



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:16 am BST

PDB ID : 3IQE  
Title : Structure of F420 dependent methylene-tetrahydromethanopterin dehydrogenase in complex with methylene-tetrahydromethanopterin and coenzyme F420  
Authors : Ceh, K.E.; Demmer, U.; Warkentin, E.; Moll, J.; Thauer, R.K.; Shima, S.; Ermler, U.  
Deposited on : 2009-08-20  
Resolution : 1.80 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

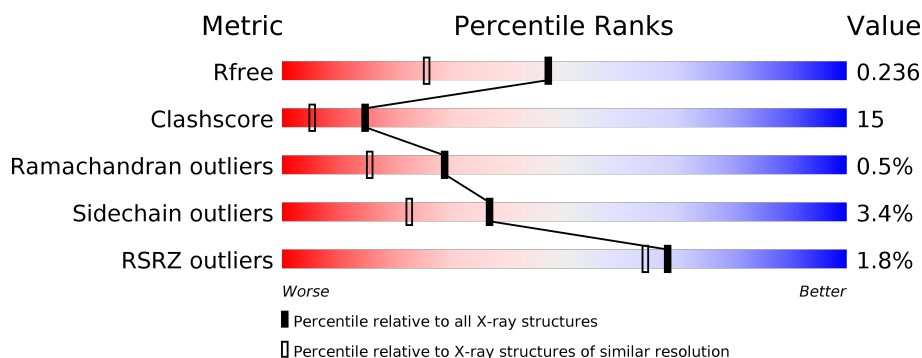
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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>2%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	283	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	283	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	283	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	E	283	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
1	F	283	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>

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
2	H4M	A	284	X	-	-	-
3	F42	C	285	-	X	-	-

## 2 Entry composition [i](#)

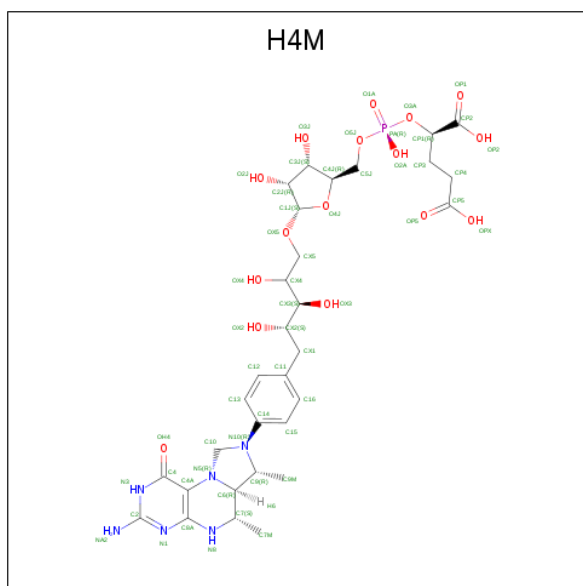
There are 6 unique types of molecules in this entry. The entry contains 14210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

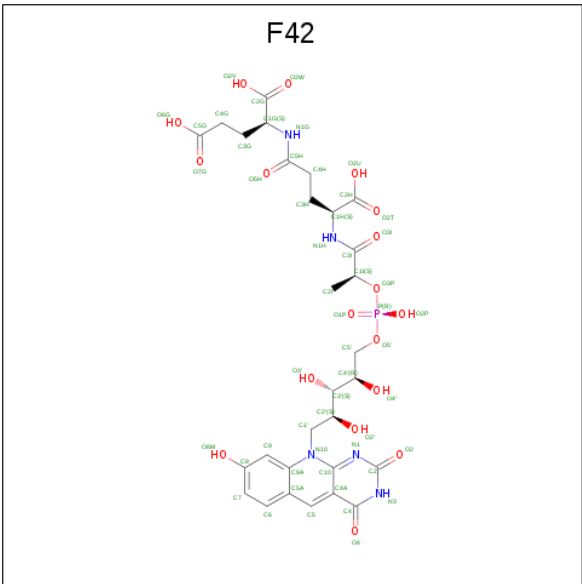
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2187	1373	357	437	20			
1	B	282	Total	C	N	O	S	0	1	0
			2190	1373	358	440	19			
1	C	282	Total	C	N	O	S	0	2	0
			2196	1378	359	439	20			
1	D	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	E	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			
1	F	282	Total	C	N	O	S	0	0	0
			2182	1369	357	437	19			

- Molecule 2 is 5,10-DIMETHYLENE TETRAHYDROMETHANOPTERIN (three-letter code: H4M) (formula:  $C_{31}H_{45}N_6O_{16}P$ ).



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 COENZYME F420 (three-letter code: F42) (formula: C<sub>29</sub>H<sub>36</sub>N<sub>5</sub>O<sub>18</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	16	3	10	1		
3	B	1	Total	C	N	O	P	0	0
			30	16	3	10	1		
3	C	1	Total	C	N	O	P	0	0
			30	16	3	10	1		
3	D	1	Total	C	N	O	P	0	0
			30	16	3	10	1		
3	E	1	Total	C	N	O	P	0	0
			30	16	3	10	1		
3	F	1	Total	C	N	O	P	0	0
			30	16	3	10	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ca 2	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

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

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

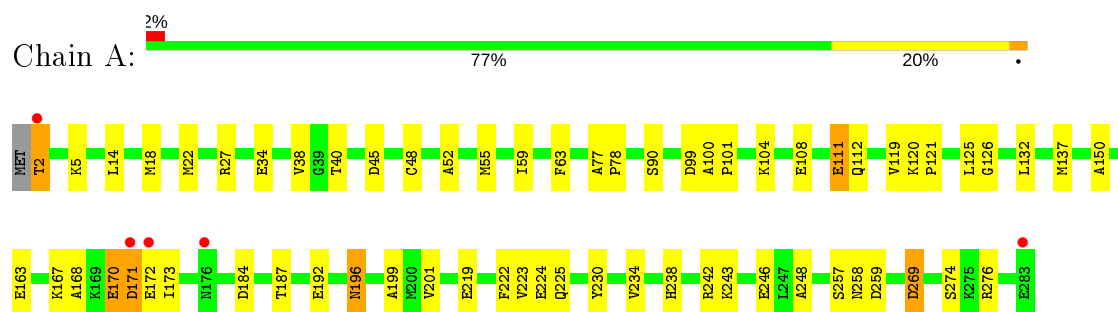
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total 85	O 85	0	0
6	B	115	Total 115	O 115	0	0
6	C	107	Total 107	O 107	0	0
6	D	106	Total 106	O 106	0	0
6	E	109	Total 109	O 109	0	0
6	F	112	Total 112	O 112	0	0

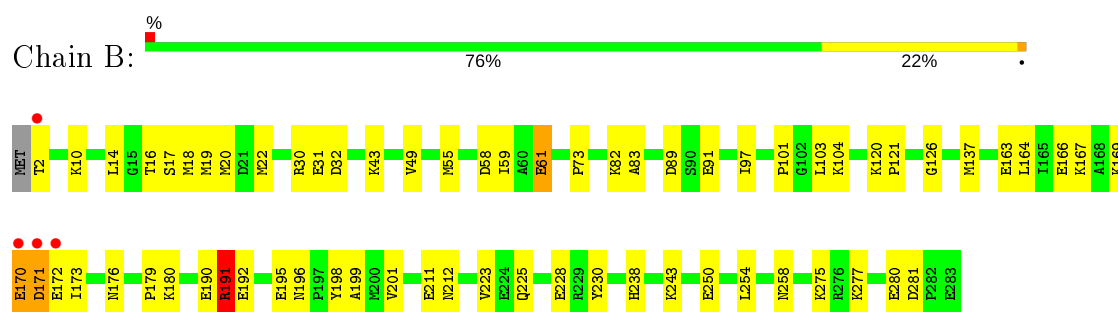
### 3 Residue-property plots

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.

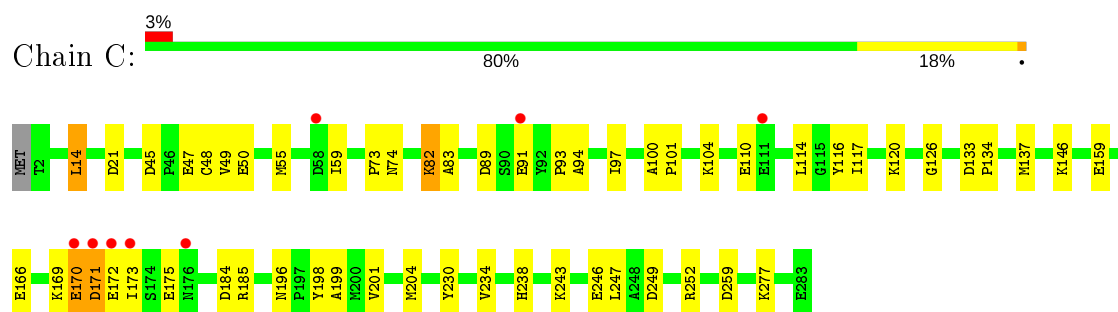
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



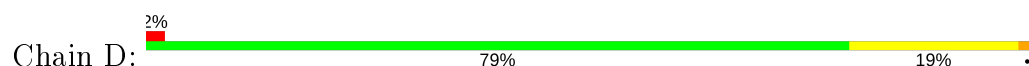
- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

