CD2	6.02	124.61	121.00
12	F	15	DT	C6-C5-C7	-6.00	119.30	122.90
14	X	497	ASP	CB-CA-C	-6.00	98.41	110.40
12	F	45	DT	C6-C5-C7	-5.99	119.31	122.90
15	Y	108	PHE	CB-CG-CD2	5.99	124.99	120.80
1	2	434	TYR	CB-CG-CD2	5.93	124.56	121.00
4	5	298	TYR	CB-CG-CD2	5.93	124.56	121.00
12	F	25	DT	C6-C5-C7	-5.93	119.34	122.90
2	3	456	ARG	CD-NE-CZ	5.92	131.88	123.60
4	5	485	MET	CA-CB-CG	5.91	123.35	113.30
12	F	54	DT	C6-C5-C7	-5.91	119.35	122.90
13	G	6	DT	C6-C5-C7	-5.90	119.36	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	19	DG	P-O3'-C3'	5.89	126.77	119.70
12	F	28	DT	O4'-C1'-N1	5.86	112.10	108.00
1	2	336	TYR	CB-CG-CD2	5.84	124.50	121.00
4	5	301	TYR	CB-CG-CD2	5.83	124.50	121.00
5	6	184	ARG	CD-NE-CZ	5.81	131.73	123.60
13	G	0	DA	C4-C5-C6	-5.78	114.11	117.00
12	F	54	DT	N3-C2-O2	-5.77	118.84	122.30
12	F	24	DG	N1-C6-O6	-5.76	116.44	119.90
13	G	8	DT	C6-C5-C7	-5.73	119.46	122.90
12	F	17	DG	N1-C6-O6	-5.72	116.47	119.90
12	F	30	DT	C6-C5-C7	-5.70	119.48	122.90
12	F	53	DT	C6-C5-C7	-5.68	119.49	122.90
12	F	36	DT	C6-C5-C7	-5.66	119.50	122.90
4	5	482	PHE	CB-CG-CD2	5.66	124.76	120.80
12	F	62	DT	N3-C2-O2	-5.66	118.91	122.30
12	F	49	DT	N3-C2-O2	-5.65	118.91	122.30
1	2	351	PHE	CB-CG-CD2	5.60	124.72	120.80
12	F	18	DT	N3-C2-O2	-5.59	118.94	122.30
12	F	41	DT	N3-C2-O2	-5.57	118.96	122.30
12	F	55	DG	N1-C6-O6	-5.55	116.57	119.90
12	F	42	DG	O4'-C1'-N9	5.54	111.88	108.00
4	5	149	ARG	CD-NE-CZ	5.53	131.35	123.60
12	F	28	DT	O4'-C1'-C2'	-5.52	101.48	105.90
5	6	703	ARG	CG-CD-NE	5.51	123.38	111.80
12	F	31	DC	N1-C2-O2	5.51	122.21	118.90
12	F	36	DT	N3-C2-O2	-5.45	119.03	122.30
9	C	3	TYR	N-CA-CB	5.43	120.38	110.60
13	G	16	DC	N1-C2-O2	5.43	122.16	118.90
13	G	10	DA	O4'-C1'-N9	5.41	111.79	108.00
1	2	360	ARG	CG-CD-NE	5.39	123.13	111.80
13	G	8	DT	N3-C2-O2	-5.38	119.07	122.30
14	X	569	ARG	CD-NE-CZ	5.36	131.10	123.60
12	F	21	DT	N3-C2-O2	-5.35	119.09	122.30
2	3	317	PHE	CB-CG-CD2	5.34	124.54	120.80
13	G	13	DC	N1-C2-O2	5.33	122.10	118.90
12	F	20	DC	N1-C2-O2	5.31	122.09	118.90
1	2	363	PHE	CB-CG-CD2	5.31	124.52	120.80
14	X	401	ARG	NE-CZ-NH2	5.29	122.95	120.30
5	6	402	MET	CA-CB-CG	5.29	122.29	113.30
14	X	778	ARG	CG-CD-NE	5.28	122.89	111.80
14	X	521	TYR	CB-CG-CD2	5.26	124.16	121.00
13	G	9	DC	N1-C2-O2	5.25	122.05	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	617	ARG	CD-NE-CZ	5.25	130.95	123.60
4	5	324	ARG	CD-NE-CZ	5.24	130.93	123.60
12	F	22	DG	N1-C6-O6	-5.21	116.77	119.90
13	G	4	DG	O4'-C4'-C3'	5.21	109.13	106.00
12	F	32	DT	C6-C5-C7	-5.20	119.78	122.90
12	F	60	DA	O4'-C4'-C3'	5.20	109.12	106.00
13	G	14	DA	C6-C5-N7	5.19	135.94	132.30
13	G	2	DC	N1-C2-O2	5.17	122.00	118.90
15	Y	58	LYS	CA-CB-CG	5.16	124.75	113.40
13	G	19	DG	N1-C6-O6	-5.16	116.81	119.90
6	7	260	TYR	CB-CG-CD2	5.16	124.09	121.00
5	6	535	ARG	NE-CZ-NH2	5.13	122.87	120.30
15	Y	133	PHE	CB-CG-CD2	5.11	124.38	120.80
12	F	30	DT	N3-C2-O2	-5.11	119.23	122.30
14	X	763	LEU	CA-CB-CG	5.05	126.93	115.30
14	X	765	PHE	CB-CG-CD2	5.05	124.34	120.80
4	5	327	TYR	CB-CG-CD2	5.04	124.02	121.00
14	X	533	MET	CA-CB-CG	5.03	121.86	113.30
12	F	16	DC	N1-C2-O2	5.03	121.92	118.90
12	F	62	DT	O4'-C1'-N1	5.02	111.51	108.00
2	3	483	ARG	CA-CB-CG	5.01	124.43	113.40
12	F	45	DT	O4'-C1'-C2'	-5.01	101.89	105.90
12	F	15	DT	N3-C2-O2	-5.01	119.30	122.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	274	VAL	Mainchain
1	2	374	ARG	Sidechain
1	2	509	ARG	Sidechain
2	3	687	ARG	Sidechain
3	4	526	ARG	Sidechain
3	4	721	ARG	Sidechain
3	4	991	ARG	Sidechain
3	4	994	ARG	Sidechain
4	5	39	ARG	Sidechain
4	5	460	ARG	Sidechain
8	B	30	ARG	Sidechain
11	E	365	ARG	Sidechain
12	F	16	DC	Sidechain
12	F	17	DG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	F	18	DT	Sidechain
12	F	24	DG	Sidechain
12	F	26	DG	Sidechain
12	F	32	DT	Sidechain
12	F	34	DC	Sidechain
12	F	36	DT	Sidechain
12	F	38	DG	Sidechain
12	F	39	DG	Sidechain
12	F	52	DG	Sidechain
13	G	1	DG	Sidechain
13	G	11	DC	Sidechain
13	G	14	DA	Sidechain
13	G	15	DG	Sidechain
13	G	9	DC	Sidechain
15	Y	48	ARG	Sidechain
15	Y	49	ARG	Sidechain

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	2	5267	5309	5311	28	0
2	3	4825	4893	4897	29	0
3	4	4879	4933	4949	57	0
4	5	4671	4746	4742	34	0
5	6	5005	5035	5035	47	0
6	7	4865	4921	4919	42	0
7	A	1600	1602	1602	16	0
8	B	1577	1618	1625	18	0
9	C	1396	1409	1410	14	0
10	D	1828	1843	1842	20	0
11	E	4569	4560	4562	38	0
12	F	1003	544	545	2	0
13	G	430	234	235	1	0
14	X	5715	5828	5833	69	0
15	Y	768	771	801	16	0
16	2	27	12	12	2	0
17	2	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	3	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
18	2	1	0	0	0	0
18	4	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
19	3	31	12	12	1	0
19	4	31	12	12	0	0
19	5	31	12	12	0	0
19	6	31	12	12	0	0
19	7	31	12	12	0	0
All	All	48591	48318	48380	375	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 4.

