



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:22 PM UTC

PDB ID : 5XO7 / pdb_00005xo7
Title : Crystal structure of a novel ZEN lactonase mutant with ligand a
Authors : Zheng, Y.Y.; Liu, W.T.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2017-05-27
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

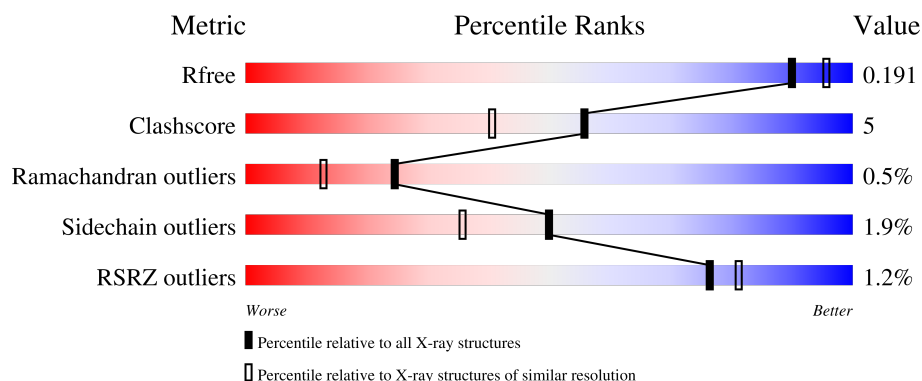
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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.



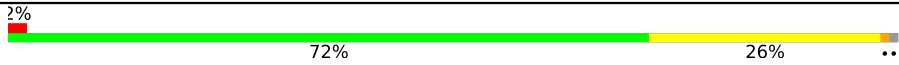
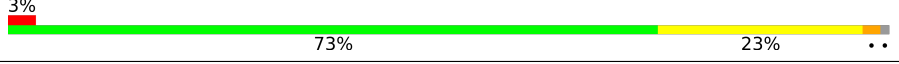
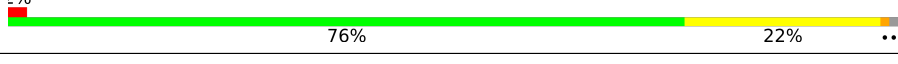
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	266	<div> <div>%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	C	266	<div> <div>%</div> <div>72%</div> <div>22%</div> <div>5%</div> <div>.</div> </div>
1	D	266	<div> <div>%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	E	266	<div> <div>68%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	266	 2% 72% 26% ..
1	G	266	 3% 73% 23% ..
1	H	266	 2% 76% 22% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

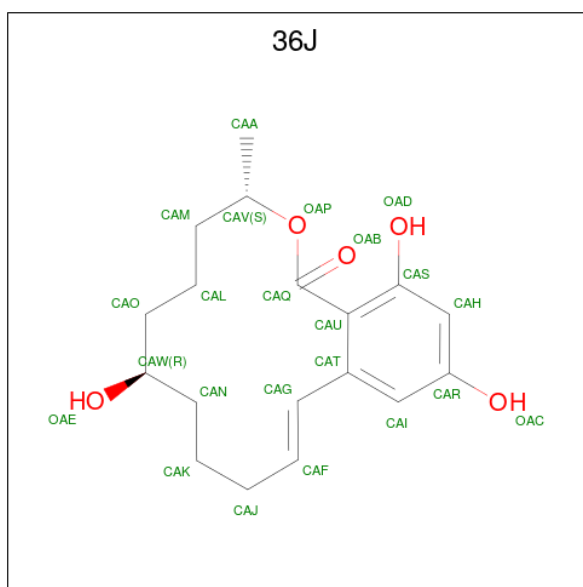
- Molecule 1 is a protein called lactonase for protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	B	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	C	263	Total	C	N	O	S	0	1	0
			2061	1310	347	395	9			
1	D	262	Total	C	N	O	S	0	0	0
			2045	1300	345	391	9			
1	E	263	Total	C	N	O	S	0	0	0
			2054	1306	347	392	9			
1	F	264	Total	C	N	O	S	0	0	0
			2060	1309	348	394	9			
1	G	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	H	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
B	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
C	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
D	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
E	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
F	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
G	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
H	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1

- Molecule 2 is (3S,7R,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (CCD ID: 36J) (formula: C₁₈H₂₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		
2	C	1	Total	C	O	0	0
			23	18	5		
2	D	1	Total	C	O	0	0
			23	18	5		
2	E	1	Total	C	O	0	0
			23	18	5		
2	F	1	Total	C	O	0	0
			23	18	5		
2	G	1	Total	C	O	0	0
			23	18	5		
2	H	1	Total	C	O	0	0
			23	18	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	354	Total	O	0	0
			354	354		
3	B	345	Total	O	0	0
			345	345		
3	C	274	Total	O	0	0
			274	274		
3	D	249	Total	O	0	0
			249	249		

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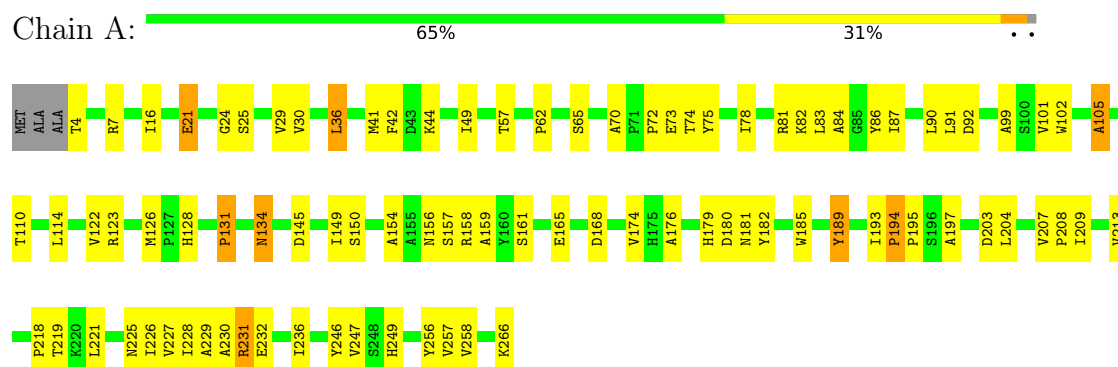
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	328	Total 328	O 328	0	0
3	F	277	Total 277	O 277	0	0
3	G	184	Total 184	O 184	0	0
3	H	199	Total 199	O 199	0	0

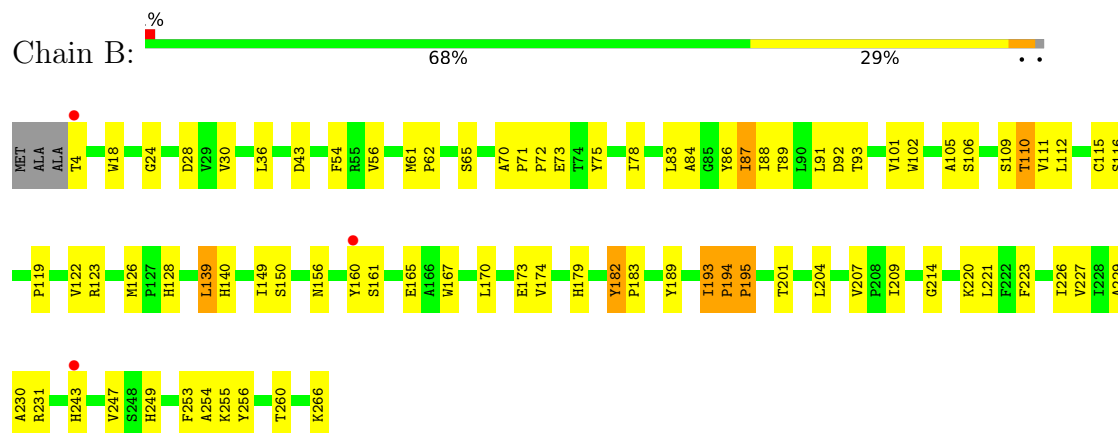
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

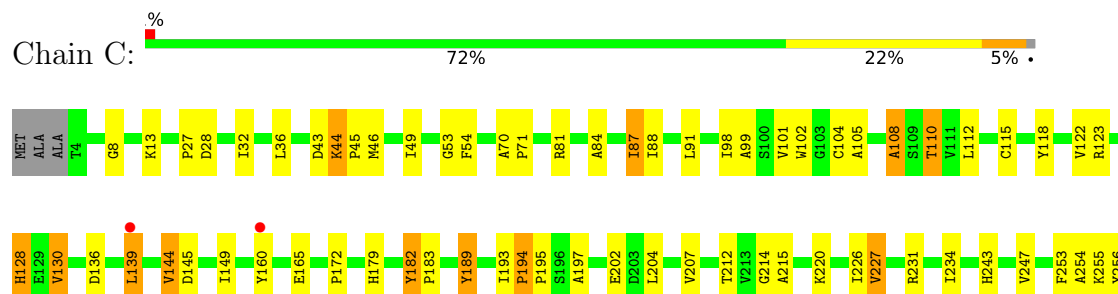
- Molecule 1: lactonase for protein



- Molecule 1: lactonase for protein

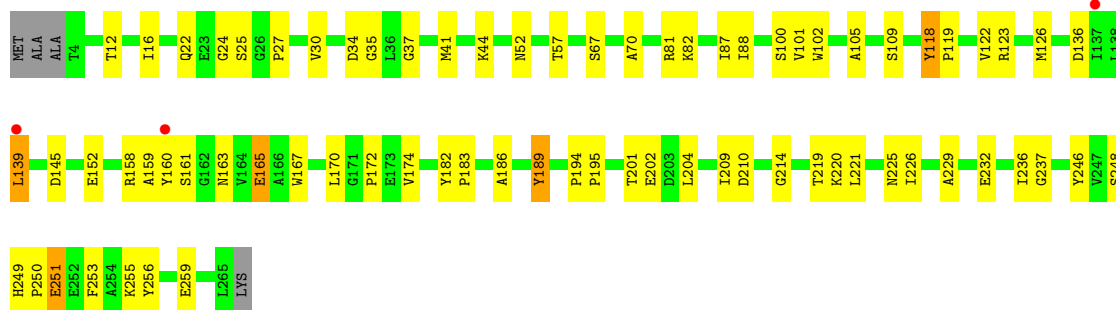


- Molecule 1: lactonase for protein





- Molecule 1: lactonase for protein



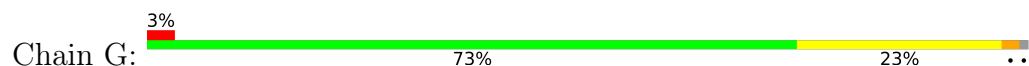
- Molecule 1: lactonase for protein

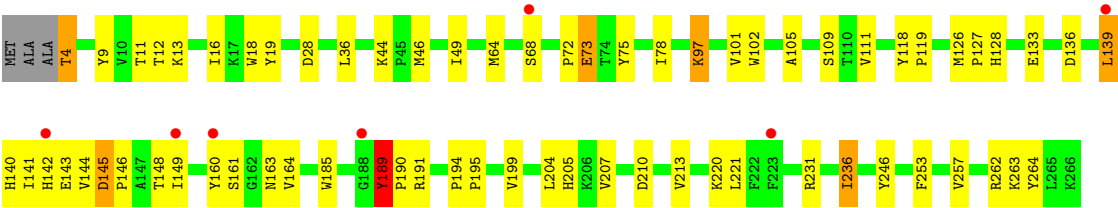


- Molecule 1: lactonase for protein

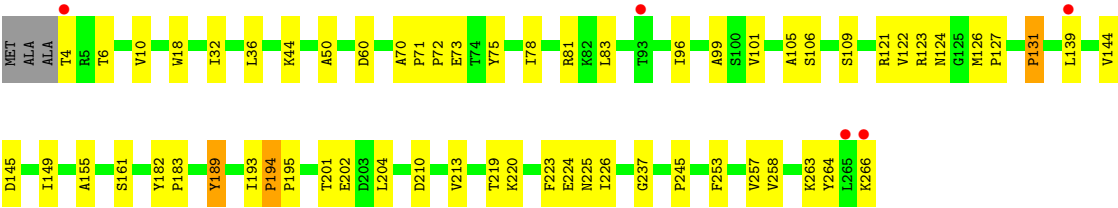
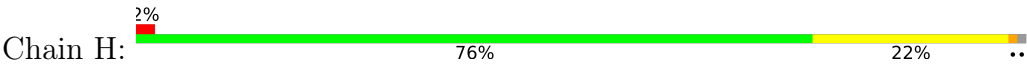


- Molecule 1: lactonase for protein





● Molecule 1: lactonase for protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.46Å 95.16Å 101.44Å 90.20° 92.13° 91.60°	Depositor
Resolution (Å)	24.93 – 1.88 24.93 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.93-1.88) 97.4 (24.93-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.156 , 0.195 (Not available) , 0.191	Depositor DCC
R_{free} test set	2038 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l 0.012 for -h,k,-l 0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18834	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 36J

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	1.94	72/2114 (3.4%)	1.14	14/2886 (0.5%)
1	B	1.92	60/2114 (2.8%)	1.09	10/2886 (0.3%)
1	C	1.84	48/2123 (2.3%)	1.13	20/2898 (0.7%)
1	D	1.84	44/2104 (2.1%)	1.10	14/2875 (0.5%)
1	E	1.86	58/2113 (2.7%)	1.11	11/2884 (0.4%)
1	F	1.86	52/2119 (2.5%)	1.10	11/2893 (0.4%)
1	G	1.68	18/2114 (0.9%)	1.10	13/2886 (0.5%)
1	H	1.75	35/2114 (1.7%)	1.09	10/2886 (0.3%)
All	All	1.84	387/16915 (2.3%)	1.11	103/23094 (0.4%)