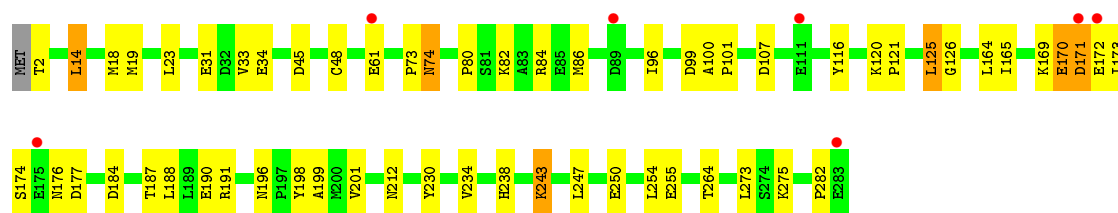


- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

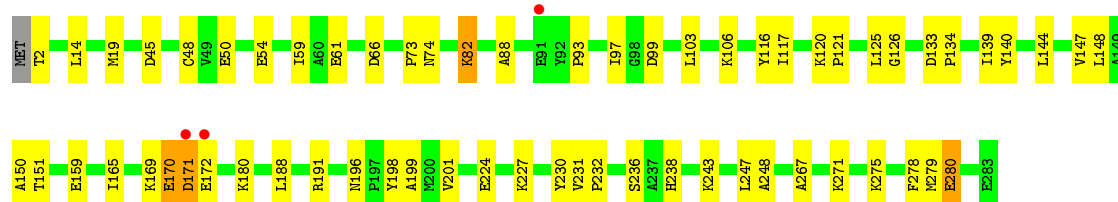
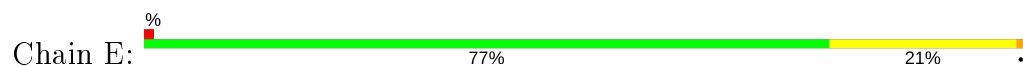


- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase

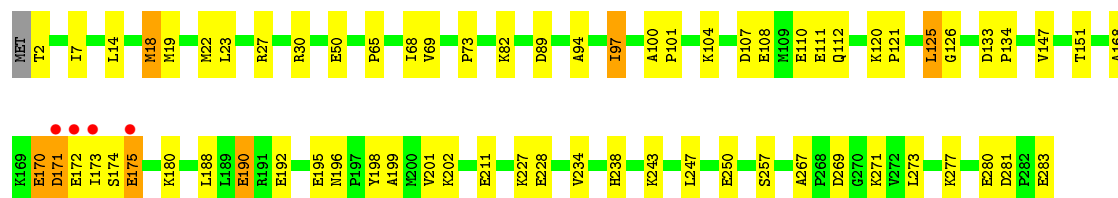
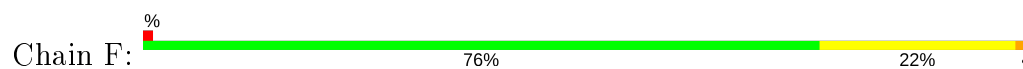




- Molecule 1: F420-dependent methylenetetrahydromethanopterin dehydrogenase



- 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, $\alpha$ , $\beta$ , $\gamma$	61.15Å 165.54Å 93.55Å 90.00° 99.14° 90.00°	Depositor
Resolution (Å)	92.45 – 1.80 47.22 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (92.45-1.80) 95.7 (47.22-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.190 , 0.228 0.198 , 0.236	Depositor DCC
$R_{free}$ test set	8157 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NA, H4M, F42, CA

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	0.65	0/2223	0.77	3/2999 (0.1%)
1	B	0.73	0/2223	0.81	2/3000 (0.1%)
1	C	0.70	0/2232	0.74	0/3011
1	D	0.68	0/2215	0.74	0/2989
1	E	0.71	0/2215	0.77	0/2989
1	F	0.74	0/2215	0.79	1/2989 (0.0%)
All	All	0.70	0/13323	0.77	6/17977 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	30	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	259	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	191	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	132	LEU	CB-CG-CD2	5.24	119.92	111.00
1	A	242	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	76	3
1	B	2190	0	2160	73	3
1	C	2196	0	2173	68	1
1	D	2182	0	2157	68	0
1	E	2182	0	2157	64	2
1	F	2182	0	2157	73	0
2	A	45	0	36	9	0
2	B	45	0	37	5	0
2	C	45	0	37	6	0
2	D	45	0	37	10	0
2	E	45	0	37	7	0
2	F	45	0	37	7	0
3	A	30	0	15	8	0
3	B	30	0	15	12	0
3	C	30	0	16	10	0
3	D	30	0	15	7	0
3	E	30	0	15	6	0
3	F	30	0	16	9	0
4	B	2	0	0	0	1
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	85	0	0	9	1
6	B	115	0	0	15	0
6	C	107	0	0	10	0
6	D	106	0	0	5	2
6	E	109	0	0	5	0
6	F	112	0	0	18	3
All	All	14210	0	13283	412	8

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 15.

