Full wwPDB EM Validation Report

Nov 19, 2022 – 08:15 PM EST

PDB ID	:	7LW1
EMDB ID	:	EMD-23544
Title	:	Human phosphofructokinase-1 liver type bound to activator NA-11
Authors	:	Lynch, E.M.; Kollman, J.M.; Webb, B.
Deposited on	:	2021-02-27
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

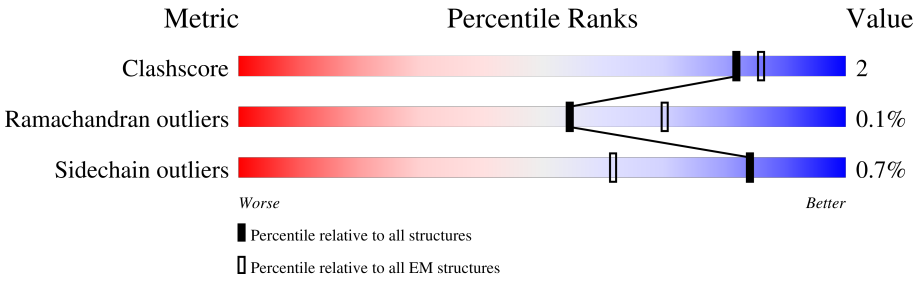
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	780	89% 6% • 5%
1	D	780	89% 6% • 5%
1	E	780	88% 6% • 5%
1	F	780	88% 6% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F6P	A	803	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F6P	D	803	-	-	X	-
4	F6P	E	803	-	-	X	-
4	F6P	F	803	-	-	X	-

2 Entry composition

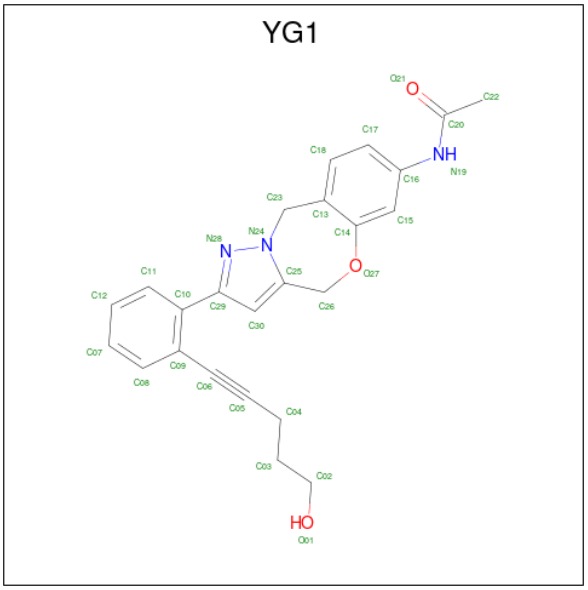
There are 5 unique types of molecules in this entry. The entry contains 45884 atoms, of which 22796 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent 6-phosphofructokinase, liver type.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	744	Total	C	H	N	O	S	0	0
			11355	3570	5676	1005	1067	37		
1	D	744	Total	C	H	N	O	S	0	0
			11355	3570	5676	1005	1067	37		
1	E	744	Total	C	H	N	O	S	0	0
			11355	3570	5676	1005	1067	37		
1	F	744	Total	C	H	N	O	S	0	0
			11355	3570	5676	1005	1067	37		

- Molecule 2 is N-{(11S)-2-[2-(5-hydroxypent-1-yn-1-yl)phenyl]-4H,10H-pyrazolo[5,1-c][1,4]benzoxazepin-7-yl}acetamide (three-letter code: YG1) (formula: $C_{24}H_{23}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	N	O	0
			53	24	23	3	3	
2	D	1	Total	C	H	N	O	0
			53	24	23	3	3	

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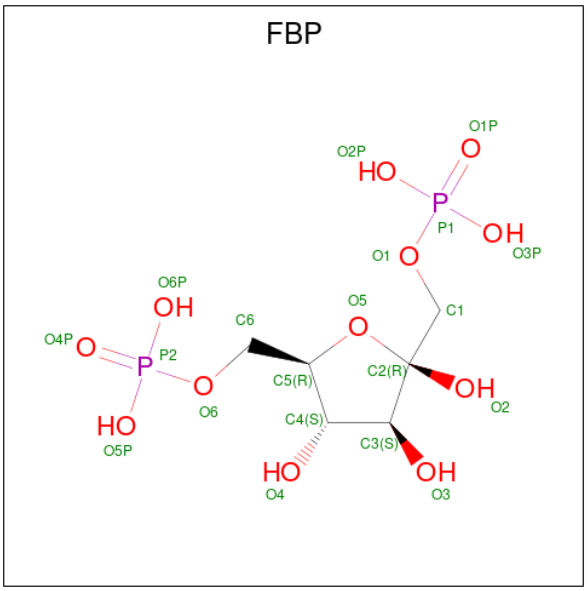
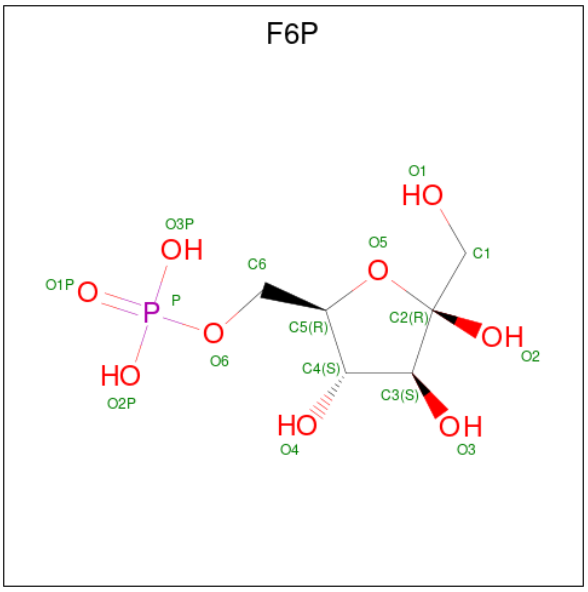
Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	H	N	O	0
			53	24	23	3	3	
2	F	1	Total	C	H	N	O	0
			53	24	23	3	3	

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



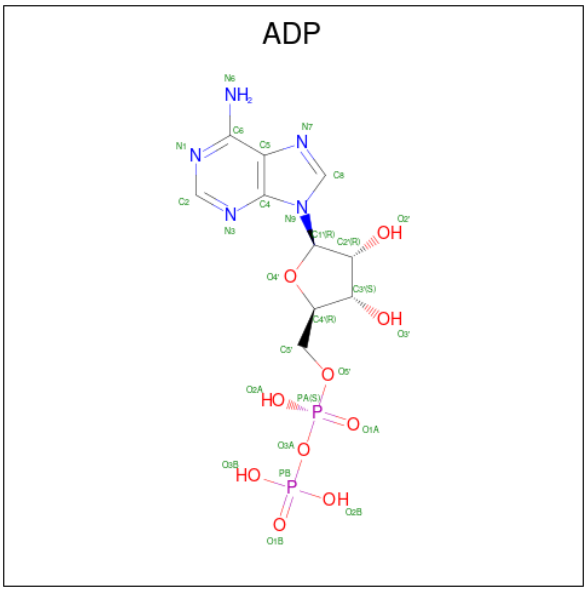
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			20	6	12	2	
3	D	1	Total	C	O	P	0
			20	6	12	2	
3	E	1	Total	C	O	P	0
			20	6	12	2	
3	F	1	Total	C	O	P	0
			20	6	12	2	

- Molecule 4 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 16 6 9 1	0
4	D	1	Total C O P 16 6 9 1	0
4	E	1	Total C O P 16 6 9 1	0
4	F	1	Total C O P 16 6 9 1	0

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



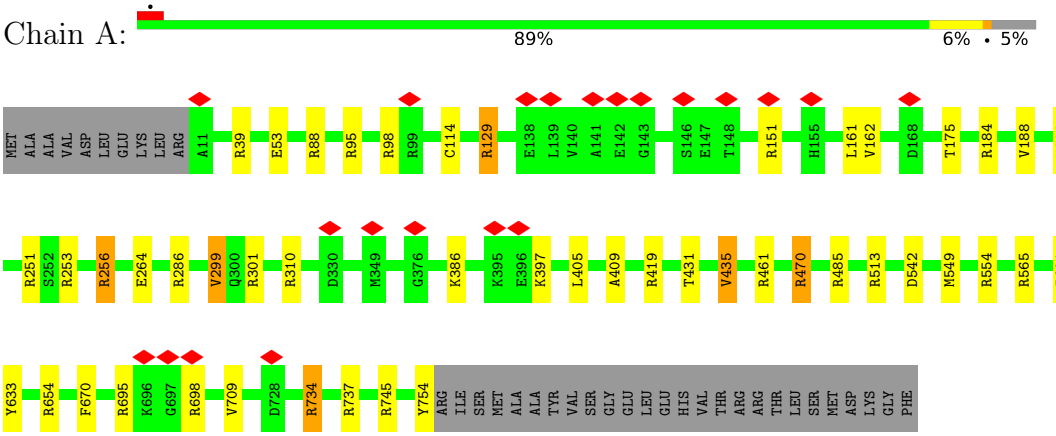
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

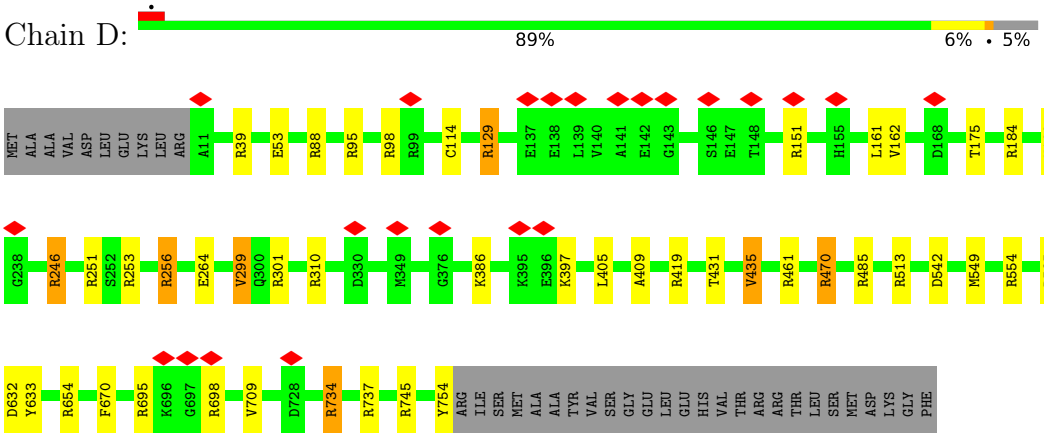
• Molecule 1: ATP-dependent 6-phosphofructokinase, liver type

Chain A:



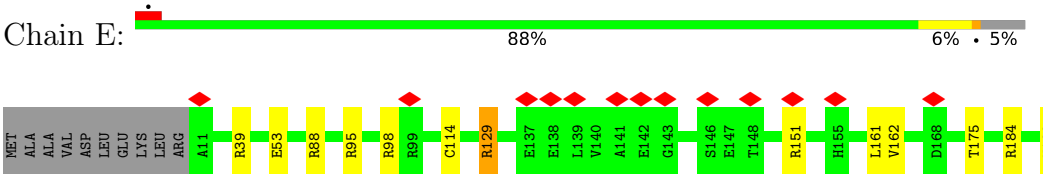
• Molecule 1: ATP-dependent 6-phosphofructokinase, liver type

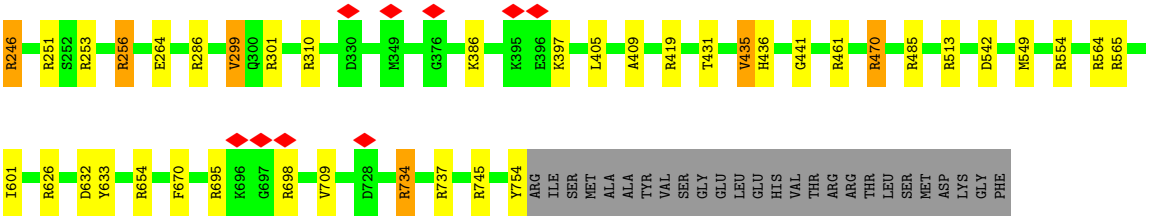
Chain D:



• Molecule 1: ATP-dependent 6-phosphofructokinase, liver type

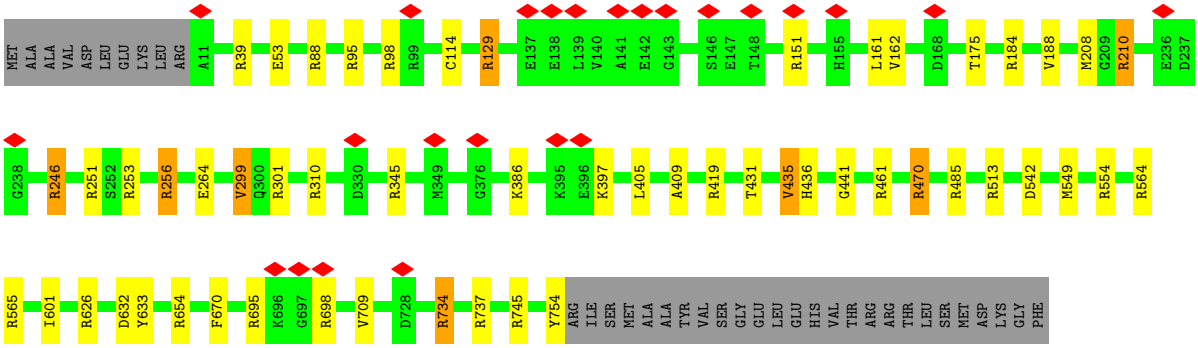
Chain E:





• Molecule 1: ATP-dependent 6-phosphofructokinase, liver type

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	63296	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.239	Depositor
Minimum map value	-9.378	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.334	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: YG1, ADP, FBP, F6P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	3/5781 (0.1%)	1.12	35/7814 (0.4%)
1	D	0.68	3/5781 (0.1%)	1.12	34/7814 (0.4%)
1	E	0.68	3/5781 (0.1%)	1.12	36/7814 (0.5%)
1	F	0.68	3/5781 (0.1%)	1.12	36/7814 (0.5%)
All	All	0.68	12/23124 (0.1%)	1.12	141/31256 (0.5%)