All (387) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	VAL	C-O	-9.58	1.16	1.24
1	B	105	ALA	C-O	-9.10	1.16	1.24
1	A	44	LYS	C-O	-9.02	1.16	1.24
1	A	207	VAL	C-O	-8.18	1.17	1.24
1	G	207	VAL	C-O	-8.05	1.18	1.24
1	D	105	ALA	C-O	-7.97	1.17	1.24
1	B	193	ILE	C-O	-7.84	1.18	1.24
1	D	22	GLN	C-N	-7.77	1.24	1.33
1	F	207	VAL	C-O	-7.50	1.18	1.24
1	B	122	VAL	C-O	-7.47	1.16	1.24
1	C	105	ALA	C-O	-7.31	1.17	1.24
1	H	44	LYS	C-O	-7.22	1.18	1.24
1	C	44	LYS	C-O	-7.20	1.18	1.24
1	A	231	ARG	C-N	-7.03	1.24	1.33
1	C	226	ILE	C-O	-6.96	1.16	1.24
1	F	230	ALA	C-O	-6.95	1.16	1.24
1	A	62	PRO	C-O	-6.88	1.15	1.23
1	B	260	THR	C-O	-6.86	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	VAL	C-O	-6.83	1.17	1.23
1	A	209	ILE	C-O	-6.79	1.17	1.24
1	E	105	ALA	C-O	-6.79	1.18	1.24
1	E	176	ALA	C-O	-6.75	1.16	1.24
1	H	258	VAL	C-N	-6.73	1.25	1.33
1	D	67	SER	C-O	-6.65	1.15	1.24
1	H	213	VAL	C-O	-6.64	1.17	1.23
1	E	168	ASP	C-O	-6.63	1.16	1.24
1	A	193	ILE	C-O	-6.62	1.19	1.24
1	D	41	MET	C-O	-6.59	1.15	1.24
1	E	57	THR	C-O	-6.58	1.15	1.23
1	A	70	ALA	C-O	-6.55	1.18	1.24
1	A	126	MET	C-O	-6.55	1.16	1.24
1	A	257	VAL	C-O	-6.54	1.16	1.24
1	F	126	MET	C-O	-6.52	1.16	1.24
1	E	207	VAL	C-O	-6.51	1.16	1.24
1	D	161	SER	C-O	-6.50	1.15	1.24
1	C	122	VAL	C-O	-6.49	1.17	1.24
1	B	89	THR	C-O	-6.46	1.16	1.24
1	A	105	ALA	C-O	-6.45	1.18	1.24
1	E	182	TYR	C-O	-6.45	1.18	1.24
1	G	128	HIS	C-O	-6.42	1.16	1.24
1	B	65	SER	C-O	-6.42	1.18	1.24
1	F	227	VAL	C-O	-6.40	1.16	1.24
1	F	256	TYR	C-O	-6.38	1.16	1.24
1	B	149	ILE	C-O	-6.38	1.17	1.24
1	B	86	TYR	C-O	-6.35	1.16	1.24
1	C	87	ILE	C-O	-6.35	1.16	1.24
1	H	96	ILE	C-O	-6.34	1.17	1.24
1	B	71	PRO	C-O	-6.32	1.19	1.25
1	B	70	ALA	C-O	-6.30	1.17	1.24
1	E	170	LEU	C-O	-6.30	1.15	1.24
1	F	228	ILE	C-O	-6.27	1.17	1.24
1	F	105	ALA	C-O	-6.25	1.18	1.24
1	E	256	TYR	C-O	-6.24	1.16	1.24
1	F	71	PRO	C-O	-6.21	1.19	1.24
1	B	87	ILE	C-O	-6.21	1.16	1.24
1	A	161	SER	C-O	-6.20	1.16	1.24
1	C	128	HIS	C-O	-6.20	1.17	1.24
1	G	257	VAL	C-O	-6.18	1.17	1.24
1	A	229	ALA	C-O	-6.17	1.17	1.24
1	A	156	ASN	C-O	-6.15	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202[A]	GLU	CA-C	6.14	1.61	1.52
1	C	202[B]	GLU	CA-C	6.14	1.61	1.52
1	D	172	PRO	C-O	-6.12	1.16	1.24
1	A	249	HIS	C-O	-6.12	1.17	1.24
1	H	71	PRO	C-O	-6.12	1.19	1.25
1	E	87	ILE	C-O	-6.10	1.17	1.24
1	B	123	ARG	C-O	-6.09	1.17	1.24
1	A	36	LEU	C-O	-6.09	1.16	1.24
1	D	256	TYR	C-O	-6.09	1.17	1.24
1	F	70	ALA	C-O	-6.08	1.18	1.24
1	D	44	LYS	C-O	-6.07	1.19	1.24
1	E	227	VAL	C-O	-6.06	1.17	1.24
1	A	74	THR	C-O	-6.05	1.15	1.24
1	B	179	HIS	C-O	-6.03	1.17	1.24
1	B	226	ILE	C-O	-6.03	1.17	1.24
1	F	194	PRO	C-O	-6.02	1.17	1.24
1	E	154	ALA	C-O	-6.01	1.17	1.24
1	G	220	LYS	C-O	-6.01	1.16	1.24
1	G	213	VAL	C-O	-6.00	1.17	1.23
1	F	81	ARG	C-O	-5.98	1.17	1.24
1	H	194	PRO	C-O	-5.98	1.17	1.24
1	A	179	HIS	C-O	-5.96	1.17	1.24
1	A	158	ARG	C-O	-5.94	1.17	1.24
1	E	46	MET	C-O	-5.94	1.17	1.24
1	F	203	ASP	C-O	-5.94	1.16	1.24
1	B	201	THR	C-O	-5.94	1.17	1.24
1	C	54	PHE	C-O	-5.94	1.16	1.23
1	D	16	ILE	C-O	-5.93	1.17	1.24
1	E	62	PRO	C-O	-5.92	1.16	1.23
1	F	115	CYS	C-O	-5.91	1.16	1.24
1	D	165	GLU	C-O	-5.91	1.17	1.24
1	C	115	CYS	C-O	-5.90	1.17	1.24
1	F	86	TYR	C-O	-5.90	1.17	1.24
1	A	149	ILE	C-O	-5.88	1.17	1.24
1	B	91	LEU	C-O	-5.88	1.17	1.24
1	B	170	LEU	C-O	-5.87	1.16	1.24
1	D	226	ILE	C-O	-5.87	1.17	1.24
1	F	220	LYS	C-O	-5.86	1.17	1.24
1	E	158	ARG	C-O	-5.85	1.17	1.24
1	A	228	ILE	C-O	-5.84	1.17	1.24
1	B	223	PHE	C-O	-5.83	1.17	1.24
1	C	112	LEU	C-O	-5.83	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	THR	C-O	-5.82	1.17	1.24
1	B	84	ALA	C-O	-5.82	1.17	1.24
1	A	189	TYR	C-O	-5.82	1.16	1.24
1	C	227	VAL	C-O	-5.80	1.17	1.24
1	A	122	VAL	C-O	-5.78	1.17	1.24
1	E	122	VAL	C-O	-5.77	1.17	1.24
1	A	258	VAL	C-O	-5.76	1.17	1.24
1	E	153	MET	C-O	-5.76	1.16	1.24
1	E	59	PHE	C-O	-5.75	1.16	1.23
1	B	253	PHE	C-O	-5.75	1.17	1.24
1	A	176	ALA	C-O	-5.74	1.17	1.24
1	C	49	ILE	C-O	-5.73	1.17	1.24
1	F	122	VAL	C-O	-5.73	1.18	1.24
1	D	249	HIS	C-O	-5.72	1.17	1.24
1	G	46	MET	C-O	-5.72	1.17	1.24
1	B	229	ALA	C-O	-5.71	1.17	1.24
1	A	194	PRO	C-O	-5.70	1.18	1.24
1	D	186	ALA	C-O	-5.70	1.17	1.24
1	F	257	VAL	C-O	-5.70	1.17	1.24
1	E	71	PRO	C-O	-5.69	1.20	1.24
1	E	131	PRO	C-O	-5.69	1.18	1.23
1	B	54	PHE	C-O	-5.69	1.16	1.23
1	E	56	VAL	C-O	-5.68	1.17	1.24
1	B	247	VAL	C-O	-5.68	1.17	1.23
1	C	254	ALA	C-O	-5.67	1.17	1.24
1	D	52	ASN	C-O	-5.67	1.16	1.24
1	H	83	LEU	C-O	-5.67	1.17	1.24
1	B	220	LYS	C-O	-5.67	1.17	1.24
1	G	111	VAL	C-O	-5.67	1.17	1.24
1	D	122	VAL	C-O	-5.67	1.18	1.24
1	D	210	ASP	C-O	-5.66	1.17	1.24
1	B	83	LEU	C-O	-5.66	1.17	1.24
1	C	220	LYS	C-O	-5.65	1.17	1.24
1	D	87	ILE	C-O	-5.65	1.17	1.24
1	C	70	ALA	C-O	-5.65	1.18	1.24
1	A	73	GLU	C-O	-5.65	1.17	1.24
1	G	105	ALA	C-O	-5.65	1.19	1.24
1	B	111	VAL	C-O	-5.63	1.17	1.24
1	G	161	SER	C-O	-5.63	1.17	1.24
1	A	110	THR	C-O	-5.63	1.17	1.24
1	C	182	TYR	C-O	-5.62	1.19	1.24
1	D	27	PRO	C-O	-5.62	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ILE	C-O	-5.62	1.17	1.24
1	E	226	ILE	C-O	-5.61	1.17	1.24
1	D	30	VAL	C-O	-5.61	1.18	1.24
1	E	152	GLU	C-O	-5.61	1.17	1.24
1	E	185	TRP	C-O	-5.60	1.17	1.24
1	E	249	HIS	C-O	-5.60	1.17	1.24
1	B	109	SER	C-O	-5.60	1.17	1.24
1	E	47	SER	C-O	-5.60	1.17	1.24
1	F	236	ILE	C-O	-5.60	1.18	1.24
1	B	30	VAL	C-O	-5.59	1.18	1.24
1	A	42	PHE	C-O	-5.59	1.16	1.24
1	B	182	TYR	C-O	-5.59	1.19	1.24
1	F	123	ARG	C-O	-5.59	1.17	1.24
1	E	213	VAL	C-O	-5.59	1.18	1.23
1	F	141	ILE	C-O	-5.59	1.17	1.24
1	B	230	ALA	C-O	-5.58	1.17	1.24
1	A	41	MET	C-O	-5.58	1.16	1.24
1	F	128	HIS	C-O	-5.58	1.17	1.24
1	C	247	VAL	C-O	-5.58	1.17	1.23
1	E	123	ARG	C-O	-5.57	1.17	1.24
1	D	159	ALA	C-O	-5.57	1.17	1.24
1	F	213	VAL	C-O	-5.57	1.18	1.23
1	C	234	ILE	C-O	-5.57	1.17	1.24
1	A	49	ILE	C-O	-5.56	1.17	1.24
1	D	70	ALA	C-O	-5.56	1.18	1.24
1	E	98	ILE	C-O	-5.56	1.18	1.24
1	A	174	VAL	C-O	-5.56	1.17	1.24
1	A	123	ARG	C-O	-5.55	1.17	1.24
1	B	110	THR	C-O	-5.55	1.17	1.24
1	F	221	LEU	C-O	-5.55	1.17	1.24
1	F	130	VAL	C-O	-5.54	1.17	1.24
1	F	234	ILE	C-O	-5.54	1.17	1.24
1	C	123	ARG	C-O	-5.54	1.17	1.24
1	F	29	VAL	C-O	-5.54	1.18	1.24
1	D	35	GLY	C-O	-5.54	1.17	1.23
1	D	109	SER	C-O	-5.54	1.17	1.24
1	F	258	VAL	C-O	-5.54	1.17	1.24
1	A	128	HIS	C-O	-5.53	1.17	1.23
1	E	16	ILE	C-O	-5.53	1.17	1.24
1	B	174	VAL	C-O	-5.53	1.17	1.24
1	E	101	VAL	C-O	-5.52	1.18	1.24
1	B	116	SER	C-O	-5.52	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	ASP	C-O	-5.51	1.17	1.24
1	C	253	PHE	C-O	-5.51	1.17	1.24
1	C	84	ALA	C-O	-5.51	1.17	1.24
1	G	126	MET	C-O	-5.51	1.17	1.24
1	F	193	ILE	C-O	-5.50	1.20	1.24
1	G	210	ASP	C-O	-5.50	1.17	1.23
1	H	109	SER	C-O	-5.50	1.17	1.24
1	D	101	VAL	C-O	-5.50	1.18	1.24
1	B	150	SER	C-O	-5.49	1.17	1.24
1	B	56	VAL	C-O	-5.49	1.17	1.24
1	H	106	SER	C-O	-5.49	1.17	1.24
1	B	126	MET	C-O	-5.48	1.18	1.24
1	A	92	ASP	C-O	-5.48	1.17	1.24
1	F	114	LEU	C-O	-5.48	1.17	1.24
1	H	126	MET	C-O	-5.48	1.18	1.24
1	B	209	ILE	C-O	-5.47	1.18	1.24
1	B	195	PRO	C-O	-5.47	1.17	1.24
1	A	208	PRO	C-O	-5.47	1.17	1.23
1	E	220	LYS	C-O	-5.46	1.17	1.24
1	C	215	ALA	C-O	-5.46	1.17	1.24
1	H	32	ILE	N-CA	-5.46	1.42	1.46
1	F	229	ALA	C-O	-5.45	1.17	1.24
1	B	92	ASP	C-O	-5.45	1.17	1.24
1	E	35	GLY	C-O	-5.45	1.16	1.23
1	E	132	THR	C-O	-5.44	1.17	1.24
1	D	57	THR	C-O	-5.44	1.17	1.23
1	B	73	GLU	C-O	-5.44	1.17	1.24
1	H	257	VAL	C-O	-5.43	1.17	1.24
1	E	223	PHE	C-O	-5.42	1.17	1.24
1	B	115	CYS	C-O	-5.42	1.17	1.24
1	C	172	PRO	C-O	-5.41	1.17	1.24
1	B	214	GLY	C-O	-5.41	1.18	1.23
1	D	225	ASN	C-O	-5.40	1.17	1.24
1	C	8	GLY	C-O	-5.40	1.18	1.23
1	D	220	LYS	C-O	-5.40	1.17	1.24
1	H	245	PRO	C-O	-5.40	1.17	1.24
1	G	49	ILE	C-O	-5.39	1.17	1.24
1	C	88	ILE	C-O	-5.39	1.17	1.24
1	D	158	ARG	C-O	-5.39	1.17	1.24
1	A	225	ASN	C-O	-5.39	1.17	1.24
1	B	112	LEU	C-O	-5.38	1.17	1.24
1	F	111	VAL	C-O	-5.37	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	155	ALA	C-O	-5.36	1.18	1.24
1	A	86	TYR	C-O	-5.36	1.17	1.24
1	A	114	LEU	C-O	-5.36	1.17	1.24
1	D	229	ALA	C-O	-5.35	1.17	1.24
1	B	167	TRP	C-O	-5.35	1.18	1.24
1	F	176	ALA	C-O	-5.34	1.17	1.24
1	A	87	ILE	C-O	-5.34	1.17	1.24
1	D	123	ARG	C-O	-5.34	1.17	1.24
1	F	184	ARG	C-O	-5.33	1.17	1.24
1	G	127	PRO	C-O	-5.33	1.18	1.23
1	H	220	LYS	C-O	-5.33	1.17	1.24
1	G	221	LEU	C-O	-5.32	1.18	1.24
1	H	253	PHE	C-O	-5.32	1.18	1.24
1	A	81	ARG	C-O	-5.32	1.17	1.24
1	F	254	ALA	C-O	-5.32	1.17	1.24
1	A	24	GLY	C-O	-5.31	1.18	1.24
1	E	90	LEU	C-O	-5.31	1.17	1.24
1	A	91	LEU	C-O	-5.31	1.18	1.24
1	B	249	HIS	C-O	-5.31	1.18	1.24
1	F	44	LYS	C-O	-5.31	1.20	1.24
1	B	88	ILE	C-O	-5.31	1.18	1.24
1	E	147	ALA	C-O	-5.30	1.18	1.24
1	E	201	THR	C-O	-5.30	1.18	1.24
1	F	96	ILE	C-O	-5.30	1.18	1.24
1	B	256	TYR	C-O	-5.30	1.18	1.24
1	C	136	ASP	C-O	-5.29	1.17	1.24
1	D	22	GLN	C-O	-5.29	1.17	1.23
1	E	194	PRO	C-O	-5.29	1.18	1.24
1	H	237	GLY	C-O	-5.29	1.17	1.23
1	D	250	PRO	C-O	-5.29	1.17	1.24
1	E	70	ALA	C-O	-5.29	1.18	1.24
1	A	134	ASN	C-O	-5.29	1.17	1.23
1	F	113	ALA	C-O	-5.29	1.18	1.24
1	F	88	ILE	C-O	-5.28	1.18	1.24
1	F	101	VAL	C-O	-5.28	1.18	1.24
1	C	214	GLY	C-O	-5.27	1.19	1.24
1	C	255	LYS	C-O	-5.27	1.18	1.24
1	C	108	ALA	C-O	-5.27	1.17	1.24
1	H	224	GLU	C-O	-5.27	1.17	1.24
1	C	207	VAL	C-O	-5.26	1.17	1.24
1	D	237	GLY	C-O	-5.26	1.17	1.23
1	C	193	ILE	C-O	-5.26	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	SER	C-O	-5.26	1.17	1.24
1	B	62	PRO	C-O	-5.26	1.17	1.24
1	G	44	LYS	C-O	-5.25	1.19	1.24
1	H	225	ASN	C-O	-5.25	1.18	1.24
1	C	194	PRO	C-O	-5.25	1.18	1.24
1	C	260	THR	C-O	-5.25	1.18	1.24
1	C	262	ARG	C-O	-5.24	1.17	1.24
1	F	108	ALA	C-O	-5.24	1.17	1.24
1	D	167	TRP	C-O	-5.24	1.18	1.24
1	H	131	PRO	C-O	-5.24	1.17	1.23
1	A	157	SER	C-O	-5.23	1.18	1.24
1	E	167	TRP	C-O	-5.23	1.18	1.24
1	D	152	GLU	C-O	-5.23	1.18	1.24
1	F	56	VAL	C-O	-5.23	1.18	1.24
1	A	236	ILE	C-O	-5.22	1.18	1.24
1	B	254	ALA	C-O	-5.22	1.18	1.24
1	F	79	THR	C-O	-5.22	1.17	1.23
1	F	263	LYS	C-O	-5.21	1.17	1.24
1	A	197	ALA	C-O	-5.21	1.17	1.24
1	H	122	VAL	C-O	-5.21	1.18	1.24
1	A	83	LEU	C-O	-5.21	1.18	1.24
1	C	81	ARG	C-O	-5.20	1.18	1.24
1	D	209	ILE	C-O	-5.20	1.18	1.24
1	E	236	ILE	C-O	-5.20	1.18	1.24
1	E	237	GLY	C-O	-5.20	1.18	1.23
1	C	202[A]	GLU	C-O	-5.20	1.17	1.24
1	C	202[B]	GLU	C-O	-5.20	1.17	1.24
1	A	180	ASP	C-O	-5.19	1.17	1.24
1	H	127	PRO	C-O	-5.19	1.18	1.23
1	D	248	SER	C-O	-5.19	1.18	1.24
1	A	185	TRP	C-O	-5.18	1.18	1.24
1	A	181	ASN	C-O	-5.18	1.18	1.24
1	E	49	ILE	C-O	-5.18	1.18	1.24
1	H	223	PHE	C-O	-5.18	1.17	1.24
1	B	18	TRP	C-O	-5.18	1.17	1.23
1	A	256	TYR	C-O	-5.17	1.18	1.24
1	H	123	ARG	C-O	-5.17	1.17	1.24
1	A	159	ALA	C-O	-5.17	1.17	1.24
1	A	29	VAL	C-O	-5.17	1.18	1.24
1	B	61	MET	C-O	-5.16	1.17	1.23
1	B	128	HIS	C-O	-5.16	1.18	1.24
1	E	215	ALA	C-O	-5.16	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	ALA	C-O	-5.16	1.18	1.24
1	C	91	LEU	C-O	-5.16	1.18	1.24
1	D	25	SER	C-O	-5.15	1.17	1.23
1	F	210	ASP	C-O	-5.15	1.18	1.24
1	B	106	SER	C-O	-5.15	1.17	1.24
1	H	226	ILE	C-O	-5.15	1.18	1.24
1	D	170	LEU	C-O	-5.15	1.17	1.24
1	A	16	ILE	C-O	-5.14	1.18	1.24
1	E	163	ASN	C-O	-5.14	1.17	1.24
1	F	27	PRO	C-O	-5.14	1.17	1.23
1	F	189	TYR	C-O	-5.13	1.17	1.24
1	C	98	ILE	C-O	-5.13	1.18	1.24
1	H	10	VAL	C-O	-5.13	1.18	1.23
1	B	255	LYS	C-O	-5.12	1.18	1.24
1	C	256	TYR	C-O	-5.12	1.18	1.24
1	E	99	ALA	C-O	-5.12	1.17	1.23
1	A	203	ASP	C-O	-5.12	1.17	1.24
1	D	174	VAL	C-O	-5.12	1.18	1.24
1	E	257	VAL	C-O	-5.12	1.18	1.24
1	A	150	SER	C-O	-5.12	1.18	1.24
1	H	81	ARG	C-O	-5.12	1.18	1.24
1	A	101	VAL	C-O	-5.11	1.18	1.24
1	C	43	ASP	C-O	-5.11	1.18	1.24
1	F	214	GLY	C-O	-5.11	1.17	1.23
1	A	57	THR	C-O	-5.11	1.17	1.23
1	E	184	ARG	C-O	-5.11	1.18	1.24
1	A	82	LYS	C-O	-5.11	1.18	1.24
1	E	255	LYS	C-O	-5.11	1.18	1.24
1	H	70	ALA	C-O	-5.11	1.18	1.24
1	E	165	GLU	C-O	-5.10	1.18	1.24
1	A	182	TYR	C-O	-5.10	1.19	1.24
1	B	24	GLY	C-O	-5.10	1.18	1.24
1	A	247	VAL	C-O	-5.10	1.18	1.23
1	H	193	ILE	C-O	-5.09	1.18	1.24
1	F	84	ALA	C-O	-5.09	1.18	1.24
1	G	253	PHE	C-O	-5.09	1.18	1.24
1	E	247	VAL	C-O	-5.09	1.18	1.23
1	H	155	ALA	C-O	-5.09	1.18	1.24
1	B	173	GLU	C-O	-5.08	1.18	1.24
1	H	201	THR	C-O	-5.08	1.18	1.24
1	C	118	TYR	C-O	-5.08	1.17	1.24
1	E	6	THR	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	99	ALA	C-O	-5.07	1.17	1.23
1	C	179	HIS	C-O	-5.07	1.18	1.24
1	E	96	ILE	C-O	-5.07	1.18	1.24
1	F	62	PRO	C-O	-5.07	1.16	1.23
1	H	210	ASP	C-O	-5.07	1.18	1.24
1	D	81	ARG	C-O	-5.06	1.18	1.24
1	A	230	ALA	C-O	-5.06	1.18	1.24
1	C	130	VAL	C-O	-5.06	1.18	1.24
1	E	250	PRO	C-O	-5.06	1.18	1.24
1	A	84	ALA	C-O	-5.05	1.18	1.24
1	H	50	ALA	C-O	-5.04	1.18	1.24
1	A	131	PRO	C-O	-5.04	1.18	1.23
1	A	226	ILE	C-O	-5.04	1.18	1.24
1	F	215	ALA	C-O	-5.04	1.18	1.24
1	C	110	THR	C-O	-5.04	1.18	1.24
1	A	30	VAL	C-O	-5.04	1.18	1.24
1	B	43	ASP	C-O	-5.03	1.18	1.24
1	E	149	ILE	C-O	-5.03	1.18	1.24
1	E	181	ASN	C-O	-5.03	1.18	1.24
1	F	37	GLY	C-N	-5.03	1.25	1.33
1	H	124	ASN	C-O	-5.03	1.17	1.23
1	G	109	SER	C-O	-5.02	1.18	1.24
1	G	236	ILE	C-O	-5.02	1.19	1.24
1	A	90	LEU	C-O	-5.02	1.18	1.24
1	A	65	SER	C-O	-5.01	1.17	1.24
1	B	119	PRO	C-O	-5.01	1.18	1.24
1	H	60	ASP	C-O	-5.01	1.17	1.23
1	D	214	GLY	C-O	-5.01	1.18	1.23
1	D	126	MET	C-O	-5.01	1.18	1.24
1	E	225	ASN	C-O	-5.01	1.18	1.24
1	C	257	VAL	C-O	-5.00	1.18	1.24
1	C	197	ALA	C-O	-5.00	1.17	1.24
1	D	253	PHE	C-O	-5.00	1.18	1.24

