



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:28 pm BST

PDB ID : 3IQZ  
Title : Structure of F420 dependent methylene-tetrahydromethanopterin dehydrogenase in complex with methylene-tetrahydromethanopterin  
Authors : Ceh, K.E.; Demmer, U.; Warkentin, E.; Moll, J.; Thauer, R.K.; Shima, S.; Ermler, U.  
Deposited on : 2009-08-21  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

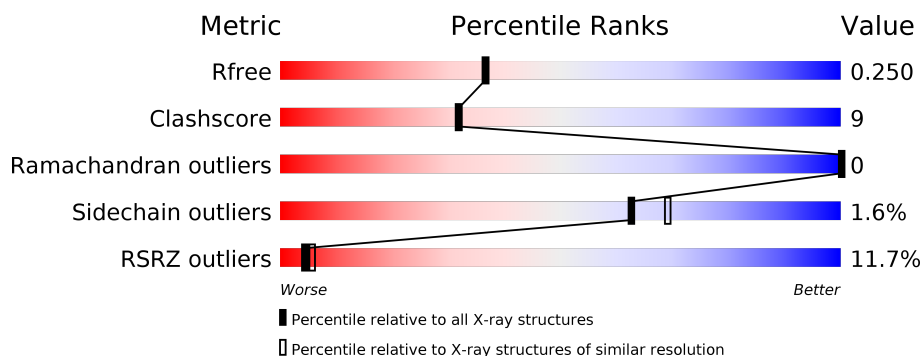
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	283	<div> <div>20%</div> <div> <div>88%</div> <div>12%</div> </div> </div>
1	B	283	<div> <div>4%</div> <div> <div>85%</div> <div>13%</div> </div> </div>
1	C	283	<div> <div>9%</div> <div> <div>83%</div> <div>16%</div> </div> </div>
1	D	283	<div> <div>18%</div> <div> <div>86%</div> <div>14%</div> </div> </div>
1	E	283	<div> <div>10%</div> <div> <div>82%</div> <div>16%</div> </div> </div>
1	F	283	<div> <div>8%</div> <div> <div>85%</div> <div>14%</div> </div> </div>

2 Entry composition ⓘ

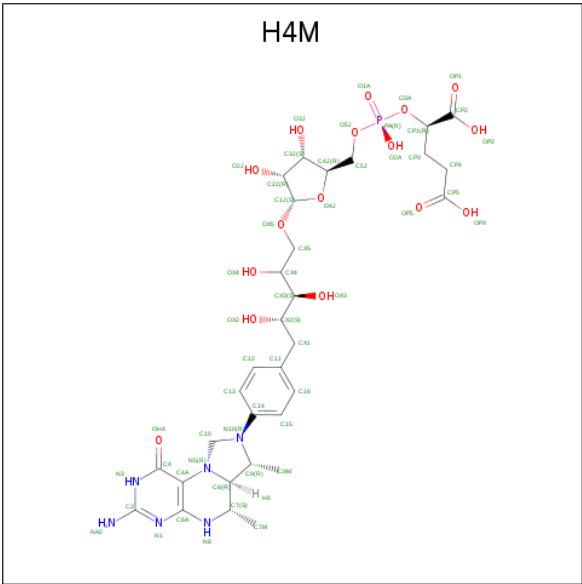
There are 6 unique types of molecules in this entry. The entry contains 13675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 F420-dependent methylenetetrahydromethanopterin dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2187	1373	357	437	20			
1	B	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	C	282	Total	C	N	O	S	0	3	0
			2202	1382	358	442	20			
1	D	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	E	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	F	282	Total	C	N	O	S	0	1	0
			2188	1373	357	439	19			

- Molecule 2 is 5,10-DIMETHYLENE TETRAHYDROMETHANOPTERIN (three-letter code: H4M) (formula: C<sub>31</sub>H<sub>45</sub>N<sub>6</sub>O<sub>16</sub>P).

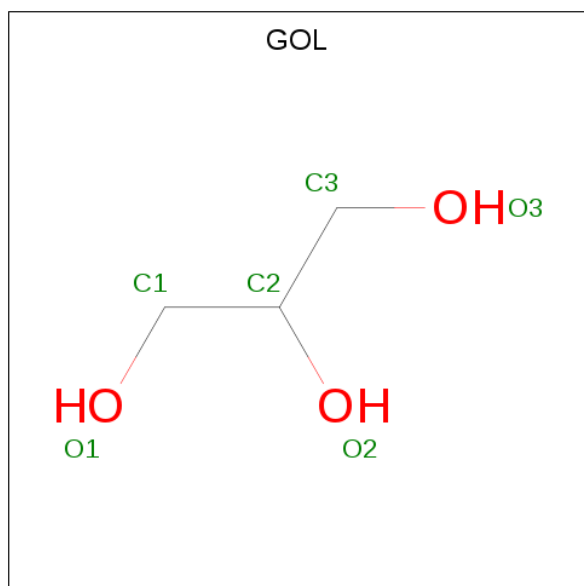


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	B	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	C	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	D	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	E	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
2	F	1	Total	C	N	O	P	0	0
			45	26	6	12	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0

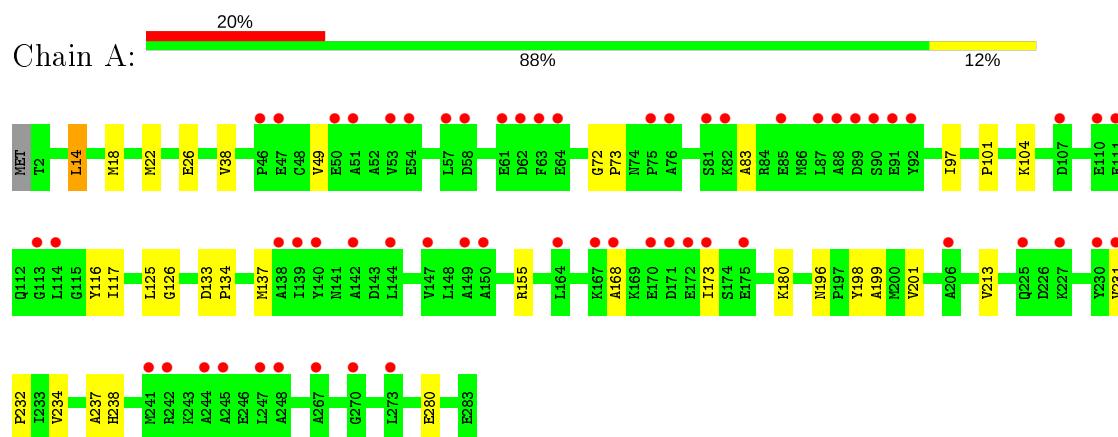
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	79	Total O 79 79	0	0
6	C	56	Total O 56 56	0	0
6	D	18	Total O 18 18	0	0
6	E	42	Total O 42 42	0	0
6	F	48	Total O 48 48	0	0

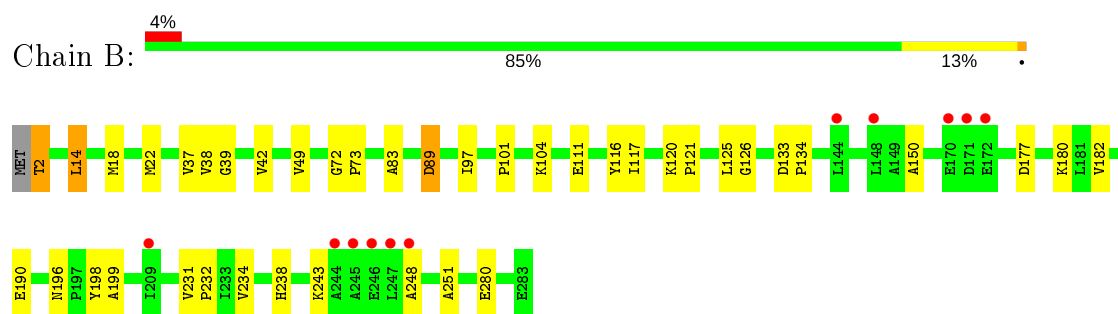
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

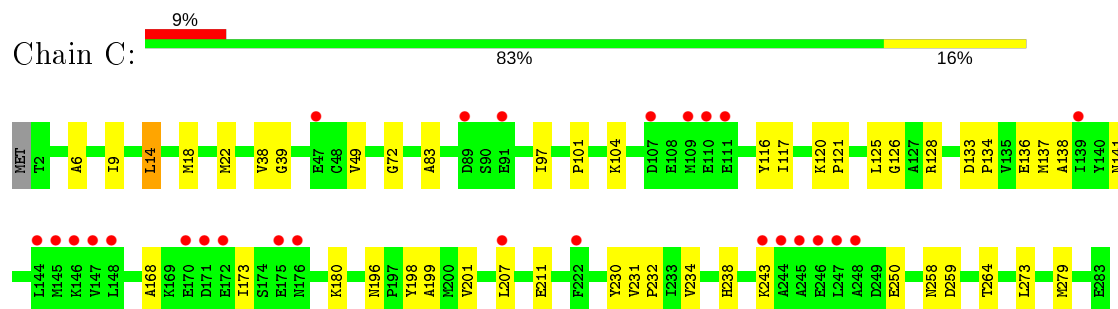
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



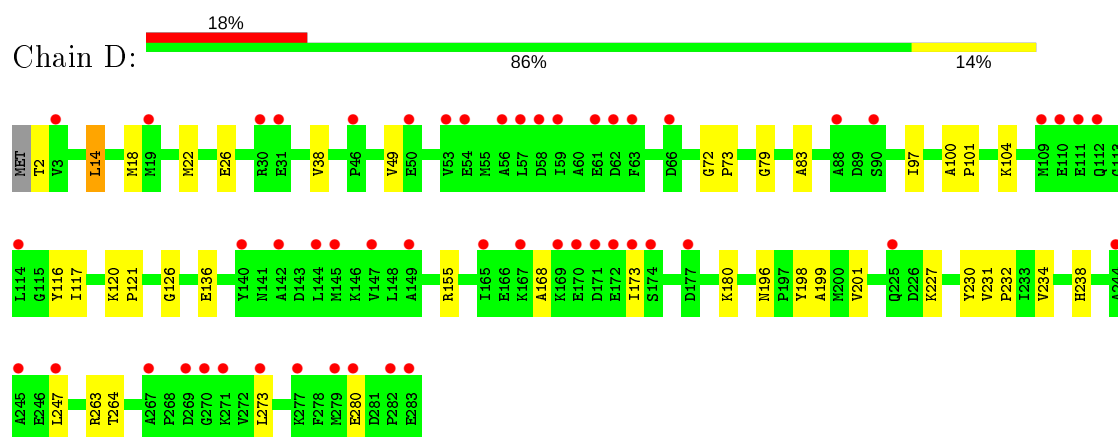
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