All (412) 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)
2:A:284:H4M:H16	3:A:285:F42:C5	1.62	1.29
2:D:284:H4M:H16	3:D:285:F42:C5	1.65	1.23
2:F:284:H4M:H16	3:F:285:F42:C5	1.69	1.21
1:F:171:ASP:HB2	6:F:371:HOH:O	1.41	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:284:H4M:H16	3:C:285:F42:C5	1.76	1.16
1:C:50:GLU:HB2	1:C:82:LYS:NZ	1.59	1.16
2:A:284:H4M:H16	3:A:285:F42:H5	1.25	1.15
1:C:171:ASP:O	1:C:172:GLU:HG3	1.48	1.14
1:A:171:ASP:O	1:A:172:GLU:HG3	1.45	1.13
1:B:171:ASP:O	1:B:172:GLU:HG3	1.47	1.13
1:F:171:ASP:O	1:F:172:GLU:HG3	1.46	1.13
2:E:284:H4M:H16	3:E:285:F42:C5	1.78	1.13
1:D:171:ASP:O	1:D:172:GLU:HG3	1.47	1.12
1:A:223:VAL:O	1:A:225:GLN:NE2	1.85	1.10
1:E:171:ASP:O	1:E:172:GLU:HG3	1.46	1.10
2:D:284:H4M:H16	3:D:285:F42:H5	1.17	1.07
2:C:284:H4M:H16	3:C:285:F42:H5	1.35	1.07
1:B:18:MET:HE1	1:F:22:MET:CE	1.84	1.07
2:F:284:H4M:H16	3:F:285:F42:H5	1.33	1.06
1:E:50:GLU:OE1	1:E:82:LYS:NZ	1.87	1.05
1:C:50:GLU:HB2	1:C:82:LYS:HZ2	0.91	1.05
1:C:166:GLU:O	1:C:170:GLU:HG2	1.60	1.02
1:B:22:MET:HE1	1:F:18:MET:HE3	1.39	1.02
1:E:45:ASP:OD1	1:E:48:CYS:SG	2.18	1.01
1:E:54:GLU:OE2	6:E:292:HOH:O	1.79	1.01
1:F:126:GLY:H	1:F:238:HIS:HE1	1.04	1.00
1:F:175:GLU:OE1	6:F:329:HOH:O	1.78	1.00
1:B:18:MET:HE1	1:F:22:MET:HE1	1.43	0.99
2:E:284:H4M:H16	3:E:285:F42:H5	1.42	0.99
1:B:22:MET:HE1	1:F:18:MET:CE	1.94	0.97
1:D:164:LEU:HD11	1:D:173:ILE:HD13	1.45	0.97
1:C:50:GLU:OE1	1:C:82:LYS:NZ	1.98	0.97
1:E:126:GLY:H	1:E:238:HIS:HE1	1.12	0.97
1:F:172:GLU:OE2	6:F:485:HOH:O	1.83	0.97
1:B:18:MET:CE	1:F:22:MET:CE	2.43	0.96
1:B:18:MET:CE	1:F:22:MET:HE1	1.96	0.95
1:C:126:GLY:H	1:C:238:HIS:HE1	1.09	0.94
1:A:243:LYS:HE2	1:E:247:LEU:HG	1.45	0.94
1:D:126:GLY:H	1:D:238:HIS:HE1	1.15	0.94
1:E:88:ALA:O	6:E:287:HOH:O	1.86	0.94
1:A:126:GLY:H	1:A:238:HIS:HE1	1.16	0.89
1:F:192:GLU:N	6:F:447:HOH:O	1.63	0.89
1:A:137[A]:MET:CE	1:D:19:MET:HE1	2.02	0.89
2:D:284:H4M:C10	3:D:285:F42:H5	2.01	0.89
1:C:169:LYS:C	1:C:170:GLU:OE1	2.12	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:H4M:H18	2:D:284:H4M:H12	1.56	0.87
1:B:22:MET:CE	1:F:18:MET:HE3	2.04	0.87
2:A:284:H4M:C10	3:A:285:F42:H5	2.03	0.87
1:A:111:GLU:OE2	1:A:111:GLU:C	2.13	0.86
1:B:61:GLU:OE2	6:B:674:HOH:O	1.94	0.86
2:B:284:H4M:H16	3:B:285:F42:C5	2.04	0.86
6:C:747:HOH:O	1:E:279:MET:HE2	1.76	0.85
1:C:166:GLU:O	1:C:170:GLU:CG	2.25	0.84
1:B:126:GLY:H	1:B:238:HIS:HE1	1.18	0.84
1:B:211:GLU:OE2	6:B:752:HOH:O	1.96	0.82
1:B:228:GLU:OE1	6:B:337:HOH:O	1.98	0.82
1:E:278:PHE:CD1	1:E:279:MET:HE3	2.15	0.82
1:A:137[A]:MET:HE3	1:D:19:MET:HE1	1.61	0.82
2:A:284:H4M:C10	3:A:285:F42:C5	2.53	0.81
1:A:223:VAL:C	1:A:225:GLN:NE2	2.35	0.81
1:D:107:ASP:OD1	6:D:632:HOH:O	2.00	0.80
1:F:211:GLU:OE2	6:F:575:HOH:O	1.99	0.79
1:A:22:MET:HE1	1:D:18:MET:CE	2.13	0.79
1:B:61:GLU:OE1	6:B:674:HOH:O	2.00	0.78
1:A:137[B]:MET:SD	2:A:284:H4M:H8	2.24	0.76
1:E:159:GLU:OE2	1:E:191:ARG:NH2	2.19	0.76
1:F:126:GLY:H	1:F:238:HIS:CE1	1.97	0.76
1:B:61:GLU:CD	6:B:674:HOH:O	2.22	0.76
1:B:18:MET:HE1	1:F:22:MET:HE3	1.67	0.75
2:F:284:H4M:C10	3:F:285:F42:C5	2.59	0.75
1:A:274:SER:HB3	6:A:298:HOH:O	1.85	0.75
1:F:196:ASN:HD22	1:F:199:ALA:H	1.34	0.75
1:C:243:LYS:NZ	1:C:246:GLU:OE1	2.18	0.74
1:C:93:PRO:HG2	1:C:173:ILE:HG21	1.70	0.74
1:C:259:ASP:OD2	6:C:312:HOH:O	2.05	0.74
1:C:45:ASP:OD1	1:C:48:CYS:SG	2.44	0.74
2:F:284:H4M:C10	3:F:285:F42:H5	2.17	0.73
2:B:284:H4M:H13	3:B:285:F42:C4	2.18	0.73
1:A:22:MET:CE	1:D:18:MET:CE	2.66	0.73
1:C:238:HIS:HD2	6:C:657:HOH:O	1.71	0.72
2:E:284:H4M:H12	2:E:284:H4M:H18	1.69	0.72
1:B:180:LYS:HD2	6:B:667:HOH:O	1.90	0.72
2:B:284:H4M:H16	3:B:285:F42:H5	1.72	0.72
2:D:284:H4M:C10	3:D:285:F42:C5	2.58	0.72
1:E:279:MET:CE	1:E:279:MET:HA	2.20	0.71
1:F:97:ILE:O	1:F:97:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:H4M:OX2	2:A:284:H4M:OX4	2.06	0.71
1:B:22:MET:CE	1:F:18:MET:CE	2.65	0.71
1:C:74:ASN:HD22	3:C:285:F42:H5'1	1.55	0.70
1:E:278:PHE:HD1	1:E:279:MET:HE3	1.52	0.70
1:E:196:ASN:HD22	1:E:199:ALA:H	1.38	0.70
1:A:137[B]:MET:HE2	1:D:19:MET:HE1	1.73	0.70
1:A:137[A]:MET:CE	1:D:19:MET:CE	2.69	0.70
1:A:172:GLU:OE1	6:A:351:HOH:O	2.09	0.70
1:C:91:GLU:HG2	6:C:568:HOH:O	1.92	0.69
1:C:133:ASP:HB2	1:C:134:PRO:HD2	1.75	0.69
1:C:159:GLU:OE1	6:C:326:HOH:O	2.11	0.69
2:A:284:H4M:H13	3:A:285:F42:C4	2.23	0.68
1:F:111:GLU:OE1	6:F:294:HOH:O	2.10	0.68
1:E:126:GLY:H	1:E:238:HIS:CE1	2.03	0.68
1:E:224:GLU:OE2	6:E:434:HOH:O	2.10	0.68
1:C:133:ASP:HB2	1:C:134:PRO:CD	2.24	0.68
1:C:196:ASN:HD22	1:C:199:ALA:H	1.42	0.68
1:F:195:GLU:HG2	6:F:496:HOH:O	1.93	0.68
1:A:258:ASN:HB3	6:A:430:HOH:O	1.94	0.67
1:C:169:LYS:O	1:C:170:GLU:OE1	2.11	0.67
1:E:231:VAL:HB	1:E:232:PRO:HD3	1.75	0.67
1:B:18:MET:HE3	1:F:22:MET:CE	2.23	0.67
1:B:169:LYS:C	1:B:170:GLU:OE1	2.32	0.67
1:E:278:PHE:CD1	1:E:279:MET:CE	2.78	0.66
1:D:82:LYS:O	1:D:86:MET:HG3	1.95	0.66
1:B:73:PRO:HB3	3:B:285:F42:C5A	2.26	0.66
1:D:196:ASN:HD22	1:D:199:ALA:H	1.41	0.66
1:B:250:GLU:OE2	1:D:243:LYS:NZ	2.29	0.65
1:C:47:GLU:HB2	6:C:683:HOH:O	1.96	0.65
2:E:284:H4M:C10	3:E:285:F42:C5	2.68	0.65
1:C:243:LYS:HG3	1:F:247:LEU:HG	1.78	0.65
1:F:175:GLU:CD	6:F:329:HOH:O	2.29	0.65
1:D:184:ASP:OD1	6:D:542:HOH:O	2.13	0.65
1:D:164:LEU:CD1	1:D:173:ILE:HD13	2.22	0.65
6:B:335:HOH:O	1:F:134:PRO:HD2	1.95	0.65
1:C:74:ASN:ND2	3:C:285:F42:H5'1	2.12	0.65
1:A:137[A]:MET:HE1	1:D:19:MET:CE	2.27	0.65
1:A:223:VAL:C	1:A:225:GLN:HE21	1.95	0.64
1:B:20:MET:SD	1:B:97:ILE:HD12	2.36	0.64
1:E:125:LEU:HD12	1:E:125:LEU:C	2.17	0.64
1:B:126:GLY:H	1:B:238:HIS:CE1	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:PRO:HB3	3:C:285:F42:C7	2.27	0.63
1:C:146:LYS:HZ3	1:C:249:ASP:HB2	1.63	0.63
1:C:93:PRO:CG	1:C:173:ILE:HG21	2.29	0.63
1:B:196:ASN:HD22	1:B:199:ALA:H	1.47	0.63
2:B:284:H4M:H18	2:B:284:H4M:H12	1.81	0.62
1:A:137[B]:MET:CE	1:D:19:MET:CE	2.78	0.62
1:C:126:GLY:H	1:C:238:HIS:CE1	2.02	0.62
1:B:163:GLU:O	1:B:167:LYS:HG3	2.00	0.61
1:C:49:VAL:CG1	1:C:83:ALA:HB2	2.30	0.61
1:E:150:ALA:HB3	1:E:248:ALA:HB1	1.82	0.61
1:B:126:GLY:N	1:B:238:HIS:HE1	1.96	0.61
1:E:171:ASP:OD2	6:E:323:HOH:O	2.16	0.61
1:A:269:ASP:HB3	6:A:539:HOH:O	2.00	0.61
1:B:73:PRO:HG2	3:B:285:F42:C5	2.31	0.60
1:D:196:ASN:HD21	1:D:198:TYR:HB2	1.67	0.60
1:D:45:ASP:OD1	1:D:48:CYS:SG	2.59	0.60
1:C:146:LYS:NZ	1:C:249:ASP:OD1	2.34	0.60
1:A:137[A]:MET:HE1	1:D:19:MET:HE3	1.84	0.60
1:D:99:ASP:OD1	3:D:285:F42:O8M	2.18	0.60
1:E:267:ALA:HB3	1:E:271:LYS:HG2	1.84	0.60
1:F:195:GLU:CG	6:F:496:HOH:O	2.50	0.59
1:F:269:ASP:OD1	6:F:658:HOH:O	2.17	0.59
1:B:190:GLU:CD	6:B:293:HOH:O	2.40	0.59
1:A:45:ASP:OD1	1:A:48:CYS:SG	2.61	0.59
1:B:258:ASN:HA	6:B:583:HOH:O	2.03	0.59
1:D:173:ILE:HG23	1:D:177:ASP:HB2	1.85	0.59
1:D:187:THR:O	1:D:190:GLU:HG2	2.02	0.59
2:E:284:H4M:C10	3:E:285:F42:H5	2.27	0.59
1:C:277:LYS:HE3	6:C:686:HOH:O	2.03	0.59
1:D:174:SER:N	1:D:177:ASP:OD1	2.33	0.59
1:A:196:ASN:HD22	1:A:199:ALA:H	1.50	0.58
1:C:73:PRO:HB3	3:C:285:F42:C6	2.34	0.58
1:C:137[A]:MET:SD	1:E:19:MET:HE1	2.44	0.58
1:C:198:TYR:HA	1:C:201:VAL:HG22	1.84	0.58
6:C:747:HOH:O	1:E:279:MET:CE	2.43	0.58
1:A:222:PHE:CZ	3:A:285:F42:H5'2	2.39	0.58
1:A:22:MET:CE	1:D:18:MET:HE3	2.32	0.58
1:C:170:GLU:OE1	1:C:170:GLU:N	2.36	0.58
1:A:38:VAL:HG11	1:A:59:ILE:CD1	2.33	0.57
1:C:238:HIS:CD2	6:C:657:HOH:O	2.52	0.57
1:D:31:GLU:OE2	6:D:312:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:PRO:HB3	3:D:285:F42:C6	2.34	0.57
1:E:278:PHE:HD1	1:E:279:MET:CE	2.17	0.57
1:F:168:ALA:HB2	1:F:173:ILE:HD11	1.86	0.57
1:D:74:ASN:O	1:D:80:PRO:HG2	2.04	0.57
1:B:137:MET:HE3	1:F:19:MET:HE1	1.86	0.56
1:E:97:ILE:HD13	1:E:117:ILE:HB	1.87	0.56
1:B:101:PRO:O	1:B:104:LYS:HE3	2.06	0.56
1:F:271:LYS:NZ	6:F:404:HOH:O	2.16	0.56
1:E:165:ILE:O	1:E:169:LYS:HG3	2.06	0.56
2:F:284:H4M:H13	3:F:285:F42:C4	2.34	0.56
1:B:170:GLU:N	1:B:170:GLU:OE1	2.37	0.56
1:A:111:GLU:OE2	1:A:112:GLN:N	2.38	0.55
1:D:100:ALA:N	1:D:101:PRO:CD	2.69	0.55
1:F:180:LYS:HD2	6:F:455:HOH:O	2.05	0.55
2:F:284:H4M:H14	2:F:284:H4M:H9	1.89	0.55
1:A:108:GLU:O	1:A:112:GLN:HG3	2.07	0.55
1:A:137[B]:MET:CE	1:D:19:MET:HE1	2.30	0.55
2:C:284:H4M:C10	3:C:285:F42:H5	2.24	0.55
1:A:22:MET:HE1	1:D:18:MET:HE3	1.89	0.55
1:D:73:PRO:HB3	3:D:285:F42:C7	2.37	0.54
1:A:2:THR:HA	6:A:509:HOH:O	2.07	0.54
1:E:196:ASN:ND2	1:E:198:TYR:H	2.06	0.54
1:C:14:LEU:HD13	1:C:73:PRO:HG3	1.89	0.54
1:A:201:VAL:CG1	1:E:236:SER:HA	2.38	0.54
1:C:133:ASP:CB	1:C:134:PRO:CD	2.84	0.54
3:B:285:F42:O2'	3:B:285:F42:N1	2.33	0.53
1:C:170:GLU:CD	1:C:170:GLU:N	2.61	0.53
1:C:50:GLU:CB	1:C:82:LYS:NZ	2.53	0.53
1:E:99:ASP:HB2	6:E:306:HOH:O	2.07	0.53
1:A:126:GLY:H	1:A:238:HIS:CE1	2.09	0.53
1:A:246:GLU:OE1	6:A:684:HOH:O	2.19	0.53
1:D:61:GLU:HG2	6:D:649:HOH:O	2.07	0.53
1:B:22:MET:HE1	1:F:18:MET:HE2	1.84	0.53
1:B:243:LYS:NZ	1:D:250:GLU:OE2	2.32	0.53
1:A:22:MET:HE3	1:D:18:MET:CE	2.37	0.53
1:C:170:GLU:CA	1:C:170:GLU:OE1	2.54	0.53
1:A:101:PRO:O	1:A:104:LYS:CE	2.57	0.53