All (375) 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)
14:X:720:ARG:NH2	15:Y:92:ILE:HG21	1.32	1.41
14:X:720:ARG:HH22	15:Y:92:ILE:CG2	1.51	1.20
14:X:720:ARG:NH2	15:Y:92:ILE:CG2	2.06	1.19
14:X:66:ASP:OD1	14:X:74:VAL:HB	1.47	1.13
14:X:511:ILE:HG21	14:X:563:ARG:NH1	1.72	1.05
14:X:393:ASP:OD2	15:Y:96:GLN:NE2	2.05	0.90
15:Y:79:SER:OG	15:Y:82:LYS:HB2	1.72	0.90
2:3:217:ALA:HB1	2:3:301:LEU:HD22	1.55	0.89
14:X:190:ASP:O	14:X:194:ARG:HG3	1.73	0.88
10:D:157:TYR:C	10:D:158:LEU:CA	2.43	0.87
1:2:589:TRP:HD1	4:5:454:GLN:HE22	1.22	0.85
14:X:720:ARG:HH22	15:Y:92:ILE:HG21	0.94	0.83
5:6:857:GLU:OE1	5:6:857:GLU:N	2.12	0.83
2:3:217:ALA:HB1	2:3:301:LEU:CD2	2.09	0.82
11:E:521:HIS:HE1	11:E:565:LEU:HD12	1.44	0.82
3:4:698:GLU:N	3:4:698:GLU:OE1	2.12	0.82
3:4:515:VAL:CG1	5:6:186:LEU:HD23	2.11	0.80
14:X:511:ILE:CG2	14:X:563:ARG:NH1	2.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:79:LEU:CB	8:B:85:CYS:SG	2.70	0.80
6:7:685:THR:O	6:7:688:THR:OG1	1.99	0.80
1:2:190:LYS:NZ	14:X:87:ASP:OD1	2.15	0.79
14:X:251:ASN:OD1	14:X:433:ASN:ND2	2.16	0.79
14:X:720:ARG:CZ	15:Y:92:ILE:HG21	2.13	0.78
8:B:2:SER:O	10:D:145:ARG:NH2	2.18	0.77
3:4:497:LEU:HD23	6:7:553:ILE:HD11	1.66	0.77
14:X:15:PHE:O	14:X:19:VAL:HG23	1.85	0.77
8:B:182:ARG:NH1	10:D:294:ILE:O	2.18	0.76
14:X:197:ARG:O	14:X:201:VAL:HG23	1.86	0.76
10:D:65:LYS:NZ	10:D:289:ASP:OD2	2.18	0.76
1:2:488:SER:OG	1:2:824:ARG:O	2.02	0.76
8:B:79:LEU:HB2	8:B:85:CYS:SG	2.26	0.76
1:2:589:TRP:CD1	4:5:454:GLN:NE2	2.52	0.75
2:3:538:SER:O	2:3:542:ARG:NH2	2.19	0.75
6:7:465:ALA:O	6:7:469:LEU:HD22	1.86	0.75
11:E:154:GLU:N	11:E:154:GLU:OE1	2.20	0.75
4:5:563:GLU:N	4:5:563:GLU:OE1	2.20	0.75
5:6:222:GLU:OE1	5:6:222:GLU:N	2.20	0.74
1:2:576:LEU:O	1:2:577:THR:OG1	2.05	0.74
4:5:350:THR:OG1	4:5:353:GLU:HG3	1.88	0.73
15:Y:79:SER:OG	15:Y:82:LYS:CB	2.36	0.73
14:X:489:ARG:NH1	14:X:496:ALA:HB1	2.03	0.73
2:3:236:THR:OG1	2:3:237:GLU:OE1	2.06	0.73
11:E:12:TYR:OH	11:E:52:GLN:OE1	2.07	0.73
8:B:1:MET:SD	10:D:152:ASP:HB3	2.30	0.71
8:B:79:LEU:HB3	8:B:85:CYS:SG	2.29	0.71
4:5:535:SER:OG	4:5:538:ASP:OD2	2.07	0.71
14:X:442:ASN:OD1	14:X:485:TYR:OH	2.07	0.71
2:3:449:ASP:OD2	2:3:452:THR:OG1	2.07	0.71
1:2:356:ASN:OD1	1:2:450:ILE:HD11	1.91	0.70
5:6:279:ARG:NH2	14:X:246:ASP:OD1	2.24	0.70
2:3:416:SER:OG	19:3:1001:ATP:O1B	2.09	0.70
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.25	0.69
11:E:521:HIS:HE1	11:E:565:LEU:CD1	2.04	0.69
6:7:101:ASP:OD2	6:7:104:SER:OG	2.06	0.68
7:A:30:PRO:O	7:A:93:ARG:NH1	2.26	0.68
14:X:720:ARG:HH22	15:Y:92:ILE:HG22	1.54	0.67
8:B:57:ASP:O	8:B:61:ASN:ND2	2.27	0.67
4:5:348:MET:HE3	9:C:163:SER:OG	1.96	0.66
5:6:733:MET:O	5:6:738:GLN:NE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:146:ARG:NH1	6:7:268:GLU:O	2.28	0.66
5:6:650:GLU:N	5:6:650:GLU:OE1	2.27	0.66
6:7:527:ASP:OD1	6:7:528:LYS:N	2.29	0.66
15:Y:71:ASN:OD1	15:Y:75:ARG:NH1	2.28	0.66
1:2:589:TRP:HD1	4:5:454:GLN:NE2	1.89	0.66
10:D:123:LYS:NZ	11:E:20:SER:OG	2.29	0.65
11:E:521:HIS:CE1	11:E:565:LEU:HD12	2.30	0.65
7:A:192:ARG:NH2	10:D:130:GLU:OE1	2.29	0.65
9:C:95:LEU:O	9:C:131:ARG:NH1	2.30	0.65
1:2:544:ASP:OD2	1:2:685:ASP:N	2.29	0.65
14:X:84:LEU:HD11	14:X:132:LEU:HD21	1.79	0.65
5:6:532:LEU:HD11	5:6:537:LEU:HB2	1.79	0.65
6:7:451:ARG:O	6:7:694:ARG:NE	2.29	0.65
9:C:96:ASP:OD2	9:C:99:SER:OG	2.02	0.65
5:6:668:THR:O	5:6:669:SER:OG	2.15	0.64
2:3:676:ILE:O	2:3:680:VAL:HG13	1.97	0.64
3:4:904:ASP:OD1	3:4:905:VAL:N	2.31	0.63
14:X:66:ASP:CG	14:X:74:VAL:HB	2.19	0.63
6:7:689:LEU:O	6:7:693:ILE:HD12	1.99	0.63
11:E:485:ASP:OD1	11:E:486:ASP:N	2.32	0.63
3:4:943:LYS:NZ	5:6:810:GLU:OE2	2.29	0.63
14:X:180:ILE:HD11	14:X:262:VAL:HG22	1.81	0.63
11:E:7:GLN:N	11:E:7:GLN:OE1	2.32	0.63
4:5:211:CYS:SG	4:5:212:LEU:N	2.72	0.62
2:3:439:GLY:N	2:3:482:ASP:OD1	2.33	0.62
3:4:725:ASP:OD2	3:4:816:GLN:NE2	2.32	0.62
5:6:198:GLU:OE1	5:6:201:ARG:NH2	2.32	0.62
10:D:75:GLU:O	10:D:150:LYS:NZ	2.28	0.62
3:4:515:VAL:HG11	5:6:186:LEU:HD23	1.82	0.62
5:6:520:GLU:N	5:6:520:GLU:OE1	2.32	0.62
1:2:184:GLU:OE1	1:2:184:GLU:N	2.33	0.61
3:4:515:VAL:HG11	5:6:186:LEU:CD2	2.31	0.61
6:7:228:ARG:NH1	6:7:327:ILE:O	2.34	0.61
11:E:521:HIS:CE1	11:E:565:LEU:CD1	2.84	0.61
8:B:104:TYR:OH	8:B:111:ARG:NH2	2.33	0.60
2:3:112:SER:O	2:3:116:VAL:HG12	2.01	0.60
10:D:230:ILE:HG21	10:D:282:ILE:HD13	1.83	0.60
1:2:705:ARG:NH2	1:2:754:GLU:OE1	2.34	0.60
1:2:573:ALA:N	1:2:616:ASP:OD1	2.35	0.60
6:7:437:VAL:HG21	6:7:702:LEU:HD21	1.83	0.60
14:X:71:ARG:NH1	14:X:73:ASP:OD2	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:617:GLN:OE1	4:5:617:GLN:N	2.34	0.59
4:5:348:MET:CE	9:C:163:SER:OG	2.51	0.59
3:4:515:VAL:HG13	5:6:186:LEU:HD23	1.85	0.59
11:E:612:ILE:O	11:E:616:THR:OG1	2.17	0.59
2:3:668:ILE:HG22	2:3:668:ILE:O	2.03	0.59
14:X:597:SER:O	14:X:601:VAL:HG23	2.02	0.58
3:4:604:ARG:NH1	14:X:359:ARG:O	2.36	0.58
7:A:173:GLU:HG2	7:A:182:ASN:HB2	1.85	0.58
11:E:281:ASP:OD2	11:E:406:ARG:NH2	2.36	0.58
11:E:155:GLN:OE1	11:E:155:GLN:N	2.37	0.58
10:D:125:PRO:O	10:D:129:MET:HG2	2.04	0.58
14:X:603:GLU:OE1	14:X:699:ARG:NH1	2.37	0.58
14:X:511:ILE:HG21	14:X:563:ARG:HH12	1.64	0.58
11:E:579:TYR:CE2	11:E:637:LEU:HD22	2.39	0.58
3:4:755:THR:HG21	3:4:765:LEU:HD21	1.86	0.57
14:X:62:PHE:CD1	14:X:66:ASP:OD2	2.57	0.57
2:3:544:ASP:OD2	2:3:707:ARG:NH2	2.37	0.57
4:5:370:LEU:HD12	4:5:666:LEU:HD11	1.85	0.57
3:4:873:LEU:HD12	3:4:873:LEU:O	2.05	0.56
5:6:703:ARG:NE	5:6:708:GLY:O	2.38	0.56
11:E:102:GLU:N	11:E:102:GLU:OE1	2.39	0.56
5:6:192:VAL:HG22	14:X:422:GLN:HE22	1.71	0.56
2:3:486:ILE:O	2:3:490:MET:HG3	2.06	0.56
4:5:354:GLU:O	4:5:358:LEU:HD23	2.05	0.56
5:6:831:ILE:HG22	5:6:833:PRO:HD3	1.88	0.56
6:7:152:ARG:NH2	14:X:372:THR:OG1	2.38	0.56
1:2:670:THR:HG22	1:2:671:GLU:H	1.70	0.55
11:E:286:GLN:NE2	11:E:597:THR:O	2.39	0.55
2:3:169:ARG:NH2	2:3:260:GLU:OE1	2.39	0.55
3:4:872:VAL:O	3:4:872:VAL:HG13	2.07	0.55
1:2:795:ARG:O	1:2:798:ILE:HG22	2.07	0.55
3:4:796:ASP:O	3:4:838:SER:OG	2.19	0.55
3:4:983:LEU:HD12	3:4:983:LEU:H	1.72	0.54
14:X:380:GLN:HA	14:X:383:VAL:HG22	1.89	0.54
4:5:346:VAL:HG13	4:5:348:MET:HE2	1.87	0.54
6:7:456:VAL:HG22	6:7:596:ILE:CG2	2.37	0.54
11:E:75:ASP:O	11:E:118:ARG:NH1	2.39	0.54
6:7:652:MET:SD	6:7:652:MET:N	2.80	0.54
3:4:852:VAL:HG11	3:4:1000:TYR:CZ	2.43	0.54
5:6:846:TYR:O	5:6:849:THR:OG1	2.24	0.54
14:X:542:LEU:O	14:X:546:THR:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:611:GLN:OE1	11:E:612:ILE:N	2.41	0.53
6:7:479:ARG:NE	6:7:517:ASP:O	2.42	0.53
6:7:693:ILE:HD12	6:7:693:ILE:H	1.72	0.53
3:4:381:ASN:ND2	3:4:384:THR:OG1	2.41	0.53
9:C:3:TYR:CG	9:C:3:TYR:O	2.59	0.53
14:X:171:GLU:O	14:X:172:SER:OG	2.23	0.53
14:X:238:THR:HG22	14:X:238:THR:O	2.09	0.52
2:3:217:ALA:CB	2:3:301:LEU:HD22	2.33	0.52
4:5:458:MET:HB3	12:F:40:DG:H2'	1.91	0.52
8:B:1:MET:SD	10:D:152:ASP:CB	2.98	0.52
1:2:241:SER:OG	1:2:413:ASP:OD2	2.23	0.52
14:X:729:ASP:OD1	14:X:730:ARG:N	2.42	0.52
2:3:462:MET:CE	2:3:486:ILE:HG12	2.40	0.52
3:4:370:ARG:NH2	3:4:408:ASP:OD2	2.40	0.52
11:E:622:ILE:O	11:E:622:ILE:HG22	2.10	0.52
3:4:568:ASP:OD1	3:4:568:ASP:O	2.28	0.51
9:C:56:ILE:HG13	9:C:57:VAL:HG23	1.92	0.51
6:7:455:ASN:N	6:7:595:ASP:OD2	2.39	0.51
4:5:541:ASP:OD1	4:5:541:ASP:C	2.49	0.51
4:5:52:ASN:ND2	9:C:142:LEU:O	2.43	0.51
5:6:348:THR:OG1	5:6:441:ARG:NH1	2.44	0.51
14:X:384:ASP:OD1	14:X:385:GLU:N	2.42	0.51
10:D:158:LEU:HB3	10:D:171:LEU:HD21	1.93	0.51
11:E:577:ASP:OD1	11:E:634:ARG:NE	2.44	0.51
3:4:175:GLU:HG2	3:4:340:PRO:HD2	1.93	0.51
2:3:92:LEU:N	2:3:92:LEU:HD12	2.26	0.50
5:6:347:GLN:O	5:6:347:GLN:NE2	2.44	0.50
6:7:89:GLN:OE1	6:7:102:LEU:N	2.41	0.50
4:5:40:LEU:HD12	4:5:45:ILE:HD11	1.92	0.50
5:6:624:PRO:HB2	5:6:831:ILE:HG23	1.93	0.50
3:4:472:VAL:H	3:4:491:ASN:HD21	1.57	0.50
6:7:20:GLU:OE2	6:7:99:ALA:HB1	2.12	0.50
11:E:76:ASP:OD2	11:E:117:ARG:NH2	2.44	0.50
7:A:55:LYS:NZ	7:A:58:GLN:OE1	2.41	0.50
8:B:115:LEU:HD11	8:B:148:LEU:HD21	1.94	0.49
4:5:346:VAL:HG13	4:5:348:MET:CE	2.42	0.49
2:3:462:MET:HE1	2:3:486:ILE:HG12	1.95	0.49
14:X:540:LEU:O	14:X:543:VAL:HG12	2.13	0.49
11:E:402:GLN:OE1	11:E:402:GLN:HA	2.12	0.49
8:B:55:THR:OG1	8:B:56:ASP:N	2.46	0.49
6:7:436:LEU:HD11	6:7:477:SER:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:248:VAL:O	11:E:290:ARG:NH1	2.46	0.49
3:4:716:PHE:CE1	5:6:827:ARG:HA	2.47	0.49
3:4:505:ASP:O	3:4:556:ALA:N	2.43	0.49
14:X:66:ASP:OD1	14:X:74:VAL:CB	2.39	0.49
5:6:869:LEU:HD22	5:6:884:ILE:HD11	1.95	0.49
3:4:959:THR:OG1	5:6:667:SER:OG	2.15	0.48
5:6:920:LEU:O	5:6:923:SER:OG	2.22	0.48
16:2:1001:ADP:O3A	5:6:887:ARG:NH1	2.46	0.48
1:2:534:ARG:NH1	1:2:625:GLU:OE1	2.45	0.48
6:7:203:TYR:OH	6:7:336:ASN:O	2.28	0.48
7:A:93:ARG:NH2	7:A:127:GLU:OE1	2.46	0.48
2:3:90:ASN:OD1	2:3:90:ASN:N	2.44	0.48
14:X:677:ASN:O	14:X:681:ARG:NH2	2.46	0.48
7:A:94:THR:HG23	7:A:130:TYR:CZ	2.48	0.48
14:X:511:ILE:CG2	14:X:563:ARG:CZ	2.92	0.48
3:4:852:VAL:HG11	3:4:1000:TYR:CE2	2.49	0.48
5:6:885:THR:OG1	5:6:886:VAL:N	2.47	0.48
7:A:12:GLU:OE2	7:A:15:ARG:NH2	2.47	0.48
1:2:511:ILE:HD11	1:2:683:VAL:HG22	1.96	0.47
14:X:186:VAL:HG13	14:X:198:ASP:HB3	1.96	0.47
2:3:143:ASN:O	2:3:147:VAL:HG23	2.14	0.47