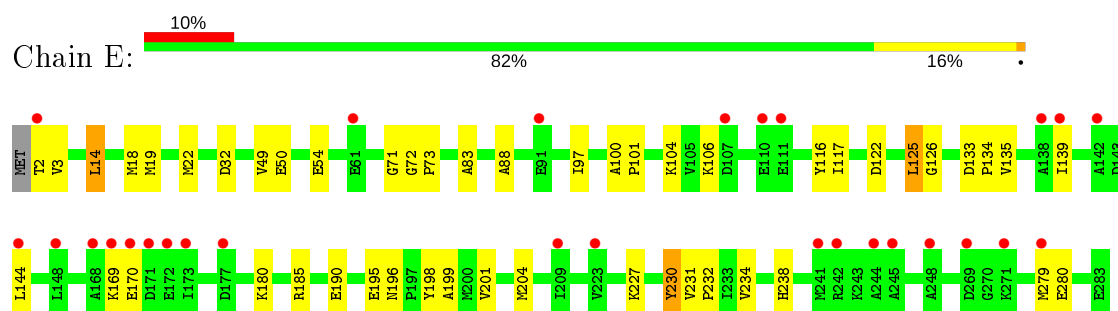
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



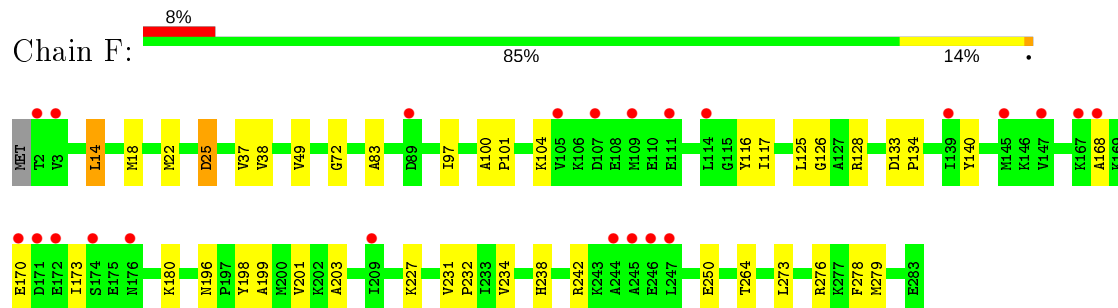
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.81Å 167.70Å 95.86Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	94.00 – 2.10 47.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (94.00-2.10) 96.9 (47.06-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.198 , 0.226 0.222 , 0.250	Depositor DCC
$R_{free}$ test set	5502 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, H4M, CA, NA

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	0.64	0/2223	0.67	0/2999
1	B	0.92	2/2215 (0.1%)	0.81	1/2989 (0.0%)
1	C	0.84	2/2241 (0.1%)	0.79	0/3023
1	D	0.62	0/2215	0.69	0/2989
1	E	0.80	0/2215	0.82	0/2989
1	F	0.84	2/2224 (0.1%)	0.80	3/3001 (0.1%)
All	All	0.79	6/13333 (0.0%)	0.77	4/17990 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	ALA	CA-CB	6.08	1.65	1.52
1	F	203	ALA	CA-CB	6.07	1.65	1.52
1	B	251	ALA	CA-CB	5.46	1.64	1.52
1	F	140	TYR	CG-CD1	5.26	1.46	1.39
1	C	250	GLU	CB-CG	-5.21	1.42	1.52
1	B	182	VAL	CB-CG2	5.02	1.63	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	242	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	F	242	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	89	ASP	CB-CG-OD2	6.03	123.73	118.30
1	F	25	ASP	CB-CG-OD1	5.56	123.30	118.30

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	2187	0	2166	39	0
1	B	2182	0	2157	43	2
1	C	2202	0	2177	53	0
1	D	2182	0	2157	40	0
1	E	2182	0	2157	55	3
1	F	2188	0	2163	40	2
2	A	45	0	37	9	0
2	B	45	0	37	0	0
2	C	45	0	37	10	0
2	D	45	0	37	6	0
2	E	45	0	37	1	0
2	F	45	0	37	7	0
3	B	1	0	0	0	1
4	B	6	0	8	3	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	29	0	0	0	0
6	B	79	0	0	8	0
6	C	56	0	0	1	0
6	D	18	0	0	1	0
6	E	42	0	0	5	0
6	F	48	0	0	2	0
All	All	13675	0	13207	236	5

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 9.