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	A	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	709	VAL	CB-CG2	-8.56	1.34	1.52
1	D	709	VAL	CB-CG2	-8.56	1.34	1.52
1	E	709	VAL	CB-CG2	-8.56	1.34	1.52
1	F	709	VAL	CB-CG2	-8.56	1.34	1.52
1	E	435	VAL	CB-CG1	-7.63	1.36	1.52
1	A	435	VAL	CB-CG1	-7.63	1.36	1.52
1	D	435	VAL	CB-CG1	-7.63	1.36	1.52
1	F	435	VAL	CB-CG1	-7.63	1.36	1.52
1	A	709	VAL	CB-CG1	-7.41	1.37	1.52
1	D	709	VAL	CB-CG1	-7.41	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	709	VAL	CB-CG1	-7.41	1.37	1.52
1	F	709	VAL	CB-CG1	-7.41	1.37	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	709	VAL	CA-CB-CG1	12.66	129.88	110.90
1	E	709	VAL	CA-CB-CG1	12.66	129.88	110.90
1	A	709	VAL	CA-CB-CG1	12.64	129.86	110.90
1	F	709	VAL	CA-CB-CG1	12.63	129.85	110.90
1	E	745	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	A	745	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	F	745	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	D	745	ARG	NE-CZ-NH1	12.46	126.53	120.30
1	A	626	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	D	626	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	F	626	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	E	626	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	299	VAL	CA-CB-CG1	8.67	123.90	110.90
1	D	299	VAL	CA-CB-CG1	8.67	123.90	110.90
1	E	299	VAL	CA-CB-CG1	8.67	123.90	110.90
1	F	299	VAL	CA-CB-CG1	8.65	123.87	110.90
1	F	98	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	98	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	98	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	151	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	D	151	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	E	151	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	151	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	E	98	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	E	745	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	F	745	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	745	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	745	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	485	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	D	485	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	E	485	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	F	485	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	698	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	698	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	D	698	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	F	698	ARG	NE-CZ-NH1	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	734	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	734	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	734	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	E	734	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	310	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	310	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	E	310	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	F	95	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	95	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	95	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	E	95	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	F	626	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	F	310	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	695	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	695	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	E	695	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	F	695	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	626	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	626	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	E	626	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	435	VAL	CA-CB-CG1	6.29	120.34	110.90
1	A	435	VAL	CA-CB-CG1	6.29	120.33	110.90
1	F	435	VAL	CA-CB-CG1	6.28	120.32	110.90
1	E	435	VAL	CA-CB-CG1	6.27	120.30	110.90
1	D	470	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	470	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	F	470	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	513	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	D	513	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	E	513	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	F	513	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	470	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	88	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	E	88	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	88	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	F	88	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	654	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	654	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	F	654	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	E	246	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	654	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	F	246	ARG	NE-CZ-NH1	5.95	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	246	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	95	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	E	565	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	565	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	95	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	95	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	E	253	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	565	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	E	737	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	565	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	253	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	253	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	253	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	210	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	D	210	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	E	210	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	F	210	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	737	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	F	737	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	E	184	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	184	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	E	95	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	184	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	184	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	E	549	MET	CA-CB-CG	5.54	122.73	113.30
1	F	549	MET	CA-CB-CG	5.54	122.71	113.30
1	D	737	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	549	MET	CA-CB-CG	5.53	122.69	113.30
1	D	549	MET	CA-CB-CG	5.52	122.68	113.30
1	F	129	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	461	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	E	461	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	461	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	F	461	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	129	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	129	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	129	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	256	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	256	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	E	256	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	F	256	ARG	NE-CZ-NH2	5.31	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	39	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	E	39	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	251	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	D	251	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	251	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	D	554	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	E	286	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	F	39	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	F	251	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	F	554	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	554	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	554	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	564	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	419	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	419	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	286	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	419	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	E	419	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	E	564	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	F	345	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	754	TYR	Sidechain
1	D	129	ARG	Sidechain
1	D	754	TYR	Sidechain
1	E	129	ARG	Sidechain
1	E	754	TYR	Sidechain
1	F	129	ARG	Sidechain
1	F	754	TYR	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	A	5679	5676	5675	28	0
1	D	5679	5676	5675	28	0
1	E	5679	5676	5675	29	0
1	F	5679	5676	5675	29	0
2	A	30	23	0	7	0
2	D	30	23	0	7	0
2	E	30	23	0	7	0
2	F	30	23	0	7	0
3	A	20	0	10	6	0
3	D	20	0	10	6	0
3	E	20	0	10	6	0
3	F	20	0	10	6	0
4	A	16	0	11	6	0
4	D	16	0	11	6	0
4	E	16	0	11	6	0
4	F	16	0	11	6	0
5	A	27	0	12	0	0
5	D	27	0	12	0	0
5	E	27	0	12	0	0
5	F	27	0	12	0	0
All	All	23088	22796	22832	114	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 2.

All (114) 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:D:264:GLU:OE2	4:D:803:F6P:O4	1.89	0.91
1:A:264:GLU:OE2	4:A:803:F6P:O4	1.89	0.91
1:E:264:GLU:OE2	4:E:803:F6P:O4	1.89	0.89
1:F:264:GLU:OE2	4:F:803:F6P:O4	1.89	0.89
1:E:734:ARG:NH2	3:E:802:FBP:O4P	2.11	0.84
1:F:734:ARG:NH2	3:F:802:FBP:O5P	2.11	0.83
1:A:734:ARG:NH2	3:A:802:FBP:O4P	2.11	0.82
1:D:734:ARG:NH2	3:D:802:FBP:O5P	2.11	0.82
1:A:208:MET:HE2	4:A:803:F6P:H4	1.65	0.76
1:D:208:MET:HE2	4:D:803:F6P:H4	1.66	0.76
2:A:801:YG1:C06	2:A:801:YG1:N28	2.49	0.76
2:D:801:YG1:C06	2:D:801:YG1:N28	2.49	0.75
2:E:801:YG1:C06	2:E:801:YG1:N28	2.49	0.74
2:F:801:YG1:C06	2:F:801:YG1:N28	2.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:MET:HE2	4:F:803:F6P:H4	1.70	0.73
1:E:208:MET:HE2	4:E:803:F6P:H4	1.76	0.68
1:D:632:ASP:OD2	1:D:633:TYR:CD1	2.50	0.64
1:A:632:ASP:OD2	1:A:633:TYR:CD1	2.50	0.64
1:E:632:ASP:OD2	1:E:633:TYR:CD1	2.51	0.63
1:F:632:ASP:OD2	1:F:633:TYR:CD1	2.51	0.63
1:D:409:ALA:CB	3:D:802:FBP:H5	2.29	0.63
1:A:409:ALA:CB	3:A:802:FBP:H5	2.29	0.63
1:F:409:ALA:CB	3:F:802:FBP:H5	2.29	0.62
1:E:409:ALA:CB	3:E:802:FBP:H5	2.29	0.62
1:D:162:VAL:CG1	1:D:175:THR:HG22	2.35	0.57
1:A:162:VAL:CG1	1:A:175:THR:HG22	2.35	0.57
1:E:162:VAL:CG1	1:E:175:THR:HG22	2.35	0.56
1:F:162:VAL:CG1	1:F:175:THR:HG22	2.35	0.56
1:D:162:VAL:HG11	1:D:175:THR:HG22	1.88	0.55
1:A:162:VAL:HG11	1:A:175:THR:HG22	1.88	0.55
1:F:162:VAL:HG11	1:F:175:THR:HG22	1.88	0.55
1:E:162:VAL:HG11	1:E:175:THR:HG22	1.88	0.55
1:A:470:ARG:NH2	3:A:802:FBP:O6	2.40	0.55
1:D:470:ARG:NH2	3:D:802:FBP:O6	2.40	0.54
1:E:470:ARG:NH2	3:E:802:FBP:O6	2.40	0.54
1:F:470:ARG:NH2	3:F:802:FBP:O6	2.40	0.54
1:A:670:PHE:HB2	2:A:801:YG1:C17	2.39	0.53
1:D:670:PHE:HB2	2:D:801:YG1:C17	2.39	0.53
1:E:670:PHE:HB2	2:E:801:YG1:C17	2.39	0.53
1:F:670:PHE:HB2	2:F:801:YG1:C17	2.39	0.53
1:E:208:MET:CE	4:E:803:F6P:H4	2.41	0.51
1:A:405:LEU:HD13	1:A:435:VAL:HB	1.95	0.49
1:D:405:LEU:HD13	1:D:435:VAL:HB	1.95	0.49
1:F:405:LEU:HD13	1:F:435:VAL:HB	1.95	0.48
1:A:208:MET:CE	4:A:803:F6P:H4	2.41	0.48
1:E:405:LEU:HD13	1:E:435:VAL:HB	1.95	0.48
1:D:208:MET:CE	4:D:803:F6P:H4	2.41	0.47
1:D:470:ARG:NH2	3:D:802:FBP:O5	2.45	0.47
1:A:470:ARG:NH2	3:A:802:FBP:O5	2.45	0.47
1:E:542:ASP:OD1	2:E:801:YG1:C02	2.63	0.47
1:F:208:MET:CE	4:F:803:F6P:H4	2.41	0.47
1:F:542:ASP:OD1	2:F:801:YG1:C02	2.63	0.47
1:A:542:ASP:OD1	2:A:801:YG1:C02	2.63	0.47
1:D:542:ASP:OD1	2:D:801:YG1:C02	2.63	0.47
1:E:208:MET:HB3	4:E:803:F6P:O3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:MET:HB3	4:F:803:F6P:O3	2.15	0.46
1:A:208:MET:HB3	4:A:803:F6P:O3	2.15	0.46
1:D:208:MET:HB3	4:D:803:F6P:O3	2.15	0.46
2:A:801:YG1:N28	2:A:801:YG1:C05	2.78	0.46
2:D:801:YG1:N28	2:D:801:YG1:C05	2.78	0.46
1:A:670:PHE:HD1	2:A:801:YG1:O21	1.99	0.46
1:D:670:PHE:HD1	2:D:801:YG1:O21	1.99	0.45
2:E:801:YG1:N28	2:E:801:YG1:C05	2.78	0.45
2:F:801:YG1:N28	2:F:801:YG1:C05	2.78	0.45
1:E:670:PHE:HD1	2:E:801:YG1:O21	1.99	0.45
1:F:670:PHE:HD1	2:F:801:YG1:O21	1.99	0.45
1:D:670:PHE:CD1	2:D:801:YG1:C16	3.00	0.44
1:E:470:ARG:NH2	3:E:802:FBP:O5	2.44	0.44
1:F:470:ARG:NH2	3:F:802:FBP:O5	2.44	0.44
1:A:670:PHE:CD1	2:A:801:YG1:C16	3.00	0.44
1:E:670:PHE:CD1	2:E:801:YG1:C16	3.00	0.44
1:F:670:PHE:CD1	2:F:801:YG1:C16	3.00	0.44
1:A:670:PHE:CD1	2:A:801:YG1:C15	3.01	0.44
1:D:670:PHE:CD1	2:D:801:YG1:C15	3.01	0.44
1:F:409:ALA:HB3	3:F:802:FBP:H5	2.00	0.44
1:E:409:ALA:HB3	3:E:802:FBP:H5	1.99	0.43
1:D:301:ARG:HD3	4:D:803:F6P:O2	2.19	0.43
1:E:670:PHE:CD1	2:E:801:YG1:C15	3.01	0.43
1:F:670:PHE:CD1	2:F:801:YG1:C15	3.01	0.43
1:A:301:ARG:HD3	4:A:803:F6P:O2	2.19	0.43
1:A:53:GLU:OE1	1:D:256:ARG:NH1	2.49	0.43
1:A:256:ARG:NH1	1:D:53:GLU:OE1	2.49	0.43
1:A:299:VAL:HG22	1:D:188:VAL:HG13	2.01	0.43
1:D:162:VAL:CG1	1:D:175:THR:CG2	2.97	0.42
1:A:162:VAL:CG1	1:A:175:THR:CG2	2.97	0.42
1:E:299:VAL:HG22	1:F:188:VAL:HG13	2.01	0.42
1:E:301:ARG:HD3	4:E:803:F6P:O2	2.19	0.42
1:F:301:ARG:HD3	4:F:803:F6P:O2	2.19	0.42
1:A:188:VAL:HG13	1:D:299:VAL:HG22	2.02	0.42
1:F:162:VAL:HG12	1:F:175:THR:CG2	2.50	0.42
1:E:162:VAL:HG12	1:E:175:THR:CG2	2.50	0.42
1:E:162:VAL:CG1	1:E:175:THR:CG2	2.97	0.41
1:F:162:VAL:CG1	1:F:175:THR:CG2	2.97	0.41
1:E:114:CYS:SG	1:E:161:LEU:HD12	2.61	0.41
1:F:114:CYS:SG	1:F:161:LEU:HD12	2.60	0.41
1:A:734:ARG:HH22	3:A:802:FBP:P2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:HG12	1:D:175:THR:CG2	2.50	0.41
1:D:734:ARG:HH22	3:D:802:FBP:P2	2.42	0.41
1:A:162:VAL:HG12	1:A:175:THR:CG2	2.50	0.41
1:E:188:VAL:HG13	1:F:299:VAL:HG22	2.02	0.41
1:E:436:HIS:O	1:E:441:GLY:HA3	2.21	0.41
1:F:436:HIS:O	1:F:441:GLY:HA3	2.21	0.41
1:E:734:ARG:CZ	3:E:802:FBP:O4P	2.67	0.41
1:A:114:CYS:SG	1:A:161:LEU:HD12	2.60	0.41
1:D:114:CYS:SG	1:D:161:LEU:HD12	2.60	0.41
1:D:409:ALA:HB3	3:D:802:FBP:H5	1.99	0.41
1:E:53:GLU:OE1	1:F:256:ARG:NH1	2.48	0.41
1:E:210:ARG:HD3	4:E:803:F6P:H5	2.03	0.41
1:E:256:ARG:NH1	1:F:53:GLU:OE1	2.48	0.41
1:F:210:ARG:HD3	4:F:803:F6P:H5	2.03	0.41
1:F:734:ARG:CZ	3:F:802:FBP:O5P	2.67	0.41
1:A:409:ALA:HB3	3:A:802:FBP:H5	1.99	0.40
1:D:210:ARG:HD3	4:D:803:F6P:H5	2.03	0.40
1:A:210:ARG:HD3	4:A:803:F6P:H5	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	742/780 (95%)	708 (95%)	33 (4%)	1 (0%)	51 82
1	D	742/780 (95%)	708 (95%)	33 (4%)	1 (0%)	51 82
1	E	742/780 (95%)	708 (95%)	33 (4%)	1 (0%)	51 82
1	F	742/780 (95%)	708 (95%)	33 (4%)	1 (0%)	51 82
All	All	2968/3120 (95%)	2832 (95%)	132 (4%)	4 (0%)	54 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	LYS
1	D	397	LYS
1	E	397	LYS
1	F	397	LYS

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	A	598/628 (95%)	594 (99%)	4 (1%)	84 95
1	D	598/628 (95%)	594 (99%)	4 (1%)	84 95
1	E	598/628 (95%)	594 (99%)	4 (1%)	84 95
1	F	598/628 (95%)	594 (99%)	4 (1%)	84 95
All	All	2392/2512 (95%)	2376 (99%)	16 (1%)	84 95

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	386	LYS
1	A	431	THR
1	A	601	ILE
1	D	246	ARG
1	D	386	LYS
1	D	431	THR
1	D	601	ILE
1	E	246	ARG
1	E	386	LYS
1	E	431	THR
1	E	601	ILE
1	F	246	ARG
1	F	386	LYS
1	F	431	THR
1	F	601	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	D	406	ASN
1	E	406	ASN
1	F	406	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	YG1	E	801	-	32,33,33	2.17	4 (12%)	37,45,45	4.06	21 (56%)
2	YG1	A	801	-	32,33,33	2.18	4 (12%)	37,45,45	4.07	21 (56%)
4	F6P	E	803	-	15,16,16	1.10	1 (6%)	17,25,25	1.85	7 (41%)
4	F6P	F	803	-	15,16,16	1.10	1 (6%)	17,25,25	1.82	6 (35%)
5	ADP	A	804	-	24,29,29	1.00	1 (4%)	29,45,45	1.67	6 (20%)
3	FBP	E	802	-	18,20,20	1.30	1 (5%)	23,32,32	1.52	1 (4%)
5	ADP	E	804	-	24,29,29	1.00	1 (4%)	29,45,45	1.67	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ADP	F	804	-	24,29,29	1.01	1 (4%)	29,45,45	1.65	6 (20%)
4	F6P	A	803	-	15,16,16	1.10	1 (6%)	17,25,25	1.85	7 (41%)
2	YG1	D	801	-	32,33,33	2.18	4 (12%)	37,45,45	4.07	21 (56%)
4	F6P	D	803	-	15,16,16	1.10	1 (6%)	17,25,25	1.81	6 (35%)
5	ADP	D	804	-	24,29,29	1.00	1 (4%)	29,45,45	1.66	6 (20%)
3	FBP	A	802	-	18,20,20	1.30	1 (5%)	23,32,32	1.52	1 (4%)
3	FBP	F	802	-	18,20,20	1.30	1 (5%)	23,32,32	1.51	1 (4%)
2	YG1	F	801	-	32,33,33	2.19	4 (12%)	37,45,45	4.06	21 (56%)
3	FBP	D	802	-	18,20,20	1.30	1 (5%)	23,32,32	1.52	1 (4%)