5:6:731:ASP:N	5:6:731:ASP:OD1	2.42	0.47
3:4:479:ARG:O	6:7:341:ARG:NH1	2.47	0.47
3:4:882:ARG:O	3:4:886:LYS:HG3	2.13	0.47
5:6:892:MET:HG3	5:6:920:LEU:HD12	1.96	0.47
6:7:689:LEU:CD1	6:7:693:ILE:HD11	2.43	0.47
3:4:515:VAL:CG1	5:6:186:LEU:CD2	2.85	0.47
7:A:29:LEU:O	7:A:122:ASN:ND2	2.47	0.47
3:4:706:LEU:HD12	3:4:968:LEU:HD12	1.95	0.47
5:6:687:THR:OG1	5:6:688:SER:N	2.47	0.47
5:6:734:ASP:OD1	5:6:735:ILE:N	2.47	0.47
11:E:572:ILE:HD11	11:E:634:ARG:NH1	2.29	0.47
11:E:343:TYR:CE2	11:E:403:ASP:HB2	2.49	0.47
11:E:165:LEU:HD22	11:E:230:ILE:HD11	1.97	0.47
14:X:497:ASP:OD1	14:X:497:ASP:O	2.33	0.47
5:6:532:LEU:HD22	5:6:535:ARG:HB2	1.96	0.47
3:4:770:THR:OG1	3:4:771:ARG:N	2.48	0.46
3:4:869:VAL:HG11	3:4:1000:TYR:OH	2.15	0.46
1:2:783:MET:SD	4:5:570:ASN:ND2	2.88	0.46
14:X:96:GLU:OE1	14:X:181:ARG:NE	2.36	0.46
3:4:451:ASN:O	3:4:452:ASN:OD1	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:522:GLN:HG3	4:5:544:THR:HG21	1.97	0.46
11:E:125:ALA:HB1	11:E:249:ASN:O	2.16	0.46
1:2:319:ARG:NH1	1:2:425:GLU:OE1	2.46	0.46
3:4:525:ASP:OD2	14:X:391:LYS:CE	2.64	0.46
10:D:243:ASP:OD2	10:D:256:TYR:OH	2.20	0.46
14:X:505:LEU:HD11	14:X:546:THR:HG21	1.98	0.46
1:2:339:PHE:O	1:2:348:LEU:N	2.46	0.46
4:5:417:ASP:OD1	4:5:417:ASP:N	2.49	0.46
4:5:453:VAL:HB	12:F:56:DA:H4'	1.98	0.46
8:B:146:GLN:O	8:B:150:GLU:HG3	2.15	0.46
3:4:757:GLY:O	3:4:800:LYS:NZ	2.43	0.46
6:7:644:TYR:O	6:7:647:THR:OG1	2.31	0.46
6:7:653:SER:OG	6:7:654:GLU:N	2.49	0.46
1:2:307:ARG:NH1	1:2:402:LEU:O	2.49	0.46
3:4:544:ASN:OD1	5:6:530:ARG:NE	2.48	0.46
11:E:274:ILE:O	11:E:278:THR:HG22	2.16	0.46
6:7:442:LYS:HG3	6:7:449:LYS:HB3	1.98	0.45
6:7:519:GLY:O	6:7:561:THR:OG1	2.33	0.45
14:X:720:ARG:NH2	15:Y:92:ILE:CB	2.74	0.45
4:5:156:VAL:O	4:5:157:SER:OG	2.31	0.45
2:3:217:ALA:HB1	2:3:301:LEU:HD21	1.93	0.45
3:4:699:ASP:OD1	3:4:699:ASP:N	2.50	0.45
6:7:721:ARG:HB3	6:7:721:ARG:NH2	2.31	0.45
14:X:729:ASP:OD1	14:X:731:MET:N	2.45	0.45
14:X:720:ARG:CZ	15:Y:92:ILE:HD13	2.46	0.45
7:A:7:ASN:O	7:A:11:LEU:HD23	2.17	0.45
8:B:15:GLU:OE2	10:D:71:ARG:NH1	2.48	0.45
3:4:755:THR:HG21	3:4:765:LEU:CD2	2.47	0.45
4:5:472:ALA:O	4:5:517:THR:HG22	2.16	0.45
1:2:781:MET:HG3	1:2:834:LEU:HD22	1.98	0.45
1:2:785:LYS:NZ	1:2:835:ASP:OD1	2.48	0.45
4:5:101:ILE:O	8:B:154:ILE:HD11	2.16	0.45
4:5:353:GLU:O	4:5:354:GLU:C	2.54	0.45
7:A:191:VAL:HG21	7:A:196:VAL:HG11	1.99	0.45
15:Y:126:ARG:O	15:Y:130:VAL:HG23	2.17	0.45
14:X:718:LEU:O	14:X:722:MET:HG3	2.17	0.44
10:D:97:LEU:O	10:D:97:LEU:HD23	2.16	0.44
4:5:346:VAL:HG23	9:C:167:LEU:CD1	2.46	0.44
2:3:156:SER:OG	2:3:325:THR:CG2	2.66	0.44
10:D:147:ARG:NE	10:D:179:GLU:OE2	2.44	0.44
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:89:LEU:HB2	14:X:90:PRO:HD3	1.98	0.44
15:Y:61:SER:OG	15:Y:62:ASP:N	2.49	0.44
6:7:230:ILE:HD11	6:7:241:VAL:HG22	1.98	0.44
7:A:170:ASP:OD1	7:A:171:ALA:N	2.51	0.44
1:2:670:THR:HG22	1:2:671:GLU:N	2.32	0.44
6:7:476:ILE:HD12	6:7:638:MET:SD	2.58	0.44
7:A:173:GLU:OE2	11:E:73:GLN:O	2.36	0.44
8:B:57:ASP:OD1	8:B:57:ASP:N	2.39	0.44
3:4:772:ASP:O	3:4:776:LYS:N	2.51	0.44
4:5:687:SER:OG	4:5:688:THR:N	2.50	0.44
5:6:278:VAL:HG13	5:6:285:LEU:HD23	2.00	0.44
11:E:333:SER:OG	11:E:336:ASP:OD1	2.30	0.44
14:X:287:LEU:HD11	14:X:474:GLU:OE1	2.18	0.44
14:X:605:TYR:HB3	14:X:611:LEU:HD11	2.00	0.43
14:X:667:MET:SD	14:X:700:VAL:HG22	2.58	0.43
6:7:450:ILE:HD12	6:7:450:ILE:H	1.82	0.43
14:X:67:ASP:OD1	14:X:67:ASP:N	2.50	0.43
5:6:401:ASP:O	5:6:404:ARG:NH1	2.51	0.43
6:7:440:VAL:HG11	6:7:452:GLY:CA	2.48	0.43
3:4:931:LYS:NZ	5:6:818:SER:OG	2.50	0.43
6:7:422:ILE:CD1	6:7:469:LEU:HD11	2.48	0.43
14:X:540:LEU:HD12	14:X:601:VAL:HG21	2.01	0.43
3:4:456:ASP:OD1	3:4:458:ASP:N	2.52	0.43
6:7:629:ASP:OD1	6:7:630:PHE:N	2.51	0.43
2:3:235:ASP:OD1	2:3:236:THR:N	2.45	0.43
11:E:624:ASN:OD1	11:E:626:GLU:N	2.49	0.43
14:X:380:GLN:HB3	14:X:387:ILE:HG21	2.00	0.43
14:X:489:ARG:CZ	14:X:496:ALA:HB1	2.47	0.43
1:2:356:ASN:OD1	1:2:450:ILE:CD1	2.63	0.43
16:2:1001:ADP:O2A	5:6:747:GLN:NE2	2.49	0.43
2:3:652:THR:HG22	2:3:654:PRO:HD2	2.00	0.43
5:6:721:ASP:OD1	5:6:722:ASN:N	2.51	0.43
6:7:13:ASP:OD1	6:7:13:ASP:N	2.47	0.43
9:C:55:ALA:HB2	9:C:74:LEU:HD13	2.01	0.43
14:X:723:LEU:O	14:X:735:ARG:NH1	2.51	0.43
8:B:17:GLN:O	8:B:21:GLU:HG3	2.18	0.42
2:3:698:THR:HG22	2:3:699:ALA:N	2.34	0.42
5:6:905:VAL:HG12	5:6:907:GLU:H	1.85	0.42
14:X:84:LEU:CD1	14:X:132:LEU:HD21	2.48	0.42
3:4:964:SER:O	3:4:968:LEU:HD23	2.20	0.42
1:2:296:ARG:NH2	1:2:454:ASN:O	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:434:VAL:O	11:E:434:VAL:HG13	2.19	0.42
3:4:863:LEU:HD21	3:4:1000:TYR:OH	2.19	0.42
3:4:873:LEU:CD1	3:4:875:LYS:HB3	2.50	0.42
6:7:455:ASN:OD1	6:7:563:ILE:N	2.43	0.42
11:E:87:GLY:O	11:E:92:LEU:HD21	2.20	0.42
3:4:785:LEU:HD13	3:4:812:VAL:HG21	2.02	0.42
5:6:242:ILE:HD12	5:6:354:ILE:HG23	2.02	0.42
6:7:20:GLU:OE2	6:7:100:ASP:N	2.53	0.42
8:B:93:LEU:HD13	8:B:134:PHE:HE1	1.85	0.42
14:X:547:LYS:NZ	14:X:608:ASP:OD2	2.42	0.42
4:5:420:THR:O	4:5:421:ALA:HB3	2.20	0.42
14:X:734:SER:O	14:X:738:VAL:HG23	2.20	0.42
4:5:41:ASP:OD2	9:C:194:LYS:HG2	2.20	0.42
5:6:518:THR:OG1	5:6:519:THR:N	2.49	0.42
7:A:23:SER:OG	7:A:26:ASP:O	2.36	0.42
3:4:852:VAL:HG21	3:4:1000:TYR:OH	2.20	0.41
8:B:156:VAL:HG11	8:B:181:LEU:HD11	2.01	0.41
11:E:568:VAL:HG22	11:E:605:PHE:HE2	1.85	0.41
2:3:400:ARG:NH2	2:3:402:ASP:O	2.52	0.41
11:E:632:ILE:HD11	11:E:640:PHE:CD2	2.55	0.41
3:4:512:LYS:HG3	3:4:519:THR:HG22	2.03	0.41
14:X:720:ARG:HD3	15:Y:92:ILE:HD12	2.02	0.41
2:3:307:ASN:OD1	2:3:308:GLN:N	2.54	0.41
3:4:852:VAL:HG21	3:4:1000:TYR:CZ	2.55	0.41
6:7:661:VAL:O	6:7:665:ILE:HG12	2.21	0.41
7:A:80:GLU:HG2	10:D:206:LEU:HD11	2.02	0.41
10:D:131:THR:O	10:D:135:ARG:HG3	2.20	0.41
11:E:579:TYR:CD2	11:E:637:LEU:HD22	2.55	0.41
1:2:247:ARG:O	1:2:251:GLU:HG2	2.21	0.41
1:2:547:THR:HB	1:2:683:VAL:HG11	2.02	0.41
4:5:348:MET:HE1	9:C:163:SER:CB	2.50	0.41
3:4:525:ASP:OD2	14:X:391:LYS:HE3	2.21	0.41
3:4:872:VAL:O	3:4:872:VAL:CG1	2.68	0.41
5:6:742:HIS:ND1	5:6:794:ILE:HD11	2.35	0.41
7:A:146:LEU:HD12	7:A:151:LEU:HD11	2.03	0.41
3:4:961:GLN:O	3:4:965:MET:HG3	2.20	0.41
6:7:66:MET:O	6:7:70:VAL:HG23	2.20	0.41
10:D:89:ASN:O	10:D:93:MET:HG2	2.21	0.41
15:Y:57:GLU:OE1	15:Y:58:LYS:N	2.54	0.41
6:7:521:CYS:N	6:7:562:SER:O	2.51	0.41
6:7:607:ASP:O	6:7:611:LYS:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:704:VAL:HG21	5:6:859:ARG:HD3	2.03	0.41
3:4:497:LEU:CD1	3:4:564:GLN:HB2	2.51	0.41
3:4:879:LYS:O	3:4:883:GLU:HG2	2.21	0.41
4:5:346:VAL:HG23	9:C:167:LEU:HD12	2.03	0.41
9:C:44:LEU:CD1	9:C:46:LEU:HD21	2.51	0.41
14:X:536:PHE:O	14:X:540:LEU:HD23	2.21	0.41
5:6:471:ARG:O	5:6:474:SER:OG	2.39	0.41
6:7:612:LEU:O	6:7:616:VAL:HG23	2.21	0.41
13:G:10:DA:H2"	13:G:11:DC:C6	2.56	0.41
2:3:354:SER:OG	2:3:659:TYR:CZ	2.72	0.40
11:E:233:TYR:O	11:E:236:VAL:HG12	2.21	0.40
11:E:502:LEU:O	11:E:506:ILE:HD13	2.21	0.40
3:4:355:THR:HG22	3:4:435:ILE:HG23	2.03	0.40
3:4:586:GLU:OE1	3:4:586:GLU:N	2.46	0.40
6:7:585:ASN:OD1	6:7:585:ASN:N	2.54	0.40
3:4:175:GLU:HG2	3:4:340:PRO:CD	2.51	0.40
14:X:129:LEU:HD22	14:X:182:LEU:HD13	2.04	0.40
14:X:156:LEU:HD12	14:X:156:LEU:HA	1.97	0.40
3:4:873:LEU:HD12	3:4:873:LEU:C	2.42	0.40
5:6:190:LYS:O	14:X:422:GLN:OE1	2.38	0.40
7:A:198:ARG:O	7:A:202:GLN:HG3	2.22	0.40
11:E:259:LEU:O	11:E:263:GLY:N	2.54	0.40
14:X:487:LEU:HD22	14:X:545:ARG:HD2	2.04	0.40
3:4:472:VAL:HG11	3:4:489:LEU:HD23	2.03	0.40
5:6:869:LEU:HD22	5:6:884:ILE:CD1	2.51	0.40
9:C:3:TYR:O	9:C:3:TYR:CD2	2.75	0.40
10:D:97:LEU:HD23	10:D:97:LEU:C	2.42	0.40
14:X:378:GLY:O	14:X:382:LEU:HD12	2.21	0.40
14:X:409:VAL:HG21	14:X:420:ASN:ND2	2.35	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	2	660/868 (76%)	645 (98%)	15 (2%)	0	100	100
2	3	608/971 (63%)	594 (98%)	14 (2%)	0	100	100
3	4	606/933 (65%)	598 (99%)	8 (1%)	0	100	100
4	5	582/775 (75%)	562 (97%)	20 (3%)	0	100	100
5	6	622/1017 (61%)	609 (98%)	12 (2%)	1 (0%)	44	71
6	7	605/845 (72%)	594 (98%)	11 (2%)	0	100	100
7	A	192/208 (92%)	190 (99%)	2 (1%)	0	100	100
8	B	185/213 (87%)	183 (99%)	2 (1%)	0	100	100
9	C	167/217 (77%)	166 (99%)	1 (1%)	0	100	100
10	D	214/294 (73%)	210 (98%)	4 (2%)	0	100	100
11	E	560/650 (86%)	548 (98%)	12 (2%)	0	100	100
14	X	699/1238 (56%)	682 (98%)	15 (2%)	2 (0%)	37	66
15	Y	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	5790/8321 (70%)	5667 (98%)	120 (2%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	707	GLY
14	X	498	ILE
14	X	495	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	582/770 (76%)	577 (99%)	5 (1%)	75	85
2	3	533/835 (64%)	531 (100%)	2 (0%)	89	93
3	4	553/848 (65%)	546 (99%)	7 (1%)	65	79
4	5	534/688 (78%)	529 (99%)	5 (1%)	75	85
5	6	552/886 (62%)	548 (99%)	4 (1%)	81	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	542/753 (72%)	532 (98%)	10 (2%)	54	74
7	A	180/193 (93%)	180 (100%)	0	100	100
8	B	178/198 (90%)	178 (100%)	0	100	100
9	C	156/192 (81%)	156 (100%)	0	100	100
10	D	213/279 (76%)	211 (99%)	2 (1%)	75	85
11	E	505/586 (86%)	503 (100%)	2 (0%)	89	93
14	X	639/1125 (57%)	630 (99%)	9 (1%)	62	78
15	Y	85/85 (100%)	84 (99%)	1 (1%)	67	80
All	All	5252/7438 (71%)	5205 (99%)	47 (1%)	74	85