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	204	LEU	N-CA-C	8.58	123.98	113.17
1	A	204	LEU	N-CA-C	8.26	123.58	113.17
1	C	204	LEU	N-CA-C	8.19	123.48	113.17
1	B	204	LEU	N-CA-C	7.82	123.78	113.30
1	D	24	GLY	N-CA-C	7.32	121.19	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	145	ASP	CA-C-N	7.22	126.75	119.24
1	F	145	ASP	C-N-CA	7.22	126.75	119.24
1	E	23	GLU	O-C-N	7.18	131.67	123.48
1	E	204	LEU	N-CA-C	7.15	121.72	112.92
1	B	101	VAL	N-CA-C	7.08	118.09	107.75
1	C	101	VAL	N-CA-C	7.08	118.02	108.11
1	H	204	LEU	N-CA-C	6.96	122.62	113.30
1	F	37	GLY	CA-C-N	6.88	132.41	122.85
1	F	37	GLY	C-N-CA	6.88	132.41	122.85
1	G	145	ASP	CA-C-N	6.76	128.29	119.84
1	G	145	ASP	C-N-CA	6.76	128.29	119.84
1	A	145	ASP	CA-C-N	6.56	126.80	119.32
1	A	145	ASP	C-N-CA	6.56	126.80	119.32
1	D	22	GLN	CA-C-N	6.52	132.72	121.64
1	D	22	GLN	C-N-CA	6.52	132.72	121.64
1	A	123	ARG	O-C-N	6.47	129.02	122.03
1	E	123	ARG	O-C-N	6.44	128.99	122.03
1	D	204	LEU	N-CA-C	6.38	121.20	113.17
1	G	101	VAL	N-CA-C	6.20	116.79	108.11
1	B	122	VAL	N-CA-C	6.14	116.71	107.75
1	H	145	ASP	CA-C-N	6.12	127.49	119.84
1	H	145	ASP	C-N-CA	6.12	127.49	119.84
1	D	101	VAL	N-CA-C	6.11	116.66	108.11
1	G	189	TYR	N-CA-C	6.07	123.22	109.81
1	D	189	TYR	N-CA-C	6.05	123.18	109.81
1	G	161	SER	N-CA-C	6.01	117.91	111.36
1	G	204	LEU	N-CA-C	5.99	120.72	113.17
1	E	78	ILE	N-CA-C	5.97	117.28	109.58
1	A	101	VAL	N-CA-C	5.97	116.46	108.11
1	C	122	VAL	N-CA-C	5.96	116.45	107.75
1	H	78	ILE	N-CA-C	5.95	117.26	109.58
1	D	145	ASP	CA-C-N	5.92	125.40	119.24
1	D	145	ASP	C-N-CA	5.92	125.40	119.24
1	C	145	ASP	CA-C-N	5.91	125.39	119.24
1	C	145	ASP	C-N-CA	5.91	125.39	119.24
1	C	32	ILE	CA-C-N	-5.89	114.56	120.21
1	C	32	ILE	C-N-CA	-5.89	114.56	120.21
1	C	139	LEU	N-CA-C	5.84	117.65	111.28
1	H	101	VAL	N-CA-C	5.83	116.27	108.11
1	C	220	LYS	N-CA-C	5.81	117.61	111.28
1	E	221	LEU	N-CA-C	5.79	118.05	111.11
1	E	99	ALA	N-CA-C	5.77	117.84	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	205	HIS	N-CA-C	5.76	119.90	112.41
1	F	100	SER	N-CA-C	-5.69	100.02	109.46
1	G	78	ILE	N-CA-C	5.65	116.35	108.89
1	G	68	SER	N-CA-C	5.62	118.18	111.71
1	H	122	VAL	N-CA-C	5.62	115.96	107.75
1	C	28	ASP	N-CA-C	5.62	119.08	110.20
1	C	71	PRO	CA-C-N	5.62	125.98	119.47
1	C	71	PRO	C-N-CA	5.62	125.98	119.47
1	B	28	ASP	N-CA-C	5.61	118.69	109.76
1	F	189	TYR	N-CA-C	5.61	122.20	109.81
1	F	101	VAL	N-CA-C	5.59	115.94	108.11
1	C	202[A]	GLU	N-CA-C	5.53	119.53	112.34
1	C	202[B]	GLU	N-CA-C	5.53	119.53	112.34
1	A	232	GLU	O-C-N	-5.46	114.92	122.46
1	G	199	VAL	N-CA-C	5.46	117.45	111.77
1	C	194	PRO	N-CA-C	5.45	117.35	110.70
1	E	101	VAL	N-CA-C	5.44	115.73	108.11
1	G	164	VAL	N-CA-C	5.43	116.16	110.62
1	D	219	THR	N-CA-C	5.42	117.88	111.33
1	H	18	TRP	N-CA-C	5.40	118.27	110.28
1	E	189	TYR	N-CA-C	5.39	121.73	109.81
1	C	189	TYR	N-CA-C	5.39	121.73	109.81
1	B	156	ASN	CB-CA-C	-5.38	102.44	110.88
1	B	170	LEU	N-CA-C	-5.34	105.56	111.71
1	A	189	TYR	N-CA-C	5.34	121.60	109.81
1	D	100	SER	N-CA-C	-5.34	100.60	109.46
1	F	122	VAL	N-CA-C	5.33	115.53	107.75
1	A	122	VAL	N-CA-C	5.33	115.53	107.75
1	E	122	VAL	N-CA-C	5.32	115.52	107.75
1	A	21	GLU	O-C-N	-5.28	116.28	123.15
1	A	78	ILE	N-CA-C	5.28	116.40	109.58
1	B	160	TYR	CB-CA-C	5.28	119.25	111.06
1	F	194	PRO	N-CA-C	5.27	117.13	110.70
1	H	219	THR	N-CA-C	5.26	117.70	111.33
1	C	99	ALA	N-CA-C	5.25	117.05	109.07
1	B	220	LYS	N-CA-C	5.22	116.97	111.28
1	D	118	TYR	CA-C-N	5.21	125.02	119.28
1	D	118	TYR	C-N-CA	5.21	125.02	119.28
1	B	194	PRO	N-CA-C	5.18	117.02	110.70
1	B	78	ILE	N-CA-C	5.17	116.24	109.58
1	D	122	VAL	N-CA-C	5.16	115.28	107.75
1	G	19	TYR	N-CA-C	-5.15	100.84	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ARG	O-C-N	-5.14	116.67	122.12
1	E	192	THR	N-CA-C	5.10	119.77	113.50
1	A	99	ALA	N-CA-C	5.09	116.81	109.07
1	H	189	TYR	N-CA-C	5.09	121.07	109.81
1	H	161	SER	N-CA-C	5.08	117.72	111.82
1	A	231	ARG	CA-C-N	5.08	131.24	121.18
1	A	231	ARG	C-N-CA	5.08	131.24	121.18
1	C	128	HIS	CA-C-O	5.07	125.62	120.24
1	G	28	ASP	N-CA-C	5.07	118.21	110.20
1	D	37	GLY	N-CA-C	5.07	121.75	114.10
1	E	100	SER	N-CA-C	-5.06	100.91	108.96
1	C	118	TYR	CA-C-N	5.04	124.83	119.28
1	C	118	TYR	C-N-CA	5.04	124.83	119.28
1	F	220	LYS	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	1993	12	0
1	B	2055	0	1993	15	0
1	C	2061	0	1999	34	0
1	D	2045	0	1980	13	0
1	E	2054	0	1993	18	0
1	F	2060	0	1998	12	0
1	G	2055	0	1993	30	0
1	H	2055	0	1993	15	0
2	A	23	0	23	2	0
2	B	23	0	22	2	0
2	C	23	0	23	8	0
2	D	23	0	23	3	0
2	E	23	0	22	3	0
2	F	23	0	23	2	0
2	G	23	0	23	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	23	0	23	2	0
3	A	354	0	0	3	0
3	B	345	0	0	4	0
3	C	274	0	0	3	0
3	D	249	0	0	3	0
3	E	328	0	0	1	0
3	F	277	0	0	4	0
3	G	184	0	0	5	0
3	H	199	0	0	4	0
All	All	18834	0	16124	155	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 5.