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	YG1	E	801	-	-	4/13/23/23	0/3/4/4
2	YG1	A	801	-	-	4/13/23/23	0/3/4/4
4	F6P	E	803	-	-	2/9/28/28	0/1/1/1
4	F6P	F	803	-	-	2/9/28/28	0/1/1/1
5	ADP	A	804	-	-	3/12/32/32	0/3/3/3
3	FBP	E	802	-	-	5/13/32/32	0/1/1/1
5	ADP	E	804	-	-	3/12/32/32	0/3/3/3
5	ADP	F	804	-	-	2/12/32/32	0/3/3/3
4	F6P	A	803	-	-	2/9/28/28	0/1/1/1
2	YG1	D	801	-	-	3/13/23/23	0/3/4/4
4	F6P	D	803	-	-	2/9/28/28	0/1/1/1
5	ADP	D	804	-	-	2/12/32/32	0/3/3/3
3	FBP	A	802	-	-	5/13/32/32	0/1/1/1
3	FBP	F	802	-	-	5/13/32/32	0/1/1/1
2	YG1	F	801	-	-	4/13/23/23	0/3/4/4
3	FBP	D	802	-	-	5/13/32/32	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	YG1	C26-C25	-7.97	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	YG1	C26-C25	-7.97	1.43	1.50
2	F	801	YG1	C26-C25	-7.97	1.43	1.50
2	E	801	YG1	C26-C25	-7.90	1.43	1.50
2	F	801	YG1	O27-C26	-5.94	1.39	1.44
2	A	801	YG1	O27-C26	-5.90	1.39	1.44
2	D	801	YG1	O27-C26	-5.90	1.39	1.44
2	E	801	YG1	O27-C26	-5.90	1.39	1.44
2	F	801	YG1	C25-N24	-4.35	1.31	1.37
2	A	801	YG1	C25-N24	-4.31	1.31	1.37
2	E	801	YG1	C25-N24	-4.31	1.31	1.37
2	D	801	YG1	C25-N24	-4.26	1.31	1.37
3	A	802	FBP	O2-C2	4.04	1.47	1.40
3	E	802	FBP	O2-C2	4.04	1.47	1.40
3	F	802	FBP	O2-C2	4.04	1.47	1.40
3	D	802	FBP	O2-C2	4.04	1.47	1.40
2	E	801	YG1	C14-C13	-3.30	1.34	1.40
2	A	801	YG1	C14-C13	-3.25	1.34	1.40
2	D	801	YG1	C14-C13	-3.25	1.34	1.40
2	F	801	YG1	C14-C13	-3.25	1.34	1.40
4	A	803	F6P	P-O3P	-2.31	1.45	1.54
4	D	803	F6P	P-O2P	-2.31	1.45	1.54
4	E	803	F6P	P-O3P	-2.31	1.45	1.54
4	F	803	F6P	P-O2P	-2.31	1.45	1.54
5	F	804	ADP	C2'-C1'	-2.11	1.50	1.53
5	A	804	ADP	C2'-C1'	-2.05	1.50	1.53
5	E	804	ADP	C2'-C1'	-2.05	1.50	1.53
5	D	804	ADP	C2'-C1'	-2.02	1.50	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	YG1	C13-C23-N24	9.69	130.63	113.31
2	F	801	YG1	C13-C23-N24	9.69	130.63	113.31
2	D	801	YG1	C13-C23-N24	9.68	130.63	113.31
2	E	801	YG1	C13-C23-N24	9.68	130.61	113.31
2	E	801	YG1	O27-C14-C15	-9.27	103.52	116.95
2	A	801	YG1	O27-C14-C15	-9.25	103.55	116.95
2	D	801	YG1	O27-C14-C15	-9.25	103.55	116.95
2	F	801	YG1	O27-C14-C15	-9.22	103.59	116.95
2	E	801	YG1	C15-C14-C13	8.73	129.82	120.48
2	A	801	YG1	C15-C14-C13	8.72	129.82	120.48
2	D	801	YG1	C15-C14-C13	8.72	129.82	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	801	YG1	C15-C14-C13	8.72	129.82	120.48
2	A	801	YG1	C16-C15-C14	-7.58	109.22	119.45
2	D	801	YG1	C16-C15-C14	-7.58	109.22	119.45
2	E	801	YG1	C16-C15-C14	-7.57	109.23	119.45
2	F	801	YG1	C16-C15-C14	-7.57	109.24	119.45
2	F	801	YG1	C30-C29-C10	-6.88	119.89	129.44
2	A	801	YG1	C30-C29-C10	-6.87	119.89	129.44
2	D	801	YG1	C30-C29-C10	-6.87	119.89	129.44
2	E	801	YG1	C30-C29-C10	-6.86	119.90	129.44
2	A	801	YG1	C23-C13-C18	6.34	130.30	119.70
2	D	801	YG1	C23-C13-C18	6.34	130.30	119.70
2	F	801	YG1	C23-C13-C18	6.33	130.28	119.70
2	E	801	YG1	C23-C13-C18	6.31	130.25	119.70
2	F	801	YG1	O21-C20-N19	-5.46	115.85	123.04
2	A	801	YG1	O21-C20-N19	-5.45	115.88	123.04
2	D	801	YG1	O21-C20-N19	-5.45	115.88	123.04
2	E	801	YG1	O21-C20-N19	-5.42	115.92	123.04
3	D	802	FBP	O2-C2-O5	5.19	119.52	109.50
3	A	802	FBP	O2-C2-O5	5.17	119.48	109.50
3	E	802	FBP	O2-C2-O5	5.16	119.46	109.50
3	F	802	FBP	O2-C2-O5	5.14	119.44	109.50
2	E	801	YG1	C10-C29-N28	4.79	128.55	120.93
2	A	801	YG1	C10-C29-N28	4.77	128.53	120.93
2	D	801	YG1	C10-C29-N28	4.77	128.53	120.93
2	F	801	YG1	C10-C29-N28	4.77	128.53	120.93
2	F	801	YG1	C09-C10-C29	-4.75	111.17	122.56
2	A	801	YG1	C09-C10-C29	-4.75	111.17	122.56
2	D	801	YG1	C09-C10-C29	-4.75	111.17	122.56
2	E	801	YG1	C09-C10-C29	-4.75	111.17	122.56
2	A	801	YG1	C23-C13-C14	-4.32	111.53	119.67
2	D	801	YG1	C23-C13-C14	-4.32	111.53	119.67
2	E	801	YG1	C23-C13-C14	-4.30	111.55	119.67
2	F	801	YG1	C23-C13-C14	-4.30	111.56	119.67
2	F	801	YG1	C17-C16-C15	4.21	124.64	119.65
2	A	801	YG1	C17-C16-C15	4.20	124.63	119.65
2	D	801	YG1	C17-C16-C15	4.20	124.63	119.65
2	E	801	YG1	C17-C16-C15	4.17	124.59	119.65
5	F	804	ADP	N3-C2-N1	-4.06	122.33	128.68
5	A	804	ADP	N3-C2-N1	-4.06	122.33	128.68
5	D	804	ADP	N3-C2-N1	-4.06	122.33	128.68
5	E	804	ADP	N3-C2-N1	-4.06	122.33	128.68
2	A	801	YG1	C08-C09-C06	-3.90	112.58	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	YG1	C08-C09-C06	-3.90	112.58	120.11
2	E	801	YG1	C08-C09-C06	-3.90	112.58	120.11
4	E	803	F6P	O1-C1-C2	3.89	120.12	111.86
2	F	801	YG1	C08-C09-C06	-3.88	112.62	120.11
4	A	803	F6P	O1-C1-C2	3.87	120.09	111.86
4	D	803	F6P	O1-C1-C2	3.87	120.09	111.86
4	F	803	F6P	O1-C1-C2	3.87	120.08	111.86
2	E	801	YG1	C17-C18-C13	-3.69	116.53	121.39
2	A	801	YG1	C17-C18-C13	-3.66	116.56	121.39
2	D	801	YG1	C17-C18-C13	-3.66	116.56	121.39
2	F	801	YG1	C17-C18-C13	-3.66	116.56	121.39
5	A	804	ADP	C3'-C2'-C1'	3.65	106.48	100.98
5	E	804	ADP	C3'-C2'-C1'	3.65	106.48	100.98
5	F	804	ADP	C3'-C2'-C1'	3.65	106.48	100.98
5	D	804	ADP	C3'-C2'-C1'	3.64	106.46	100.98
2	E	801	YG1	C11-C10-C29	3.53	128.28	119.68
2	A	801	YG1	C11-C10-C29	3.52	128.26	119.68
2	D	801	YG1	C11-C10-C29	3.52	128.26	119.68
2	F	801	YG1	C11-C10-C29	3.52	128.26	119.68
4	D	803	F6P	O2P-P-O6	-3.45	97.56	106.73
4	A	803	F6P	O3P-P-O6	-3.44	97.59	106.73
4	E	803	F6P	O3P-P-O6	-3.44	97.59	106.73
4	F	803	F6P	O2P-P-O6	-3.44	97.59	106.73
2	A	801	YG1	C07-C08-C09	-3.12	116.33	120.36
2	D	801	YG1	C07-C08-C09	-3.12	116.33	120.36
2	F	801	YG1	C07-C08-C09	-3.11	116.35	120.36
2	E	801	YG1	C07-C08-C09	-3.10	116.35	120.36
4	F	803	F6P	O2-C2-O5	-2.86	103.98	109.50
4	A	803	F6P	O2-C2-O5	-2.84	104.02	109.50
4	D	803	F6P	O2-C2-O5	-2.84	104.02	109.50
4	E	803	F6P	O2-C2-O5	-2.84	104.02	109.50
5	F	804	ADP	C4-C5-N7	-2.82	106.47	109.40
5	A	804	ADP	C4-C5-N7	-2.79	106.49	109.40
5	D	804	ADP	C4-C5-N7	-2.79	106.49	109.40
5	E	804	ADP	C4-C5-N7	-2.79	106.49	109.40
5	D	804	ADP	PA-O3A-PB	-2.77	123.32	132.83
5	F	804	ADP	PA-O3A-PB	-2.77	123.32	132.83
5	A	804	ADP	PA-O3A-PB	-2.77	123.33	132.83
5	E	804	ADP	PA-O3A-PB	-2.77	123.33	132.83
2	D	801	YG1	C25-N24-N28	2.59	113.95	111.96
2	F	801	YG1	C25-N24-N28	2.58	113.94	111.96
2	A	801	YG1	C25-N24-N28	2.58	113.93	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	YG1	C25-N24-N28	2.56	113.92	111.96
5	D	804	ADP	O2'-C2'-C1'	-2.54	101.47	110.85
5	A	804	ADP	O2'-C2'-C1'	-2.54	101.49	110.85
5	E	804	ADP	O2'-C2'-C1'	-2.54	101.49	110.85
5	F	804	ADP	O2'-C2'-C1'	-2.53	101.50	110.85
2	F	801	YG1	C11-C10-C09	2.44	120.54	117.94
2	A	801	YG1	C11-C10-C09	2.44	120.54	117.94
2	D	801	YG1	C11-C10-C09	2.44	120.54	117.94
2	E	801	YG1	C11-C10-C09	2.41	120.51	117.94
4	F	803	F6P	O5-C5-C6	2.26	114.44	109.45
4	A	803	F6P	O5-C5-C6	2.25	114.40	109.45
4	E	803	F6P	O5-C5-C6	2.24	114.38	109.45
4	D	803	F6P	O5-C5-C6	2.23	114.36	109.45
2	F	801	YG1	C17-C16-N19	-2.20	113.00	120.40
2	A	801	YG1	C17-C16-N19	-2.20	113.02	120.40
2	E	801	YG1	C17-C16-N19	-2.20	113.02	120.40
2	D	801	YG1	C17-C16-N19	-2.19	113.05	120.40
4	E	803	F6P	C6-C5-C4	-2.18	107.02	115.18
2	F	801	YG1	O21-C20-C22	2.17	126.08	122.06
4	A	803	F6P	C6-C5-C4	-2.17	107.06	115.18
4	D	803	F6P	C6-C5-C4	-2.17	107.06	115.18
4	F	803	F6P	C6-C5-C4	-2.17	107.06	115.18
2	A	801	YG1	C08-C09-C10	2.17	122.94	120.36
2	D	801	YG1	C08-C09-C10	2.17	122.94	120.36
2	E	801	YG1	C08-C09-C10	2.17	122.94	120.36
2	F	801	YG1	C08-C09-C10	2.15	122.92	120.36
2	A	801	YG1	O21-C20-C22	2.14	126.03	122.06
2	D	801	YG1	O21-C20-C22	2.14	126.03	122.06
2	E	801	YG1	O21-C20-C22	2.14	126.03	122.06
4	A	803	F6P	O3P-P-O2P	2.13	115.77	107.64
4	E	803	F6P	O3P-P-O2P	2.13	115.77	107.64
2	A	801	YG1	C22-C20-N19	2.12	118.09	114.98
2	D	801	YG1	C22-C20-N19	2.12	118.09	114.98
2	F	801	YG1	C22-C20-N19	2.10	118.06	114.98
2	E	801	YG1	C22-C20-N19	2.09	118.05	114.98
5	A	804	ADP	C2-N1-C6	2.07	122.29	118.75
5	D	804	ADP	C2-N1-C6	2.07	122.29	118.75
5	E	804	ADP	C2-N1-C6	2.07	122.29	118.75
5	F	804	ADP	C2-N1-C6	2.06	122.27	118.75
4	A	803	F6P	O2P-P-O1P	2.02	118.58	110.68
4	D	803	F6P	O3P-P-O1P	2.02	118.58	110.68
4	E	803	F6P	O2P-P-O1P	2.02	118.58	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	803	F6P	O3P-P-O1P	2.02	118.58	110.68

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	YG1	C02-C03-C04-C05
2	A	801	YG1	C09-C10-C29-C30
2	D	801	YG1	C02-C03-C04-C05
2	D	801	YG1	C09-C10-C29-C30
2	E	801	YG1	C02-C03-C04-C05
2	E	801	YG1	C09-C10-C29-C30
2	F	801	YG1	C02-C03-C04-C05
2	F	801	YG1	C04-C05-C06-C09
2	F	801	YG1	C09-C10-C29-C30
3	A	802	FBP	O1-C1-C2-O2
3	A	802	FBP	O1-C1-C2-C3
3	A	802	FBP	O1-C1-C2-O5
3	A	802	FBP	C4-C5-C6-O6
3	D	802	FBP	O1-C1-C2-O2
3	D	802	FBP	O1-C1-C2-C3
3	D	802	FBP	O1-C1-C2-O5
3	D	802	FBP	C4-C5-C6-O6
3	E	802	FBP	O1-C1-C2-O2
3	E	802	FBP	O1-C1-C2-C3
3	E	802	FBP	O1-C1-C2-O5
3	E	802	FBP	C4-C5-C6-O6
3	F	802	FBP	O1-C1-C2-O2
3	F	802	FBP	O1-C1-C2-C3
3	F	802	FBP	O1-C1-C2-O5
3	F	802	FBP	C4-C5-C6-O6
4	A	803	F6P	C4-C5-C6-O6
4	A	803	F6P	O5-C5-C6-O6
4	D	803	F6P	C4-C5-C6-O6
4	D	803	F6P	O5-C5-C6-O6
4	E	803	F6P	C4-C5-C6-O6
4	E	803	F6P	O5-C5-C6-O6
4	F	803	F6P	C4-C5-C6-O6
4	F	803	F6P	O5-C5-C6-O6
3	A	802	FBP	O5-C5-C6-O6
3	D	802	FBP	O5-C5-C6-O6
3	E	802	FBP	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	802	FBP	O5-C5-C6-O6
5	A	804	ADP	O4'-C4'-C5'-O5'
5	D	804	ADP	O4'-C4'-C5'-O5'
5	E	804	ADP	O4'-C4'-C5'-O5'
5	F	804	ADP	O4'-C4'-C5'-O5'
2	A	801	YG1	C04-C05-C06-C09
2	E	801	YG1	C04-C05-C06-C09
2	A	801	YG1	O01-C02-C03-C04
2	D	801	YG1	O01-C02-C03-C04
2	E	801	YG1	O01-C02-C03-C04
2	F	801	YG1	O01-C02-C03-C04
5	A	804	ADP	C3'-C4'-C5'-O5'
5	D	804	ADP	C3'-C4'-C5'-O5'
5	E	804	ADP	C3'-C4'-C5'-O5'
5	F	804	ADP	C3'-C4'-C5'-O5'
5	A	804	ADP	PA-O3A-PB-O1B
5	E	804	ADP	PA-O3A-PB-O1B

There are no ring outliers.