All (236) 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:C:137[B]:MET:CE	1:E:19:MET:HE1	1.60	1.31
1:B:18:MET:CE	1:F:22:MET:HE1	1.63	1.28
4:B:286:GOL:C3	6:B:365:HOH:O	1.86	1.24
1:A:137[B]:MET:HE2	2:A:284:H4M:H4	1.10	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:H4M:H9	1:D:26:GLU:O	1.54	1.07
4:B:286:GOL:H32	6:B:365:HOH:O	1.49	1.07
1:C:22:MET:HE1	1:E:18:MET:HE3	1.41	1.02
1:B:18:MET:HE3	1:F:22:MET:CE	1.89	1.02
2:D:284:H4M:H18	2:D:284:H4M:H12	1.42	1.01
1:C:137[B]:MET:HE3	1:E:19:MET:HE1	1.03	1.01
1:C:22:MET:CE	1:E:18:MET:HE3	1.96	0.95
1:C:137[A]:MET:CE	2:C:284:H4M:H4	1.79	0.95
1:B:18:MET:HE3	1:F:22:MET:HE1	0.93	0.93
1:B:18:MET:CE	1:F:22:MET:CE	2.44	0.93
1:E:126:GLY:H	1:E:238:HIS:HE1	1.12	0.92
1:D:126:GLY:H	1:D:238:HIS:HE1	1.18	0.92
4:B:286:GOL:H31	6:B:365:HOH:O	1.58	0.91
1:C:137[A]:MET:HE2	2:C:284:H4M:H4	1.33	0.91
1:C:207:LEU:O	1:C:211[B]:GLU:HG3	1.71	0.90
1:C:137[B]:MET:CE	1:E:19:MET:CE	2.49	0.89
1:B:126:GLY:H	1:B:238:HIS:HE1	1.18	0.89
1:A:18:MET:HE3	1:D:22:MET:CE	2.01	0.88
1:A:126:GLY:H	1:A:238:HIS:HE1	1.21	0.88
1:C:126:GLY:H	1:C:238:HIS:HE1	1.17	0.88
1:F:126:GLY:H	1:F:238:HIS:HE1	1.19	0.88
1:A:22:MET:CE	1:D:18:MET:HE3	2.07	0.85
1:B:22:MET:CE	1:F:18:MET:HE3	2.08	0.84
1:C:18:MET:HE3	1:E:22:MET:CE	2.08	0.83
1:C:137[B]:MET:HE1	1:E:19:MET:HE1	1.60	0.82
1:C:22:MET:HE1	1:E:18:MET:CE	2.10	0.82
1:C:137[B]:MET:HE3	1:E:19:MET:CE	2.00	0.81
1:C:22:MET:CE	1:E:18:MET:CE	2.58	0.81
1:C:18:MET:HE3	1:E:22:MET:HE1	1.63	0.81
1:A:18:MET:CE	1:D:22:MET:CE	2.58	0.80
1:A:101:PRO:O	1:A:104:LYS:HE3	1.82	0.79
1:B:111:GLU:HG3	6:B:325:HOH:O	1.83	0.78
1:F:276:ARG:O	6:F:288:HOH:O	2.00	0.78
1:A:18:MET:CE	1:D:22:MET:HE3	2.15	0.76
2:F:284:H4M:C10	2:F:284:H4M:OH4	2.33	0.76
1:A:22:MET:HE1	1:D:18:MET:HE3	1.67	0.76
1:A:137[B]:MET:HE2	2:A:284:H4M:N8	1.95	0.76
1:F:196:ASN:HD22	1:F:199:ALA:H	1.31	0.75
1:A:22:MET:CE	1:D:18:MET:CE	2.65	0.75
1:A:18:MET:HE3	1:D:22:MET:HE1	1.67	0.75
1:B:22:MET:HE1	1:F:18:MET:HE3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLY:H	1:E:238:HIS:CE1	2.02	0.74
1:B:22:MET:CE	1:F:18:MET:CE	2.65	0.74
2:F:284:H4M:O2A	6:F:297:HOH:O	2.04	0.74
1:D:196:ASN:HD22	1:D:199:ALA:H	1.35	0.73
1:C:137[A]:MET:HE2	2:C:284:H4M:N8	2.01	0.73
2:A:284:H4M:C7M	1:D:26:GLU:O	2.34	0.73
1:E:116:TYR:CE1	1:E:180:LYS:HG2	2.23	0.73
1:A:18:MET:HE3	1:D:22:MET:HE3	1.68	0.72
1:E:88:ALA:O	6:E:320:HOH:O	2.06	0.72
1:E:126:GLY:N	1:E:238:HIS:HE1	1.87	0.72
1:C:196:ASN:HD22	1:C:199:ALA:H	1.38	0.71
1:A:18:MET:CE	1:D:22:MET:HE1	2.20	0.70
2:D:284:H4M:H12	2:D:284:H4M:C13	2.18	0.70
1:E:101:PRO:O	1:E:104:LYS:HE3	1.92	0.70
1:A:196:ASN:HD22	1:A:199:ALA:H	1.39	0.70
1:C:18:MET:CE	1:E:22:MET:CE	2.70	0.70
1:C:137[B]:MET:HE1	1:E:19:MET:CE	2.20	0.69
1:E:196:ASN:HD22	1:E:199:ALA:H	1.40	0.69
1:B:22:MET:HE3	1:F:18:MET:CE	2.23	0.69
1:B:196:ASN:HD22	1:B:199:ALA:H	1.38	0.68
1:F:101:PRO:O	1:F:104:LYS:HE3	1.94	0.68
1:B:22:MET:HE1	1:F:18:MET:CE	2.25	0.67
1:B:101:PRO:O	1:B:104:LYS:HE3	1.95	0.67
1:A:22:MET:HE3	1:D:18:MET:HE3	1.76	0.67
1:A:22:MET:HE3	1:D:18:MET:CE	2.24	0.67
1:C:18:MET:CE	1:E:22:MET:HE3	2.24	0.67
1:F:126:GLY:H	1:F:238:HIS:CE1	2.09	0.66
1:C:137[A]:MET:HE3	2:C:284:H4M:H4	1.61	0.66
1:C:137[B]:MET:HE2	1:C:138:ALA:N	2.11	0.65
1:A:22:MET:HE1	1:D:18:MET:CE	2.24	0.64
1:D:101:PRO:O	1:D:104:LYS:HE3	1.97	0.63
1:E:195:GLU:OE2	6:E:323:HOH:O	2.14	0.63
2:F:284:H4M:H12	2:F:284:H4M:H18	1.80	0.63
1:C:101:PRO:O	1:C:104:LYS:HE3	1.99	0.63
1:B:22:MET:HE3	1:F:18:MET:HE3	1.79	0.63
1:C:22:MET:HE3	1:E:18:MET:CE	2.29	0.62
1:C:126:GLY:HA3	1:C:234:VAL:HB	1.80	0.62
2:C:284:H4M:H12	2:C:284:H4M:C13	2.29	0.62
2:D:284:H4M:OH4	2:D:284:H4M:C10	2.48	0.62
2:F:284:H4M:OH4	2:F:284:H4M:H15	2.00	0.61
1:B:126:GLY:H	1:B:238:HIS:CE1	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:THR:HG22	1:E:3:VAL:N	2.16	0.61
2:C:284:H4M:H18	2:C:284:H4M:H12	1.84	0.60
1:B:14:LEU:HD22	1:B:72:GLY:C	2.21	0.60
2:C:284:H4M:OH4	2:C:284:H4M:C10	2.49	0.59
1:C:18:MET:HE3	1:E:22:MET:HE3	1.79	0.59
1:D:231:VAL:HB	1:D:232:PRO:HD3	1.85	0.59
1:D:126:GLY:H	1:D:238:HIS:CE1	2.10	0.58
1:B:73:PRO:HG2	6:B:317:HOH:O	2.03	0.58
1:E:198:TYR:HA	1:E:201:VAL:HG22	1.84	0.58
1:A:231:VAL:HB	1:A:232:PRO:HD3	1.86	0.58
1:B:38:VAL:HG12	1:F:38:VAL:HG12	1.86	0.58
1:E:101:PRO:HG2	6:E:296:HOH:O	2.04	0.57
1:C:22:MET:HE3	1:E:18:MET:HE3	1.82	0.56
1:F:279:MET:HE3	1:F:279:MET:HA	1.87	0.56
1:A:126:GLY:HA3	1:A:234:VAL:HB	1.86	0.56
2:A:284:H4M:H18	2:A:284:H4M:H12	1.88	0.56
1:A:116:TYR:CE1	1:A:180:LYS:HG2	2.40	0.56
1:C:133:ASP:HB2	1:C:134:PRO:CD	2.37	0.55
1:F:126:GLY:HA3	1:F:234:VAL:HB	1.88	0.55
1:F:116:TYR:CE1	1:F:180:LYS:HG2	2.42	0.55
1:F:128:ARG:HH21	2:F:284:H4M:H33	1.71	0.55
1:C:126:GLY:H	1:C:238:HIS:CE1	2.09	0.55
1:E:133:ASP:HB2	1:E:134:PRO:CD	2.36	0.54
1:A:26:GLU:O	2:D:284:H4M:H9	2.08	0.54
1:B:2:THR:N	6:B:349:HOH:O	2.41	0.54
1:D:263:ARG:NE	6:D:289:HOH:O	2.34	0.54
1:E:279:MET:CE	1:E:279:MET:HA	2.36	0.54
1:F:128:ARG:NH2	2:F:284:H4M:H33	2.21	0.54
1:A:126:GLY:H	1:A:238:HIS:CE1	2.13	0.54
1:A:137[B]:MET:CE	2:A:284:H4M:H4	2.02	0.54
1:B:111:GLU:CG	6:B:325:HOH:O	2.51	0.53
1:E:14:LEU:HD13	1:E:73:PRO:HG3	1.90	0.53
1:E:116:TYR:CZ	1:E:180:LYS:HG2	2.44	0.53
1:B:22:MET:HE3	1:F:18:MET:HE1	1.90	0.53
1:B:116:TYR:CE1	1:B:180:LYS:HG2	2.43	0.53
2:D:284:H4M:C9M	2:D:284:H4M:H18	2.19	0.53
1:B:126:GLY:N	1:B:238:HIS:HE1	1.98	0.52
1:C:116:TYR:CE1	1:C:180:LYS:HG2	2.44	0.52
1:B:14:LEU:HD13	1:B:73:PRO:HG3	1.91	0.52
1:E:106:LYS:HE2	6:E:293:HOH:O	2.08	0.52
1:A:196:ASN:ND2	1:A:198:TYR:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137[A]:MET:CE	1:C:141:ASN:ND2	2.72	0.52
1:F:14:LEU:HD22	1:F:72:GLY:C	2.31	0.51
1:F:97:ILE:HD12	1:F:117:ILE:HB	1.91	0.51
1:A:196:ASN:HD21	1:A:198:TYR:HB2	1.75	0.51
1:C:18:MET:CE	1:E:22:MET:HE1	2.37	0.51
1:C:136:GLU:OE1	1:C:238:HIS:HD2	1.94	0.51
1:E:100:ALA:N	1:E:101:PRO:CD	2.74	0.51
1:E:126:GLY:HA3	1:E:234:VAL:HB	1.93	0.51
1:F:196:ASN:HD21	1:F:198:TYR:HB2	1.75	0.50
1:C:128:ARG:NH2	2:C:284:H4M:H33	2.26	0.50
1:D:116:TYR:CE1	1:D:180:LYS:HG2	2.47	0.50
1:D:126:GLY:HA3	1:D:234:VAL:HB	1.93	0.50
2:F:284:H4M:C13	2:F:284:H4M:H12	2.40	0.50
1:C:18:MET:HE1	1:E:22:MET:HE3	1.93	0.49
1:E:133:ASP:HB2	1:E:134:PRO:HD2	1.95	0.49
1:C:137[A]:MET:HE2	1:C:141:ASN:HD21	1.78	0.49
1:C:198:TYR:HA	1:C:201:VAL:HG22	1.95	0.49
1:C:97:ILE:HD12	1:C:117:ILE:HB	1.95	0.48
1:D:198:TYR:HA	1:D:201:VAL:HG22	1.95	0.48
1:D:168:ALA:HB2	1:D:173:ILE:HD11	1.95	0.48
1:B:49:VAL:CG1	1:B:83:ALA:HB2	2.44	0.48
1:E:32:ASP:OD1	1:E:169:LYS:NZ	2.44	0.48
1:C:264:THR:HA	1:C:273:LEU:O	2.14	0.48
1:A:137[A]:MET:HG3	2:A:284:H4M:H8	1.95	0.48
2:D:284:H4M:C9M	2:D:284:H4M:C13	2.83	0.47
1:B:120:LYS:N	1:B:121:PRO:CD	2.78	0.47
1:C:168:ALA:HB2	1:C:173:ILE:HD11	1.96	0.47
1:C:231:VAL:HB	1:C:232:PRO:HD3	1.95	0.47
1:C:49:VAL:CG1	1:C:83:ALA:HB2	2.44	0.47
1:D:196:ASN:HD21	1:D:198:TYR:HB2	1.79	0.47
1:E:134:PRO:HD2	6:E:322:HOH:O	2.15	0.47
1:F:231:VAL:HB	1:F:232:PRO:HD3	1.96	0.47
1:A:198:TYR:HA	1:A:201:VAL:HG22	1.97	0.47
1:A:22:MET:HE3	1:D:18:MET:HE1	1.96	0.47
1:B:97:ILE:HD12	1:B:117:ILE:HB	1.96	0.47
1:D:264:THR:HA	1:D:273:LEU:O	2.14	0.47
1:A:49:VAL:CG1	1:A:83:ALA:HB2	2.44	0.47
1:B:126:GLY:HA3	1:B:234:VAL:HB	1.97	0.47
1:A:116:TYR:CZ	1:A:180:LYS:HG2	2.50	0.47
1:E:135:VAL:O	1:E:139:ILE:HG13	2.15	0.47
1:B:39:GLY:HA3	6:B:326:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG12	1:D:38:VAL:HG12	1.97	0.46
1:E:279:MET:HE3	1:E:279:MET:HA	1.96	0.46
1:C:258:ASN:O	1:C:259:ASP:C	2.54	0.46
1:B:231:VAL:HB	1:B:232:PRO:HD3	1.98	0.46
1:C:14:LEU:HD22	1:C:72:GLY:C	2.36	0.46
1:D:97:ILE:HD12	1:D:117:ILE:HB	1.96	0.46
1:E:50:GLU:O	1:E:54:GLU:HG3	2.17	0.45
1:A:14:LEU:HD22	1:A:72:GLY:C	2.37	0.45
1:B:42:VAL:HG21	1:F:25:ASP:O	2.17	0.45
1:C:22:MET:HE3	1:E:18:MET:HE1	1.98	0.45
1:E:185:ARG:HG3	1:E:204:MET:O	2.17	0.45
1:E:2:THR:HG22	1:E:3:VAL:H	1.80	0.45
1:A:168:ALA:HB2	1:A:173:ILE:HD11	1.98	0.45
1:F:168:ALA:HB2	1:F:173:ILE:HD11	1.99	0.45
1:A:18:MET:HE1	1:D:22:MET:HE3	1.94	0.45
1:B:116:TYR:CZ	1:B:180:LYS:HG2	2.51	0.45
1:A:137[B]:MET:HG3	2:A:284:H4M:H8	1.99	0.44
1:E:71:GLY:HA2	1:E:97:ILE:HB	2.00	0.44
1:F:49:VAL:CG1	1:F:83:ALA:HB2	2.47	0.44
1:D:100:ALA:N	1:D:101:PRO:CD	2.80	0.44
1:E:122:ASP:OD1	1:E:144:LEU:HD21	2.17	0.44
1:B:37:VAL:O	1:F:38:VAL:HA	2.16	0.44
1:C:137[A]:MET:HE2	1:C:141:ASN:ND2	2.32	0.44
1:C:9:ILE:HA	1:C:38:VAL:O	2.18	0.44
1:D:49:VAL:HG11	1:D:79:GLY:O	2.18	0.44
1:E:49:VAL:CG1	1:E:83:ALA:HB2	2.48	0.44
1:F:100:ALA:N	1:F:101:PRO:CD	2.81	0.44
1:A:133:ASP:HB2	1:A:134:PRO:CD	2.48	0.43
1:D:97:ILE:CD1	1:D:117:ILE:HB	2.48	0.43
2:E:284:H4M:C10	2:E:284:H4M:OH4	2.66	0.43
1:F:133:ASP:HB2	1:F:134:PRO:CD	2.48	0.43
1:F:264:THR:HA	1:F:273:LEU:O	2.18	0.43
1:B:231:VAL:HG12	1:F:278:PHE:CZ	2.54	0.43
1:E:227:LYS:HA	1:E:230:TYR:CD1	2.54	0.43
1:E:231:VAL:HB	1:E:232:PRO:HD3	2.00	0.43
1:E:2:THR:CG2	1:E:3:VAL:N	2.81	0.43
1:B:150:ALA:HB3	1:B:248:ALA:HB1	2.00	0.43
1:B:133:ASP:HB2	1:B:134:PRO:CD	2.49	0.43
2:C:284:H4M:H15	2:C:284:H4M:OH4	2.19	0.43
1:E:14:LEU:HD22	1:E:72:GLY:C	2.39	0.43
1:D:14:LEU:HD13	1:D:73:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:ALA:HB3	1:F:101:PRO:HD3	2.00	0.42
1:B:196:ASN:HD21	1:B:198:TYR:HB2	1.84	0.42
1:E:125:LEU:C	1:E:125:LEU:HD12	2.40	0.42
1:F:116:TYR:CZ	1:F:180:LYS:HG2	2.55	0.42
1:B:196:ASN:ND2	1:B:198:TYR:H	2.17	0.42
1:D:14:LEU:HD22	1:D:72:GLY:C	2.40	0.42
1:D:49:VAL:CG1	1:D:83:ALA:HB2	2.49	0.42
1:A:14:LEU:HD13	1:A:73:PRO:HG3	2.02	0.41
1:A:213:VAL:HG13	1:A:237:ALA:HB1	2.02	0.41
1:B:243:LYS:HG3	1:D:247:LEU:HG	2.02	0.41
1:F:198:TYR:HA	1:F:201:VAL:HG22	2.02	0.41
1:C:120:LYS:N	1:C:121:PRO:CD	2.83	0.41
1:B:18:MET:HE2	1:F:22:MET:CE	2.43	0.41
1:C:128:ARG:HH21	2:C:284:H4M:H33	1.85	0.41
1:C:279:MET:HA	1:C:279:MET:CE	2.51	0.41
1:D:227:LYS:O	1:D:231:VAL:HG23	2.21	0.41
1:C:39:GLY:HA3	6:C:335:HOH:O	2.21	0.41
1:A:97:ILE:HD12	1:A:117:ILE:HB	2.03	0.41
1:B:120:LYS:HB2	1:B:121:PRO:HD3	2.02	0.41
1:B:125:LEU:C	1:B:125:LEU:HD12	2.42	0.41
1:E:97:ILE:HD12	1:E:117:ILE:HB	2.03	0.40
1:C:243:LYS:NZ	1:F:250:GLU:OE2	2.51	0.40
1:D:120:LYS:N	1:D:121:PRO:CD	2.85	0.40
2:A:284:H4M:C13	2:A:284:H4M:H12	2.51	0.40
1:B:38:VAL:HA	1:F:37:VAL:O	2.21	0.40
1:C:133:ASP:HB2	1:C:134:PRO:HD2	2.02	0.40
1:D:136:GLU:OE1	1:D:238:HIS:HD2	2.05	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLU:OE2	3:B:285:CA:CA[1_454]	1.29	0.91
1:B:89:ASP:OD2	1:E:50:GLU:OE2[1_656]	1.65	0.55
1:F:170:GLU:OE1	1:F:227:LYS:NZ[1_655]	1.94	0.26
1:B:177:ASP:OD2	1:E:170:GLU:OE1[1_556]	2.16	0.04
1:F:170:GLU:OE1	1:F:227:LYS:CE[1_655]	2.16	0.04