All (155) 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)
1:E:139:LEU:HD22	3:E:575:HOH:O	1.42	1.13
1:C:160:TYR:CD1	1:C:243:HIS:NE2	2.33	0.95
1:C:160:TYR:HB3	1:C:243:HIS:HD2	1.35	0.90
1:C:160:TYR:HD2	2:C:301:36J:H24	1.24	0.83
1:B:4:THR:HA	3:B:599:HOH:O	1.80	0.82
1:F:160:TYR:CE2	3:F:502:HOH:O	2.34	0.81
1:E:266:LYS:H	1:E:266:LYS:HD2	1.45	0.80
1:G:72:PRO:HA	1:G:75:TYR:CE1	2.15	0.80
1:B:165:GLU:HG3	3:B:563:HOH:O	1.83	0.78
1:F:139:LEU:HB2	3:F:595:HOH:O	1.84	0.78
1:C:160:TYR:HB3	1:C:243:HIS:CD2	2.19	0.76
1:E:266:LYS:H	1:E:266:LYS:CD	1.99	0.75
1:C:144:VAL:CG2	1:C:149:ILE:HG13	2.18	0.74
1:G:160:TYR:CD2	2:G:301:36J:H22	2.24	0.72
1:C:165:GLU:HG3	3:C:538:HOH:O	1.89	0.72
1:G:262:ARG:HD2	3:G:525:HOH:O	1.91	0.71
1:C:160:TYR:CG	1:C:243:HIS:CD2	2.79	0.70
1:A:36:LEU:HG	2:A:301:36J:H9	1.74	0.67
1:C:160:TYR:CD2	2:C:301:36J:OAE	2.43	0.67
1:B:243:HIS:CD2	2:B:301:36J:H5	2.31	0.65
1:G:73:GLU:HB3	3:G:519:HOH:O	1.96	0.64
1:A:165:GLU:HG3	3:A:478:HOH:O	1.98	0.64
2:E:301:36J:H15	2:E:301:36J:OAP	1.97	0.63
1:H:4:THR:HG23	1:H:4:THR:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:TYR:CB	1:C:243:HIS:HD2	2.09	0.62
1:F:40:GLN:HG2	3:F:546:HOH:O	1.99	0.62
1:F:4:THR:O	1:F:4:THR:HG23	1.99	0.61
2:F:301:36J:H15	2:F:301:36J:OAP	2.00	0.60
1:C:160:TYR:CD1	1:C:243:HIS:CD2	2.90	0.60
1:A:7:ARG:HG2	1:A:21:GLU:HG2	1.83	0.59
1:G:194:PRO:HB2	1:G:195:PRO:HD3	1.84	0.59
1:G:160:TYR:CE2	2:G:301:36J:H19	2.39	0.58
1:G:142:HIS:CD2	1:G:191:ARG:HD3	2.39	0.57
1:C:144:VAL:HG22	1:C:149:ILE:HG13	1.87	0.57
1:C:160:TYR:CB	1:C:243:HIS:CD2	2.88	0.56
1:G:194:PRO:HB2	1:G:195:PRO:CD	2.35	0.56
1:H:121:ARG:HD3	3:H:467:HOH:O	2.04	0.56
1:B:36:LEU:HG	2:B:301:36J:H9	1.87	0.56
1:C:160:TYR:CD2	2:C:301:36J:H22	2.41	0.56
1:D:182:TYR:HB2	1:D:183:PRO:HD3	1.87	0.56
1:C:182:TYR:HB2	1:C:183:PRO:HD3	1.88	0.56
1:E:138:LEU:HD11	2:E:301:36J:H18	1.88	0.55
1:H:6:THR:HG23	3:H:539:HOH:O	2.06	0.55
2:C:301:36J:H15	2:C:301:36J:OAP	2.07	0.55
1:G:97:LYS:N	1:G:97:LYS:HD2	2.17	0.55
1:D:160:TYR:CD2	2:D:301:36J:OAE	2.59	0.55
1:G:118:TYR:N	1:G:119:PRO:CD	2.70	0.55
1:C:160:TYR:CE1	3:C:561:HOH:O	2.60	0.54
1:C:194:PRO:HB2	1:C:195:PRO:HD3	1.89	0.54
1:C:227:VAL:CG1	1:C:231:ARG:CZ	2.85	0.54
1:G:72:PRO:HA	1:G:75:TYR:CZ	2.42	0.54
1:H:36:LEU:HG	2:H:301:36J:H9	1.89	0.54
1:A:194:PRO:HB2	1:A:195:PRO:HD3	1.89	0.54
1:H:144:VAL:HG23	1:H:149:ILE:HG13	1.90	0.54
1:H:182:TYR:HB2	1:H:183:PRO:HD3	1.89	0.53
1:G:145:ASP:HB2	1:G:146:PRO:HD2	1.90	0.53
1:D:136:ASP:HA	1:D:139:LEU:HD22	1.91	0.53
1:G:36:LEU:HG	2:G:301:36J:H9	1.90	0.52
1:D:118:TYR:N	1:D:119:PRO:CD	2.73	0.52
1:C:160:TYR:CE2	2:C:301:36J:OAE	2.55	0.52
2:H:301:36J:H15	2:H:301:36J:OAP	2.10	0.52
1:D:255:LYS:HE2	1:D:259:GLU:OE2	2.11	0.51
1:G:160:TYR:CE2	2:G:301:36J:H22	2.45	0.51
1:H:149:ILE:HG21	1:H:183:PRO:HA	1.91	0.51
2:D:301:36J:OAP	2:D:301:36J:H15	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:TYR:HD2	2:C:301:36J:OAE	1.85	0.51
1:G:145:ASP:OD1	1:G:148:THR:HB	2.11	0.50
1:A:165:GLU:HG3	3:A:666:HOH:O	2.10	0.50
1:A:218:PRO:HD2	1:A:221:LEU:HD12	1.93	0.50
1:F:160:TYR:CZ	3:F:502:HOH:O	2.53	0.50
1:C:128:HIS:HD2	1:C:212:THR:OG1	1.95	0.50
1:F:182:TYR:HB2	1:F:183:PRO:HD3	1.94	0.50
1:D:201:THR:HG23	1:D:232:GLU:OE2	2.13	0.49
1:C:44:LYS:HB2	1:C:45:PRO:HD3	1.95	0.49
1:G:4:THR:N	3:G:406:HOH:O	2.46	0.49
1:A:4:THR:N	3:A:406:HOH:O	2.46	0.48
2:G:301:36J:OAP	2:G:301:36J:H15	2.12	0.48
1:G:263:LYS:HE3	1:G:264:TYR:CZ	2.48	0.48
1:H:194:PRO:HB2	1:H:195:PRO:HD3	1.95	0.48
1:B:227:VAL:CG1	1:B:231:ARG:CZ	2.91	0.48
1:D:34:ASP:HB2	2:D:301:36J:H8	1.95	0.48
1:F:36:LEU:HG	2:F:301:36J:H9	1.95	0.48
1:H:263:LYS:HE3	1:H:264:TYR:CZ	2.48	0.48
1:B:4:THR:N	3:B:404:HOH:O	2.47	0.47
1:H:266:LYS:HE2	3:H:567:HOH:O	2.13	0.47
1:A:227:VAL:CG1	1:A:231:ARG:CZ	2.92	0.47
1:G:189:TYR:HB2	1:G:190:PRO:HD3	1.97	0.47
1:G:142:HIS:NE2	1:G:191:ARG:HD3	2.30	0.47
1:B:72:PRO:HA	1:B:75:TYR:CZ	2.50	0.47
1:B:87:ILE:HD12	1:B:110:THR:HG21	1.96	0.46
1:B:139:LEU:HD13	1:B:140:HIS:NE2	2.30	0.46
1:D:165:GLU:HG3	3:D:551:HOH:O	2.15	0.46
1:A:72:PRO:HA	1:A:75:TYR:CZ	2.50	0.46
1:C:144:VAL:HG23	1:C:149:ILE:HG13	1.93	0.46
1:C:87:ILE:HD12	1:C:110:THR:HG21	1.96	0.46
1:H:266:LYS:HG3	3:H:402:HOH:O	2.15	0.46
1:F:144:VAL:HG23	1:F:149:ILE:HG13	1.96	0.46
1:E:9:TYR:HA	1:E:18:TRP:O	2.16	0.46
1:B:102:TRP:CD1	1:B:102:TRP:C	2.94	0.46
1:H:72:PRO:HA	1:H:75:TYR:CE1	2.51	0.45
1:C:36:LEU:HG	2:C:301:36J:H9	1.97	0.45
1:G:102:TRP:CD1	1:G:102:TRP:C	2.94	0.45
1:H:105:ALA:HA	1:H:131:PRO:HD3	1.97	0.45
1:E:87:ILE:HD12	1:E:110:THR:HG21	1.97	0.45
1:E:194:PRO:HB2	1:E:195:PRO:HD3	1.98	0.45
1:D:82:LYS:NZ	3:D:407:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:THR:HG21	3:B:505:HOH:O	2.17	0.44
1:G:9:TYR:HA	1:G:18:TRP:O	2.17	0.44
1:G:136:ASP:HA	1:G:139:LEU:HD23	1.99	0.44
1:G:144:VAL:HG23	1:G:149:ILE:HG13	1.99	0.44
1:C:266:LYS:O	1:C:266:LYS:HG3	2.12	0.44
1:E:266:LYS:H	1:E:266:LYS:CE	2.30	0.44
1:G:231:ARG:NH2	3:G:410:HOH:O	2.50	0.44
1:G:262:ARG:CD	3:G:525:HOH:O	2.60	0.43
1:C:160:TYR:CG	1:C:243:HIS:NE2	2.82	0.43
1:D:251:GLU:HG2	3:D:637:HOH:O	2.18	0.43
1:E:44:LYS:HB2	1:E:45:PRO:HD3	2.00	0.43
1:F:72:PRO:HA	1:F:75:TYR:CZ	2.53	0.43
1:G:140:HIS:O	1:G:143:GLU:HB2	2.19	0.43
1:A:105:ALA:HA	1:A:131:PRO:HD3	2.01	0.43
1:C:144:VAL:HG22	1:C:149:ILE:CG1	2.48	0.43
1:C:160:TYR:CE2	2:C:301:36J:H22	2.53	0.43
1:H:202:GLU:H	1:H:202:GLU:CD	2.26	0.43
1:E:108:ALA:HB1	1:E:130:VAL:HG22	2.01	0.43
1:D:88:ILE:HD13	1:D:88:ILE:HA	1.94	0.42
1:G:97:LYS:N	1:G:97:LYS:CD	2.82	0.42
1:E:197:ALA:HA	1:E:198:PRO:HD3	1.89	0.42
1:C:13:LYS:HE2	1:E:4:THR:HG21	2.02	0.42
1:C:104:CYS:HA	1:C:128:HIS:O	2.19	0.42
1:C:160:TYR:CD1	3:C:561:HOH:O	2.57	0.42
1:E:182:TYR:HB2	1:E:183:PRO:HD3	2.02	0.42
1:A:102:TRP:CD1	1:A:102:TRP:C	2.98	0.41
1:B:194:PRO:HB2	1:B:195:PRO:HD3	2.02	0.41
1:C:102:TRP:CD1	1:C:102:TRP:C	2.97	0.41
1:G:64:MET:HE1	1:G:185:TRP:HB2	2.02	0.41
1:B:193:ILE:HB	1:B:194:PRO:HD3	2.01	0.41
1:E:266:LYS:N	1:E:266:LYS:HE2	2.35	0.41
1:D:194:PRO:HB2	1:D:195:PRO:HD3	2.02	0.41
1:E:266:LYS:CD	1:E:266:LYS:N	2.72	0.41
1:F:38:GLU:OE1	1:F:65:SER:OG	2.33	0.41
1:B:227:VAL:CG1	1:B:231:ARG:NH2	2.84	0.41
1:H:72:PRO:HA	1:H:75:TYR:CZ	2.55	0.41
1:G:139:LEU:HD13	1:G:139:LEU:HA	1.86	0.41
1:E:149:ILE:HG21	1:E:183:PRO:HA	2.03	0.41
1:A:134:ASN:HD21	2:A:301:36J:H13	1.67	0.41
1:B:182:TYR:HB2	1:B:183:PRO:HD3	2.03	0.41
1:D:102:TRP:CD1	1:D:102:TRP:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:THR:HA	1:G:16:ILE:O	2.20	0.41
1:C:27:PRO:HD2	1:C:53:GLY:O	2.21	0.40
1:E:71:PRO:HA	1:E:72:PRO:HD3	1.97	0.40
1:F:71:PRO:HA	1:F:72:PRO:HD3	1.92	0.40
1:E:201:THR:HG23	1:E:232:GLU:OE2	2.21	0.40
1:F:105:ALA:HA	1:F:131:PRO:HD3	2.02	0.40
1:C:108:ALA:HB1	1:C:130:VAL:HG22	2.03	0.40
2:E:301:36J:CAG	2:E:301:36J:H21	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	261/266 (98%)	255 (98%)	5 (2%)	1 (0%)	30	18
1	B	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	30	18
1	C	262/266 (98%)	255 (97%)	6 (2%)	1 (0%)	30	18
1	D	260/266 (98%)	252 (97%)	6 (2%)	2 (1%)	16	5
1	E	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	30	18
1	F	262/266 (98%)	254 (97%)	6 (2%)	2 (1%)	16	5
1	G	261/266 (98%)	251 (96%)	8 (3%)	2 (1%)	16	5
1	H	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	30	18
All	All	2089/2128 (98%)	2026 (97%)	52 (2%)	11 (0%)	24	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	ASN
1	F	163	ASN

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Mol	Chain	Res	Type
1	A	189	TYR
1	B	189	TYR
1	D	189	TYR
1	E	189	TYR
1	F	189	TYR
1	G	189	TYR
1	H	189	TYR
1	C	189	TYR
1	G	163	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	223/224 (100%)	220 (99%)	3 (1%)	61	50
1	B	223/224 (100%)	220 (99%)	3 (1%)	61	50
1	C	224/224 (100%)	220 (98%)	4 (2%)	51	38
1	D	222/224 (99%)	215 (97%)	7 (3%)	34	17
1	E	223/224 (100%)	220 (99%)	3 (1%)	61	50
1	F	223/224 (100%)	221 (99%)	2 (1%)	70	63
1	G	223/224 (100%)	213 (96%)	10 (4%)	24	9
1	H	223/224 (100%)	221 (99%)	2 (1%)	70	63
All	All	1784/1792 (100%)	1750 (98%)	34 (2%)	50	36

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	246	TYR
1	A	266	LYS
1	B	139	LEU
1	B	221	LEU
1	B	266	LYS

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Mol	Chain	Res	Type
1	C	46	MET
1	C	139	LEU
1	C	144	VAL
1	C	266	LYS
1	D	12	THR
1	D	139	LEU
1	D	202	GLU
1	D	221	LEU
1	D	236	ILE
1	D	246	TYR
1	D	251	GLU
1	E	46	MET
1	E	139	LEU
1	E	266	LYS
1	F	246	TYR
1	F	266	LYS
1	G	4	THR
1	G	12	THR
1	G	13	LYS
1	G	73	GLU
1	G	97	LYS
1	G	133	GLU
1	G	139	LEU
1	G	141	ILE
1	G	236	ILE
1	G	246	TYR
1	H	73	GLU
1	H	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	134	ASN
1	B	22	GLN
1	C	76	GLN
1	C	128	HIS
1	D	22	GLN
1	D	124	ASN
1	D	134	ASN
1	E	140	HIS
1	F	140	HIS