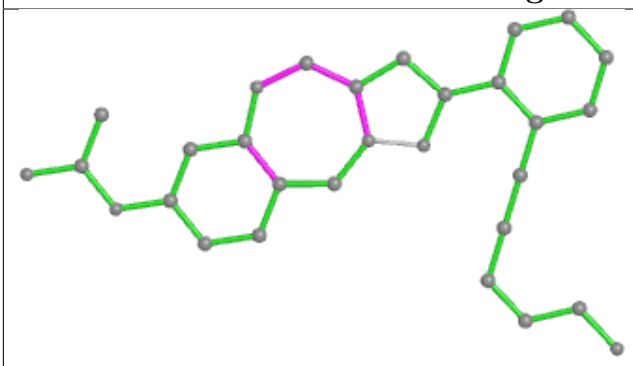
12 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	YG1	7	0
2	A	801	YG1	7	0
4	E	803	F6P	6	0
4	F	803	F6P	6	0
3	E	802	FBP	6	0
4	A	803	F6P	6	0
2	D	801	YG1	7	0
4	D	803	F6P	6	0
3	A	802	FBP	6	0
3	F	802	FBP	6	0
2	F	801	YG1	7	0
3	D	802	FBP	6	0

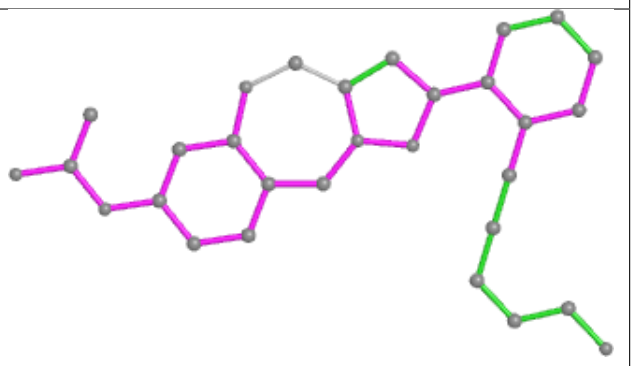
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

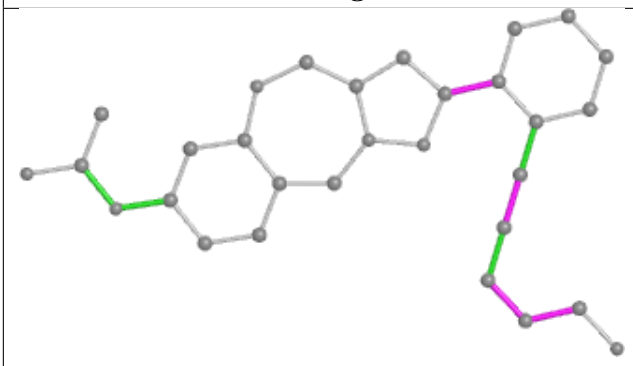
Ligand YG1 E 801



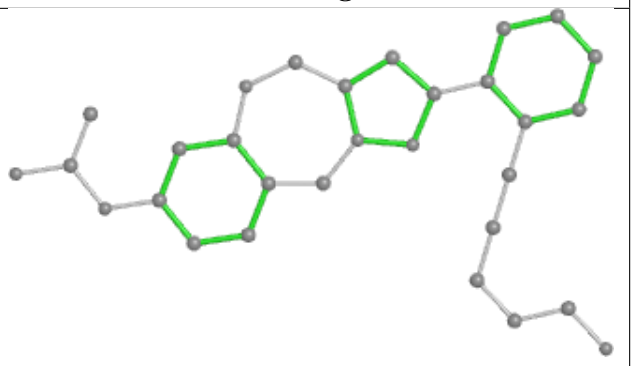
Bond lengths



Bond angles

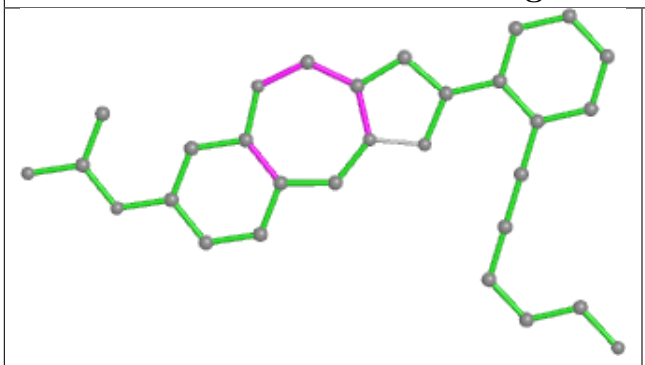


Torsions

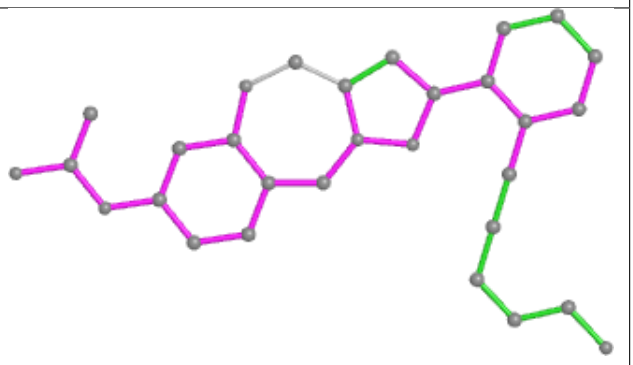


Rings

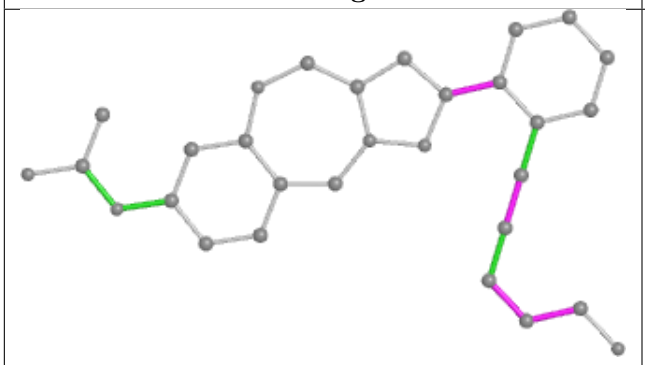
Ligand YG1 A 801



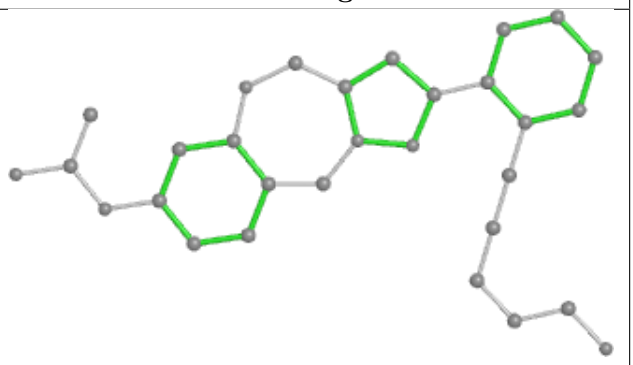
Bond lengths



Bond angles

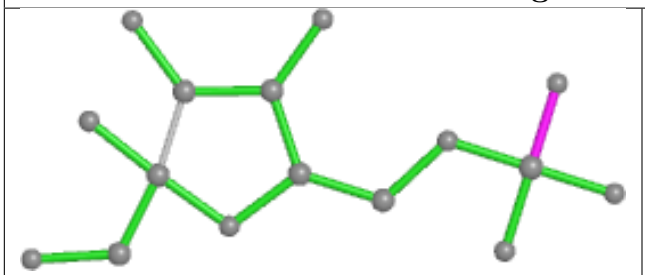


Torsions



Rings

Ligand F6P E 803



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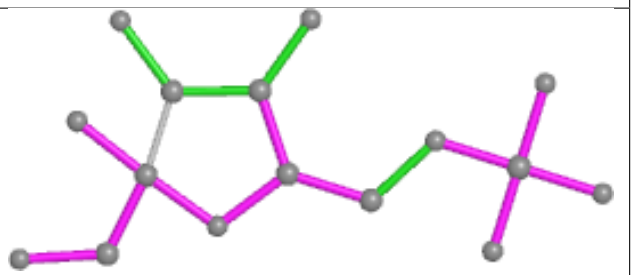
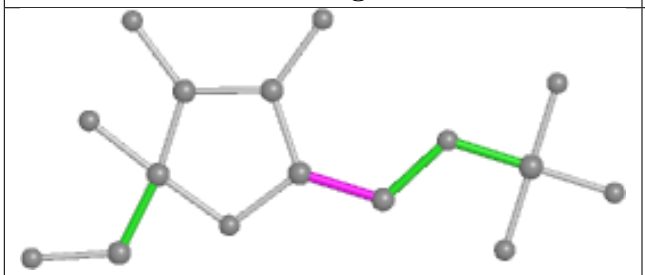


Bond angles



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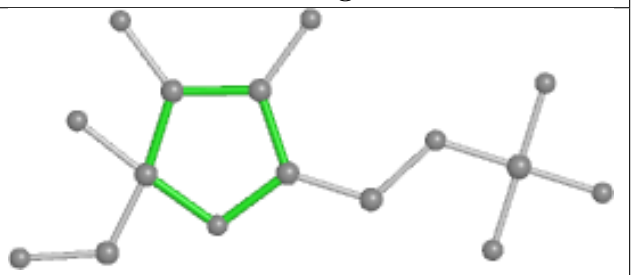
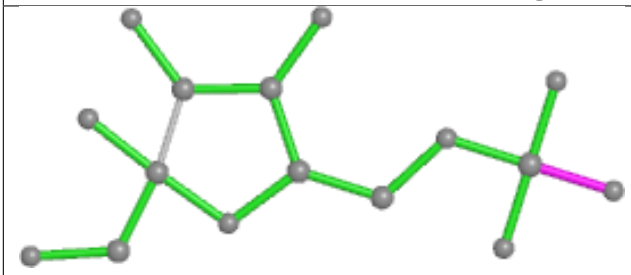


Rings

Ligand F6P F 803



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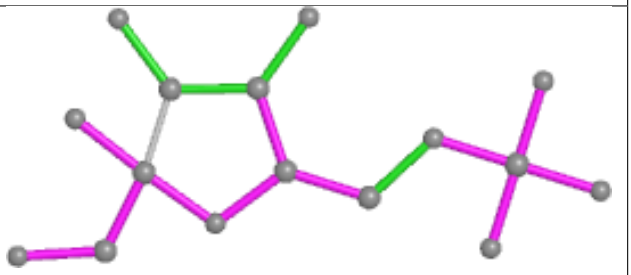
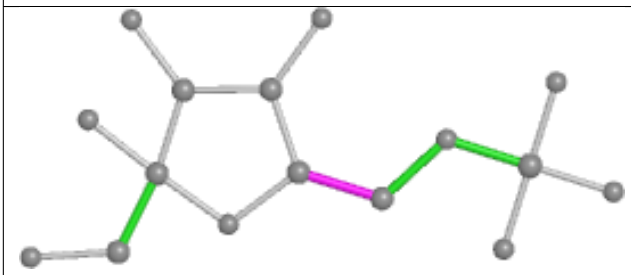


Bond angles



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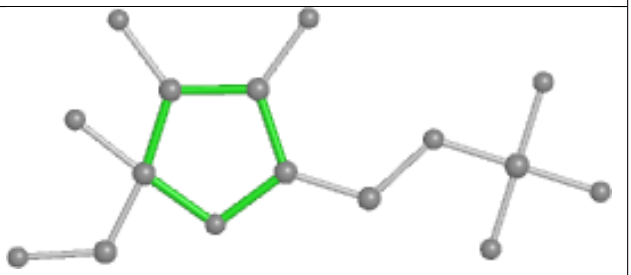
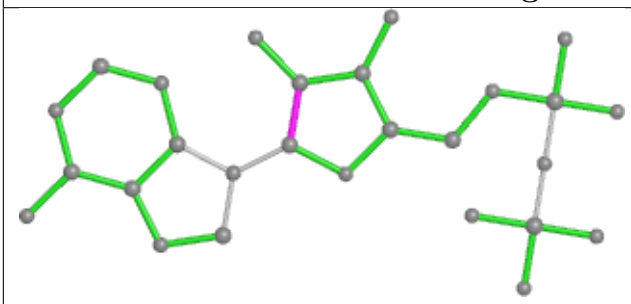


Rings

Ligand ADP A 804



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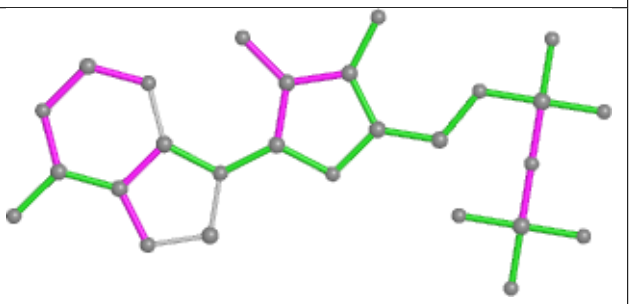

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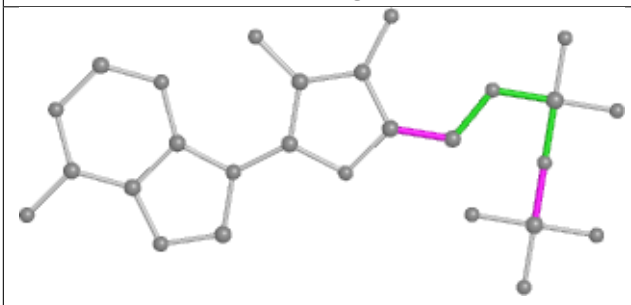

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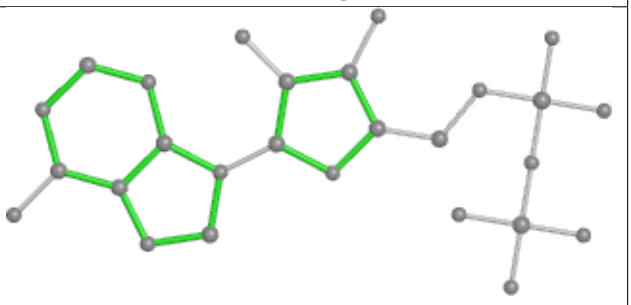
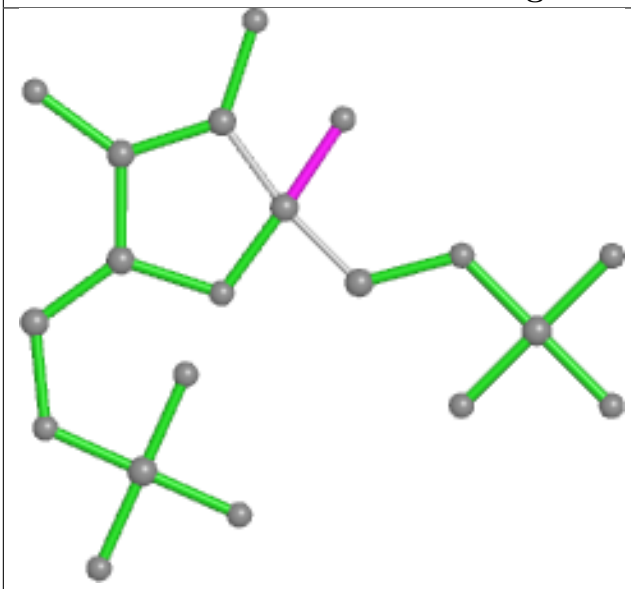