## 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	281/283 (99%)	271 (96%)	10 (4%)	0	100	100
1	B	280/283 (99%)	270 (96%)	10 (4%)	0	100	100
1	C	283/283 (100%)	275 (97%)	8 (3%)	0	100	100
1	D	280/283 (99%)	273 (98%)	7 (2%)	0	100	100
1	E	280/283 (99%)	269 (96%)	11 (4%)	0	100	100
1	F	281/283 (99%)	271 (96%)	10 (4%)	0	100	100
All	All	1685/1698 (99%)	1629 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	234/234 (100%)	230 (98%)	4 (2%)	60	67
1	B	233/234 (100%)	229 (98%)	4 (2%)	60	67
1	C	236/234 (101%)	233 (99%)	3 (1%)	69	75
1	D	233/234 (100%)	228 (98%)	5 (2%)	53	59
1	E	233/234 (100%)	228 (98%)	5 (2%)	53	59
1	F	234/234 (100%)	232 (99%)	2 (1%)	78	84
All	All	1403/1404 (100%)	1380 (98%)	23 (2%)	62	69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	125	LEU
1	A	155	ARG
1	A	280	GLU
1	B	2	THR
1	B	14	LEU
1	B	190	GLU
1	B	280	GLU
1	C	14	LEU
1	C	125	LEU
1	C	230	TYR
1	D	2	THR
1	D	14	LEU
1	D	155	ARG
1	D	230	TYR
1	D	280	GLU
1	E	14	LEU
1	E	125	LEU
1	E	190	GLU
1	E	230	TYR
1	E	280	GLU
1	F	14	LEU
1	F	125	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	238	HIS
1	B	196	ASN
1	B	212	ASN
1	B	238	HIS
1	C	196	ASN
1	C	238	HIS
1	D	196	ASN
1	D	212	ASN
1	D	238	HIS
1	E	196	ASN
1	E	238	HIS
1	E	258	ASN
1	F	196	ASN

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Mol	Chain	Res	Type
1	F	212	ASN
1	F	238	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GOL	B	286	-	5,5,5	0.29	0	5,5,5	0.87	0
2	H4M	C	284	-	47,49,58	1.09	3 (6%)	61,74,86	1.83	10 (16%)
2	H4M	E	284	-	47,49,58	1.08	2 (4%)	61,74,86	1.91	15 (24%)
2	H4M	F	284	-	47,49,58	1.16	2 (4%)	61,74,86	2.40	10 (16%)
2	H4M	D	284	-	47,49,58	0.99	1 (2%)	61,74,86	2.50	17 (27%)
2	H4M	A	284	-	47,49,58	0.71	1 (2%)	61,74,86	1.61	11 (18%)
2	H4M	B	284	-	47,49,58	1.14	4 (8%)	61,74,86	2.24	21 (34%)

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
4	GOL	B	286	-	-	2/4/4/4	-
2	H4M	C	284	-	-	5/27/71/85	0/5/5/5
2	H4M	E	284	-	-	7/27/71/85	0/5/5/5
2	H4M	F	284	-	-	5/27/71/85	0/5/5/5
2	H4M	D	284	-	-	4/27/71/85	0/5/5/5
2	H4M	A	284	-	-	9/27/71/85	0/5/5/5
2	H4M	B	284	-	-	12/27/71/85	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	284	H4M	C4-C4A	-4.80	1.35	1.41
2	E	284	H4M	C4-C4A	-3.60	1.36	1.41
2	C	284	H4M	C6-N5	-3.34	1.44	1.47
2	D	284	H4M	C4-C4A	-3.30	1.37	1.41
2	C	284	H4M	CX1-CX2	3.05	1.56	1.53
2	C	284	H4M	C4-C4A	-3.03	1.37	1.41
2	B	284	H4M	C4-N3	2.69	1.37	1.33
2	F	284	H4M	C6-N5	-2.67	1.44	1.47
2	A	284	H4M	C6-N5	-2.32	1.45	1.47
2	B	284	H4M	OX5-C1J	2.19	1.43	1.40
2	B	284	H4M	C2-NA2	2.08	1.38	1.33
2	E	284	H4M	OX5-C1J	2.06	1.43	1.40
2	B	284	H4M	C4-C4A	-2.00	1.38	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	284	H4M	O4J-C1J-OX5	-12.25	98.51	111.95
2	F	284	H4M	O4J-C1J-OX5	-10.80	100.10	111.95
2	F	284	H4M	C4-C4A-C8A	9.67	122.00	114.44
2	B	284	H4M	O4J-C1J-OX5	-8.89	102.19	111.95
2	D	284	H4M	C4-C4A-C8A	8.18	120.83	114.44
2	C	284	H4M	C4-C4A-C8A	7.19	120.06	114.44
2	E	284	H4M	C4-C4A-C8A	6.05	119.17	114.44
2	A	284	H4M	C4-C4A-C8A	5.97	119.11	114.44
2	D	284	H4M	C7-C6-N5	-5.83	102.79	108.61
2	C	284	H4M	C9M-C9-N10	-5.55	103.48	112.68
2	F	284	H4M	C7-C6-N5	-5.24	103.39	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	284	H4M	O4J-C1J-OX5	-5.07	106.39	111.95
2	C	284	H4M	C7-C6-N5	-5.01	103.61	108.61
2	A	284	H4M	C7-C6-N5	-4.96	103.66	108.61
2	B	284	H4M	C7-C6-N5	-4.92	103.70	108.61
2	F	284	H4M	OX5-C1J-C2J	4.69	115.41	107.76
2	B	284	H4M	CX4-CX3-CX2	-4.13	104.78	113.36
2	B	284	H4M	C7M-C7-N8	-4.12	104.87	109.55
2	B	284	H4M	N3-C2-N1	-3.98	119.18	125.42
2	C	284	H4M	O4J-C1J-OX5	-3.97	107.59	111.95
2	E	284	H4M	C4-N3-C2	3.82	122.01	115.93
2	B	284	H4M	OX3-CX3-CX4	-3.55	100.24	108.81
2	E	284	H4M	OX5-C1J-C2J	3.53	113.52	107.76
2	A	284	H4M	C4-N3-C2	3.46	121.42	115.93
2	B	284	H4M	C4-N3-C2	3.27	121.12	115.93
2	A	284	H4M	O4J-C1J-OX5	-3.26	108.37	111.95
2	E	284	H4M	C7-C6-N5	-3.18	105.44	108.61
2	F	284	H4M	C4-N3-C2	3.13	120.90	115.93
2	B	284	H4M	O3A-PA-O2A	3.12	119.55	107.64
2	E	284	H4M	CX4-CX3-CX2	-3.11	106.88	113.36
2	E	284	H4M	OX5-CX5-CX4	-3.11	102.02	109.27
2	D	284	H4M	N3-C2-N1	-3.08	120.59	125.42
2	E	284	H4M	C9M-C9-N10	-3.04	107.63	112.68
2	C	284	H4M	OX4-CX4-CX5	-3.04	103.08	109.92
2	B	284	H4M	C9M-C9-N10	-3.04	107.64	112.68
2	D	284	H4M	C2-N1-C8A	3.03	121.32	114.54
2	A	284	H4M	N3-C2-N1	-2.99	120.73	125.42
2	E	284	H4M	C4A-C4-N3	-2.93	117.12	123.14
2	F	284	H4M	C4A-C4-N3	-2.82	117.34	123.14
2	D	284	H4M	OX4-CX4-CX5	-2.78	103.66	109.92
2	C	284	H4M	C4-N3-C2	2.76	120.31	115.93
2	A	284	H4M	C5J-C4J-C3J	-2.72	104.97	115.18
2	B	284	H4M	C9-C6-N5	2.72	104.91	102.36
2	E	284	H4M	C4A-C8A-N8	2.72	121.72	119.08
2	B	284	H4M	O3J-C3J-C2J	-2.69	103.11	111.82
2	D	284	H4M	OX5-C1J-C2J	2.69	112.15	107.76
2	E	284	H4M	C7M-C7-N8	-2.67	106.51	109.55
2	F	284	H4M	CX4-CX3-CX2	-2.63	107.89	113.36
2	D	284	H4M	O2A-PA-O5J	-2.62	99.77	106.73
2	B	284	H4M	OX5-C1J-C2J	2.61	112.03	107.76
2	D	284	H4M	O3A-PA-O2A	2.61	117.60	107.64
2	B	284	H4M	O3A-PA-O5J	-2.60	99.81	106.73
2	B	284	H4M	C2-N1-C8A	2.58	120.33	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	284	H4M	N3-C2-N1	-2.56	121.41	125.42
2	E	284	H4M	OX2-CX2-CX3	-2.52	102.98	109.10
2	B	284	H4M	O3J-C3J-C4J	-2.47	103.90	111.05
2	A	284	H4M	C2-N1-C8A	2.47	120.07	114.54
2	D	284	H4M	OX4-CX4-CX3	-2.44	103.16	109.10
2	D	284	H4M	C7M-C7-N8	2.44	112.31	109.55
2	E	284	H4M	N3-C2-N1	-2.43	121.61	125.42
2	F	284	H4M	C7M-C7-N8	-2.42	106.80	109.55
2	B	284	H4M	C4-C4A-C8A	2.42	116.33	114.44
2	D	284	H4M	CX5-CX4-CX3	2.42	116.87	112.20
2	B	284	H4M	O2A-PA-O5J	-2.35	100.47	106.73
2	E	284	H4M	O3J-C3J-C4J	-2.33	104.31	111.05
2	C	284	H4M	NA2-C2-N1	2.30	120.83	117.25
2	A	284	H4M	C9M-C9-N10	-2.29	108.89	112.68
2	A	284	H4M	NA2-C2-N1	2.26	120.76	117.25
2	B	284	H4M	C2J-C3J-C4J	2.25	107.02	102.64
2	D	284	H4M	C5J-C4J-C3J	-2.24	106.77	115.18
2	E	284	H4M	O3A-PA-O2A	2.24	116.21	107.64
2	C	284	H4M	C10-N10-C14	2.22	127.55	120.34
2	B	284	H4M	OX3-CX3-CX2	2.17	114.05	108.81
2	F	284	H4M	O3A-PA-O2A	2.16	115.90	107.64
2	B	284	H4M	C15-C14-N10	-2.12	117.12	121.14
2	D	284	H4M	O3J-C3J-C4J	-2.12	104.92	111.05
2	C	284	H4M	N3-C2-N1	-2.10	122.13	125.42
2	B	284	H4M	NA2-C2-N3	2.08	120.48	117.25
2	D	284	H4M	NA2-C2-N3	2.08	120.48	117.25
2	D	284	H4M	CX5-OX5-C1J	2.07	117.79	113.74
2	A	284	H4M	O5J-PA-O1A	-2.07	100.66	106.47
2	D	284	H4M	C9M-C9-N10	-2.06	109.26	112.68
2	A	284	H4M	C4A-C4-N3	-2.03	118.96	123.14
2	C	284	H4M	C9-C6-N5	-2.01	100.47	102.36