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Mol	Chain	Res	Type
1	G	134	ASN
1	H	134	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
2	36J	H	301	-	24,24,24	1.30	2 (8%)	32,32,32	1.81	7 (21%)
2	36J	B	301	-	24,24,24	1.77	6 (25%)	32,32,32	1.71	8 (25%)
2	36J	C	301	-	24,24,24	1.40	4 (16%)	32,32,32	1.37	6 (18%)
2	36J	D	301	-	24,24,24	2.11	5 (20%)	32,32,32	3.01	9 (28%)
2	36J	F	301	-	24,24,24	2.06	9 (37%)	32,32,32	1.65	6 (18%)
2	36J	A	301	-	24,24,24	2.13	7 (29%)	32,32,32	1.94	6 (18%)
2	36J	G	301	-	24,24,24	1.39	4 (16%)	32,32,32	1.71	6 (18%)
2	36J	E	301	-	24,24,24	2.13	6 (25%)	32,32,32	1.71	6 (18%)

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
2	36J	H	301	-	-	5/22/22/22	0/2/2/2
2	36J	B	301	-	-	6/22/22/22	0/2/2/2
2	36J	C	301	-	-	8/22/22/22	0/2/2/2
2	36J	D	301	-	-	8/22/22/22	1/2/2/2
2	36J	F	301	-	-	6/22/22/22	0/2/2/2
2	36J	A	301	-	-	5/22/22/22	0/2/2/2
2	36J	G	301	-	-	7/22/22/22	1/2/2/2
2	36J	E	301	-	-	7/22/22/22	1/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	36J	OAP-CAV	6.57	1.58	1.47
2	E	301	36J	OAP-CAV	6.33	1.58	1.47
2	A	301	36J	OAP-CAV	5.20	1.56	1.47
2	B	301	36J	OAP-CAV	4.74	1.55	1.47
2	A	301	36J	CAH-CAS	4.48	1.45	1.38
2	D	301	36J	CAM-CAV	4.20	1.66	1.52
2	A	301	36J	CAN-CAW	3.95	1.63	1.52
2	F	301	36J	CAN-CAW	3.87	1.63	1.52
2	F	301	36J	CAU-CAQ	-3.84	1.41	1.50
2	F	301	36J	CAG-CAF	3.82	1.43	1.31
2	F	301	36J	OAP-CAV	3.75	1.53	1.47
2	E	301	36J	CAJ-CAF	-3.66	1.30	1.50
2	D	301	36J	CAG-CAF	3.62	1.42	1.31
2	E	301	36J	CAT-CAG	-3.61	1.41	1.47
2	G	301	36J	CAT-CAG	-3.33	1.41	1.47
2	C	301	36J	CAN-CAW	3.26	1.61	1.52
2	A	301	36J	CAL-CAO	3.19	1.65	1.52
2	B	301	36J	CAN-CAW	3.15	1.61	1.52
2	C	301	36J	CAG-CAF	3.15	1.41	1.31
2	D	301	36J	CAN-CAW	3.14	1.61	1.52
2	E	301	36J	CAU-CAQ	-3.07	1.43	1.50
2	H	301	36J	CAU-CAQ	-3.00	1.43	1.50
2	H	301	36J	CAG-CAF	2.93	1.40	1.31
2	G	301	36J	CAO-CAW	2.85	1.60	1.52
2	F	301	36J	OAE-CAW	2.82	1.51	1.43
2	B	301	36J	CAG-CAF	2.69	1.40	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	36J	CAN-CAW	2.69	1.60	1.52
2	B	301	36J	CAU-CAQ	-2.60	1.44	1.50
2	F	301	36J	CAL-CAM	2.45	1.62	1.52
2	F	301	36J	CAO-CAW	2.44	1.59	1.52
2	A	301	36J	CAO-CAW	-2.42	1.45	1.52
2	A	301	36J	CAG-CAF	2.36	1.39	1.31
2	C	301	36J	CAU-CAQ	-2.36	1.45	1.50
2	G	301	36J	CAU-CAQ	-2.34	1.45	1.50
2	G	301	36J	CAG-CAF	2.32	1.38	1.31
2	D	301	36J	CAU-CAQ	-2.28	1.45	1.50
2	A	301	36J	OAE-CAW	2.26	1.49	1.43
2	F	301	36J	CAM-CAV	2.14	1.59	1.52
2	B	301	36J	OAC-CAR	-2.14	1.32	1.37
2	F	301	36J	CAL-CAO	2.10	1.61	1.52
2	E	301	36J	CAK-CAN	2.09	1.60	1.52
2	C	301	36J	OAC-CAR	-2.07	1.32	1.37
2	B	301	36J	CAL-CAO	2.05	1.60	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	36J	CAV-OAP-CAQ	10.54	137.30	117.67
2	D	301	36J	OAP-CAV-CAM	8.43	124.49	106.75
2	E	301	36J	CAT-CAG-CAF	6.81	139.91	125.55
2	A	301	36J	CAN-CAK-CAJ	-6.08	101.30	114.47
2	D	301	36J	CAN-CAK-CAJ	-5.90	101.67	114.47
2	A	301	36J	CAV-OAP-CAQ	5.18	127.33	117.67
2	H	301	36J	CAN-CAK-CAJ	-5.09	103.44	114.47
2	B	301	36J	CAN-CAK-CAJ	-4.91	103.83	114.47
2	F	301	36J	CAV-OAP-CAQ	4.83	126.67	117.67
2	G	301	36J	CAN-CAK-CAJ	-4.49	104.74	114.47
2	F	301	36J	CAN-CAK-CAJ	-4.43	104.86	114.47
2	G	301	36J	CAV-OAP-CAQ	4.21	125.51	117.67
2	H	301	36J	CAH-CAS-CAU	3.64	124.99	120.92
2	C	301	36J	CAN-CAK-CAJ	-3.50	106.89	114.47
2	D	301	36J	CAL-CAO-CAW	-3.28	105.65	114.68
2	A	301	36J	CAT-CAI-CAR	3.20	124.27	120.92
2	D	301	36J	CAT-CAI-CAR	3.18	124.25	120.92
2	F	301	36J	CAT-CAI-CAR	3.14	124.22	120.92
2	A	301	36J	CAS-CAH-CAR	-3.14	116.77	119.67
2	B	301	36J	CAV-OAP-CAQ	3.09	123.43	117.67
2	G	301	36J	CAA-CAV-CAM	-3.05	106.01	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	36J	CAK-CAN-CAW	-3.04	106.32	114.68
2	H	301	36J	CAT-CAI-CAR	2.93	123.99	120.92
2	B	301	36J	CAT-CAI-CAR	2.91	123.97	120.92
2	D	301	36J	CAA-CAV-CAM	-2.87	106.47	113.90
2	E	301	36J	CAS-CAH-CAR	2.80	122.25	119.67
2	H	301	36J	CAS-CAH-CAR	-2.80	117.09	119.67
2	D	301	36J	CAU-CAT-CAG	2.73	126.05	121.92
2	A	301	36J	OAE-CAW-CAO	-2.69	102.18	109.35
2	G	301	36J	OAP-CAV-CAA	2.68	113.97	107.96
2	B	301	36J	CAA-CAV-CAM	-2.66	107.00	113.90
2	F	301	36J	CAI-CAT-CAU	-2.61	116.65	119.94
2	F	301	36J	CAT-CAG-CAF	2.58	130.99	125.55
2	B	301	36J	CAK-CAN-CAW	-2.57	107.59	114.68
2	C	301	36J	CAV-OAP-CAQ	2.57	122.45	117.67
2	B	301	36J	CAI-CAT-CAU	-2.56	116.73	119.94
2	D	301	36J	CAH-CAS-CAU	2.54	123.76	120.92
2	B	301	36J	OAP-CAV-CAM	2.52	112.07	106.75
2	E	301	36J	OAP-CAV-CAM	2.44	111.89	106.75
2	H	301	36J	CAV-OAP-CAQ	2.40	122.13	117.67
2	A	301	36J	CAH-CAS-CAU	2.38	123.58	120.92
2	C	301	36J	OAP-CAQ-OAB	-2.35	119.72	123.55
2	B	301	36J	CAU-CAT-CAG	2.32	125.43	121.92
2	D	301	36J	CAI-CAR-CAH	-2.28	117.34	120.47
2	H	301	36J	CAI-CAT-CAU	-2.23	117.13	119.94
2	E	301	36J	CAA-CAV-CAM	-2.23	108.13	113.90
2	C	301	36J	CAL-CAO-CAW	-2.20	108.63	114.68
2	E	301	36J	CAT-CAU-CAS	-2.14	116.56	118.73
2	C	301	36J	OAD-CAS-CAU	-2.12	117.22	121.14
2	C	301	36J	CAI-CAR-CAH	-2.09	117.60	120.47
2	E	301	36J	CAV-OAP-CAQ	2.06	121.50	117.67
2	H	301	36J	CAL-CAO-CAW	-2.04	109.07	114.68
2	F	301	36J	OAP-CAV-CAM	2.01	110.98	106.75
2	G	301	36J	CAN-CAW-CAO	2.00	117.92	113.56

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	36J	CAA-CAV-OAP-CAQ
2	D	301	36J	CAA-CAV-OAP-CAQ
2	E	301	36J	CAA-CAV-OAP-CAQ
2	E	301	36J	CAU-CAQ-OAP-CAV

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Mol	Chain	Res	Type	Atoms
2	E	301	36J	CAJ-CAF-CAG-CAT
2	F	301	36J	CAA-CAV-OAP-CAQ
2	G	301	36J	CAL-CAM-CAV-OAP
2	G	301	36J	CAA-CAV-OAP-CAQ
2	G	301	36J	CAU-CAQ-OAP-CAV
2	G	301	36J	OAB-CAQ-OAP-CAV
2	E	301	36J	OAB-CAQ-OAP-CAV
2	C	301	36J	CAM-CAV-OAP-CAQ
2	H	301	36J	CAM-CAV-OAP-CAQ
2	G	301	36J	CAL-CAM-CAV-CAA
2	H	301	36J	CAA-CAV-OAP-CAQ
2	F	301	36J	CAU-CAQ-OAP-CAV
2	F	301	36J	CAL-CAO-CAW-CAN
2	G	301	36J	CAL-CAO-CAW-CAN
2	C	301	36J	CAL-CAM-CAV-CAA
2	D	301	36J	CAU-CAQ-OAP-CAV
2	B	301	36J	CAF-CAJ-CAK-CAN
2	C	301	36J	CAF-CAJ-CAK-CAN
2	D	301	36J	CAF-CAJ-CAK-CAN
2	H	301	36J	CAF-CAJ-CAK-CAN
2	G	301	36J	CAF-CAJ-CAK-CAN
2	D	301	36J	CAG-CAF-CAJ-CAK
2	D	301	36J	CAK-CAN-CAW-OAE
2	E	301	36J	CAJ-CAK-CAN-CAW
2	H	301	36J	CAU-CAQ-OAP-CAV
2	A	301	36J	CAL-CAM-CAV-CAA
2	B	301	36J	CAK-CAN-CAW-OAE
2	A	301	36J	CAF-CAJ-CAK-CAN
2	B	301	36J	CAK-CAN-CAW-CAO
2	D	301	36J	CAK-CAN-CAW-CAO
2	H	301	36J	CAM-CAL-CAO-CAW
2	F	301	36J	CAM-CAV-OAP-CAQ
2	D	301	36J	CAM-CAL-CAO-CAW
2	C	301	36J	CAL-CAM-CAV-OAP
2	E	301	36J	CAM-CAL-CAO-CAW
2	C	301	36J	CAJ-CAK-CAN-CAW
2	B	301	36J	CAM-CAL-CAO-CAW
2	A	301	36J	OAP-CAQ-CAU-CAS
2	C	301	36J	CAM-CAL-CAO-CAW
2	B	301	36J	OAP-CAQ-CAU-CAT
2	C	301	36J	CAL-CAO-CAW-OAE
2	D	301	36J	CAL-CAO-CAW-OAE

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Mol	Chain	Res	Type	Atoms
2	B	301	36J	OAP-CAQ-CAU-CAS
2	F	301	36J	CAF-CAJ-CAK-CAN
2	A	301	36J	CAM-CAL-CAO-CAW
2	E	301	36J	CAF-CAJ-CAK-CAN
2	A	301	36J	CAA-CAV-OAP-CAQ
2	F	301	36J	CAL-CAM-CAV-CAA

All (3) ring outliers are listed below:

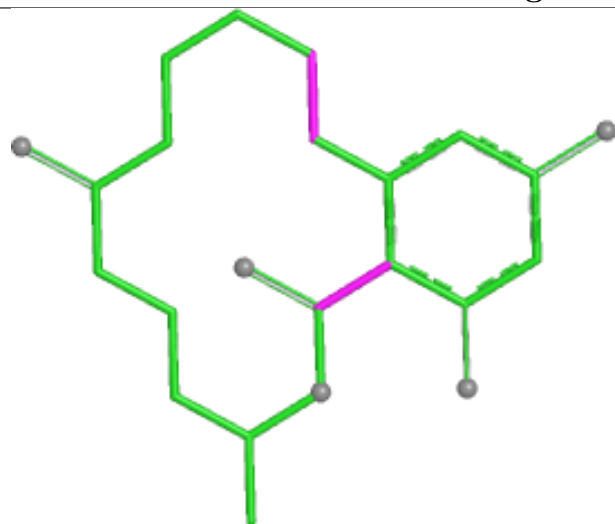
Mol	Chain	Res	Type	Atoms
2	G	301	36J	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C
2	E	301	36J	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C
2	D	301	36J	CAF-CAG-CAJ-CAK-CAL-CAM-CAN-CAO-CAQ-CAT-CAU-CAV-CAW-C

8 monomers are involved in 27 short contacts:

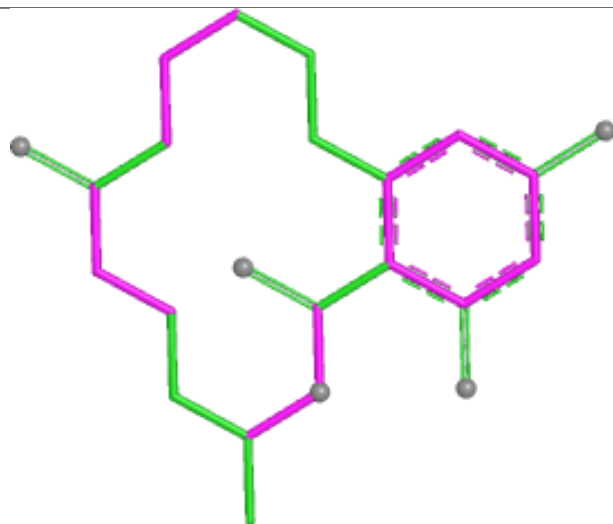
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	36J	2	0
2	B	301	36J	2	0
2	C	301	36J	8	0
2	D	301	36J	3	0
2	F	301	36J	2	0
2	A	301	36J	2	0
2	G	301	36J	5	0
2	E	301	36J	3	0