Rings

Ligand FBP E 802



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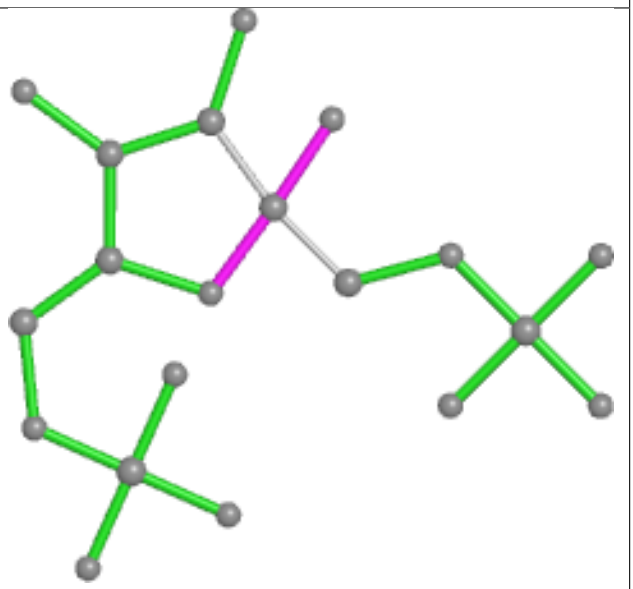

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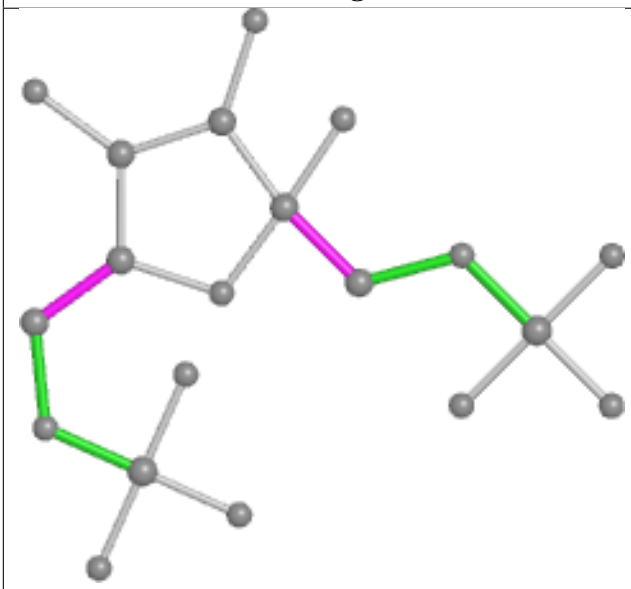

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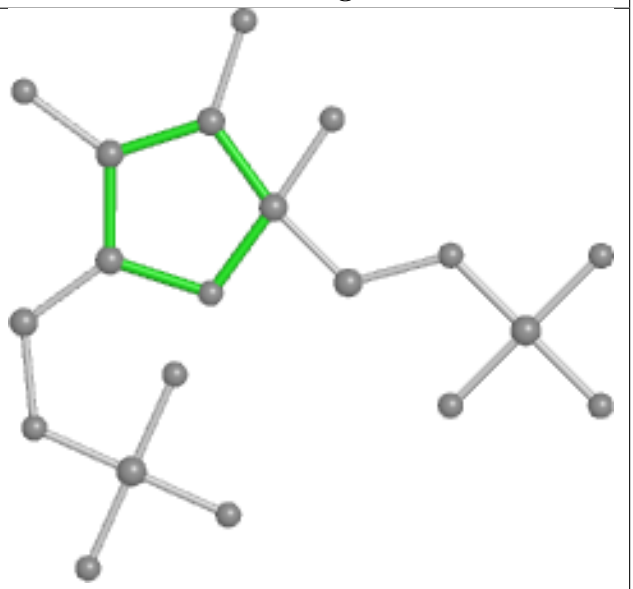
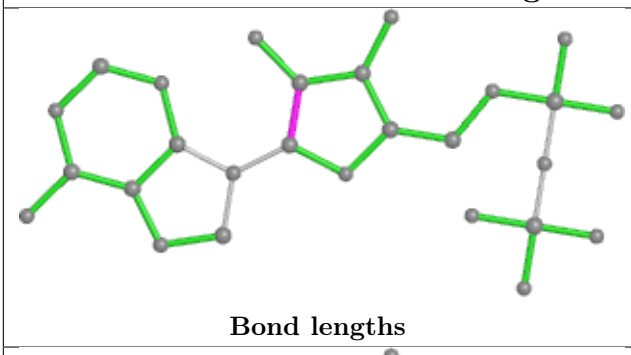


Rings

Ligand ADP E 804



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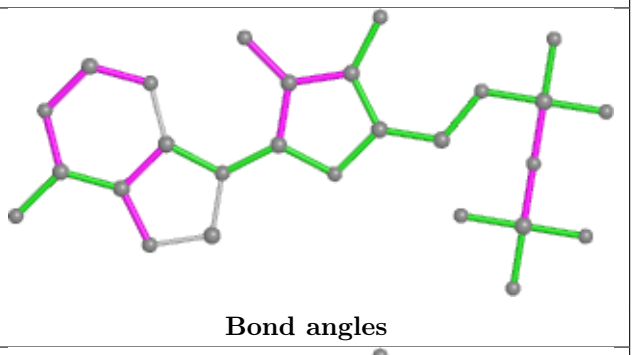
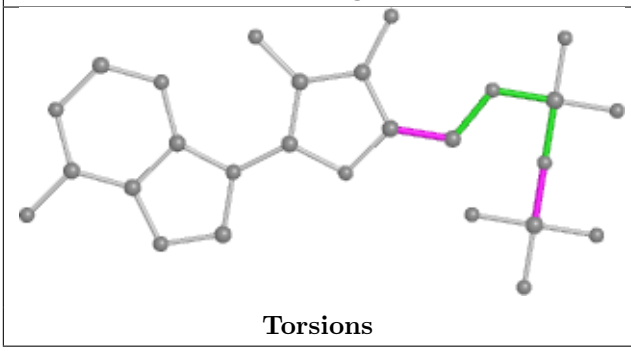


Bond angles



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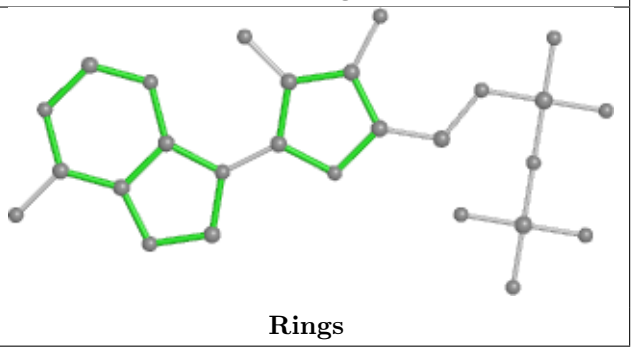
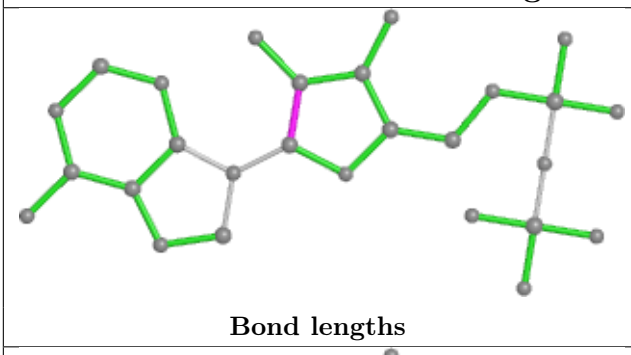


Rings

Ligand ADP F 804



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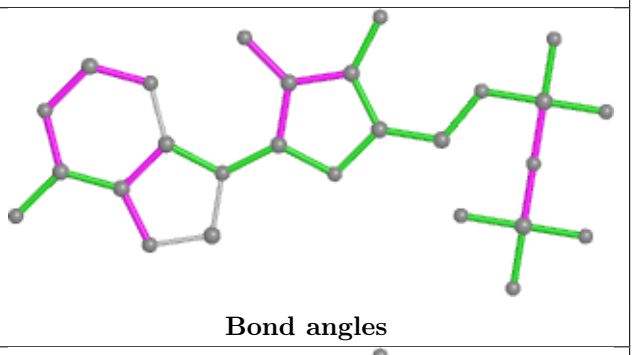
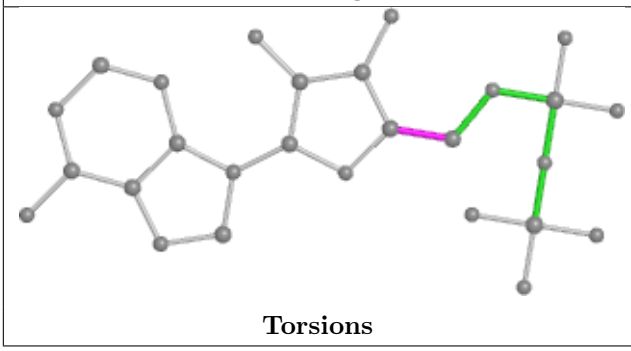


Bond angles



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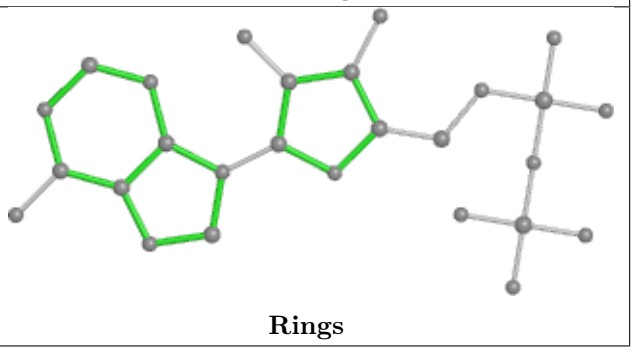
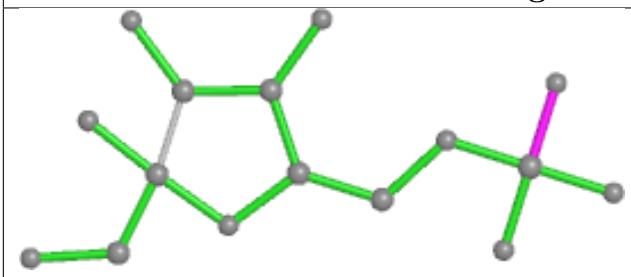


Rings

Ligand F6P A 803



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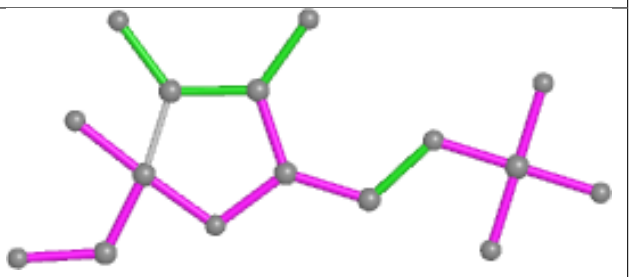

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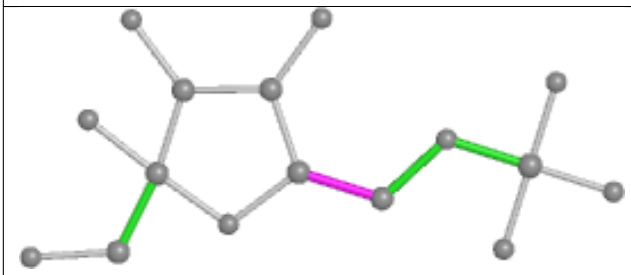

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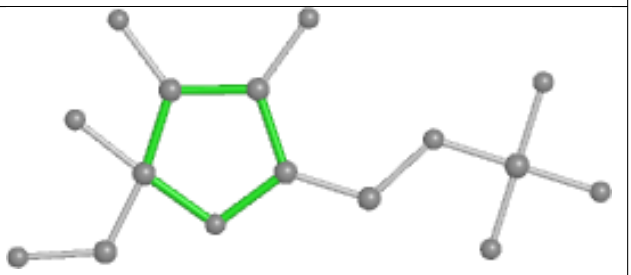
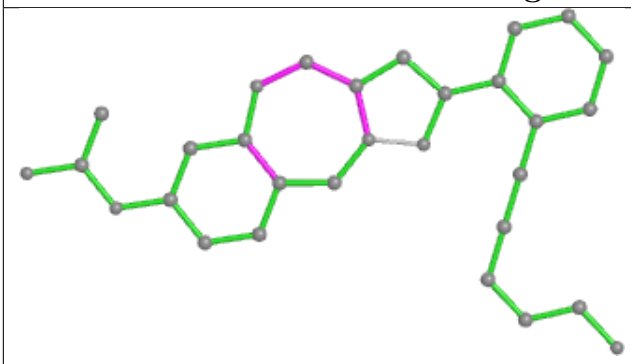


Rings

Ligand YG1 D 801



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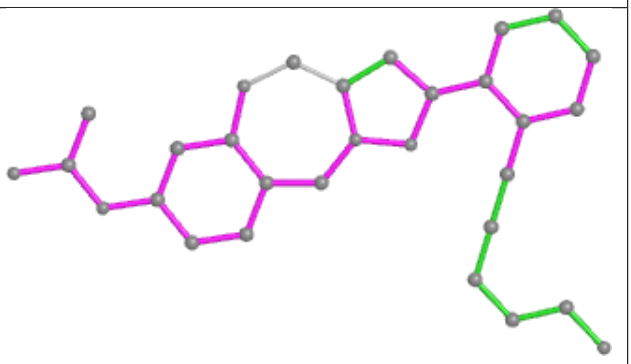
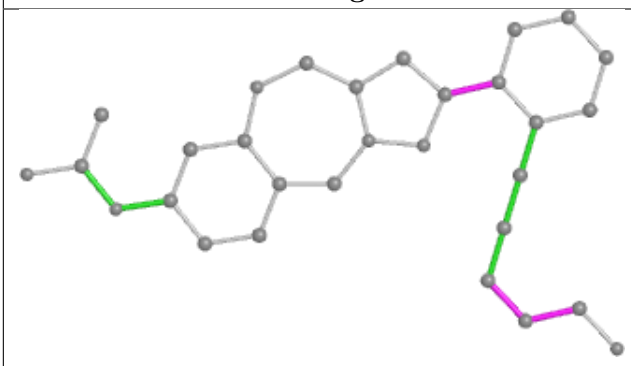


Bond angles



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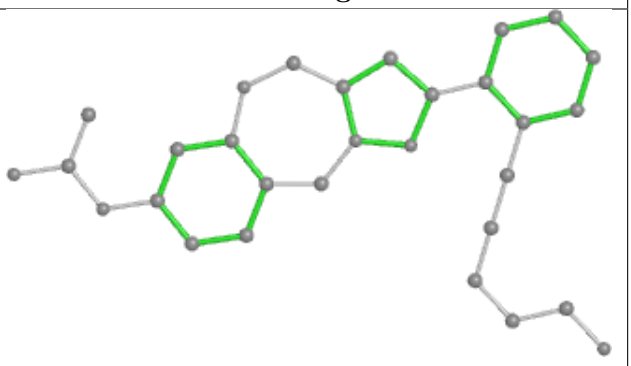
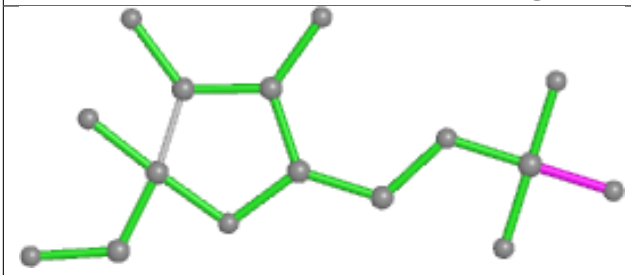