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	286	GOL	O1-C1-C2-C3
2	C	284	H4M	O4J-C1J-OX5-CX5
2	C	284	H4M	C2J-C1J-OX5-CX5
2	C	284	H4M	C5J-O5J-PA-O1A
2	C	284	H4M	C5J-O5J-PA-O2A
2	E	284	H4M	O4J-C1J-OX5-CX5

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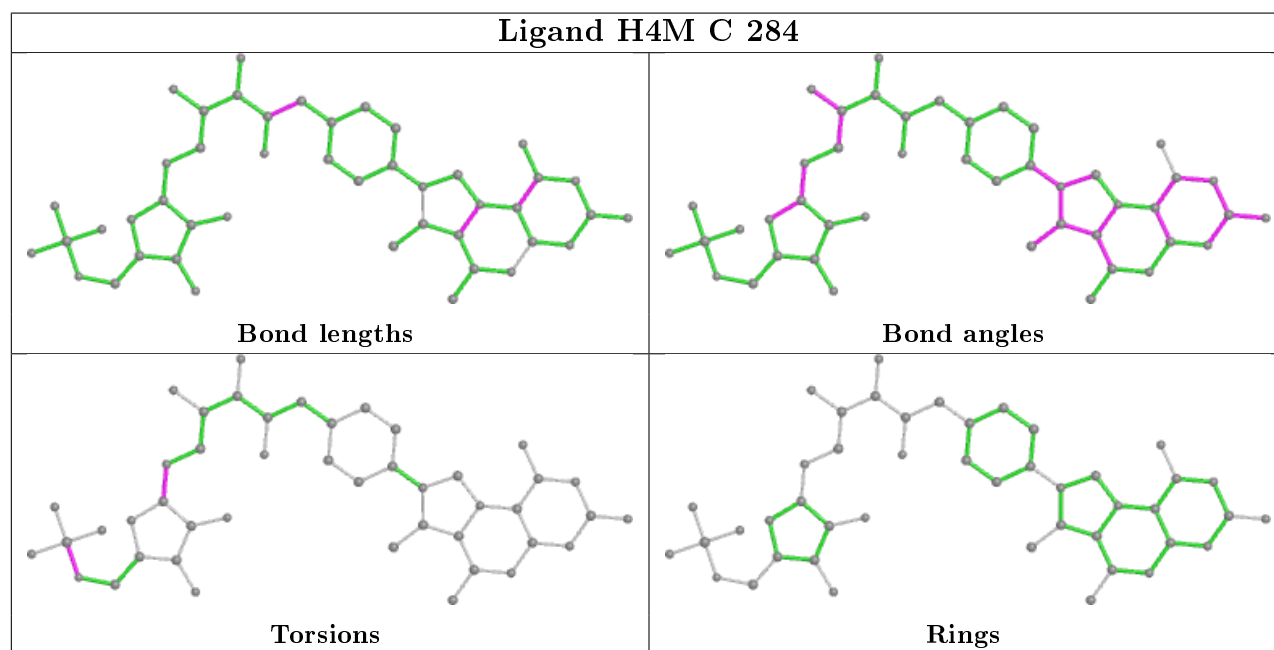
Mol	Chain	Res	Type	Atoms
2	E	284	H4M	C2J-C1J-OX5-CX5
2	E	284	H4M	C5J-O5J-PA-O1A
2	E	284	H4M	C5J-O5J-PA-O2A
2	E	284	H4M	C5J-O5J-PA-O3A
2	F	284	H4M	O4J-C1J-OX5-CX5
2	F	284	H4M	C2J-C1J-OX5-CX5
2	F	284	H4M	C5J-O5J-PA-O2A
2	F	284	H4M	C5J-O5J-PA-O3A
2	D	284	H4M	O4J-C1J-OX5-CX5
2	D	284	H4M	C2J-C1J-OX5-CX5
2	A	284	H4M	O4J-C1J-OX5-CX5
2	A	284	H4M	C2J-C1J-OX5-CX5
2	A	284	H4M	C5J-O5J-PA-O2A
2	A	284	H4M	C5J-O5J-PA-O3A
2	B	284	H4M	O4J-C1J-OX5-CX5
2	B	284	H4M	C2J-C1J-OX5-CX5
2	B	284	H4M	C5J-O5J-PA-O2A
2	B	284	H4M	C5J-O5J-PA-O3A
2	A	284	H4M	OX3-CX3-CX4-OX4
2	B	284	H4M	OX3-CX3-CX4-OX4
2	A	284	H4M	CX2-CX3-CX4-OX4
2	A	284	H4M	OX3-CX3-CX4-CX5
2	B	284	H4M	OX3-CX3-CX4-CX5
2	A	284	H4M	CX2-CX3-CX4-CX5
2	B	284	H4M	CX2-CX3-CX4-CX5
4	B	286	GOL	O1-C1-C2-O2
2	B	284	H4M	CX2-CX3-CX4-OX4
2	F	284	H4M	C5J-O5J-PA-O1A
2	A	284	H4M	C5J-O5J-PA-O1A
2	B	284	H4M	C5J-O5J-PA-O1A
2	E	284	H4M	O4J-C4J-C5J-O5J
2	D	284	H4M	CX2-CX3-CX4-CX5
2	B	284	H4M	OX2-CX2-CX3-OX3
2	D	284	H4M	C5J-O5J-PA-O1A
2	E	284	H4M	C13-C14-N10-C10
2	C	284	H4M	C5J-O5J-PA-O3A
2	B	284	H4M	CX1-CX2-CX3-OX3
2	B	284	H4M	C16-C11-CX1-CX2

There are no ring outliers.

6 monomers are involved in 36 short contacts:

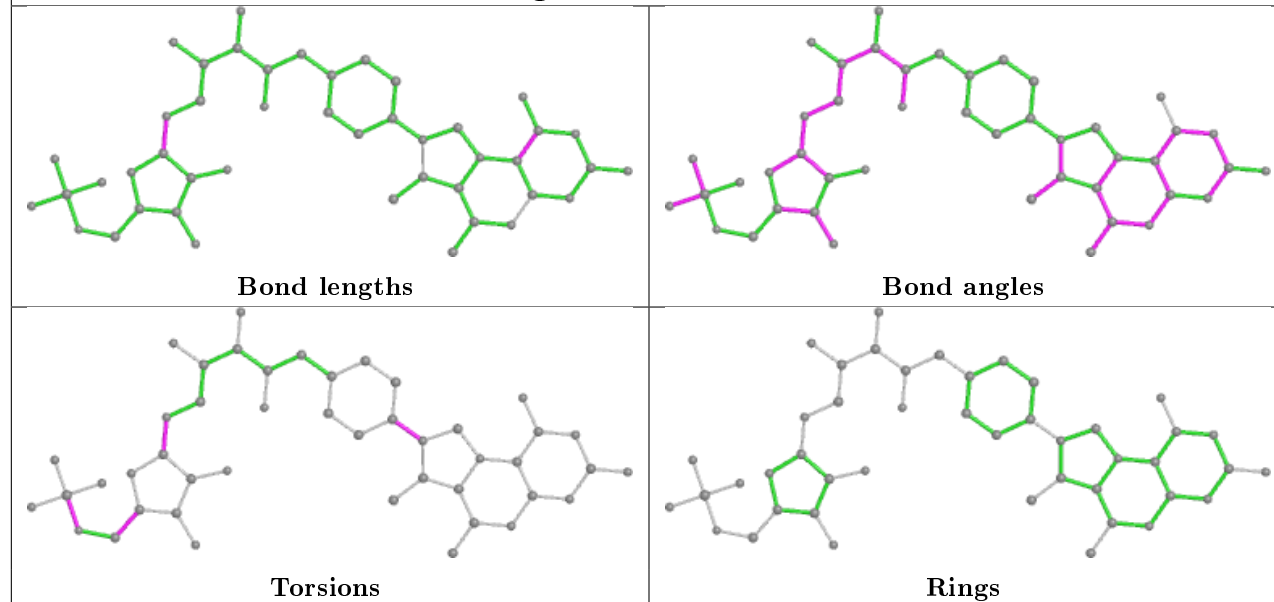
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	286	GOL	3	0
2	C	284	H4M	10	0
2	E	284	H4M	1	0
2	F	284	H4M	7	0
2	D	284	H4M	6	0
2	A	284	H4M	9	0

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.