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

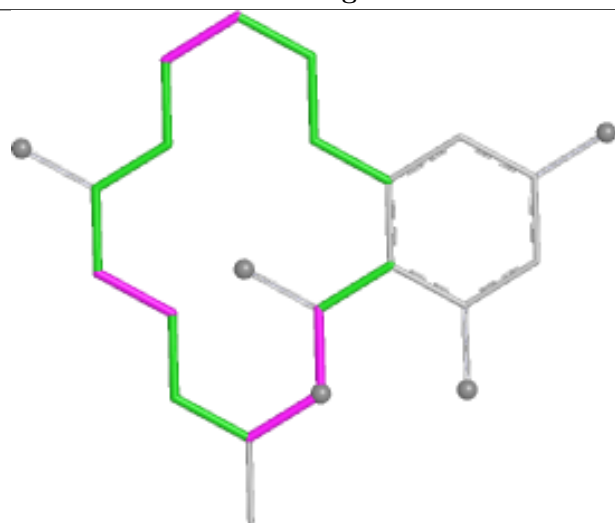
Ligand 36J H 301



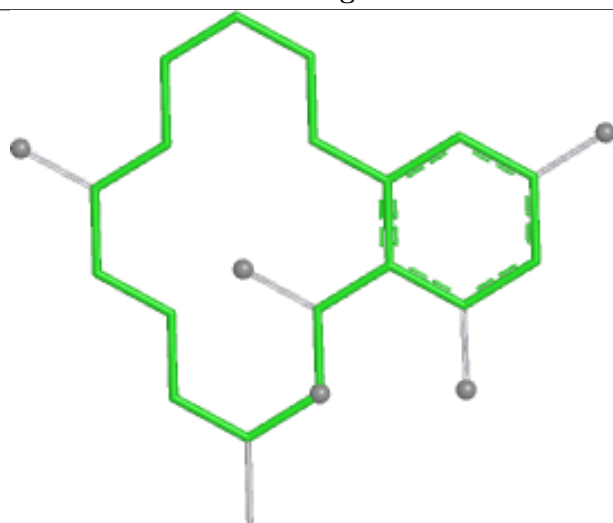
Bond lengths



Bond angles

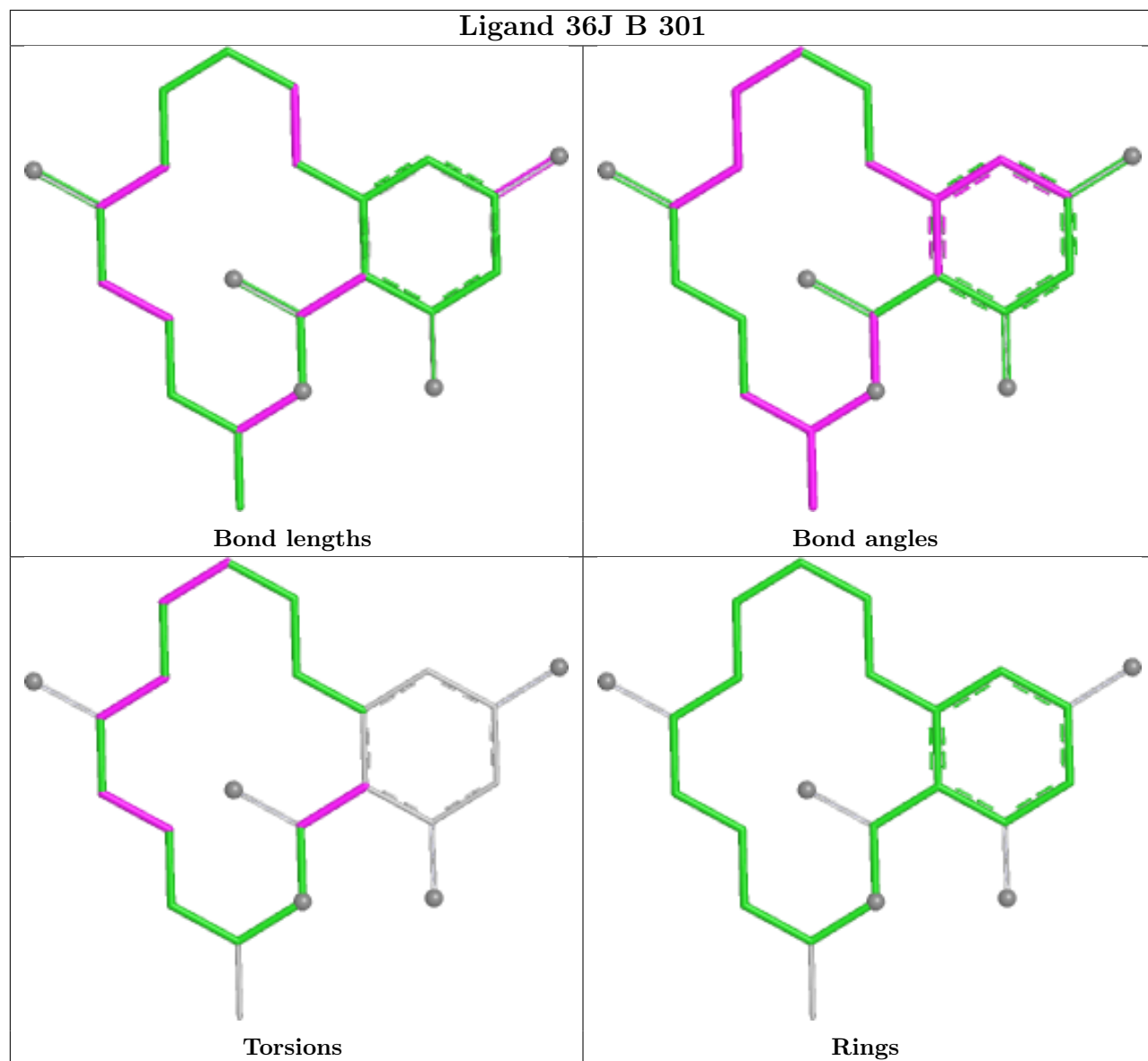


Torsions

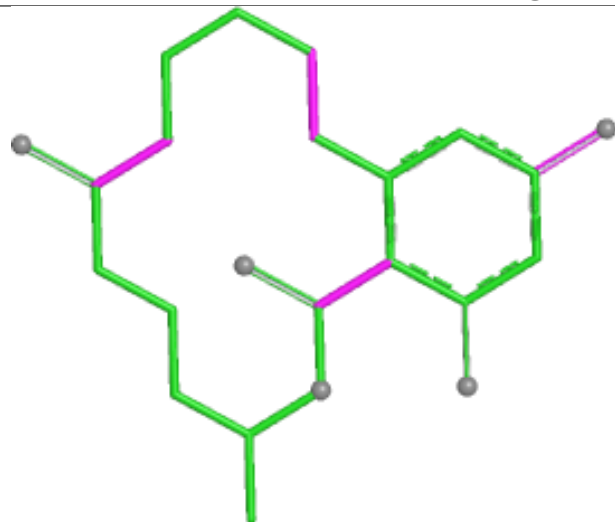


Rings

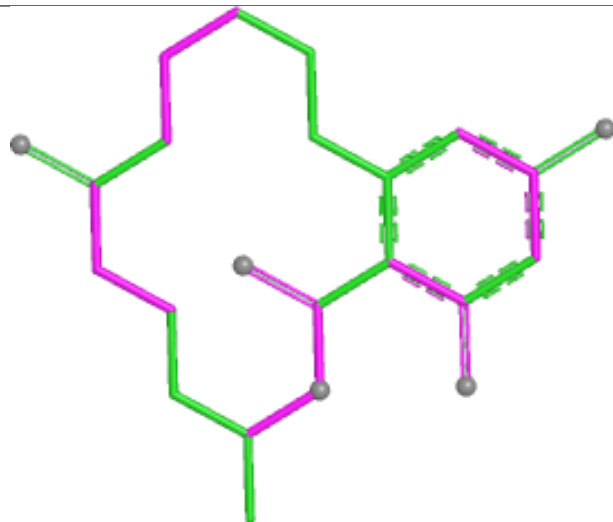
Ligand 36J B 301



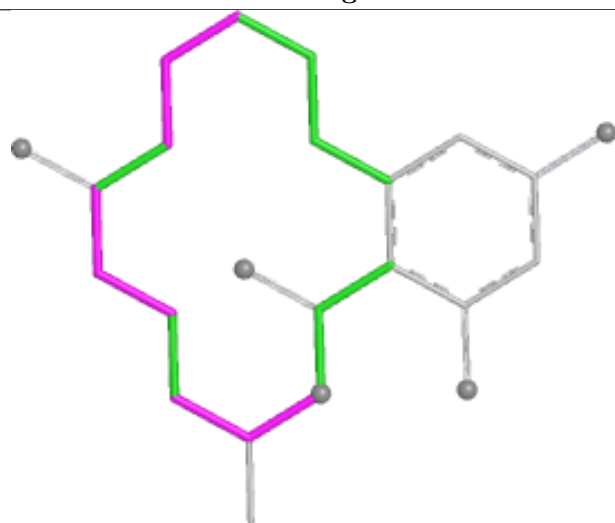
Ligand 36J C 301



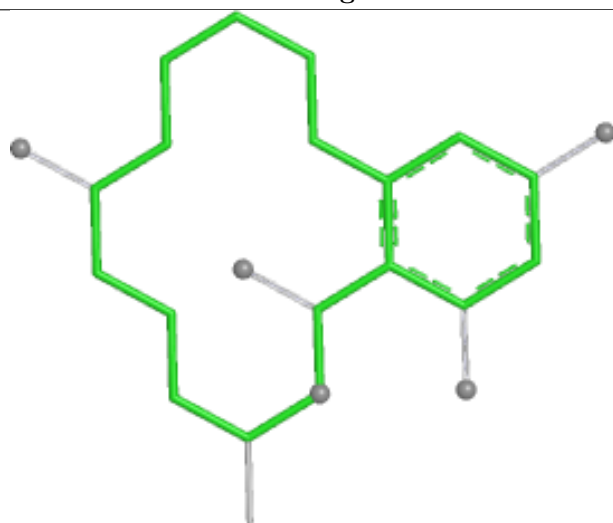
Bond lengths



Bond angles

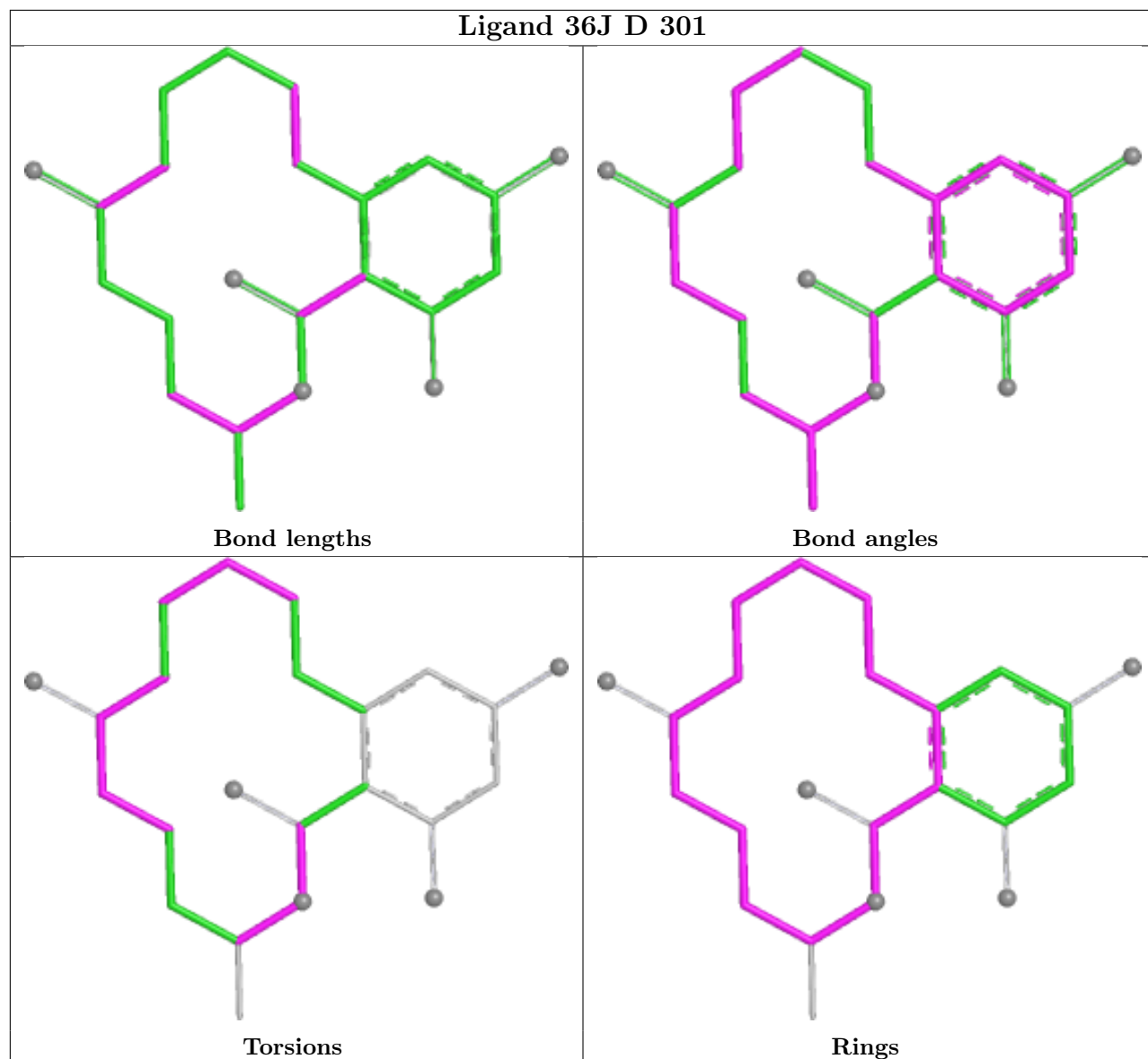


Torsions

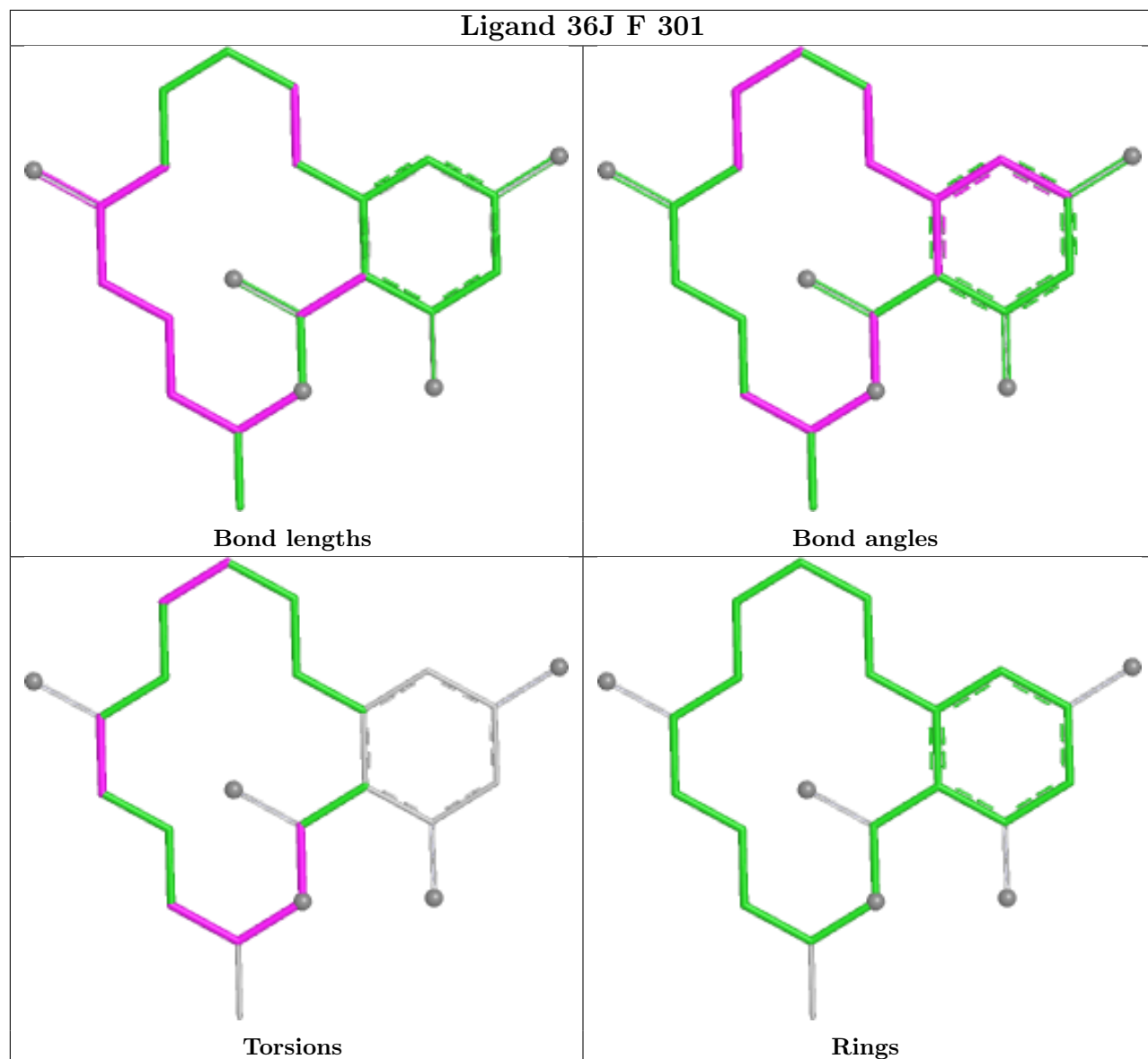


Rings

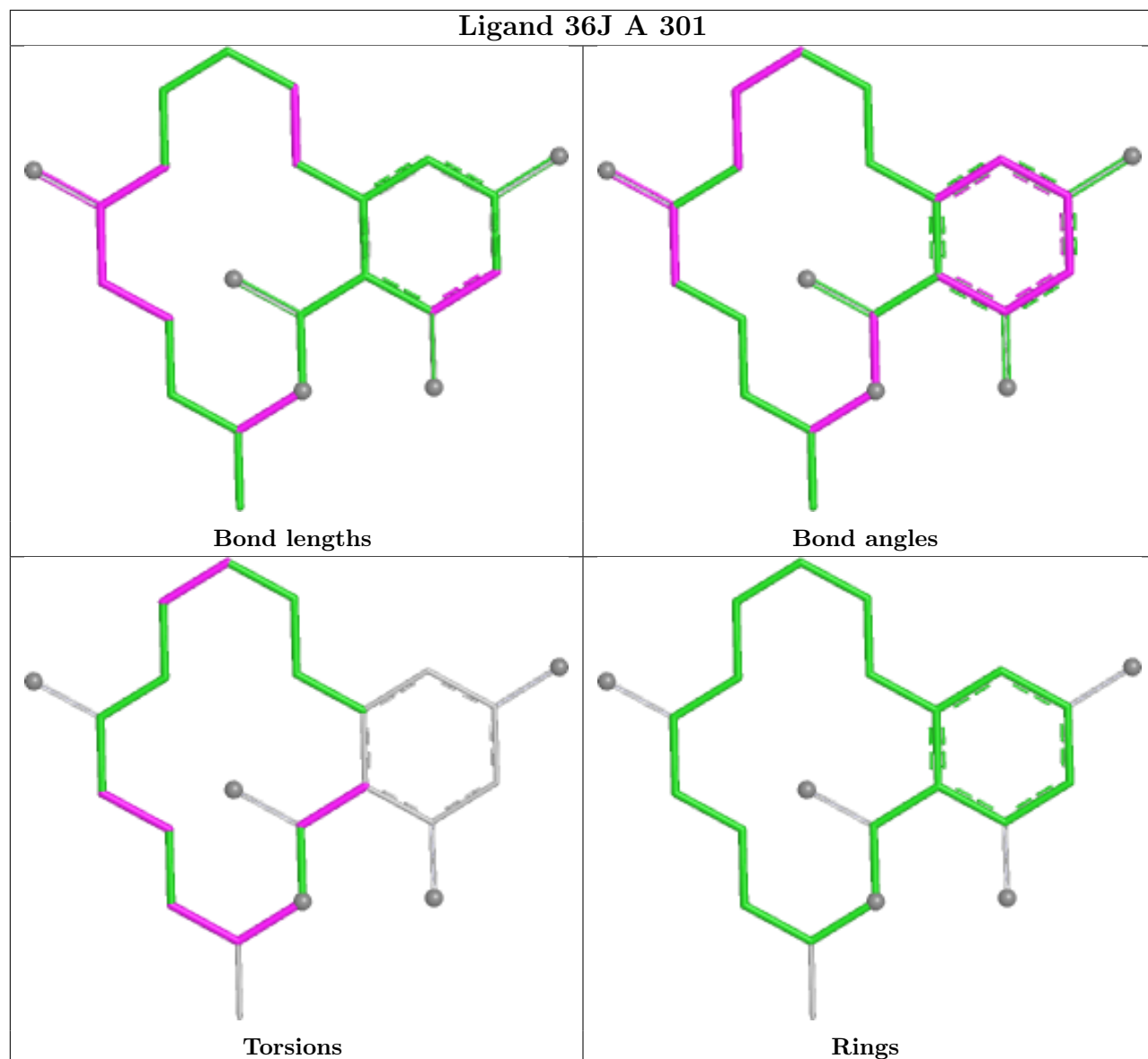
Ligand 36J D 301



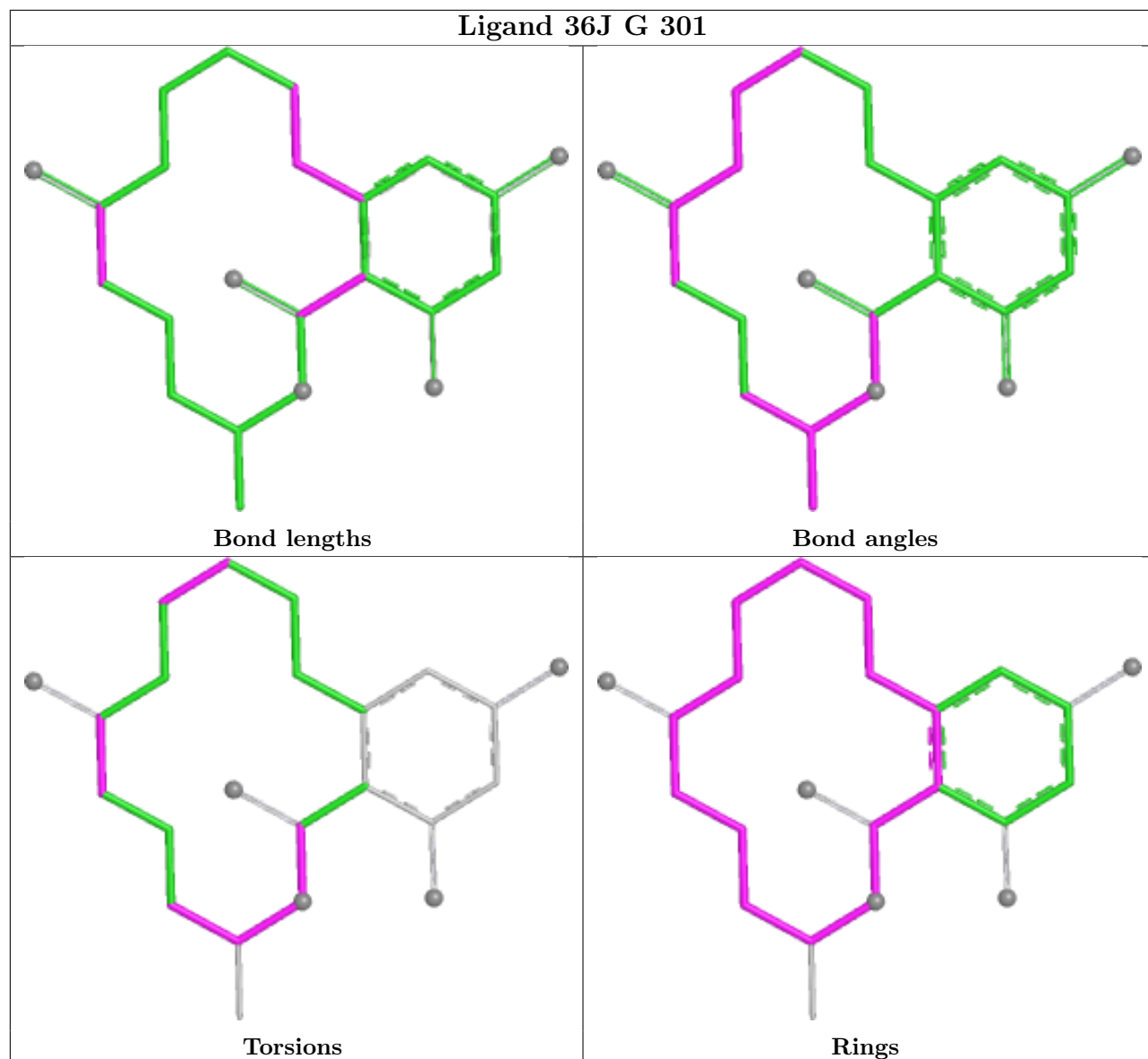
Ligand 36J F 301

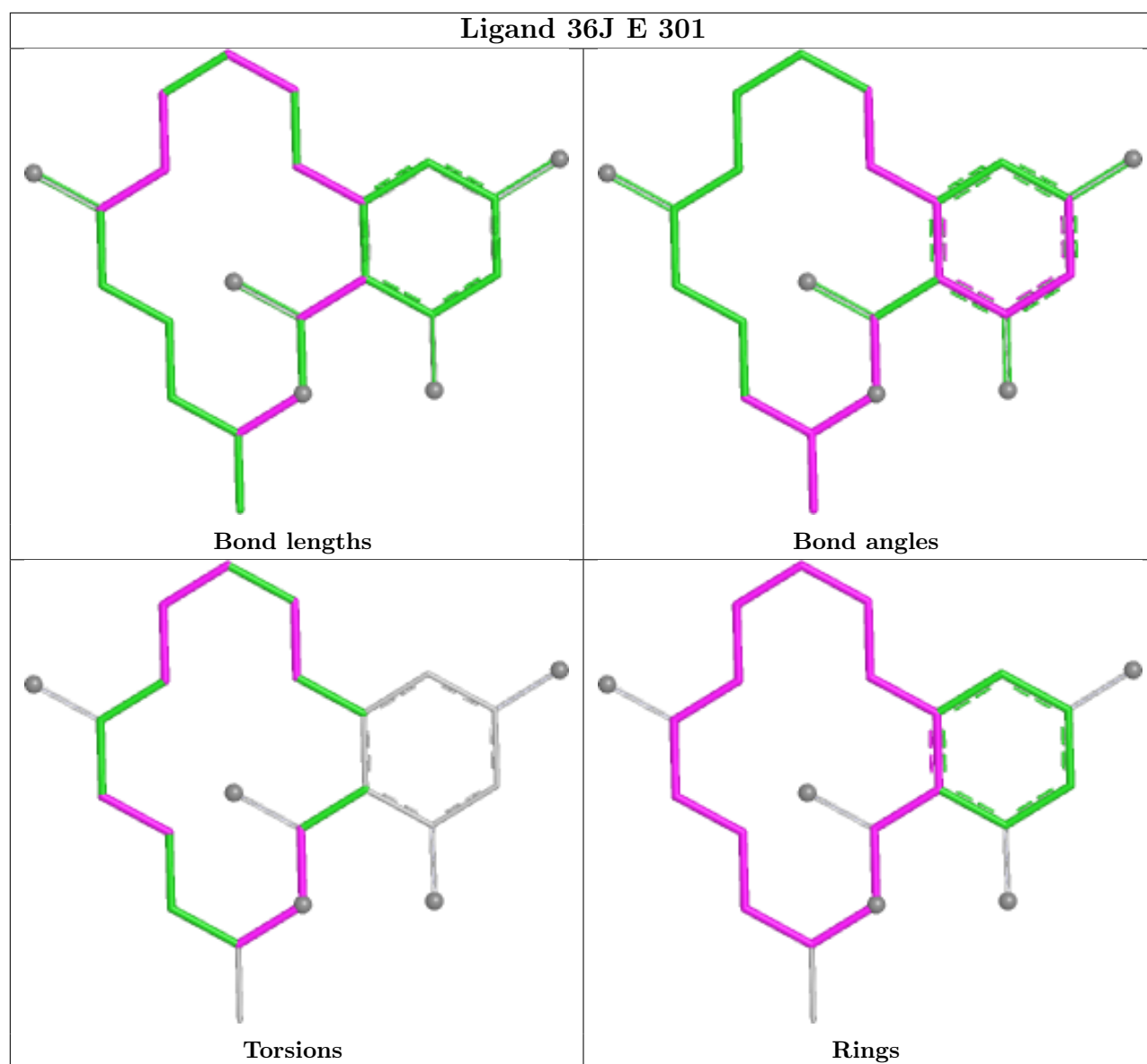


Ligand 36J A 301



Ligand 36J G 301





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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/266 (98%)	-0.30	0 100 100	16, 23, 36, 54	0