Rings

Ligand F6P D 803



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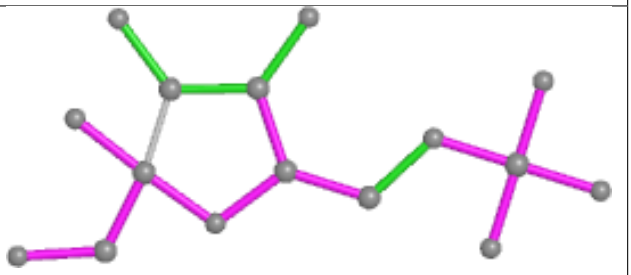
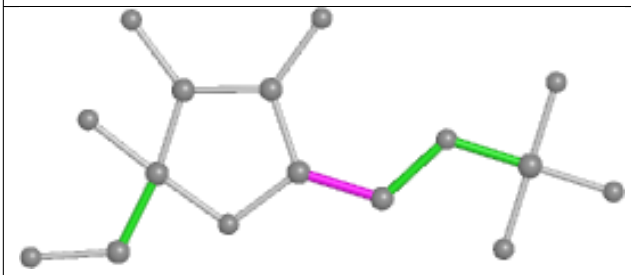


Bond angles



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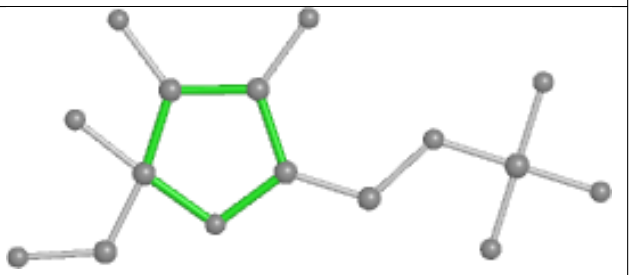
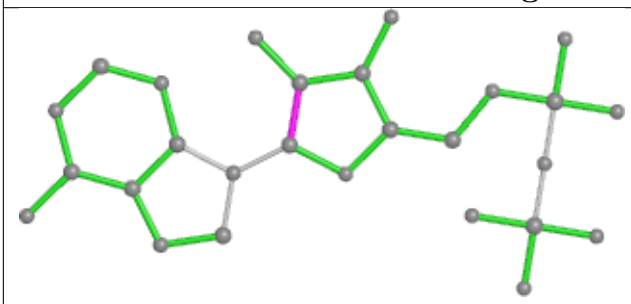


Rings

Ligand ADP D 804



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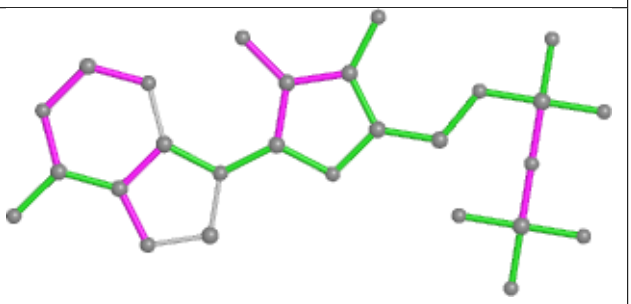
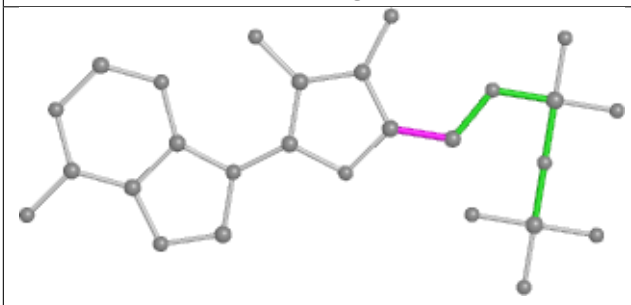


Bond angles



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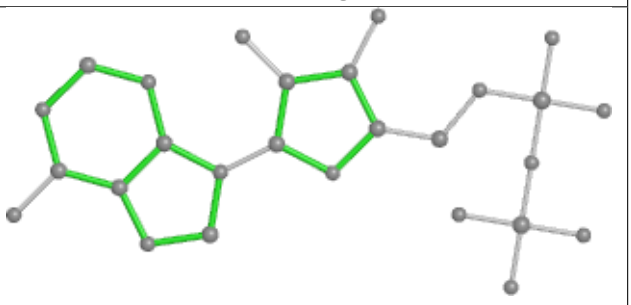
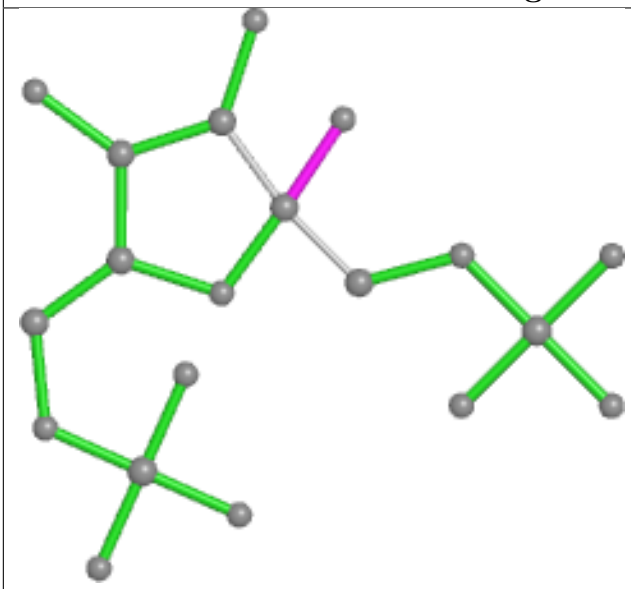


Rings

Ligand FBP A 802



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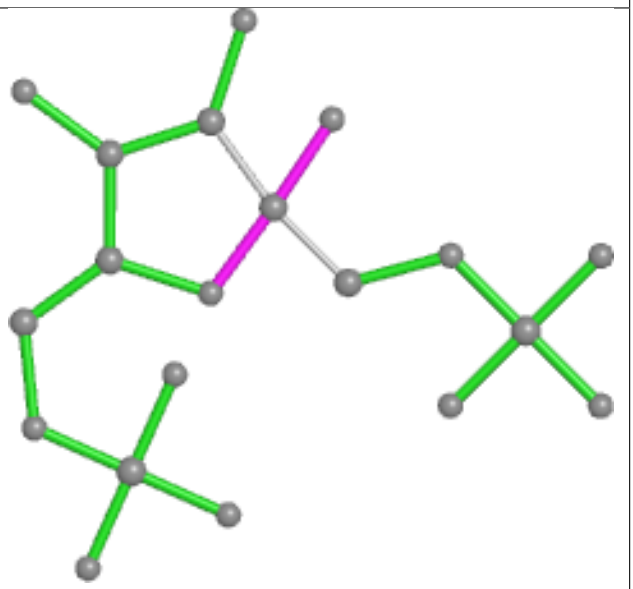

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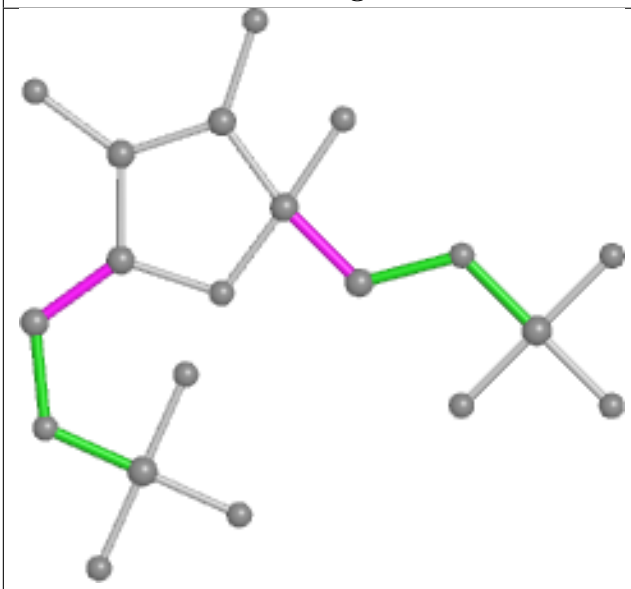

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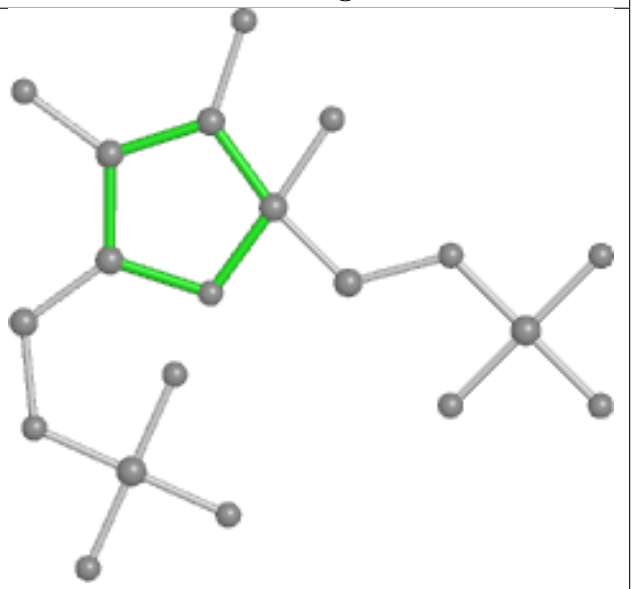
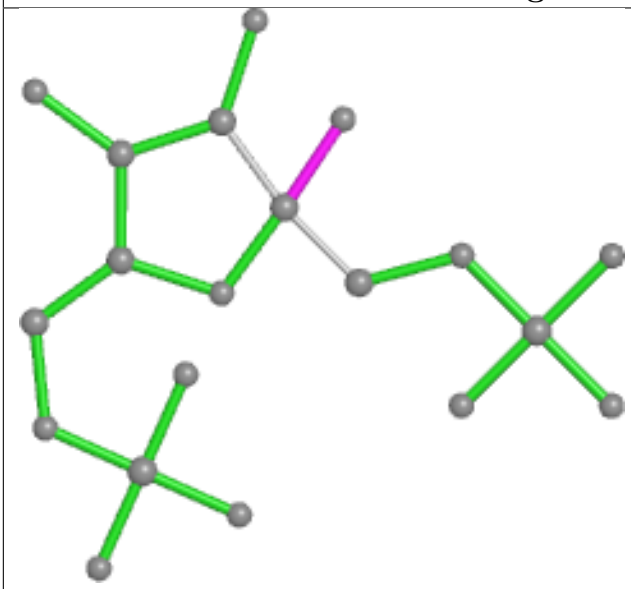


Rings

Ligand FBP F 802



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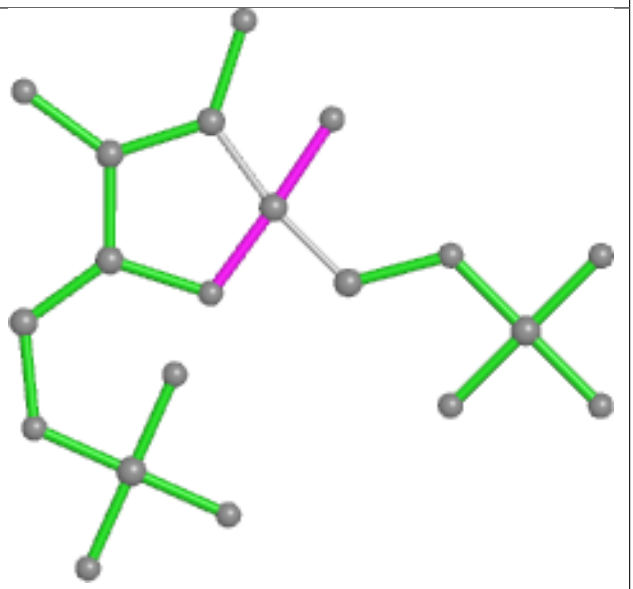
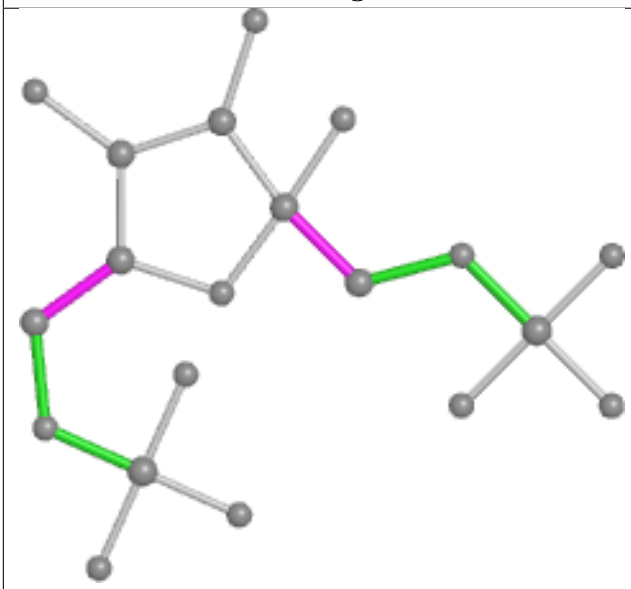


Bond angles



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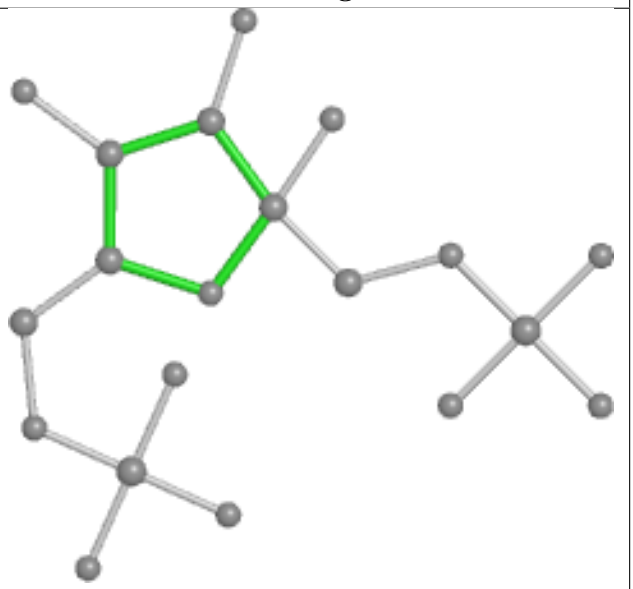
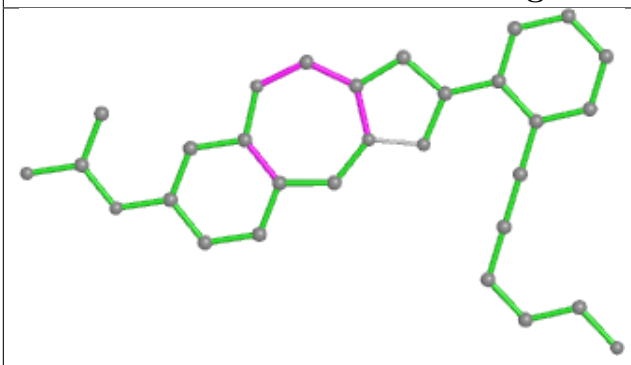


Rings

Ligand YG1 F 801



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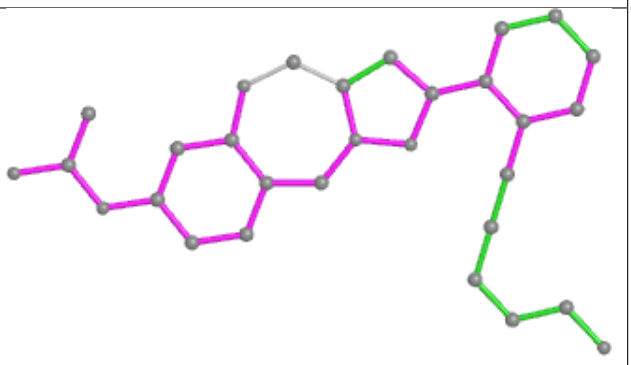
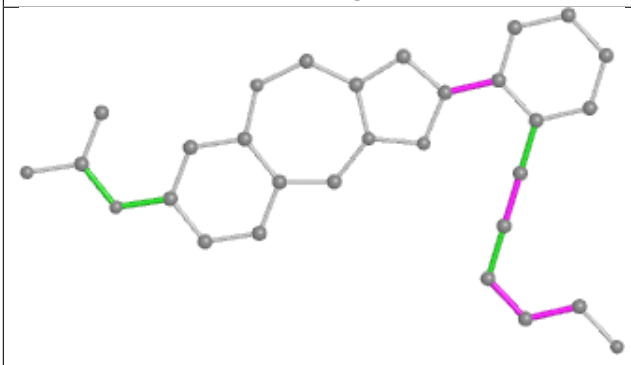