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	187	SER
1	2	238	ASN
1	2	271	PHE
1	2	362	SER
1	2	621	HIS
2	3	51	ASN
2	3	110	PHE
3	4	410	ARG
3	4	419	GLU
3	4	683	TYR
3	4	716	PHE
3	4	814	GLU
3	4	983	LEU
3	4	994	ARG
4	5	90	PHE
4	5	170	SER
4	5	343	TRP
4	5	541	ASP
4	5	678	ASP
5	6	183	SER
5	6	212	SER
5	6	742	HIS
5	6	761	LEU
6	7	20	GLU
6	7	334	HIS
6	7	474	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	7	573	ARG
6	7	598	PHE
6	7	608	ASP
6	7	620	HIS
6	7	621	MET
6	7	644	TYR
6	7	719	LEU
10	D	80	PRO
10	D	83	LEU
11	E	554	GLU
11	E	640	PHE
14	X	115	PHE
14	X	256	SER
14	X	293	PHE
14	X	431	GLU
14	X	498	ILE
14	X	604	GLN
14	X	713	PHE
14	X	726	ASP
14	X	770	ASN
15	Y	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	E	521	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
16	ADP	2	1001	17	24,29,29	0.89	0	29,45,45	1.28	2 (6%)
19	ATP	6	1201	17	28,33,33	0.63	0	34,52,52	1.18	2 (5%)
19	ATP	3	1001	17	28,33,33	0.63	0	34,52,52	1.18	2 (5%)
19	ATP	7	1001	17	28,33,33	0.62	0	34,52,52	1.20	2 (5%)
19	ATP	4	1101	17	28,33,33	0.61	0	34,52,52	0.93	3 (8%)
19	ATP	5	1001	17	28,33,33	0.63	0	34,52,52	0.93	2 (5%)