1	B	263/266 (98%)	-0.26	3 (1%) 78 82	16, 23, 39, 54	0
1	C	263/266 (98%)	-0.09	2 (0%) 82 86	15, 26, 48, 79	1 (0%)
1	D	262/266 (98%)	0.02	3 (1%) 78 82	20, 29, 46, 65	0
1	E	263/266 (98%)	-0.18	1 (0%) 88 92	18, 26, 39, 90	0
1	F	264/266 (99%)	-0.01	5 (1%) 66 72	17, 28, 49, 88	0
1	G	263/266 (98%)	0.41	7 (2%) 56 61	22, 36, 61, 77	0
1	H	263/266 (98%)	0.30	5 (1%) 66 72	21, 34, 54, 66	0
All	All	2104/2128 (98%)	-0.02	26 (1%) 76 81	15, 28, 50, 90	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	160	TYR	6.2
1	C	160	TYR	4.9
1	D	160	TYR	4.6
1	F	3	ALA	4.2
1	G	139	LEU	4.1
1	B	160	TYR	3.7
1	G	160	TYR	3.3
1	D	137	ILE	3.2
1	E	139	LEU	2.7
1	G	68	SER	2.6
1	H	266	LYS	2.5
1	G	142	HIS	2.4
1	G	149	ILE	2.4
1	G	223	PHE	2.3
1	C	139	LEU	2.3
1	H	139	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	137	ILE	2.2
1	H	4	THR	2.2
1	F	159	ALA	2.2
1	D	139	LEU	2.2
1	G	188	GLY	2.2
1	B	4	THR	2.2
1	H	93	THR	2.2
1	H	265	LEU	2.2
1	B	243	HIS	2.1
1	F	243	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