1:A:22:MET:HE1	1:D:18:MET:HE2	1.89	0.53
1:E:279:MET:HE3	1:E:279:MET:HA	1.88	0.53
1:F:120:LYS:N	1:F:121:PRO:CD	2.72	0.53
1:E:170:GLU:CA	1:E:170:GLU:OE1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD12	1:A:125:LEU:C	2.30	0.53
1:C:247:LEU:HG	1:F:243:LYS:HG3	1.92	0.52
1:B:32:ASP:HB2	1:B:169:LYS:HE3	1.90	0.52
1:C:100:ALA:N	1:C:101:PRO:CD	2.72	0.52
1:B:73:PRO:HB3	3:B:285:F42:C6	2.39	0.52
2:C:284:H4M:C10	3:C:285:F42:C5	2.70	0.52
1:A:111:GLU:OE2	1:A:111:GLU:O	2.27	0.52
1:B:228:GLU:CD	6:B:337:HOH:O	2.45	0.52
1:C:97:ILE:HD12	1:C:117:ILE:HB	1.92	0.52
1:E:106:LYS:HG3	1:E:116:TYR:CZ	2.45	0.52
1:D:170:GLU:CA	1:D:170:GLU:OE1	2.57	0.52
2:D:284:H4M:C13	2:D:284:H4M:H12	2.36	0.52
2:A:284:H4M:H12	2:A:284:H4M:H18	1.92	0.52
1:A:170:GLU:CA	1:A:170:GLU:OE1	2.58	0.51
1:F:73:PRO:HB3	3:F:285:F42:C5A	2.40	0.51
1:A:168:ALA:HB2	1:A:173:ILE:HD11	1.92	0.51
1:C:49:VAL:HG11	1:C:83:ALA:HB2	1.92	0.51
1:B:82:LYS:HE2	6:B:458:HOH:O	2.10	0.51
1:E:66:ASP:O	1:E:93:PRO:HG2	2.11	0.51
1:B:170:GLU:CA	1:B:170:GLU:OE1	2.56	0.51
1:A:201:VAL:HG13	1:E:236:SER:CA	2.40	0.51
1:F:170:GLU:CA	1:F:170:GLU:OE1	2.57	0.51
1:D:120:LYS:HD3	1:D:184:ASP:HB3	1.92	0.51
1:E:278:PHE:CE1	1:E:279:MET:HE1	2.46	0.51
1:B:73:PRO:HB3	3:B:285:F42:C9A	2.41	0.51
1:A:101:PRO:O	1:A:104:LYS:HE3	2.11	0.51
1:F:19:MET:HE2	1:F:23:LEU:HD21	1.91	0.51
1:F:73:PRO:HB3	3:F:285:F42:C6	2.41	0.51
1:A:119:VAL:HG12	1:A:121:PRO:HD2	1.93	0.50
1:F:100:ALA:N	1:F:101:PRO:CD	2.73	0.50
1:A:99:ASP:OD1	3:A:285:F42:O8M	2.30	0.50
1:B:164:LEU:HD11	1:B:173:ILE:HD13	1.93	0.50
1:B:170:GLU:N	1:B:170:GLU:CD	2.65	0.50
1:C:110:GLU:OE2	1:C:116:TYR:OH	2.25	0.50
1:A:120:LYS:N	1:A:121:PRO:CD	2.75	0.50
1:A:40:THR:HG23	1:A:52:ALA:HB2	1.93	0.50
1:B:103:LEU:HD11	1:B:120:LYS:HD3	1.94	0.50
1:B:223:VAL:O	1:B:225:GLN:NE2	2.37	0.50
1:D:173:ILE:HA	1:D:177:ASP:OD1	2.12	0.50
1:E:275:LYS:NZ	1:E:280:GLU:O	2.40	0.49
1:B:169:LYS:O	1:B:170:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:284:H4M:H18	2:C:284:H4M:H12	1.94	0.49
1:D:275:LYS:HD2	1:D:282:PRO:HD3	1.95	0.49
1:E:133:ASP:HB2	1:E:134:PRO:CD	2.42	0.49
1:B:10:LYS:HE2	1:B:17:SER:O	2.13	0.49
1:C:169:LYS:C	1:C:170:GLU:CD	2.71	0.49
1:C:126:GLY:HA3	1:C:234:VAL:HB	1.94	0.49
1:D:126:GLY:H	1:D:238:HIS:CE1	2.08	0.49
1:E:103:LEU:HD11	1:E:120:LYS:HD3	1.93	0.49
1:A:77:ALA:HB1	1:A:78:PRO:HD2	1.94	0.49
1:B:73:PRO:CG	3:B:285:F42:C5	2.91	0.49
1:C:50:GLU:CD	1:C:82:LYS:HZ1	2.05	0.49
1:B:91:GLU:HG2	6:B:546:HOH:O	2.12	0.49
1:F:50:GLU:OE2	1:F:82:LYS:HE2	2.13	0.49
1:D:99:ASP:CG	1:D:101:PRO:HD2	2.33	0.49
1:A:224:GLU:C	1:A:225:GLN:NE2	2.67	0.48
1:B:212:ASN:ND2	1:D:212:ASN:ND2	2.61	0.48
1:C:93:PRO:HG2	1:C:173:ILE:CG2	2.42	0.48
1:F:190:GLU:HG2	6:F:330:HOH:O	2.12	0.48
1:E:196:ASN:HD21	1:E:198:TYR:HB2	1.78	0.48
1:F:111:GLU:CD	6:F:294:HOH:O	2.52	0.48
1:F:107:ASP:HB2	6:F:338:HOH:O	2.13	0.48
1:B:55:MET:O	1:B:59:ILE:HG12	2.13	0.48
1:D:254:LEU:HD22	1:F:257:SER:HA	1.96	0.48
1:B:73:PRO:CB	3:B:285:F42:C5A	2.92	0.48
1:D:170:GLU:N	1:D:170:GLU:OE1	2.47	0.48
1:C:169:LYS:HB2	1:C:170:GLU:OE2	2.14	0.48
1:E:169:LYS:C	1:E:171:ASP:H	2.16	0.48
1:F:101:PRO:O	1:F:104:LYS:HE3	2.13	0.48
1:A:258:ASN:CB	6:A:430:HOH:O	2.59	0.47
2:A:284:H4M:H13	3:A:285:F42:N3	2.29	0.47
1:C:93:PRO:CB	1:C:173:ILE:HG21	2.44	0.47
1:D:80:PRO:O	1:D:84:ARG:HG3	2.14	0.47
1:E:198:TYR:HA	1:E:201:VAL:HG22	1.95	0.47
1:E:279:MET:HE2	1:E:279:MET:HA	1.94	0.47
1:D:126:GLY:HA3	1:D:234:VAL:HB	1.96	0.47
1:D:264:THR:HA	1:D:273:LEU:O	2.15	0.47
1:E:171:ASP:O	1:E:172:GLU:CG	2.40	0.47
1:B:243:LYS:HG3	1:D:247:LEU:HG	1.97	0.47
1:A:170:GLU:N	1:A:170:GLU:OE1	2.47	0.47
1:B:166:GLU:O	1:B:170:GLU:OE2	2.33	0.47
1:D:243:LYS:HD2	1:D:243:LYS:HA	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:OD1	1:A:184:ASP:C	2.53	0.46
1:C:166:GLU:O	1:C:170:GLU:OE2	2.33	0.46
1:F:170:GLU:N	1:F:170:GLU:OE1	2.47	0.46
1:A:201:VAL:HG13	1:E:236:SER:N	2.30	0.46
1:B:198:TYR:HA	1:B:201:VAL:HG22	1.97	0.46
1:A:223:VAL:C	1:A:225:GLN:HE22	2.16	0.46
2:B:284:H4M:C13	2:B:284:H4M:H12	2.46	0.46
1:E:231:VAL:HB	1:E:232:PRO:CD	2.43	0.46
1:A:257:SER:HA	1:B:254:LEU:HD22	1.96	0.46
1:C:196:ASN:HD21	1:C:198:TYR:HB2	1.81	0.46
1:F:174:SER:HB3	6:F:442:HOH:O	2.16	0.46
2:C:284:H4M:H13	3:C:285:F42:C4	2.45	0.46
1:B:179:PRO:HB3	6:B:707:HOH:O	2.16	0.46
1:F:196:ASN:HD21	1:F:198:TYR:HB2	1.81	0.46
1:D:125:LEU:HG	2:D:284:H4M:C4	2.46	0.45
1:F:19:MET:HE2	1:F:19:MET:HB3	1.65	0.45
1:D:96:ILE:O	1:D:116:TYR:HA	2.16	0.45
1:E:170:GLU:N	1:E:170:GLU:OE1	2.49	0.45
1:B:16:THR:O	1:B:20:MET:HB3	2.16	0.45
1:C:55:MET:SD	1:E:59:ILE:HD12	2.57	0.45
1:B:73:PRO:HG2	3:B:285:F42:C4A	2.46	0.45
1:F:198:TYR:HA	1:F:201:VAL:HG22	1.99	0.45
1:D:198:TYR:HA	1:D:201:VAL:HG22	1.98	0.45
1:A:150:ALA:HB3	1:A:248:ALA:HB1	1.99	0.45
1:D:19:MET:HE2	1:D:23:LEU:HD21	1.99	0.45
1:B:19:MET:HE2	1:B:19:MET:HB3	1.72	0.45
1:C:170:GLU:O	1:C:171:ASP:C	2.55	0.45
1:D:165:ILE:O	1:D:169:LYS:HG3	2.17	0.45
1:D:255:GLU:OE2	6:D:562:HOH:O	2.21	0.45
1:A:137[B]:MET:CE	1:D:19:MET:HE3	2.47	0.44
1:C:252:ARG:NE	1:E:139:ILE:HD13	2.31	0.44
1:B:137:MET:CE	1:F:19:MET:HE1	2.47	0.44
1:E:227:LYS:HA	1:E:230:TYR:CD1	2.52	0.44
1:F:147:VAL:O	1:F:151:THR:HG23	2.17	0.44
1:B:170:GLU:O	1:B:171:ASP:C	2.56	0.44
1:C:166:GLU:O	1:C:170:GLU:CD	2.56	0.44
1:D:170:GLU:O	1:D:171:ASP:C	2.55	0.44
1:D:125:LEU:C	1:D:125:LEU:HD12	2.37	0.44
1:A:201:VAL:CG1	1:E:236:SER:CA	2.94	0.44
1:F:133:ASP:HB2	1:F:134:PRO:CD	2.48	0.44
1:F:228:GLU:CD	6:F:464:HOH:O	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:ND2	1:B:176:ASN:H	2.16	0.44
1:D:120:LYS:N	1:D:121:PRO:HD2	2.33	0.44
1:A:201:VAL:CG1	1:E:236:SER:N	2.80	0.44
1:A:5:LYS:NZ	1:A:63:PHE:O	2.38	0.44
1:F:108:GLU:O	1:F:112:GLN:HG3	2.18	0.44
1:A:137[B]:MET:HE3	1:D:19:MET:CE	2.48	0.44
1:B:49:VAL:CG1	1:B:83:ALA:HB2	2.47	0.44
1:A:104:LYS:HB2	1:A:104:LYS:HE3	1.71	0.43
1:B:243:LYS:HA	1:B:243:LYS:HD3	1.75	0.43
1:A:170:GLU:O	1:A:171:ASP:C	2.55	0.43
1:A:5:LYS:HB3	1:A:63:PHE:CE2	2.53	0.43
1:A:171:ASP:O	1:A:172:GLU:CG	2.39	0.43
1:F:170:GLU:O	1:F:171:ASP:C	2.56	0.43
1:B:120:LYS:N	1:B:121:PRO:CD	2.81	0.43
1:B:281:ASP:OD2	1:F:227:LYS:NZ	2.50	0.43
1:A:126:GLY:HA3	1:A:234:VAL:HB	2.01	0.43
1:E:170:GLU:O	1:E:171:ASP:C	2.56	0.43
1:F:110:GLU:HG2	1:F:180:LYS:HE3	2.01	0.43
2:E:284:H4M:H9	2:E:284:H4M:H14	2.01	0.43
1:F:126:GLY:HA3	1:F:234:VAL:HB	1.99	0.43
1:F:277:LYS:HB2	1:F:280:GLU:HB3	2.00	0.43
1:A:101:PRO:HB3	1:A:104:LYS:NZ	2.33	0.43
1:B:73:PRO:CG	3:B:285:F42:C5A	2.97	0.43
1:E:120:LYS:N	1:E:121:PRO:CD	2.82	0.43
1:F:188:LEU:HD23	1:F:188:LEU:HA	1.77	0.43
1:B:43:LYS:NZ	1:F:30:ARG:O	2.48	0.43
1:A:27:ARG:HA	2:D:284:H4M:H12	2.01	0.42
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.85	0.42
2:E:284:H4M:C13	2:E:284:H4M:H12	2.46	0.42
1:F:68:ILE:HG22	1:F:69:VAL:N	2.33	0.42
2:D:284:H4M:H14	2:D:284:H4M:H9	2.00	0.42
1:E:73:PRO:HB3	3:E:285:F42:C5A	2.50	0.42
1:F:283:GLU:O	6:F:404:HOH:O	2.20	0.42
1:C:93:PRO:CG	1:C:173:ILE:CG2	2.97	0.42
1:C:73:PRO:HG2	3:C:285:F42:C5	2.50	0.42
1:D:164:LEU:CD1	1:D:173:ILE:CD1	2.96	0.42
1:A:187:THR:HG23	6:A:492:HOH:O	2.20	0.41
1:C:21:ASP:OD2	6:C:525:HOH:O	2.22	0.41
1:F:202:LYS:NZ	1:F:250:GLU:OE1	2.47	0.41
1:C:185:ARG:HG3	1:C:204:MET:O	2.19	0.41
1:A:100:ALA:HB3	1:A:101:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HE3	1:B:277:LYS:O	2.20	0.41
1:D:188:LEU:HA	1:D:188:LEU:HD23	1.80	0.41
1:E:125:LEU:CD1	1:E:125:LEU:C	2.87	0.41
1:F:243:LYS:HD3	1:F:243:LYS:HA	1.82	0.41
2:F:284:H4M:H16	3:F:285:F42:C5A	2.38	0.41
1:A:163:GLU:O	1:A:167:LYS:HG3	2.20	0.41
1:B:22:MET:CE	1:F:18:MET:HE2	2.45	0.41
1:C:55:MET:O	1:C:59:ILE:HD12	2.21	0.41
1:D:125:LEU:HG	2:D:284:H4M:C4A	2.50	0.41
1:F:125:LEU:C	1:F:125:LEU:HD12	2.41	0.41
1:F:7:ILE:HD12	1:F:65:PRO:HG3	2.03	0.41
1:E:147:VAL:O	1:E:151:THR:HG23	2.21	0.41
1:F:68:ILE:O	1:F:94:ALA:HA	2.21	0.41
1:A:52:ALA:HA	1:A:55:MET:HE2	2.02	0.41
1:D:170:GLU:N	1:D:170:GLU:CD	2.74	0.41
1:A:170:GLU:N	1:A:170:GLU:CD	2.74	0.41
1:B:191:ARG:HD2	6:B:339:HOH:O	2.20	0.41
1:B:61:GLU:OE2	6:B:625:HOH:O	2.22	0.41
1:D:187:THR:O	1:D:191:ARG:HG2	2.21	0.41
1:E:125:LEU:HB3	1:E:140:TYR:CE2	2.56	0.41
3:E:285:F42:H9	3:E:285:F42:C2'	2.50	0.41
1:F:267:ALA:HB2	1:F:273:LEU:HD11	2.02	0.41
3:F:285:F42:H1'2	3:F:285:F42:H4'	1.86	0.41
1:A:201:VAL:HG12	1:E:236:SER:HA	2.04	0.41
1:F:171:ASP:O	1:F:172:GLU:CG	2.39	0.41
1:E:243:LYS:HA	1:E:243:LYS:HD3	1.70	0.40
1:A:192:GLU:O	1:A:276:ARG:NH1	2.54	0.40
1:A:219:GLU:OE1	6:A:366:HOH:O	2.22	0.40
1:C:104:LYS:HE2	1:C:104:LYS:HB2	1.86	0.40
1:C:94:ALA:HB3	1:C:114:LEU:CD2	2.52	0.40
1:E:2:THR:HG22	1:E:2:THR:O	2.21	0.40
1:D:174:SER:OG	1:D:176:ASN:HB2	2.22	0.40
1:C:171:ASP:O	1:C:172:GLU:CG	2.41	0.40
1:D:14:LEU:HD13	1:D:73:PRO:HG3	2.03	0.40
1:C:252:ARG:CD	1:E:139:ILE:HD13	2.51	0.40
1:E:144:LEU:O	1:E:148:LEU:HG	2.21	0.40
1:B:18:MET:HE3	1:F:22:MET:HE2	2.00	0.40
1:C:120:LYS:HD3	1:C:184:ASP:HB3	2.03	0.40
1:C:137[A]:MET:CE	1:E:19:MET:HE1	2.51	0.40