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
16	ADP	2	1001	17	-	3/12/32/32	0/3/3/3
19	ATP	6	1201	17	-	8/18/38/38	0/3/3/3
19	ATP	3	1001	17	-	8/18/38/38	0/3/3/3
19	ATP	7	1001	17	-	5/18/38/38	0/3/3/3
19	ATP	4	1101	17	-	1/18/38/38	0/3/3/3
19	ATP	5	1001	17	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	7	1001	ATP	C4'-O4'-C1'	-4.51	105.79	109.92
19	3	1001	ATP	C4'-O4'-C1'	-4.37	105.92	109.92
19	6	1201	ATP	C4'-O4'-C1'	-4.30	105.98	109.92
16	2	1001	ADP	N3-C2-N1	-4.16	123.03	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	2	1001	ADP	C4-C5-N7	-2.52	106.67	109.34
19	6	1201	ATP	C5-C6-N6	2.33	123.85	120.31
19	4	1101	ATP	C5-C6-N6	2.31	123.83	120.31
19	7	1001	ATP	C5-C6-N6	2.31	123.83	120.31
19	3	1001	ATP	C5-C6-N6	2.30	123.81	120.31
19	5	1001	ATP	C5-C6-N6	2.29	123.81	120.31
19	4	1101	ATP	O2'-C2'-C3'	-2.11	105.05	111.82
19	4	1101	ATP	O4'-C1'-N9	-2.10	105.97	108.75
19	5	1001	ATP	O4'-C1'-N9	-2.05	106.03	108.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	2	1001	ADP	C5'-O5'-PA-O1A
16	2	1001	ADP	C5'-O5'-PA-O3A
19	3	1001	ATP	PB-O3B-PG-O2G
19	3	1001	ATP	C5'-O5'-PA-O3A
19	3	1001	ATP	O4'-C4'-C5'-O5'
19	6	1201	ATP	C5'-O5'-PA-O1A
19	6	1201	ATP	C5'-O5'-PA-O2A
19	6	1201	ATP	C5'-O5'-PA-O3A
19	7	1001	ATP	PB-O3A-PA-O5'
19	7	1001	ATP	C5'-O5'-PA-O2A
19	7	1001	ATP	C5'-O5'-PA-O3A
19	3	1001	ATP	C3'-C4'-C5'-O5'
19	7	1001	ATP	O4'-C4'-C5'-O5'
19	6	1201	ATP	PG-O3B-PB-O1B
19	6	1201	ATP	PB-O3A-PA-O5'
19	5	1001	ATP	O4'-C4'-C5'-O5'
19	4	1101	ATP	O4'-C4'-C5'-O5'
19	7	1001	ATP	C4'-C5'-O5'-PA
16	2	1001	ADP	C5'-O5'-PA-O2A
19	3	1001	ATP	C5'-O5'-PA-O1A
19	6	1201	ATP	C4'-C5'-O5'-PA
19	3	1001	ATP	PB-O3B-PG-O1G
19	3	1001	ATP	PG-O3B-PB-O1B
19	3	1001	ATP	PG-O3B-PB-O2B
19	6	1201	ATP	PG-O3B-PB-O2B
19	6	1201	ATP	PB-O3A-PA-O1A
19	5	1001	ATP	PG-O3B-PB-O2B
19	5	1001	ATP	PA-O3A-PB-O2B