Bond angles



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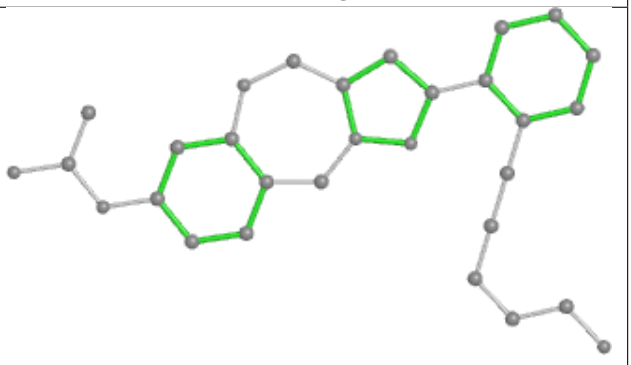
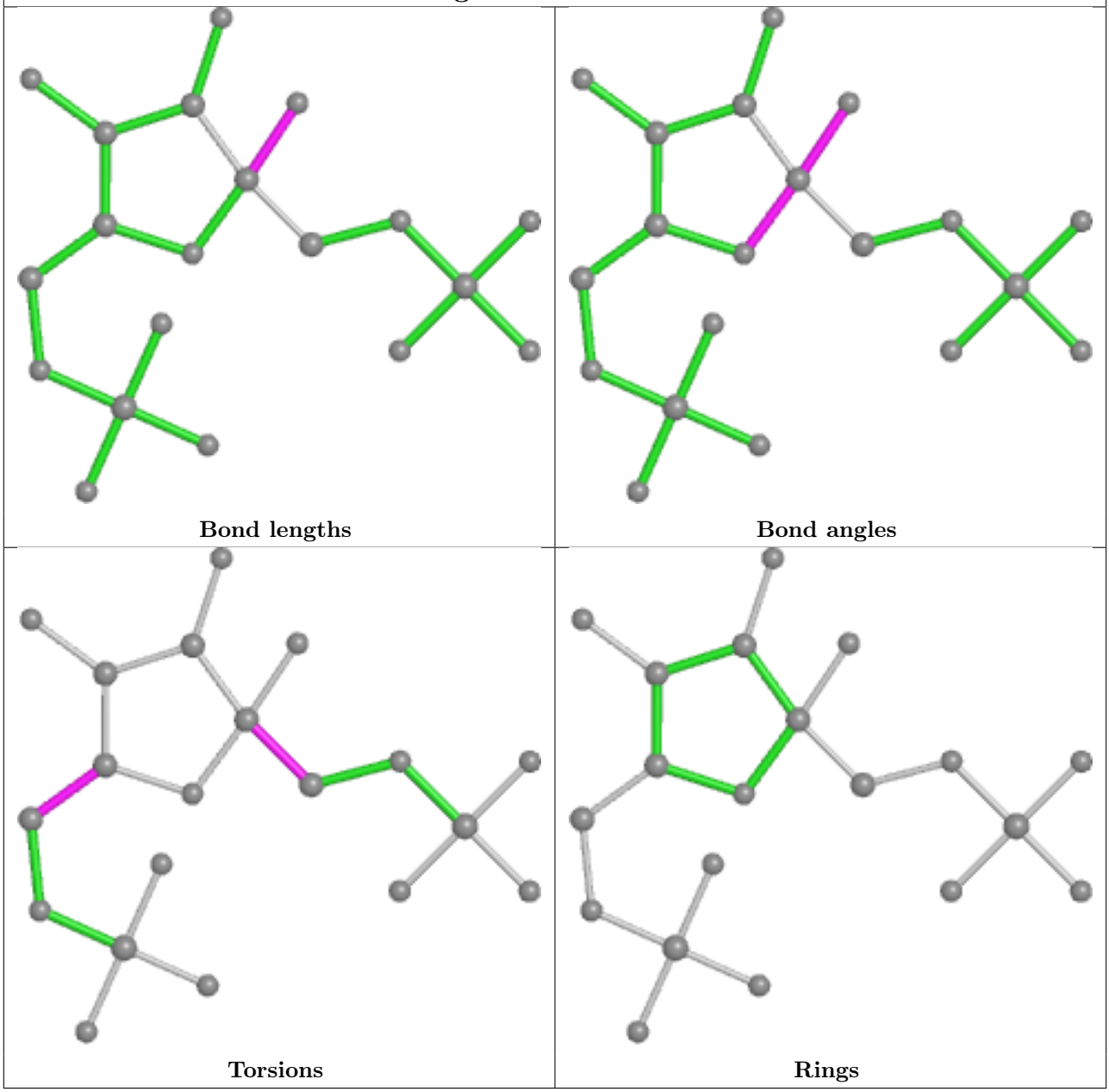


Rings

Ligand FBP D 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

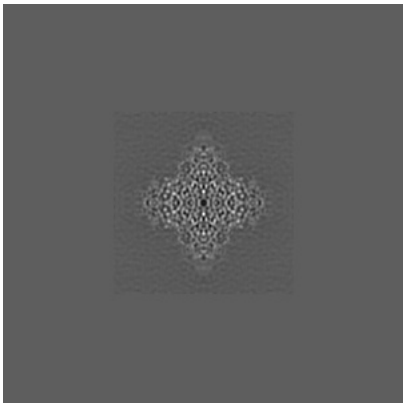
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23544. These allow visual inspection of the internal detail of the map and identification of artifacts.

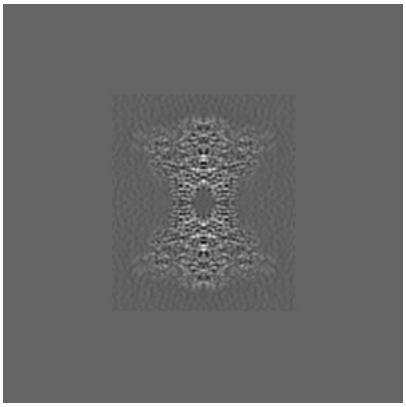
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

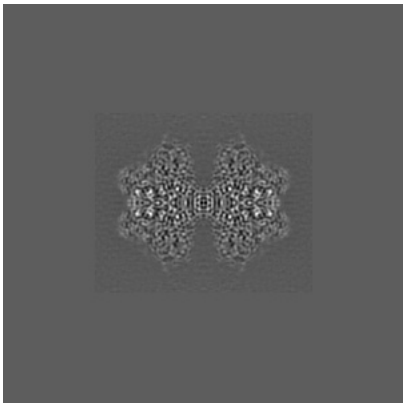
6.1.1 Primary map



X



Y

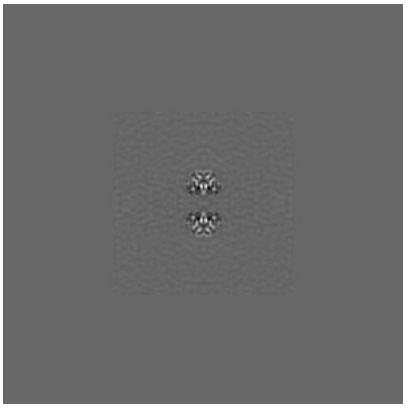


Z

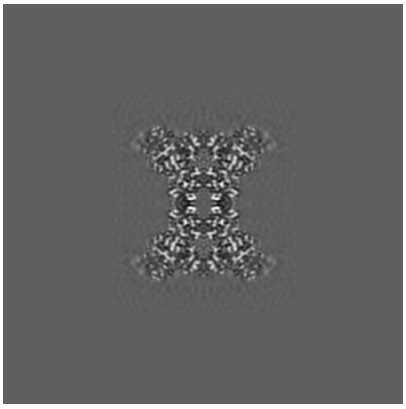
The images above show the map projected in three orthogonal directions.

6.2 Central slices

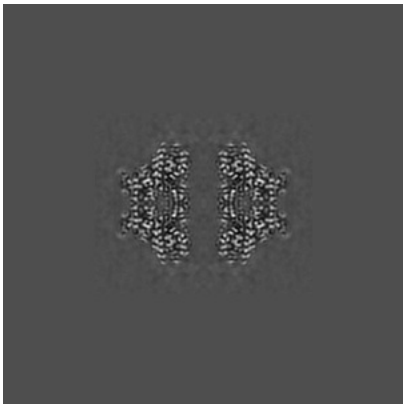
6.2.1 Primary map



X Index: 150



Y Index: 150

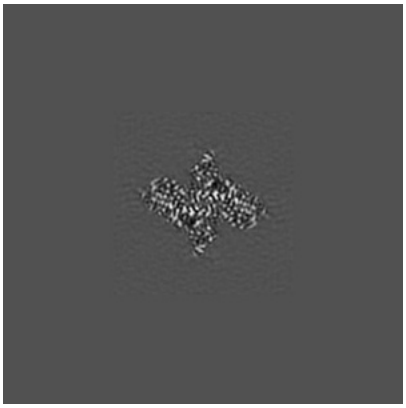


Z Index: 150

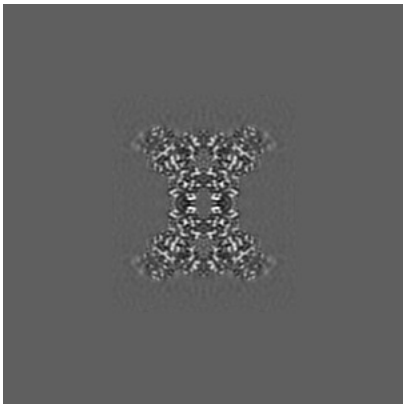
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

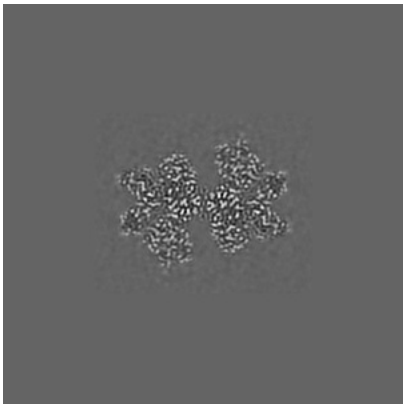
6.3.1 Primary map



X Index: 125



Y Index: 150

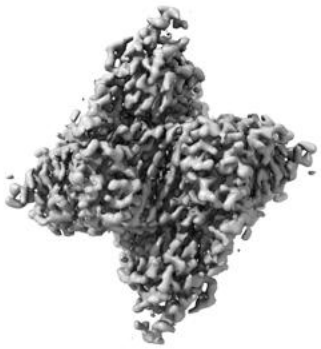


Z Index: 158

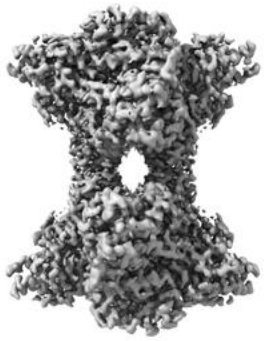
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

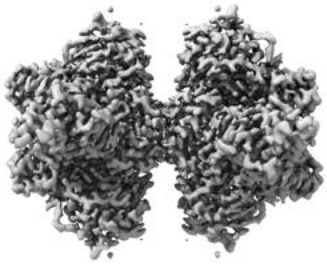
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

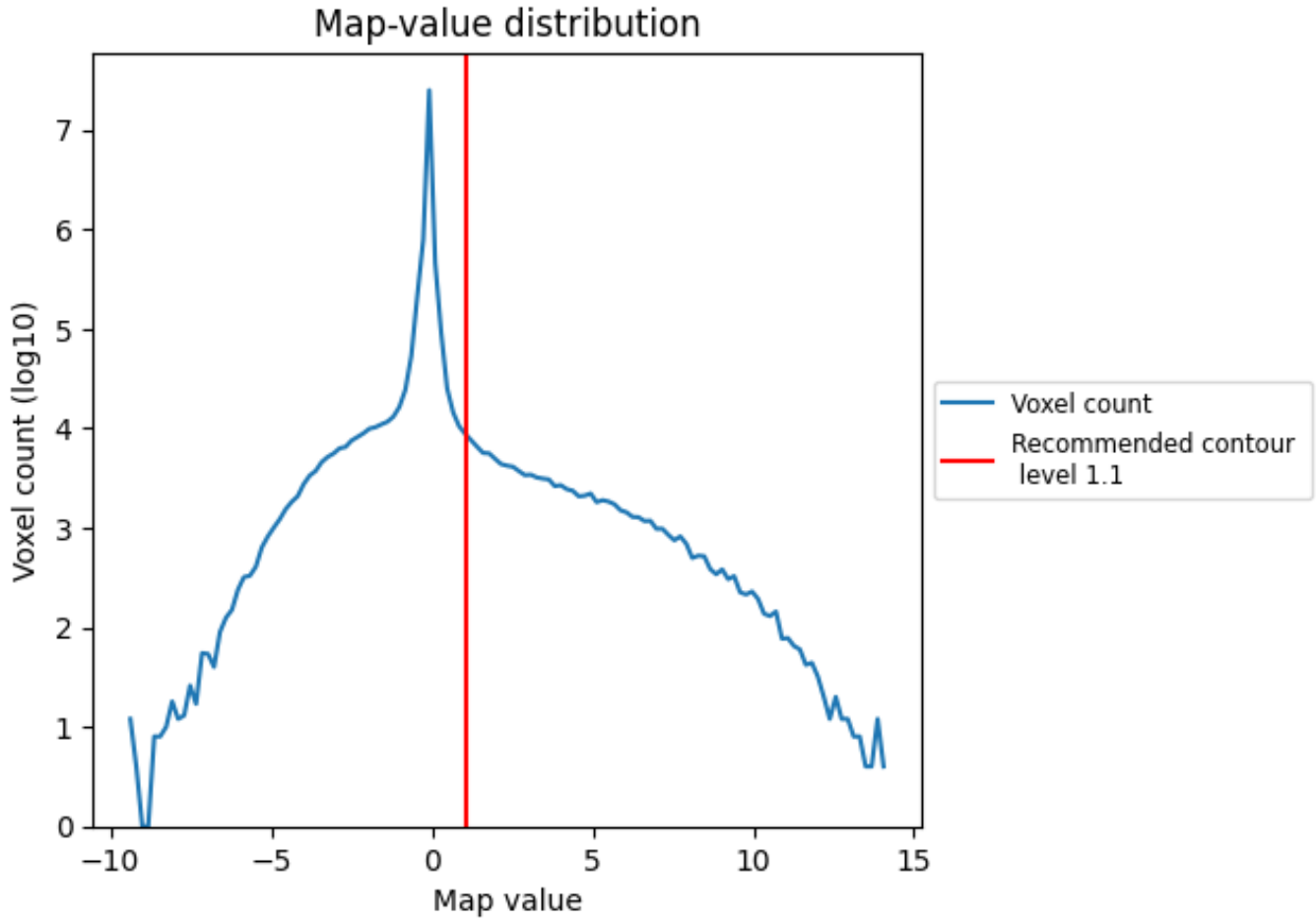
6.5 Mask visualisation (i)