All (8) 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:B:2:THR:CG2	6:A:289:HOH:O[2_556]	1.51	0.69
1:E:50:GLU:OE2	4:B:286:CA:CA[1_454]	1.54	0.66
1:A:34:GLU:OE1	6:F:379:HOH:O[2_546]	1.85	0.35
1:C:89:ASP:OD1	6:D:309:HOH:O[2_555]	1.89	0.31
1:A:34:GLU:OE2	6:F:379:HOH:O[2_546]	1.93	0.27
1:A:34:GLU:CD	6:F:379:HOH:O[2_546]	2.04	0.16
1:B:89:ASP:OD2	1:E:50:GLU:OE2[1_656]	2.04	0.16
1:B:31:GLU:OE1	6:D:714:HOH:O[2_556]	2.16	0.04

## 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 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%)	9 (3%)	1 (0%)	34	21
1	B	281/283 (99%)	269 (96%)	11 (4%)	1 (0%)	34	21
1	C	282/283 (100%)	270 (96%)	11 (4%)	1 (0%)	34	21
1	D	280/283 (99%)	272 (97%)	6 (2%)	2 (1%)	22	10
1	E	280/283 (99%)	268 (96%)	10 (4%)	2 (1%)	22	10
1	F	280/283 (99%)	271 (97%)	8 (3%)	1 (0%)	34	21
All	All	1684/1698 (99%)	1621 (96%)	55 (3%)	8 (0%)	29	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	B	171	ASP
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP
1	F	171	ASP
1	E	74	ASN
1	D	74	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/234 (100%)	225 (96%)	9 (4%)	33	18
1	B	234/234 (100%)	224 (96%)	10 (4%)	29	14
1	C	235/234 (100%)	230 (98%)	5 (2%)	53	42
1	D	233/234 (100%)	225 (97%)	8 (3%)	37	22
1	E	233/234 (100%)	227 (97%)	6 (3%)	46	32
1	F	233/234 (100%)	223 (96%)	10 (4%)	29	14
All	All	1402/1404 (100%)	1354 (97%)	48 (3%)	37	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	14	LEU
1	A	18	MET
1	A	90	SER
1	A	111	GLU
1	A	170	GLU
1	A	196	ASN
1	A	230	TYR
1	A	269	ASP
1	B	14	LEU
1	B	58[A]	ASP
1	B	58[B]	ASP
1	B	61	GLU
1	B	170	GLU
1	B	191	ARG
1	B	192	GLU
1	B	195	GLU
1	B	230	TYR
1	B	280	GLU
1	C	14	LEU
1	C	82	LYS
1	C	170	GLU