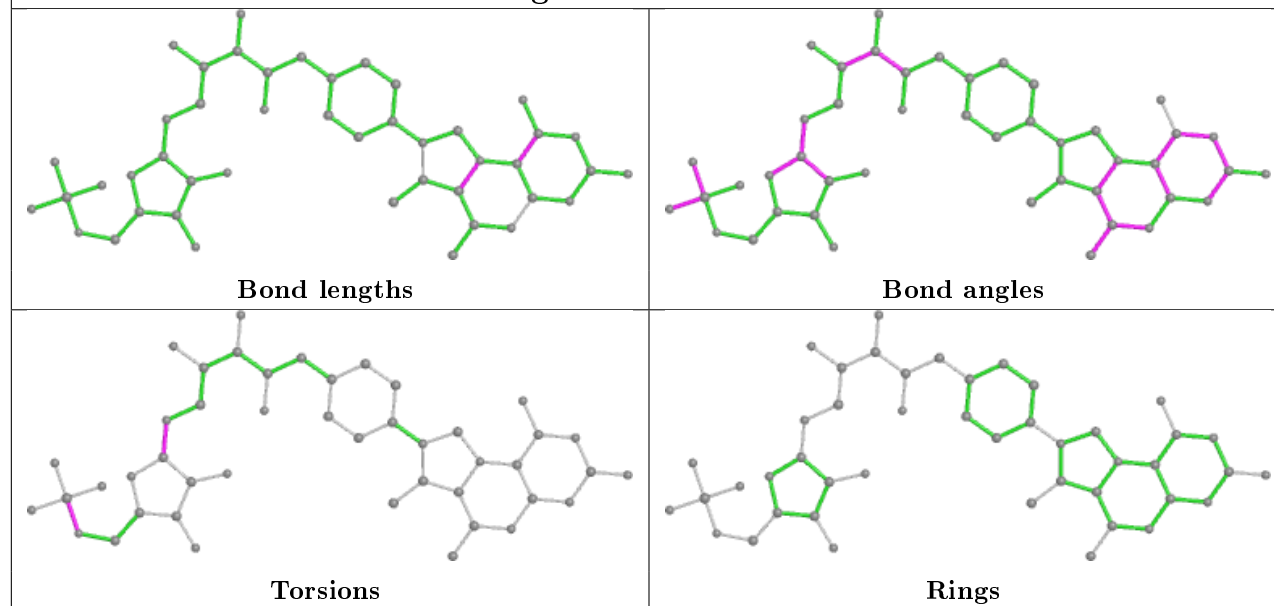


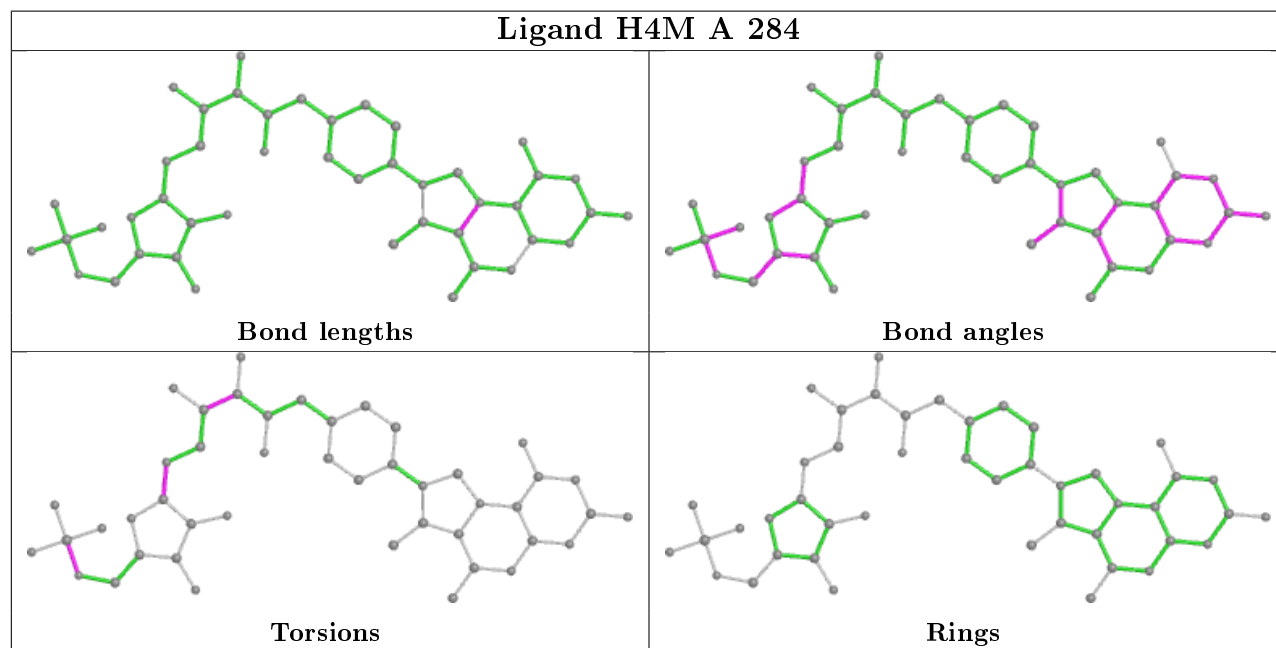
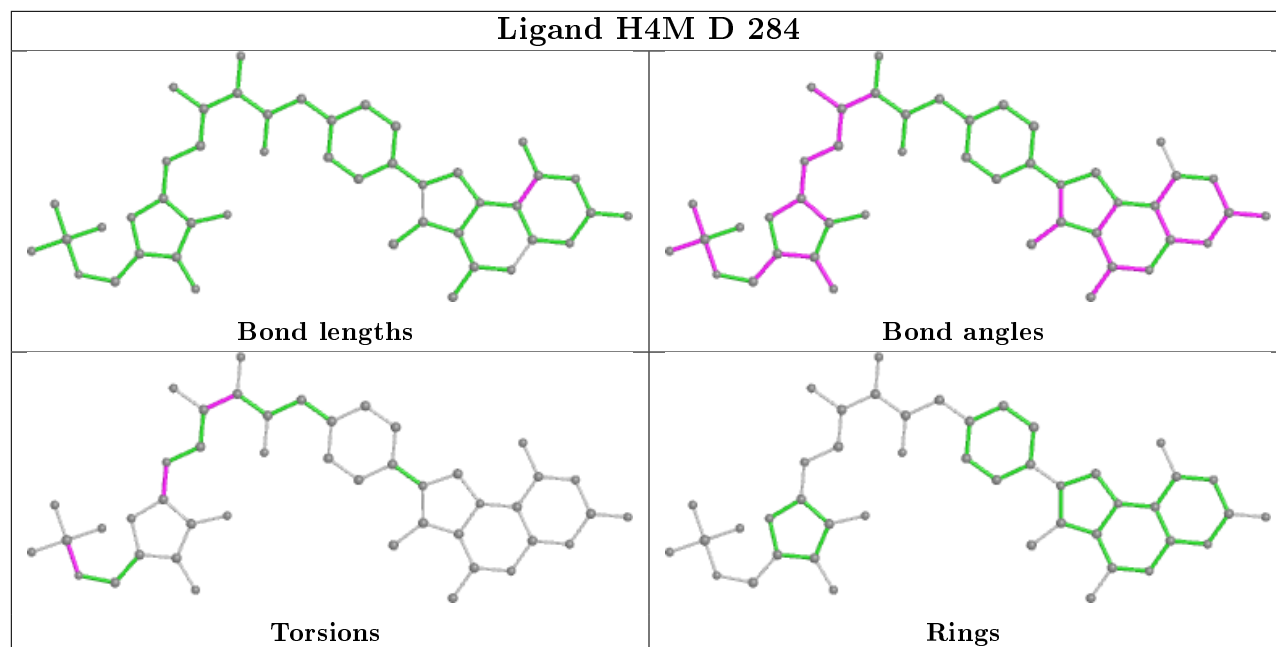