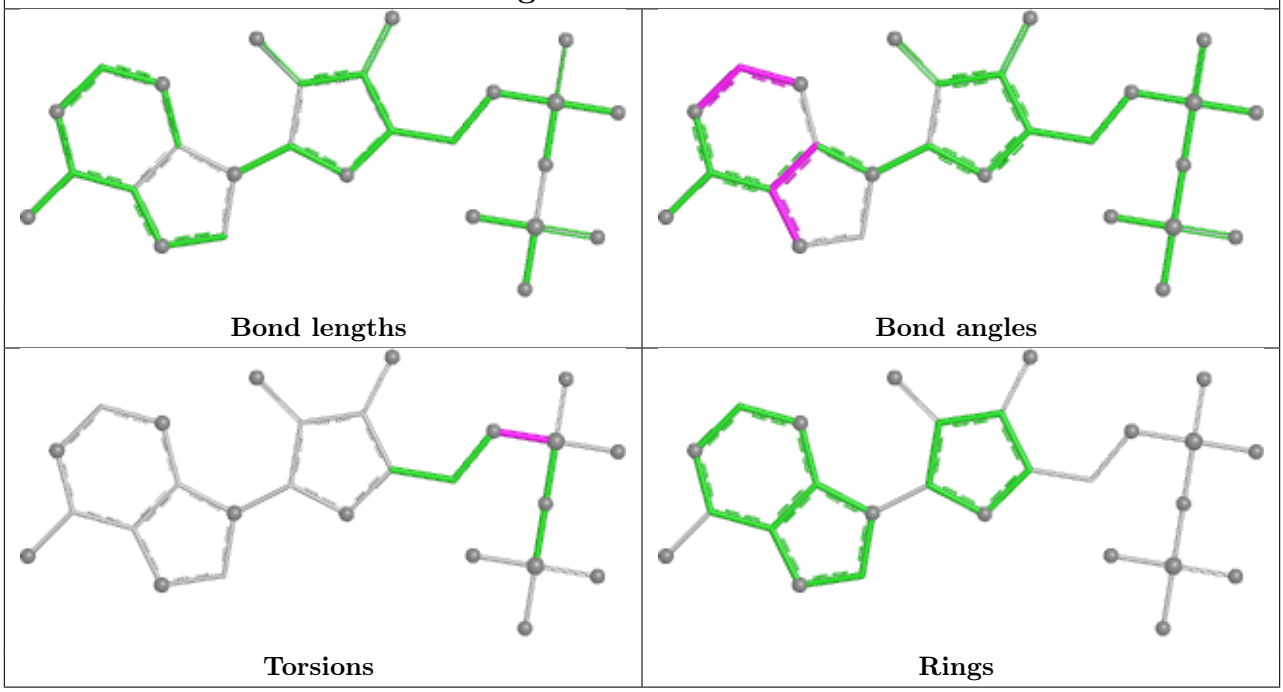
There are no ring outliers.