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Mol	Chain	Res	Type
1	C	175	GLU
1	C	230	TYR
1	D	2	THR
1	D	14	LEU
1	D	33	VAL
1	D	34	GLU
1	D	125	LEU
1	D	170	GLU
1	D	230	TYR
1	D	243	LYS
1	E	14	LEU
1	E	61	GLU
1	E	82	LYS
1	E	170	GLU
1	E	180	LYS
1	E	280	GLU
1	F	2	THR
1	F	14	LEU
1	F	18	MET
1	F	89	ASP
1	F	97	ILE
1	F	125	LEU
1	F	170	GLU
1	F	175	GLU
1	F	190	GLU
1	F	281	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	212	ASN
1	A	225	GLN
1	A	238	HIS
1	B	176	ASN
1	B	196	ASN
1	B	212	ASN
1	B	238	HIS
1	C	196	ASN
1	C	212	ASN
1	C	238	HIS
1	C	258	ASN

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Mol	Chain	Res	Type
1	D	196	ASN
1	D	212	ASN
1	D	238	HIS
1	E	13	ASN
1	E	196	ASN
1	E	238	HIS
1	F	196	ASN
1	F	238	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\# Z  > 2$
3	F42	F	285	-	29,32,55	4.28	13 (44%)	36,48,79	3.34	17 (47%)
3	F42	B	285	-	29,32,55	4.39	12 (41%)	36,48,79	3.31	15 (41%)
2	H4M	F	284	-	47,49,58	0.85	1 (2%)	61,74,86	2.02	13 (21%)
2	H4M	E	284	-	47,49,58	0.75	0	61,74,86	1.82	12 (19%)
2	H4M	B	284	-	47,49,58	0.80	1 (2%)	61,74,86	2.04	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	H4M	A	284	-	47,49,58	0.89	2 (4%)	61,74,86	2.31	20 (32%)
2	H4M	D	284	-	47,49,58	0.75	1 (2%)	61,74,86	1.69	12 (19%)
2	H4M	C	284	-	47,49,58	0.74	1 (2%)	61,74,86	1.82	9 (14%)
3	F42	C	285	-	29,32,55	4.20	12 (41%)	36,48,79	3.39	15 (41%)
3	F42	E	285	-	29,32,55	4.50	12 (41%)	36,48,79	3.30	16 (44%)
3	F42	A	285	-	29,32,55	4.50	12 (41%)	36,48,79	3.31	13 (36%)
3	F42	D	285	-	29,32,55	4.52	12 (41%)	36,48,79	3.27	13 (36%)

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
3	F42	F	285	-	-	1/18/18/53	0/3/3/3
3	F42	B	285	-	-	7/18/18/53	0/3/3/3
2	H4M	F	284	-	-	3/27/71/85	0/5/5/5
2	H4M	E	284	-	-	5/27/71/85	0/5/5/5
2	H4M	B	284	-	-	7/27/71/85	0/5/5/5
2	H4M	A	284	-	1/1/13/17	8/27/71/85	0/5/5/5
2	H4M	D	284	-	-	7/27/71/85	0/5/5/5
2	H4M	C	284	-	-	5/27/71/85	0/5/5/5
3	F42	C	285	-	-	14/18/18/53	0/3/3/3
3	F42	E	285	-	-	8/18/18/53	0/3/3/3
3	F42	A	285	-	-	4/18/18/53	0/3/3/3
3	F42	D	285	-	-	5/18/18/53	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	285	F42	C5-C4A	-9.74	1.39	1.53
3	B	285	F42	C5-C4A	-9.52	1.39	1.53
3	D	285	F42	C5-C4A	-9.46	1.39	1.53
3	C	285	F42	C10-N1	-9.21	1.35	1.46
3	D	285	F42	C10-N1	-9.13	1.35	1.46
3	E	285	F42	C5-C4A	-9.09	1.40	1.53
3	F	285	F42	C10-N1	-8.87	1.35	1.46
3	F	285	F42	C5-C4A	-8.85	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	285	F42	C10-N1	-8.79	1.36	1.46
3	E	285	F42	C10-N1	-8.78	1.36	1.46
3	A	285	F42	C10-N1	-8.66	1.36	1.46
3	C	285	F42	C5-C4A	-8.64	1.41	1.53
3	E	285	F42	C4A-C4	-8.51	1.39	1.51
3	A	285	F42	C9A-N10	-8.43	1.33	1.48
3	E	285	F42	C9A-N10	-8.24	1.33	1.48
3	A	285	F42	C4A-C4	-8.12	1.39	1.51
3	D	285	F42	C4A-C4	-8.10	1.39	1.51
3	C	285	F42	C4A-C4	-7.93	1.39	1.51
3	F	285	F42	C9A-N10	-7.77	1.34	1.48
3	D	285	F42	C9A-N10	-7.59	1.34	1.48
3	D	285	F42	C5A-C9A	-7.58	1.38	1.53
3	F	285	F42	C5A-C9A	-7.49	1.38	1.53
3	B	285	F42	C9A-N10	-7.45	1.35	1.48
3	E	285	F42	C5A-C9A	-7.43	1.38	1.53
3	B	285	F42	C4A-C4	-7.27	1.40	1.51
3	B	285	F42	C9-C9A	-7.18	1.38	1.53
3	A	285	F42	C5A-C9A	-7.15	1.39	1.53
3	E	285	F42	C9-C9A	-7.11	1.38	1.53
3	E	285	F42	C9-C8	-7.09	1.39	1.51
3	B	285	F42	C9-C8	-7.06	1.39	1.51
3	A	285	F42	C9-C8	-6.91	1.39	1.51
3	B	285	F42	C5A-C9A	-6.86	1.40	1.53
3	A	285	F42	C9-C9A	-6.80	1.38	1.53
3	F	285	F42	C9-C8	-6.72	1.39	1.51
3	C	285	F42	C5A-C9A	-6.71	1.40	1.53
3	C	285	F42	C9A-N10	-6.66	1.36	1.48
3	F	285	F42	C4A-C4	-6.60	1.41	1.51
3	D	285	F42	C9-C8	-6.54	1.40	1.51
3	D	285	F42	C9-C9A	-6.46	1.39	1.53
3	D	285	F42	C5-C5A	-6.31	1.38	1.53
3	B	285	F42	C5-C5A	-6.27	1.38	1.53
3	F	285	F42	C9-C9A	-6.26	1.40	1.53
3	C	285	F42	C9-C9A	-6.22	1.40	1.53
3	C	285	F42	C9-C8	-6.03	1.40	1.51
3	D	285	F42	C6-C5A	-5.92	1.39	1.53
3	A	285	F42	C6-C5A	-5.74	1.39	1.53
3	D	285	F42	C7-C6	-5.72	1.38	1.52
3	A	285	F42	C5-C5A	-5.72	1.40	1.53
3	C	285	F42	C5-C5A	-5.63	1.40	1.53
3	E	285	F42	C5-C5A	-5.61	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	285	F42	C6-C5A	-5.57	1.39	1.53
3	A	285	F42	C7-C6	-5.50	1.39	1.52
3	E	285	F42	C6-C5A	-5.49	1.40	1.53
3	E	285	F42	C7-C6	-5.49	1.39	1.52
3	B	285	F42	C7-C6	-5.49	1.39	1.52
3	B	285	F42	C6-C5A	-5.44	1.40	1.53
3	F	285	F42	C5-C5A	-5.43	1.40	1.53
3	C	285	F42	C7-C6	-5.40	1.39	1.52
3	C	285	F42	C6-C5A	-5.39	1.40	1.53
3	D	285	F42	C7-C8	-5.38	1.38	1.51
3	F	285	F42	C7-C6	-5.24	1.39	1.52
3	A	285	F42	C7-C8	-5.05	1.39	1.51
3	F	285	F42	C7-C8	-4.82	1.40	1.51
3	C	285	F42	C7-C8	-4.69	1.40	1.51
3	B	285	F42	C7-C8	-4.59	1.40	1.51
3	E	285	F42	C7-C8	-4.52	1.40	1.51
3	A	285	F42	O8M-C8	-2.53	1.35	1.43
3	D	285	F42	O8M-C8	-2.49	1.36	1.43
2	D	284	H4M	C4-C4A	-2.48	1.38	1.41
3	E	285	F42	O8M-C8	-2.45	1.36	1.43
3	B	285	F42	O8M-C8	-2.41	1.36	1.43
2	C	284	H4M	OX5-C1J	2.35	1.44	1.40
2	A	284	H4M	C4-C4A	-2.30	1.38	1.41
2	F	284	H4M	OX5-C1J	2.21	1.44	1.40
2	A	284	H4M	CX1-CX2	-2.18	1.51	1.53
2	B	284	H4M	OX5-C1J	2.17	1.43	1.40
3	F	285	F42	O4-C4	2.16	1.27	1.23
3	C	285	F42	O8M-C8	-2.14	1.37	1.43
3	F	285	F42	O8M-C8	-2.05	1.37	1.43