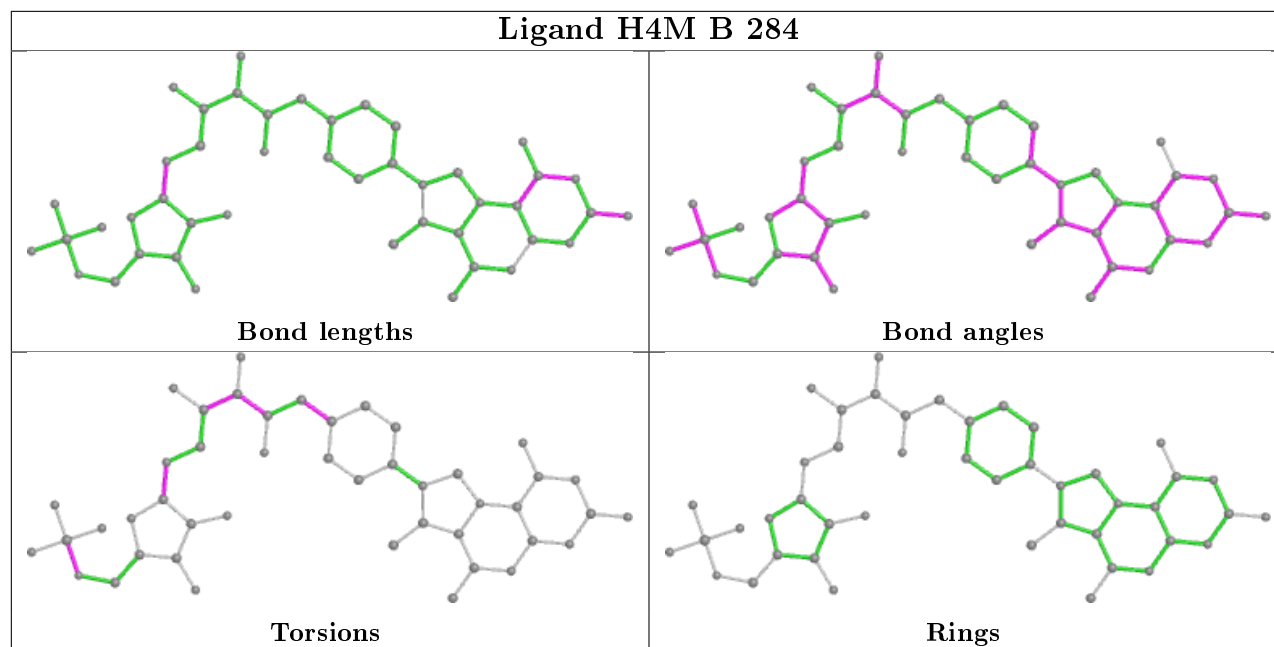
## Ligand H4M E 284



## Ligand H4M F 284







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	282/283 (99%)	1.19	58 (20%) 1 1	3, 8, 21, 43	0
1	B	282/283 (99%)	0.42	11 (3%) 39 45	2, 8, 21, 43	1 (0%)
1	C	282/283 (99%)	0.56	26 (9%) 9 11	2, 8, 21, 43	1 (0%)
1	D	282/283 (99%)	1.10	52 (18%) 1 1	2, 8, 21, 43	0
1	E	282/283 (99%)	0.64	28 (9%) 7 9	2, 8, 21, 43	0
1	F	282/283 (99%)	0.62	23 (8%) 11 15	2, 8, 21, 43	1 (0%)
All	All	1692/1698 (99%)	0.76	198 (11%) 4 6	2, 8, 22, 43	3 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASP	7.8
1	B	171	ASP	6.5
1	A	172	GLU	6.4
1	D	57	LEU	6.2
1	E	171	ASP	6.0
1	A	46	PRO	5.8
1	D	172	GLU	5.6
1	A	92	TYR	5.5
1	A	111	GLU	5.4
1	D	171	ASP	5.4
1	A	58	ASP	5.3
1	D	282	PRO	5.0
1	D	53	VAL	4.9
1	A	113	GLY	4.9
1	D	165	ILE	4.9
1	D	173	ILE	4.7
1	A	89	ASP	4.6
1	A	114	LEU	4.5
1	C	171	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	225	GLN	4.3
1	A	47	GLU	4.3
1	A	107	ASP	4.2
1	F	171	ASP	4.2
1	D	63	PHE	4.2
1	D	273	LEU	4.2
1	D	111	GLU	4.1
1	D	169	LYS	4.1
1	A	76	ALA	4.1
1	A	85	GLU	4.0
1	D	283	GLU	4.0
1	D	167	LYS	4.0
1	C	247	LEU	3.9
1	F	2	THR	3.9
1	E	169	LYS	3.9
1	F	174	SER	3.8
1	C	111	GLU	3.8
1	C	176	ASN	3.8
1	D	269	ASP	3.7
1	A	167	LYS	3.7
1	B	246	GLU	3.7
1	A	57	LEU	3.7
1	A	82	LYS	3.7
1	E	172	GLU	3.7
1	E	168	ALA	3.6
1	A	173	ILE	3.6
1	E	91	GLU	3.6
1	D	177	ASP	3.6
1	D	88	ALA	3.5
1	A	230	TYR	3.5
1	C	172	GLU	3.4
1	F	111	GLU	3.4
1	D	267	ALA	3.4
1	A	164	LEU	3.4
1	B	170	GLU	3.4
1	F	245	ALA	3.4
1	E	170	GLU	3.4
1	D	3	VAL	3.3
1	C	245	ALA	3.3
1	A	88	ALA	3.3
1	A	247	LEU	3.2
1	D	170	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	PRO	3.2
1	A	53	VAL	3.2
1	A	147	VAL	3.2
1	A	51	ALA	3.1
1	A	244	ALA	3.1
1	F	89	ASP	3.1
1	D	31	GLU	3.1
1	A	61	GLU	3.1
1	A	140	TYR	3.1
1	A	245	ALA	3.0
1	C	246[A]	GLU	3.0
1	B	172	GLU	3.0
1	D	142	ALA	2.9
1	B	209	ILE	2.9
1	F	244	ALA	2.9
1	A	144	LEU	2.9
1	E	173	ILE	2.9
1	A	175	GLU	2.9
1	F	172	GLU	2.9
1	F	246[A]	GLU	2.9
1	A	170	GLU	2.9
1	C	170	GLU	2.9
1	F	247	LEU	2.9
1	D	174	SER	2.9
1	D	59	ILE	2.9
1	A	54	GLU	2.9
1	D	244	ALA	2.9
1	E	142	ALA	2.9
1	C	248	ALA	2.8
1	E	245	ALA	2.8
1	A	50	GLU	2.8
1	A	62	ASP	2.8
1	E	244	ALA	2.8
1	F	3	VAL	2.8
1	E	111	GLU	2.8
1	D	245	ALA	2.8
1	A	63	PHE	2.8
1	A	270	GLY	2.7
1	D	270	GLY	2.7
1	A	81	SER	2.7
1	A	90	SER	2.7
1	D	61	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	110	GLU	2.6
1	F	109	MET	2.6
1	B	247	LEU	2.6
1	C	107	ASP	2.6
1	A	139	ILE	2.6
1	E	107	ASP	2.6
1	A	91	GLU	2.6
1	F	105	VAL	2.6
1	E	177	ASP	2.6
1	B	148	LEU	2.6
1	D	149	ALA	2.6
1	E	138	ALA	2.6
1	E	248	ALA	2.6
1	D	109	MET	2.6
1	D	247	LEU	2.6
1	B	245	ALA	2.5
1	C	47	GLU	2.5
1	D	280	GLU	2.5
1	E	241	MET	2.5
1	A	267	ALA	2.5
1	D	140	TYR	2.5
1	A	227	LYS	2.5
1	D	144	LEU	2.5
1	C	244	ALA	2.5
1	E	61	GLU	2.5
1	F	170	GLU	2.5
1	A	168	ALA	2.5
1	A	248	ALA	2.5
1	D	46	PRO	2.4
1	D	50	GLU	2.4
1	A	150	ALA	2.4
1	D	54	GLU	2.4
1	D	62	ASP	2.4
1	E	242	ARG	2.4
1	A	241	MET	2.4
1	F	176	ASN	2.4
1	E	139	ILE	2.4
1	D	147	VAL	2.4
1	A	64	GLU	2.4
1	A	231	VAL	2.3
1	A	138	ALA	2.3
1	B	244	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	56	ALA	2.3
1	D	271	LYS	2.3
1	E	148	LEU	2.3
1	C	175	GLU	2.3
1	F	167	LYS	2.3
1	C	147	VAL	2.3
1	D	225	GLN	2.3
1	F	147	VAL	2.3
1	C	139	ILE	2.3
1	E	271	LYS	2.2
1	A	149	ALA	2.2
1	B	144	LEU	2.2
1	A	242	ARG	2.2
1	C	146	LYS	2.2
1	A	87	LEU	2.2
1	A	206	ALA	2.2
1	D	114	LEU	2.2
1	D	90	SER	2.2
1	C	145	MET	2.2
1	E	2	THR	2.2
1	C	243	LYS	2.2
1	C	222	PHE	2.2
1	D	279	MET	2.2
1	F	145	MET	2.2
1	C	89	ASP	2.2
1	E	209	ILE	2.1
1	F	209	ILE	2.1
1	A	110	GLU	2.1
1	F	168	ALA	2.1
1	C	144	LEU	2.1
1	D	145	MET	2.1
1	E	279	MET	2.1
1	D	277	LYS	2.1
1	D	58	ASP	2.1
1	E	144	LEU	2.1
1	F	107	ASP	2.1
1	D	110	GLU	2.1
1	F	139	ILE	2.1
1	C	148	LEU	2.1
1	F	114	LEU	2.1
1	D	19	MET	2.1
1	B	248	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	66	ASP	2.1
1	A	273	LEU	2.1
1	D	30	ARG	2.0
1	D	112	GLN	2.0
1	A	142	ALA	2.0
1	E	110	GLU	2.0
1	C	207	LEU	2.0
1	C	109	MET	2.0
1	C	91	GLU	2.0
1	E	223	VAL	2.0
1	E	269	ASP	2.0

## 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](#)

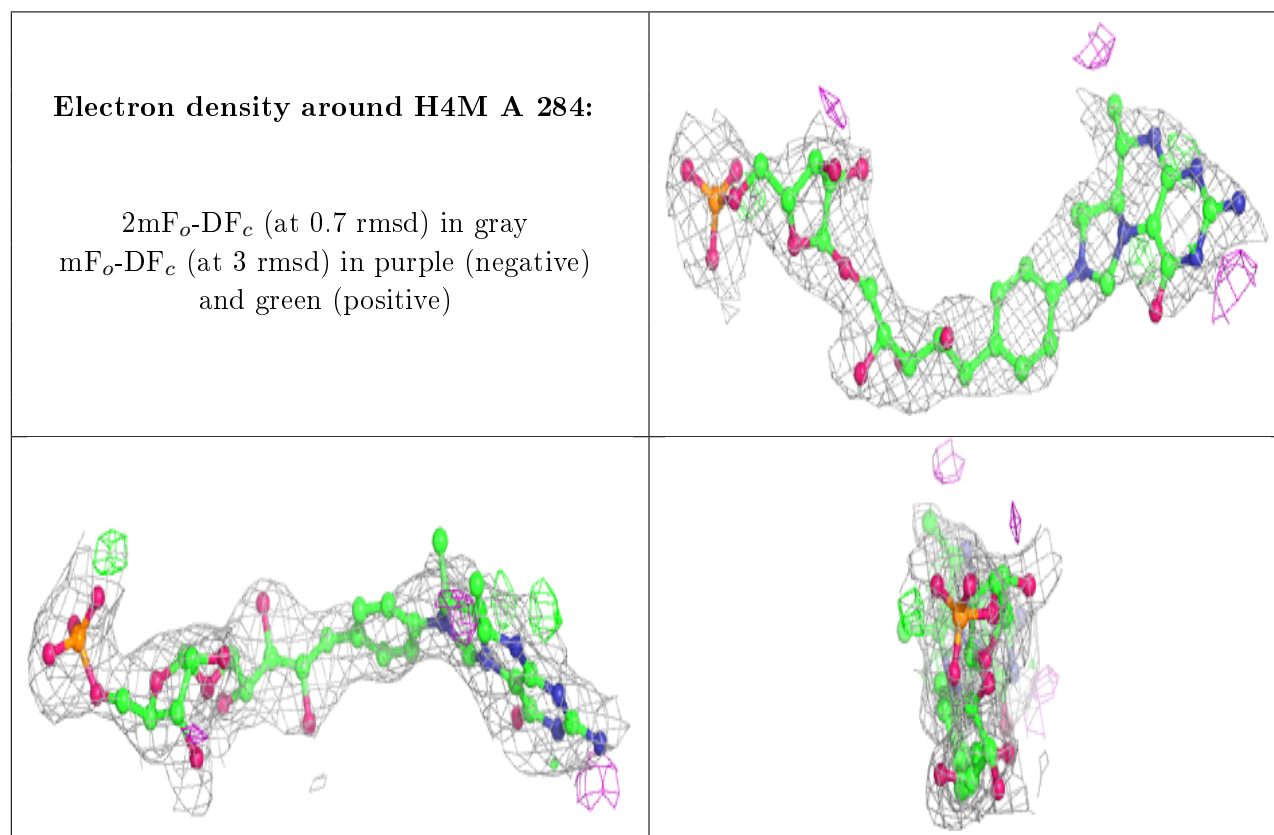
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