2 monomers are involved in 3 short contacts:

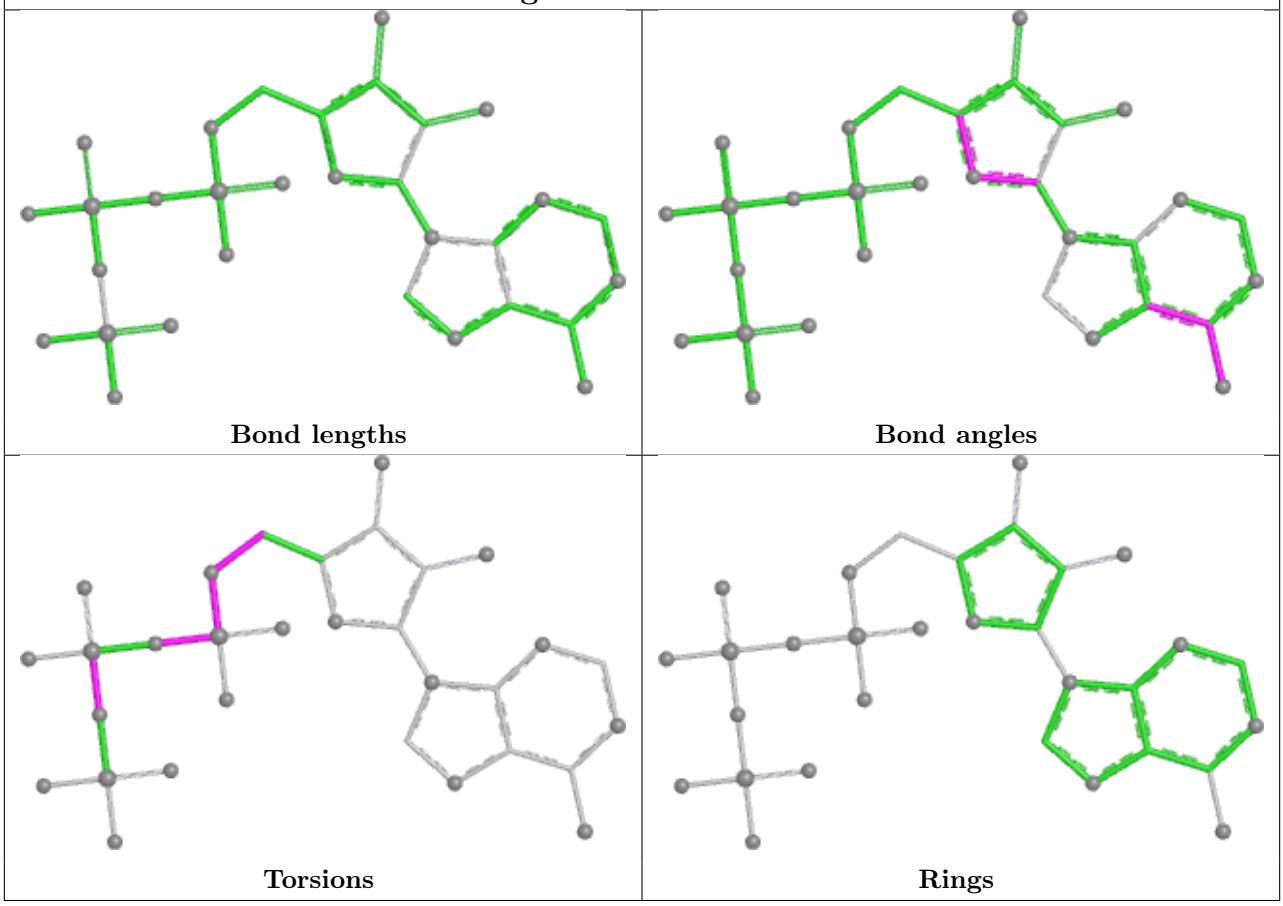
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	1001	ADP	2	0
19	3	1001	ATP	1	0