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

7 Map analysis

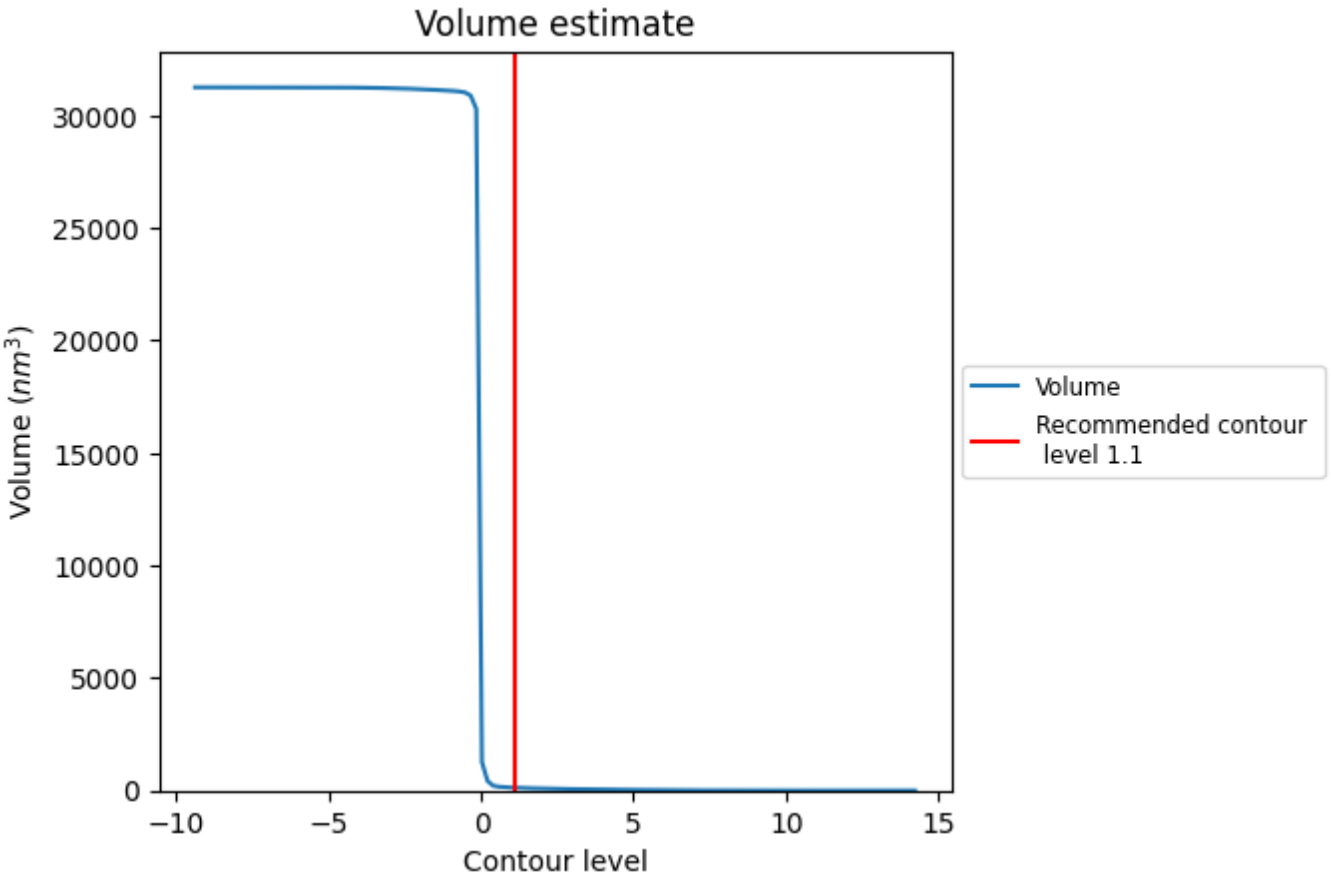
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

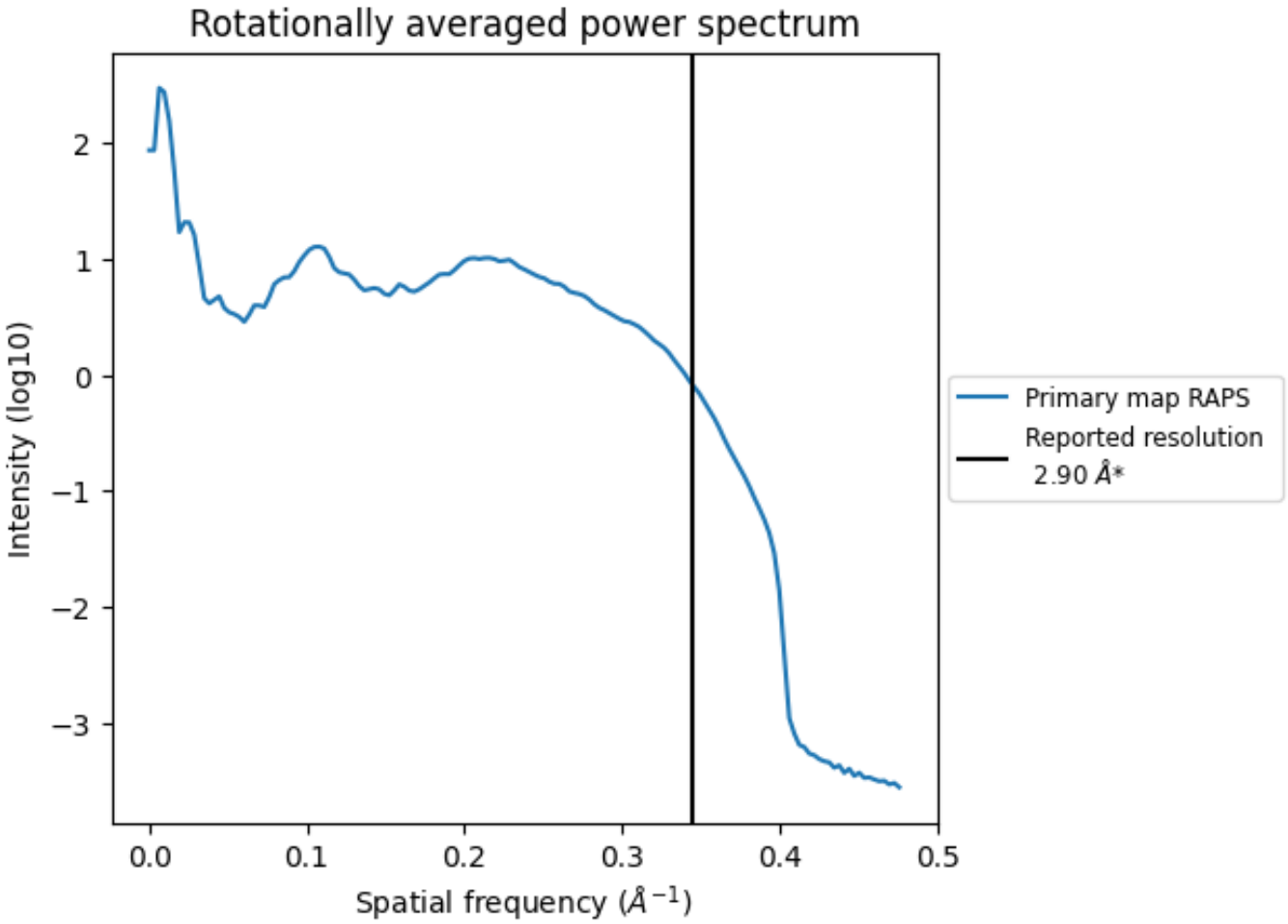
7.2 Volume estimate



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 116 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

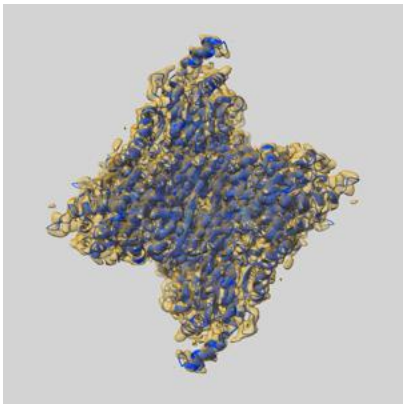
8 Fourier-Shell correlation

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

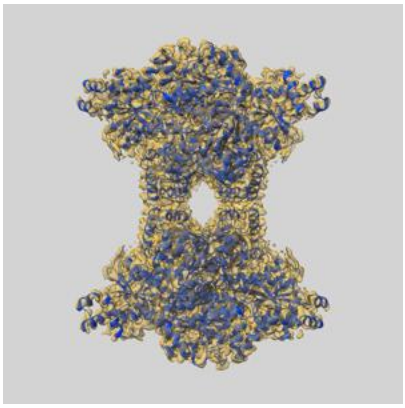
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23544 and PDB model 7LW1. Per-residue inclusion information can be found in section 3 on page 8.

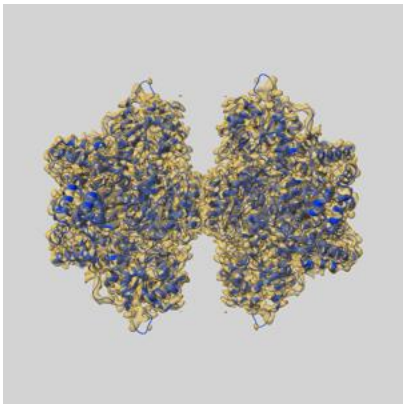
9.1 Map-model overlay



X



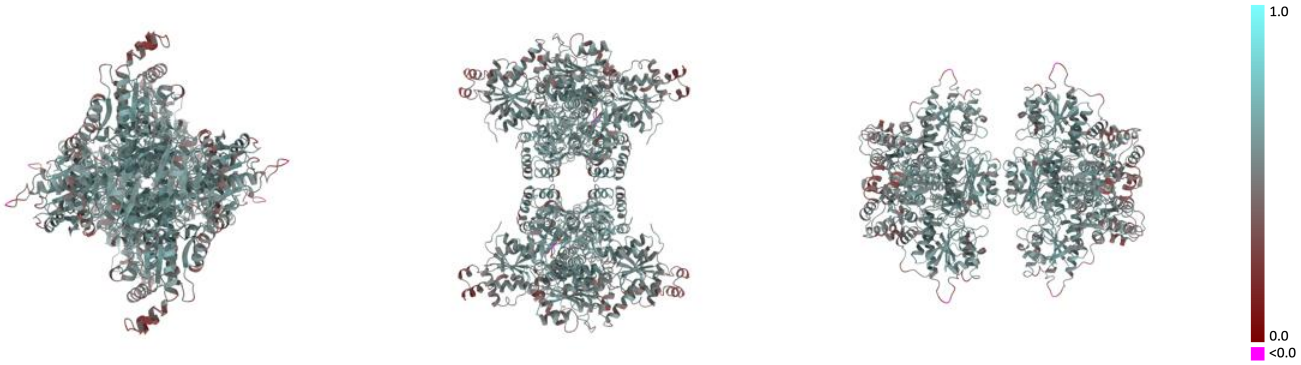
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

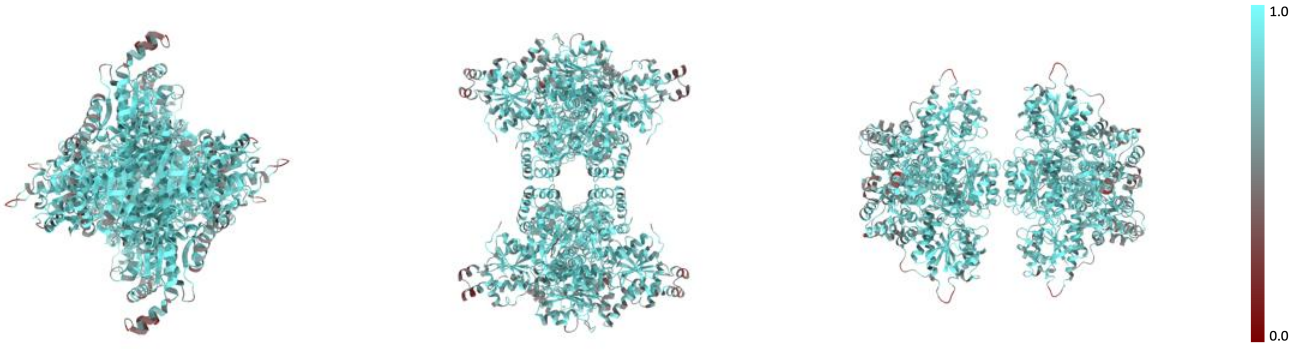
9.2 Q-score mapped to coordinate model



X Y Z

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

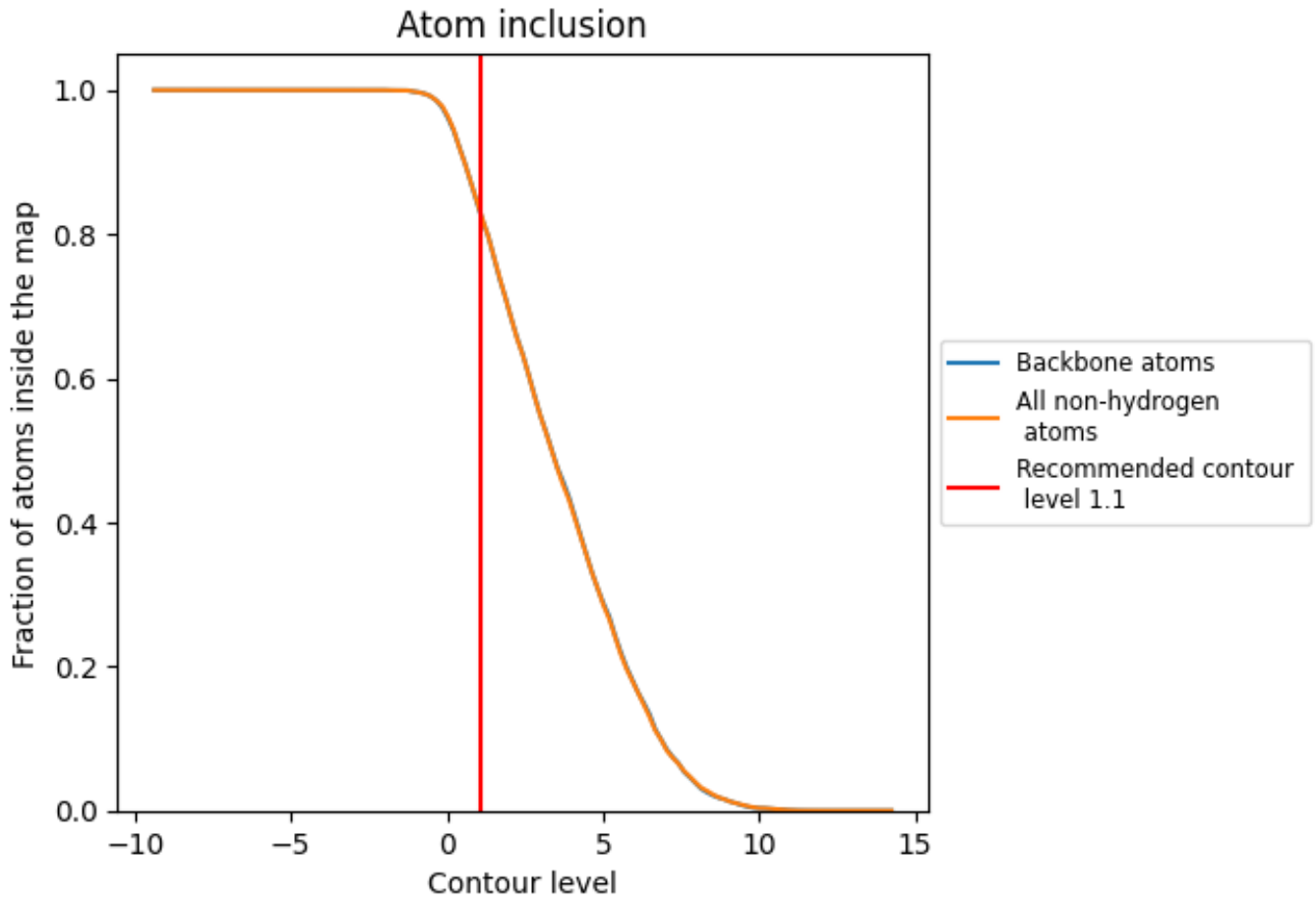
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8268	0.5430
A	0.8330	0.5430
D	0.8316	0.5420
E	0.8314	0.5430
F	0.8311	0.5430