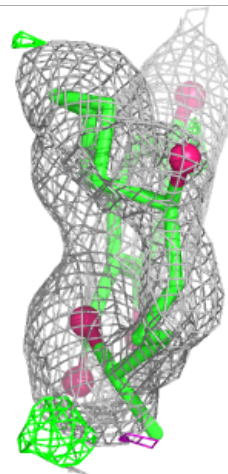
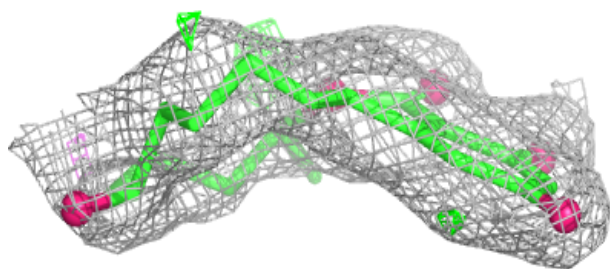
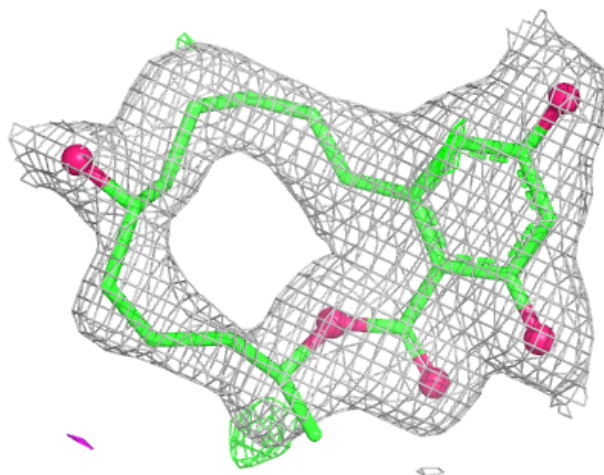
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	36J	G	301	23/23	0.92	0.12	34,45,65,69	0
2	36J	D	301	23/23	0.94	0.10	26,34,55,57	0
2	36J	H	301	23/23	0.94	0.10	29,35,57,58	0
2	36J	A	301	23/23	0.95	0.08	19,25,32,34	0
2	36J	E	301	23/23	0.95	0.07	20,24,36,40	0
2	36J	F	301	23/23	0.96	0.08	24,34,51,53	0
2	36J	B	301	23/23	0.96	0.07	18,28,46,47	0
2	36J	C	301	23/23	0.96	0.09	22,30,60,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

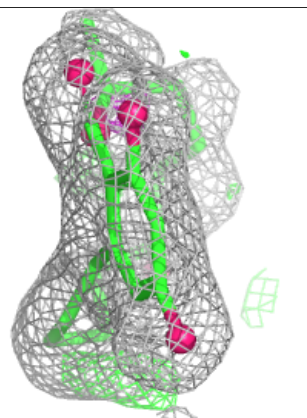
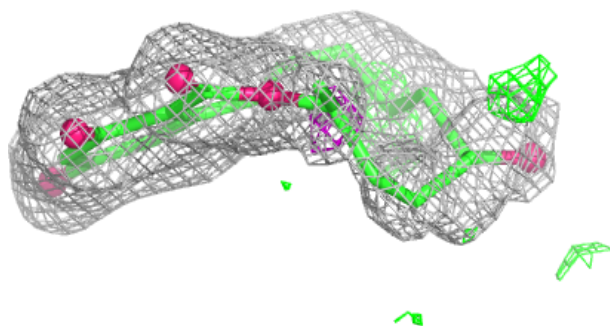
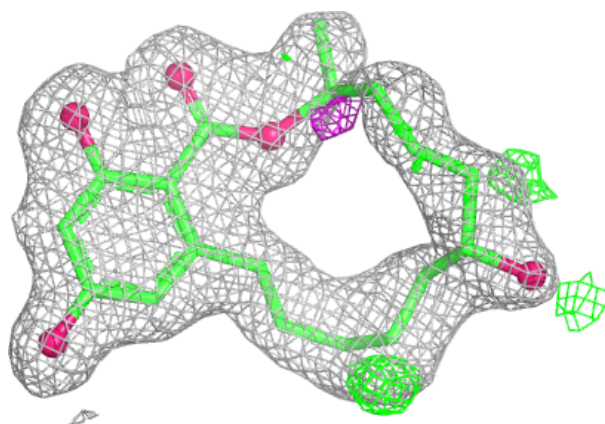
Electron density around 36J G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



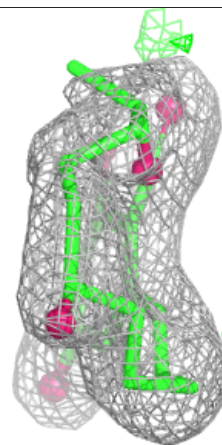
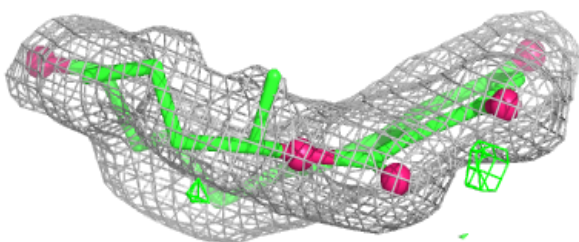
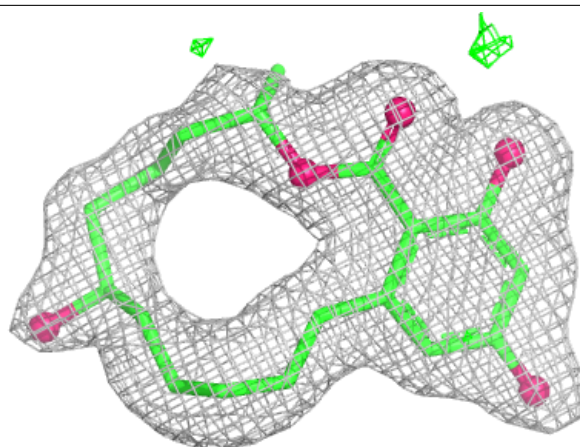
Electron density around 36J D 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



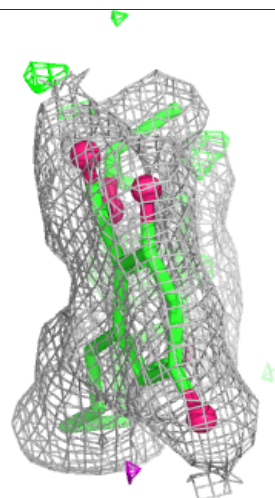
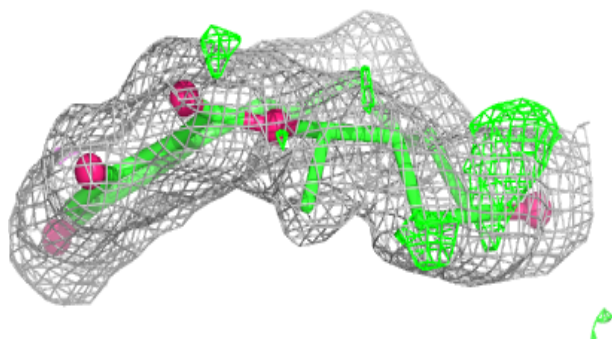
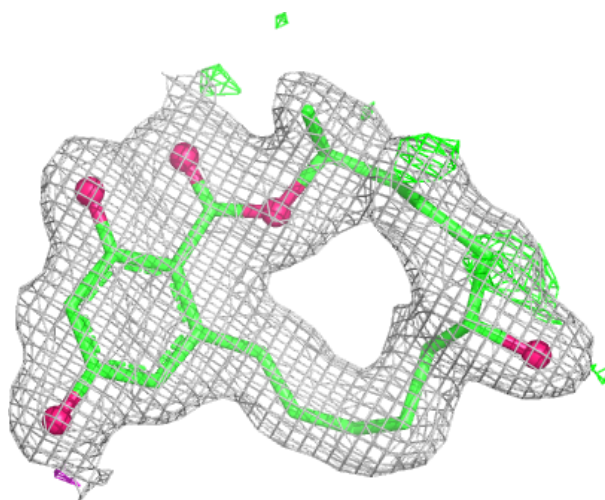
Electron density around 36J H 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



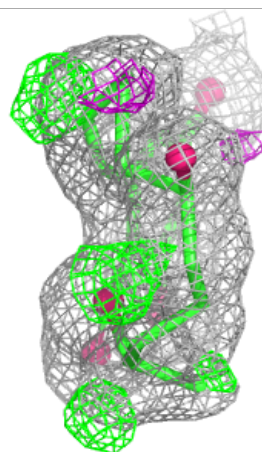
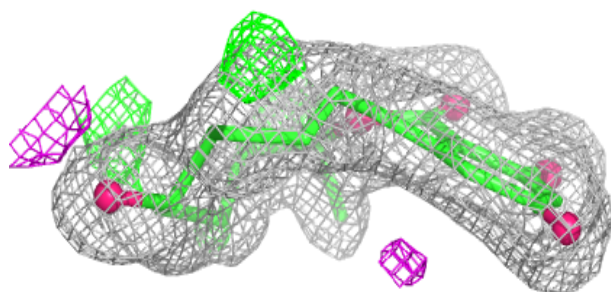
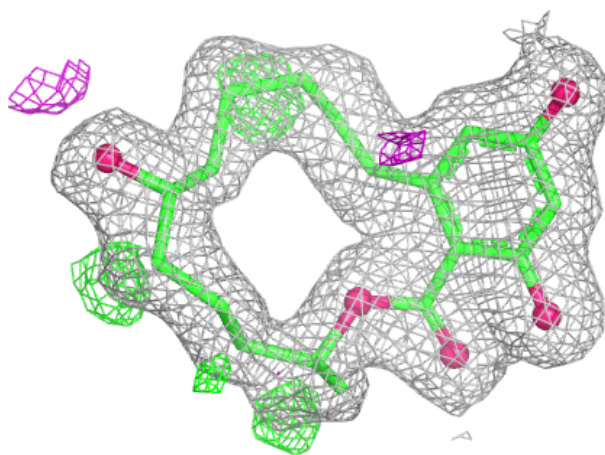
Electron density around 36J A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



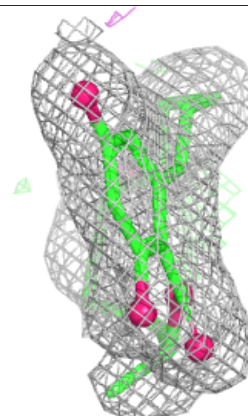
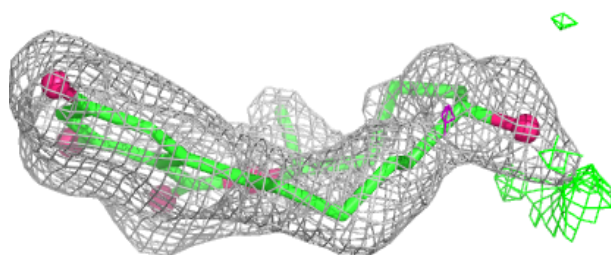
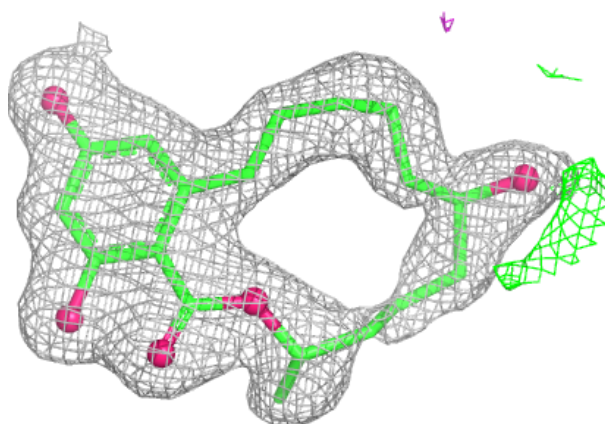
Electron density around 36J E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

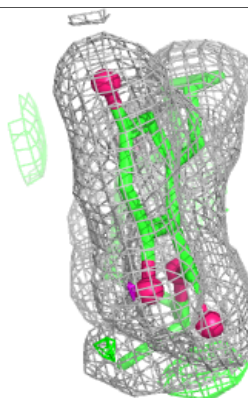
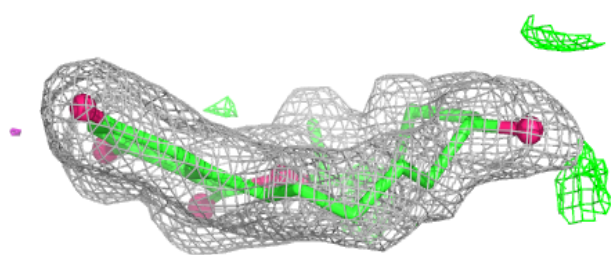
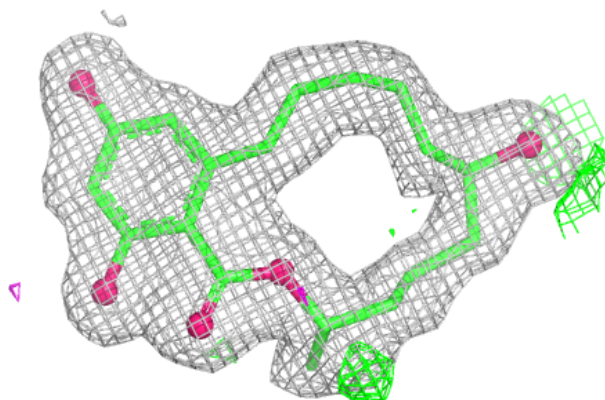


Electron density around 36J F 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

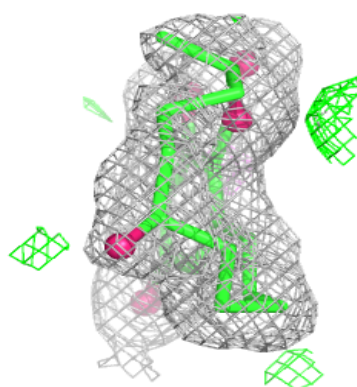
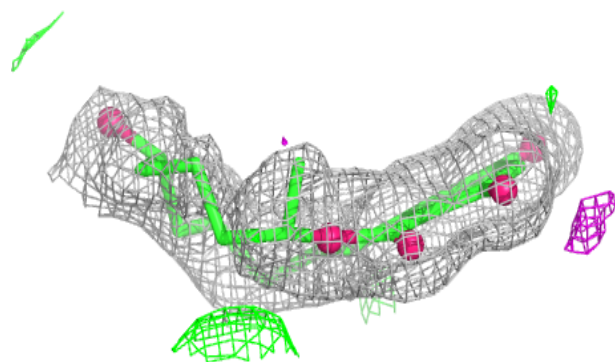
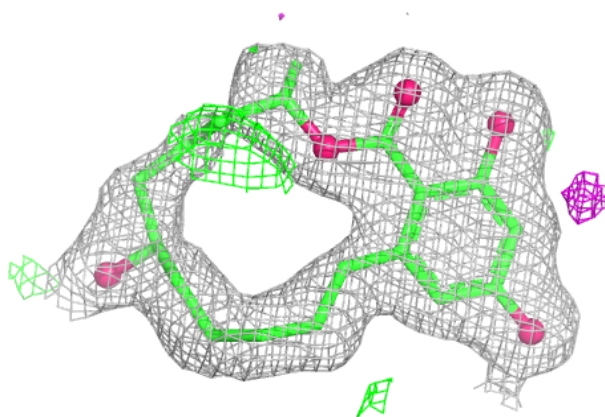
**Electron density around 36J B 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 36J C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.