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	285	F42	C5-C4A-C10	8.89	118.80	107.74
3	E	285	F42	C5-C4A-C10	8.68	118.54	107.74
3	B	285	F42	C9-C8-C7	8.46	120.65	110.55
3	B	285	F42	C5-C4A-C10	8.40	118.18	107.74
2	B	284	H4M	C4-C4A-C8A	8.39	121.00	114.44
3	D	285	F42	C9-C8-C7	8.31	120.48	110.55
3	A	285	F42	C5-C4A-C10	8.24	117.99	107.74
3	C	285	F42	C9-C8-C7	8.20	120.34	110.55
3	E	285	F42	C9-C8-C7	8.06	120.18	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	285	F42	C9-C8-C7	7.95	120.04	110.55
2	C	284	H4M	C4-C4A-C8A	7.93	120.64	114.44
2	A	284	H4M	CX4-CX3-CX2	-7.39	97.99	113.36
3	D	285	F42	C5-C4A-C10	7.25	116.76	107.74
2	E	284	H4M	C4-C4A-C8A	6.85	119.80	114.44
3	F	285	F42	C5-C5A-C9A	6.81	119.39	110.04
3	F	285	F42	C5-C4A-C10	6.77	116.16	107.74
3	F	285	F42	C9-C8-C7	6.67	118.52	110.55
2	D	284	H4M	C4-C4A-C8A	6.43	119.47	114.44
3	C	285	F42	C5-C5A-C9A	6.40	118.82	110.04
2	F	284	H4M	C4-C4A-C8A	6.32	119.38	114.44
3	A	285	F42	C5-C4A-C4	6.26	123.85	111.13
3	A	285	F42	C5-C5A-C9A	6.17	118.52	110.04
3	F	285	F42	C5-C4A-C4	5.97	123.25	111.13
3	F	285	F42	C4-N3-C2	-5.90	118.36	126.25
2	A	284	H4M	CX5-CX4-CX3	5.88	123.56	112.20
3	E	285	F42	C5-C4A-C4	5.79	122.90	111.13
3	D	285	F42	C5-C5A-C9A	5.79	117.99	110.04
3	E	285	F42	C5-C5A-C9A	5.77	117.97	110.04
2	F	284	H4M	O4J-C1J-OX5	-5.68	105.72	111.95
2	B	284	H4M	O4J-C1J-OX5	-5.67	105.73	111.95
3	D	285	F42	C5-C4A-C4	5.66	122.63	111.13
3	B	285	F42	C5-C4A-C4	5.54	122.38	111.13
3	C	285	F42	C5-C4A-C4	5.54	122.38	111.13
3	F	285	F42	C6-C7-C8	5.52	121.04	111.61
2	E	284	H4M	N10-C10-N5	5.51	110.85	103.03
3	E	285	F42	C5-C5A-C6	5.35	122.43	112.66
3	C	285	F42	O8M-C8-C9	5.34	120.48	109.85
3	F	285	F42	O8M-C8-C9	5.29	120.38	109.85
2	C	284	H4M	N10-C10-N5	5.29	110.53	103.03
3	B	285	F42	C5-C5A-C6	5.27	122.29	112.66
2	A	284	H4M	C4-C4A-C8A	5.26	118.56	114.44
3	B	285	F42	C4-N3-C2	-5.19	119.30	126.25
3	B	285	F42	C5-C5A-C9A	5.19	117.17	110.04
3	D	285	F42	O8M-C8-C9	5.18	120.15	109.85
3	A	285	F42	C5-C5A-C6	5.16	122.08	112.66
2	F	284	H4M	OX5-C1J-C2J	5.12	116.11	107.76
3	A	285	F42	O8M-C8-C9	5.00	119.80	109.85
3	A	285	F42	C6-C7-C8	4.89	119.96	111.61
2	A	284	H4M	OX4-CX4-CX5	4.89	120.91	109.92
3	C	285	F42	C4-N3-C2	-4.83	119.79	126.25
2	A	284	H4M	N10-C10-N5	4.81	109.86	103.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	285	F42	O8M-C8-C7	4.77	122.31	110.16
3	D	285	F42	C6-C7-C8	4.77	119.75	111.61
2	F	284	H4M	C4-N3-C2	4.76	123.49	115.93
3	F	285	F42	C5-C5A-C6	4.76	121.35	112.66
3	E	285	F42	C6-C7-C8	4.75	119.73	111.61
2	A	284	H4M	O4J-C1J-OX5	-4.75	106.74	111.95
3	C	285	F42	C6-C7-C8	4.75	119.72	111.61
2	D	284	H4M	N10-C10-N5	4.66	109.64	103.03
2	E	284	H4M	O4J-C1J-OX5	-4.64	106.86	111.95
3	D	285	F42	C5-C5A-C6	4.59	121.05	112.66
3	B	285	F42	C6-C7-C8	4.57	119.42	111.61
3	D	285	F42	C4-N3-C2	-4.55	120.17	126.25
3	E	285	F42	O8M-C8-C9	4.46	118.73	109.85
3	D	285	F42	N3-C2-N1	4.45	120.80	116.12
3	F	285	F42	O8M-C8-C7	4.29	121.09	110.16
3	E	285	F42	O8M-C8-C7	4.29	121.09	110.16
2	F	284	H4M	N3-C2-N1	-4.20	118.83	125.42
3	A	285	F42	C4-N3-C2	-4.20	120.63	126.25
2	C	284	H4M	C7-C6-N5	-4.17	104.45	108.61
2	B	284	H4M	C7-C6-N5	-4.16	104.46	108.61
3	C	285	F42	C5-C5A-C6	4.14	120.22	112.66
2	C	284	H4M	O4J-C1J-OX5	-4.12	107.43	111.95
3	C	285	F42	C6-C5A-C9A	4.11	120.95	109.73
3	D	285	F42	C6-C5A-C9A	4.11	120.94	109.73
3	E	285	F42	C4-N3-C2	-4.03	120.85	126.25
3	D	285	F42	C9-C9A-N10	4.02	121.37	113.83
3	B	285	F42	C6-C5A-C9A	3.96	120.53	109.73
3	A	285	F42	O8M-C8-C7	3.92	120.15	110.16
2	A	284	H4M	OX5-C1J-C2J	3.91	114.14	107.76
3	C	285	F42	C9-C9A-N10	3.89	121.12	113.83
3	E	285	F42	N3-C2-N1	3.89	120.21	116.12
2	D	284	H4M	O4J-C1J-OX5	-3.86	107.72	111.95
2	B	284	H4M	N10-C10-N5	3.84	108.48	103.03
3	F	285	F42	C9-C9A-N10	3.81	120.97	113.83
2	F	284	H4M	N10-C10-N5	3.75	108.35	103.03
3	F	285	F42	N3-C2-N1	3.71	120.02	116.12
2	A	284	H4M	C4-N3-C2	3.66	121.75	115.93
2	A	284	H4M	N3-C2-N1	-3.65	119.70	125.42
3	E	285	F42	C6-C5A-C9A	3.62	119.60	109.73
3	D	285	F42	O8M-C8-C7	3.62	119.37	110.16
3	B	285	F42	O8M-C8-C9	3.59	117.00	109.85
2	E	284	H4M	C7-C6-N5	-3.56	105.06	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	285	F42	C7-C6-C5A	3.54	120.22	112.24
3	A	285	F42	C6-C5A-C9A	3.54	119.39	109.73
3	C	285	F42	O8M-C8-C7	3.54	119.17	110.16
3	F	285	F42	C6-C5A-C9A	3.49	119.26	109.73
3	B	285	F42	N3-C2-N1	3.43	119.73	116.12
3	F	285	F42	C7-C6-C5A	3.42	119.94	112.24
3	A	285	F42	N3-C2-N1	3.42	119.72	116.12
3	C	285	F42	C7-C6-C5A	3.39	119.87	112.24
3	D	285	F42	C7-C6-C5A	3.39	119.86	112.24
2	E	284	H4M	OX5-C1J-C2J	3.36	113.25	107.76
3	E	285	F42	C7-C6-C5A	3.35	119.78	112.24
3	A	285	F42	C9-C9A-N10	3.31	120.03	113.83
2	B	284	H4M	CX4-CX3-CX2	-3.29	106.51	113.36
3	B	285	F42	C7-C6-C5A	3.22	119.48	112.24
2	F	284	H4M	C7-C6-N5	-3.16	105.45	108.61
2	A	284	H4M	C2-N1-C8A	3.09	121.47	114.54
2	F	284	H4M	C2-N1-C8A	3.05	121.37	114.54
2	B	284	H4M	C4-N3-C2	3.03	120.74	115.93
2	B	284	H4M	C4A-C4-N3	-3.01	116.95	123.14
3	B	285	F42	C9-C9A-N10	3.01	119.47	113.83
3	C	285	F42	N3-C2-N1	2.95	119.22	116.12
2	D	284	H4M	OX5-C1J-C2J	2.89	112.47	107.76
2	B	284	H4M	C4A-C8A-N8	2.86	121.86	119.08
2	E	284	H4M	C5J-C4J-C3J	-2.85	104.49	115.18
2	A	284	H4M	CX5-OX5-C1J	-2.85	108.17	113.74
2	F	284	H4M	C4A-C4-N3	-2.77	117.44	123.14
3	B	285	F42	C4A-C5-C5A	2.77	119.14	109.93
2	D	284	H4M	C4-N3-C2	2.76	120.31	115.93
2	D	284	H4M	O3A-PA-O5J	-2.72	99.49	106.73
2	E	284	H4M	O3A-PA-O2A	2.71	118.00	107.64
2	A	284	H4M	OX3-CX3-CX4	2.70	115.34	108.81
2	B	284	H4M	OX5-C1J-C2J	2.69	112.16	107.76
2	D	284	H4M	C4A-C8A-N8	2.61	121.61	119.08
2	A	284	H4M	C4A-C8A-N8	2.57	121.57	119.08
2	D	284	H4M	N3-C2-N1	-2.48	121.53	125.42
3	C	285	F42	O2-C2-N1	-2.44	118.05	122.92
2	B	284	H4M	NA2-C2-N3	2.42	121.02	117.25
2	E	284	H4M	C4-N3-C2	2.41	119.77	115.93
2	C	284	H4M	C2-N1-C8A	2.40	119.92	114.54
2	F	284	H4M	C7M-C7-N8	-2.40	106.83	109.55
2	B	284	H4M	C2-N1-C8A	2.39	119.90	114.54
2	A	284	H4M	OX4-CX4-CX3	2.38	114.88	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	284	H4M	NA2-C2-N1	2.37	120.94	117.25
3	F	285	F42	O3P-P-O5'	-2.37	100.43	106.73
2	C	284	H4M	O5J-PA-O1A	-2.34	99.92	106.47
2	C	284	H4M	C7M-C7-N8	-2.33	106.90	109.55
3	E	285	F42	C9-C9A-N10	2.31	118.17	113.83
2	B	284	H4M	N3-C2-N1	-2.29	121.83	125.42
2	B	284	H4M	O3A-PA-O2A	2.28	116.36	107.64
2	B	284	H4M	C6-C9-N10	2.26	104.25	102.56
2	A	284	H4M	C6-C9-N10	2.24	104.23	102.56
2	D	284	H4M	C2-N1-C8A	2.23	119.55	114.54
2	D	284	H4M	C4A-C4-N3	-2.23	118.55	123.14
3	F	285	F42	C4A-C5-C5A	2.22	117.31	109.93
2	F	284	H4M	NA2-C2-N1	2.21	120.69	117.25
3	F	285	F42	O4-C4-N3	-2.21	117.08	121.01
2	A	284	H4M	C7-C6-N5	-2.19	106.43	108.61
2	D	284	H4M	O3A-PA-O2A	2.18	115.98	107.64
3	C	285	F42	C5'-C4'-C3'	-2.17	108.01	112.20
2	A	284	H4M	O2A-PA-O5J	-2.16	100.99	106.73
2	F	284	H4M	O3A-PA-O2A	2.15	115.87	107.64
2	C	284	H4M	C1J-C2J-C3J	2.14	105.02	102.30
2	A	284	H4M	O3A-PA-O2A	2.11	115.72	107.64
2	E	284	H4M	O4J-C4J-C3J	2.10	109.27	105.11
2	E	284	H4M	C4A-C4-N3	-2.10	118.83	123.14
2	E	284	H4M	C10-N5-C6	-2.10	99.84	108.68
2	C	284	H4M	C4A-C8A-N8	2.10	121.11	119.08
2	D	284	H4M	CX5-OX5-C1J	-2.09	109.66	113.74
3	B	285	F42	O2-C2-N1	-2.08	118.78	122.92
2	E	284	H4M	C1J-C2J-C3J	2.08	104.93	102.30
3	F	285	F42	O3P-P-O2P	2.06	115.50	107.64
2	F	284	H4M	NA2-C2-N3	2.05	120.44	117.25
2	A	284	H4M	C4A-C4-N3	-2.05	118.94	123.14
3	E	285	F42	O3P-P-O2P	2.04	115.45	107.64
3	E	285	F42	C4A-C5-C5A	2.04	116.71	109.93
3	E	285	F42	O3P-P-O5'	-2.00	101.40	106.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	284	H4M	CX4