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

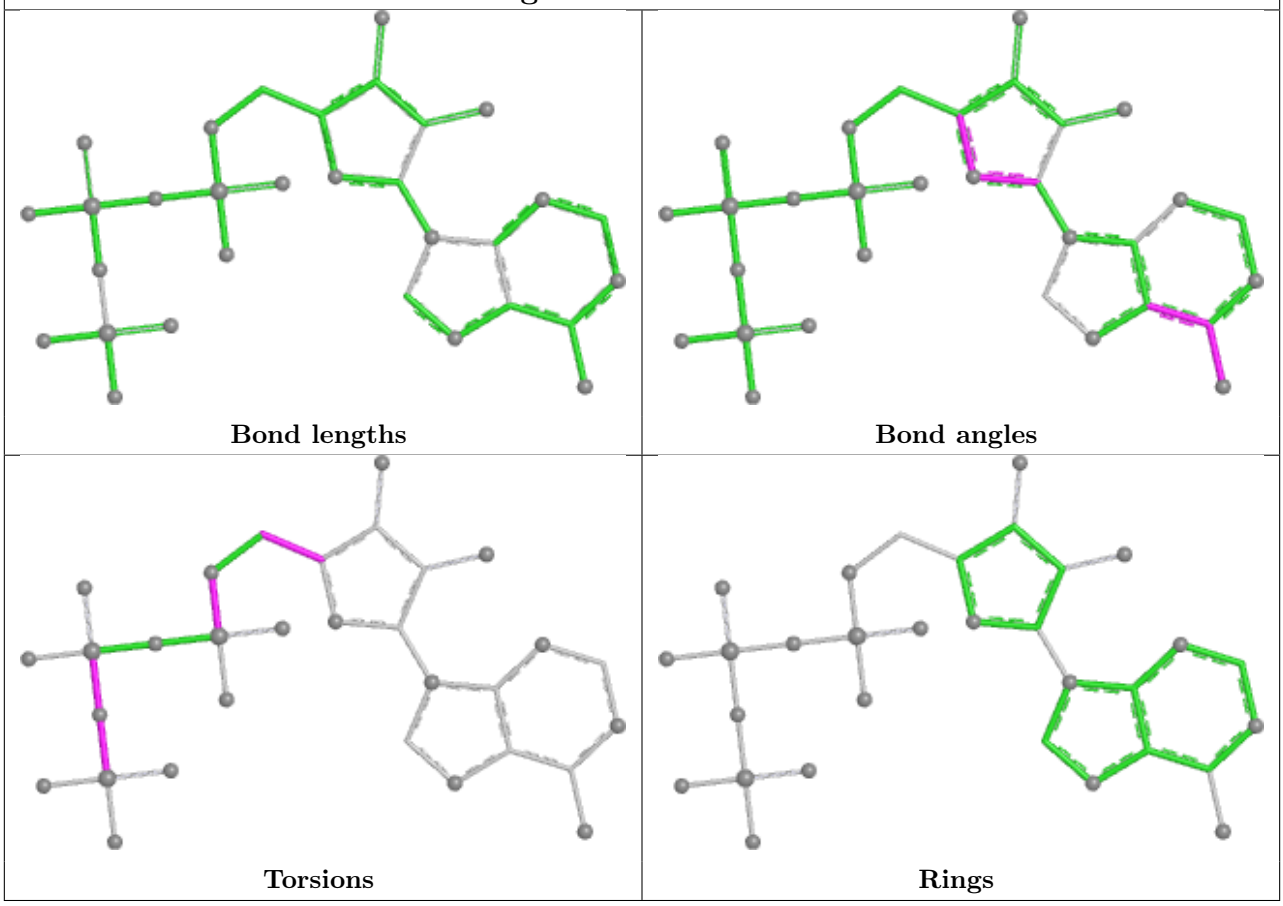
Ligand ADP 2 1001



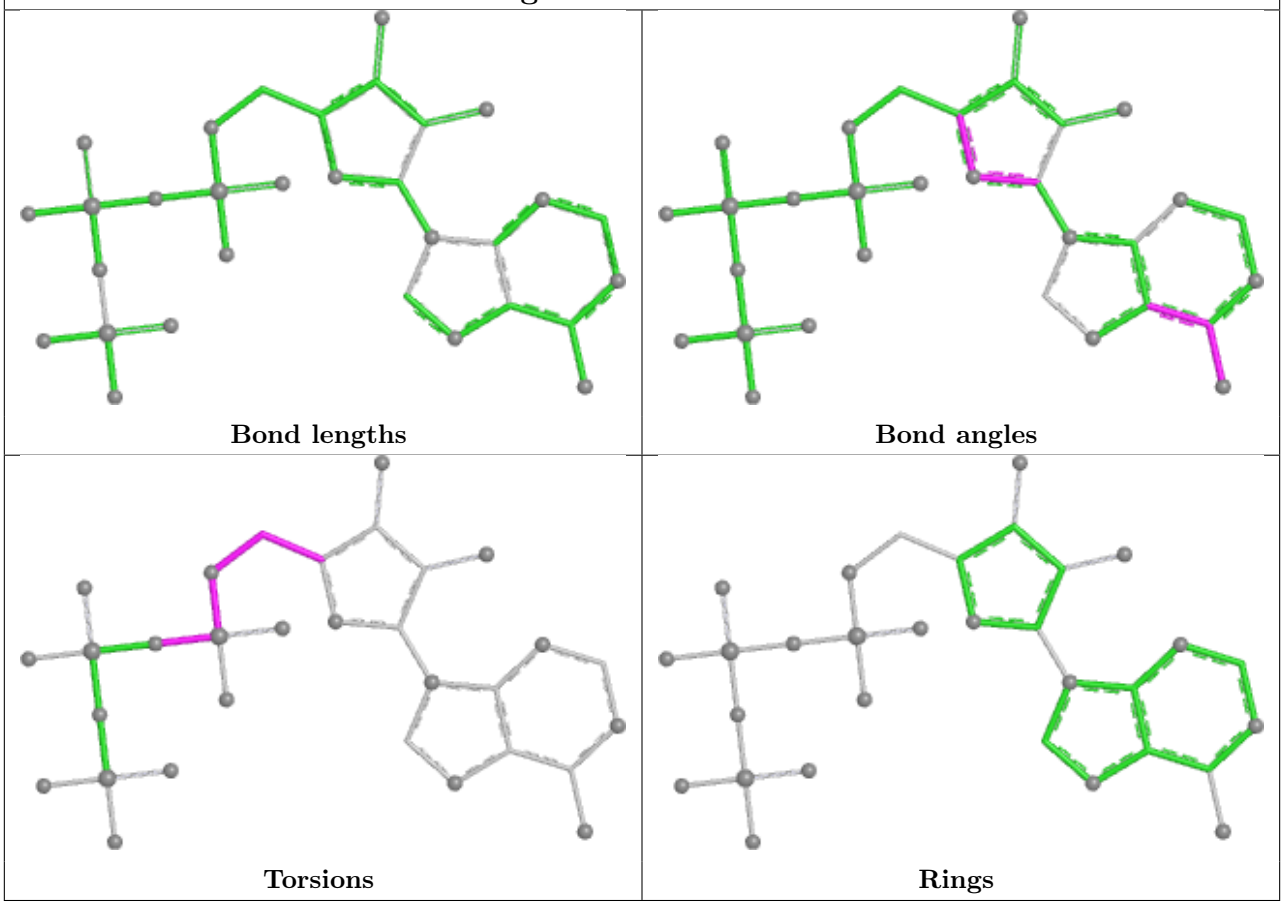
Ligand ATP 6 1201



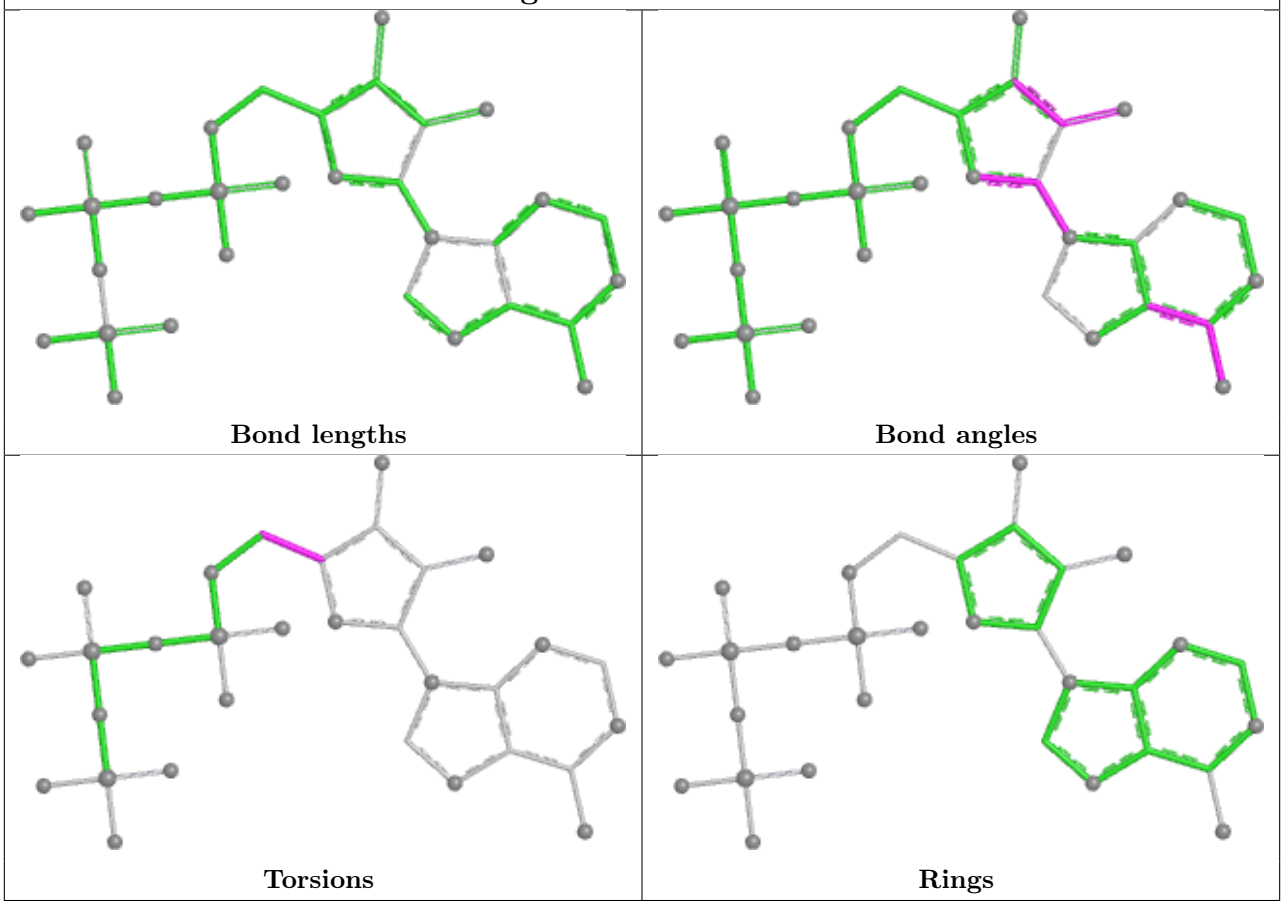
Ligand ATP 3 1001



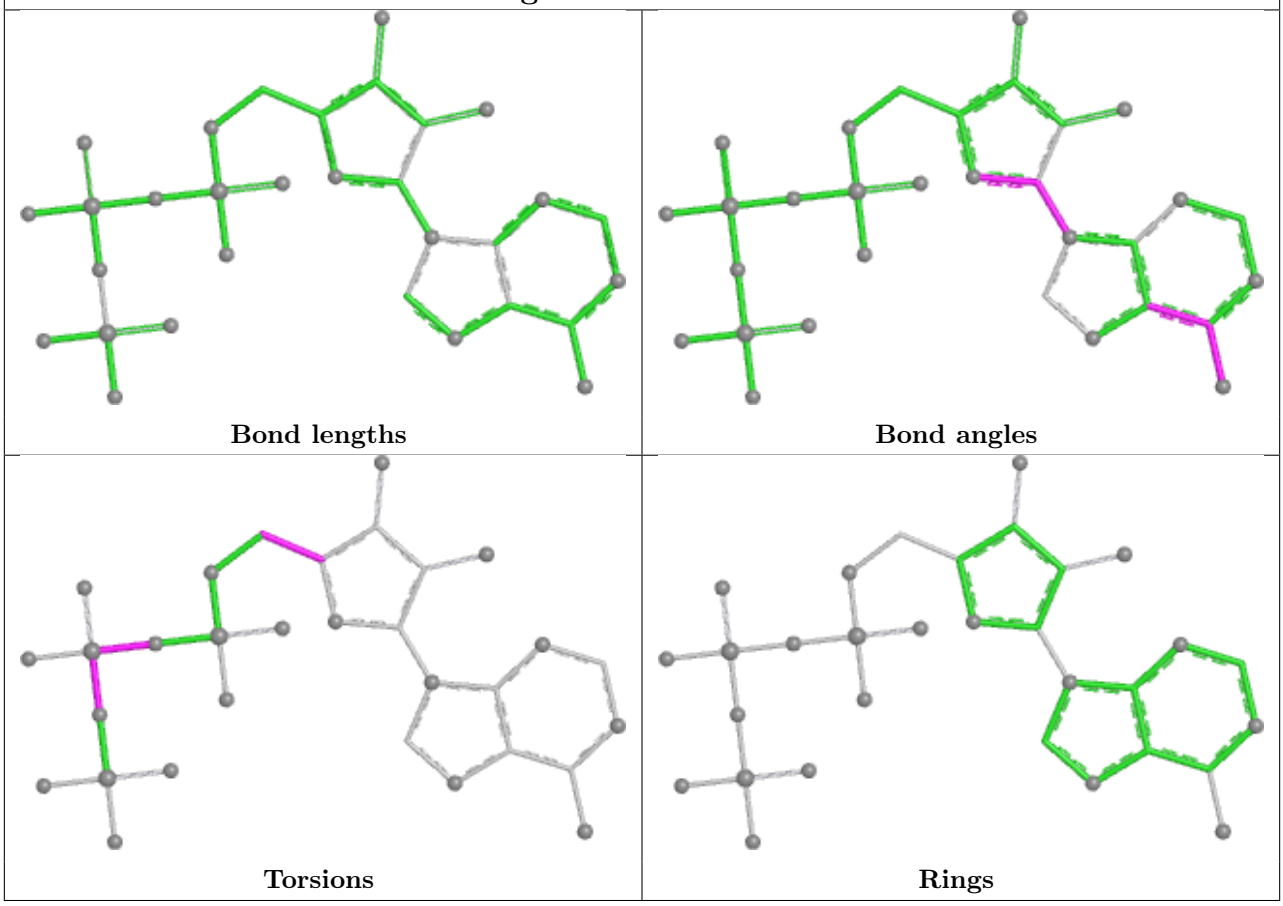
Ligand ATP 7 1001



Ligand ATP 4 1101



Ligand ATP 5 1001



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-47470. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.