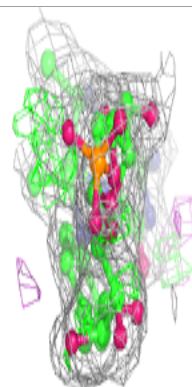
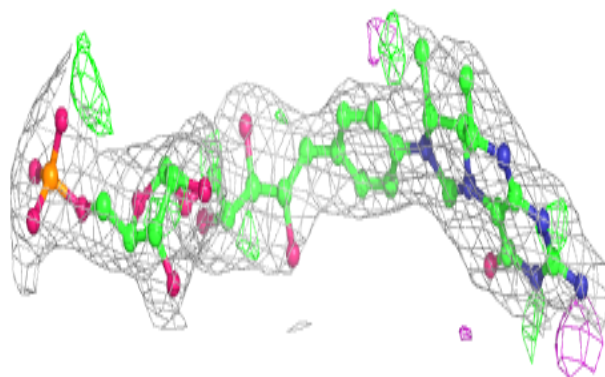
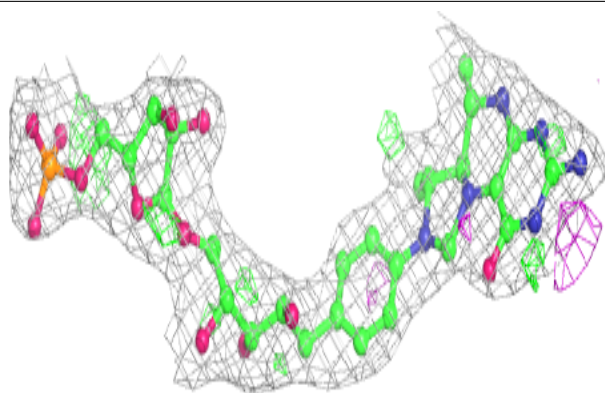
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	H4M	A	284	45/54	0.75	0.21	56,63,75,77	45
2	H4M	D	284	45/54	0.79	0.17	32,43,64,67	45
4	GOL	B	286	6/6	0.81	0.15	53,57,58,62	0
2	H4M	B	284	45/54	0.81	0.15	32,39,70,74	0
5	NA	E	285	1/1	0.82	0.52	72,72,72,72	0
2	H4M	C	284	45/54	0.85	0.15	28,38,63,65	45
2	H4M	E	284	45/54	0.85	0.15	34,41,66,72	0
5	NA	F	285	1/1	0.87	0.24	58,58,58,58	0
2	H4M	F	284	45/54	0.91	0.12	26,40,77,79	0
5	NA	D	285	1/1	0.95	0.23	45,45,45,45	0
3	CA	B	285	1/1	0.97	0.13	42,42,42,42	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.

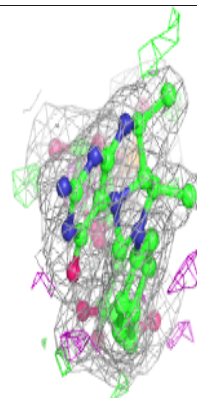
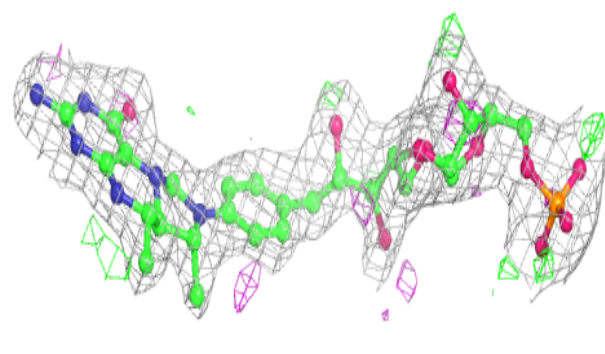
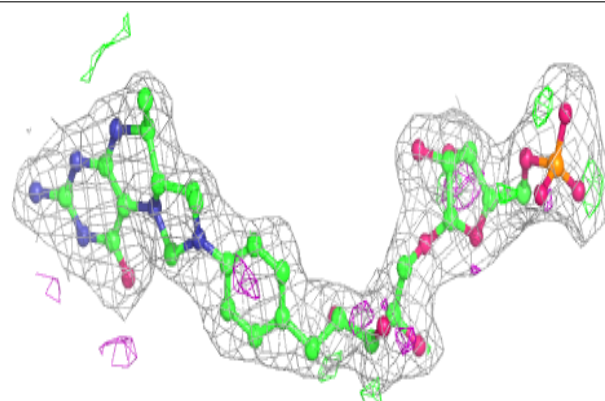


**Electron density around H4M D 284:**

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

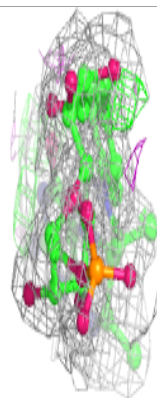
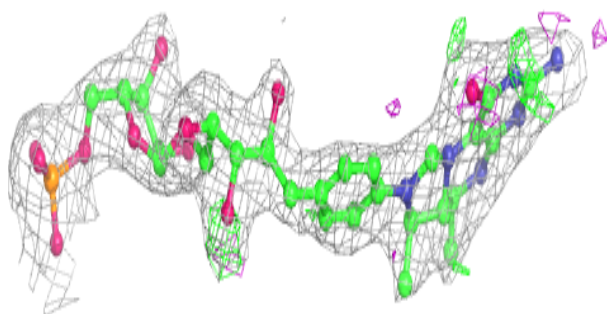
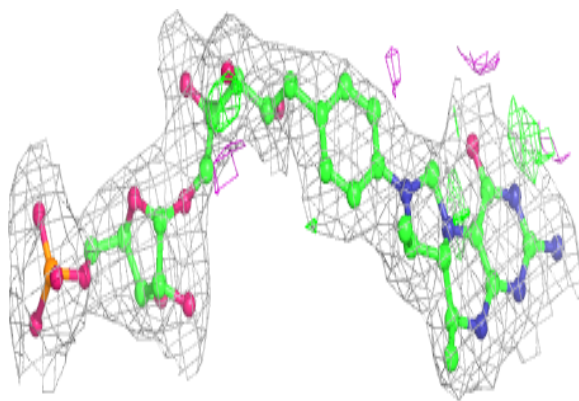
**Electron density around H4M B 284:**

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

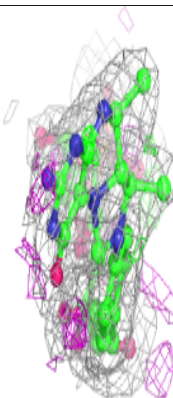
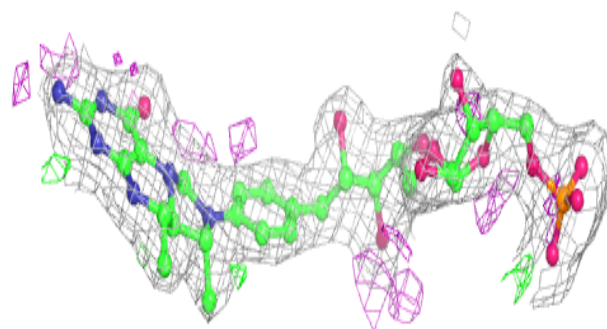
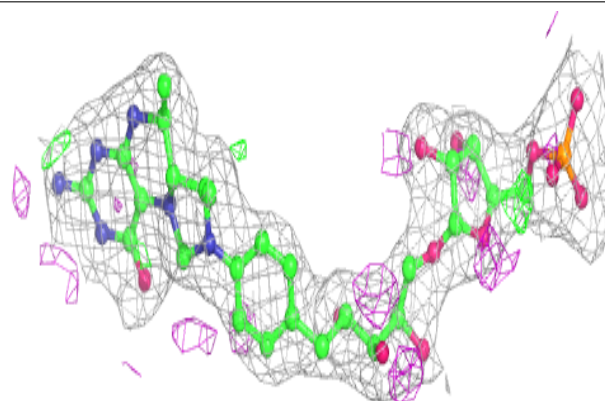


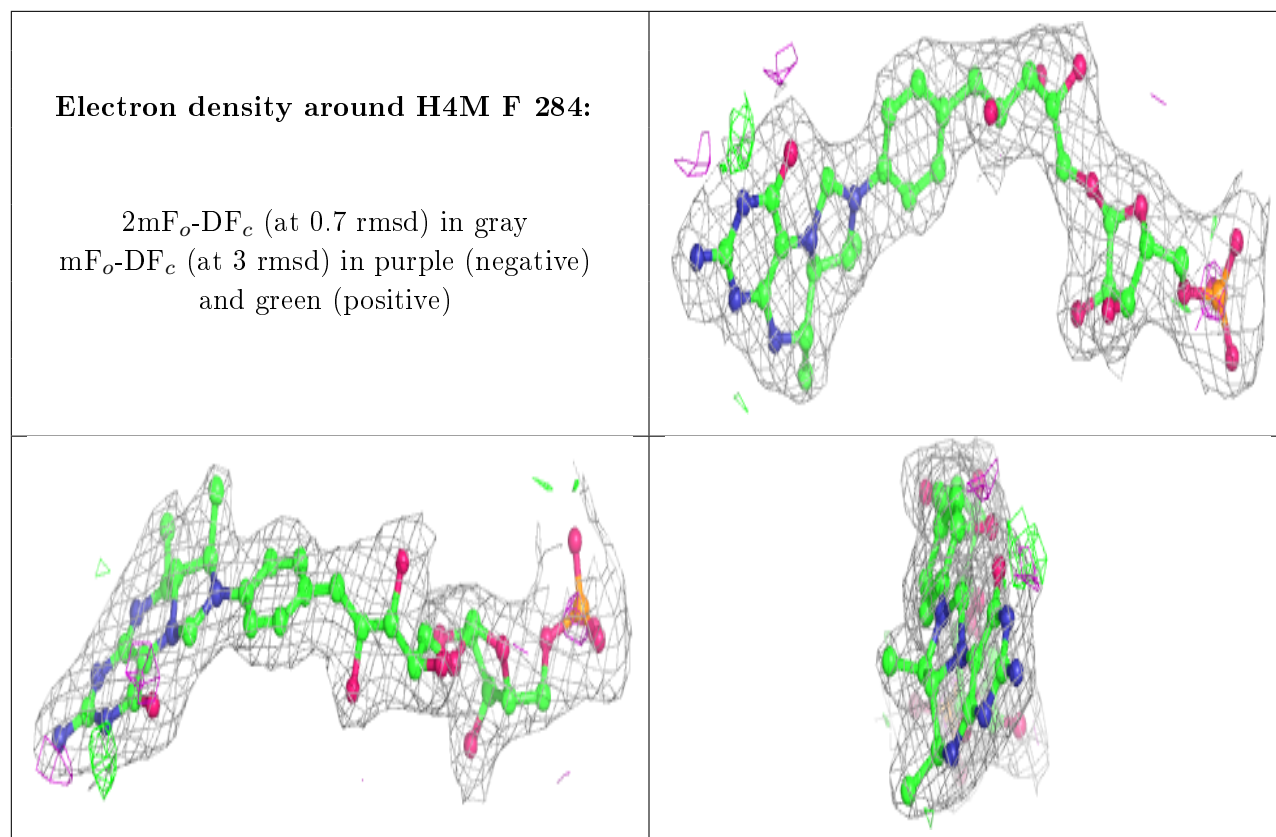
**Electron density around H4M C 284:**

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

**Electron density around H4M E 284:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.