All (74) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	B	285	F42	C3'-C4'-C5'-O5'
3	B	285	F42	O4'-C4'-C5'-O5'
2	F	284	H4M	O4J-C1J-OX5-CX5
2	F	284	H4M	C2J-C1J-OX5-CX5
2	E	284	H4M	O4J-C1J-OX5-CX5
2	E	284	H4M	C2J-C1J-OX5-CX5
2	E	284	H4M	C5J-O5J-PA-O1A
2	E	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-O1A
2	B	284	H4M	C5J-O5J-PA-O2A
2	B	284	H4M	C5J-O5J-PA-O3A
2	A	284	H4M	OX3-CX3-CX4-CX5
2	A	284	H4M	C5J-O5J-PA-O2A
2	A	284	H4M	C5J-O5J-PA-O3A
2	D	284	H4M	O4J-C1J-OX5-CX5
2	D	284	H4M	C2J-C1J-OX5-CX5
2	D	284	H4M	C5J-O5J-PA-O2A
2	D	284	H4M	C5J-O5J-PA-O3A
2	C	284	H4M	O4J-C1J-OX5-CX5
2	C	284	H4M	C2J-C1J-OX5-CX5
3	C	285	F42	C1'-C2'-C3'-C4'
3	C	285	F42	C2'-C3'-C4'-O4'
3	C	285	F42	O3'-C3'-C4'-O4'
3	C	285	F42	O3'-C3'-C4'-C5'
3	C	285	F42	C3'-C4'-C5'-O5'
3	C	285	F42	O4'-C4'-C5'-O5'
3	C	285	F42	C5'-O5'-P-O1P
3	C	285	F42	C5'-O5'-P-O2P
3	C	285	F42	C5'-O5'-P-O3P
3	E	285	F42	C1'-C2'-C3'-O3'
3	E	285	F42	C1'-C2'-C3'-C4'
3	E	285	F42	O2'-C2'-C3'-O3'
3	E	285	F42	O2'-C2'-C3'-C4'
3	E	285	F42	C5'-O5'-P-O2P
3	E	285	F42	C5'-O5'-P-O3P
3	A	285	F42	O4'-C4'-C5'-O5'
3	A	285	F42	C5'-O5'-P-O2P
3	D	285	F42	C3'-C4'-C5'-O5'
3	D	285	F42	O4'-C4'-C5'-O5'
3	D	285	F42	C5'-O5'-P-O2P
3	D	285	F42	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
3	B	285	F42	O3'-C3'-C4'-O4'
2	A	284	H4M	CX2-CX3-CX4-CX5
3	C	285	F42	C2'-C3'-C4'-C5'
3	B	285	F42	C2'-C3'-C4'-O4'
3	B	285	F42	O3'-C3'-C4'-C5'
3	B	285	F42	C2'-C3'-C4'-C5'
3	C	285	F42	O2'-C2'-C3'-C4'
3	C	285	F42	O2'-C2'-C3'-O3'
2	C	284	H4M	O4J-C4J-C5J-O5J
3	A	285	F42	C3'-C4'-C5'-O5'
2	A	284	H4M	C5J-O5J-PA-O1A
3	E	285	F42	C5'-O5'-P-O1P
3	D	285	F42	C5'-O5'-P-O1P
2	A	284	H4M	CX3-CX4-CX5-OX5
3	F	285	F42	C2'-C1'-N10-C9A
3	E	285	F42	C2'-C1'-N10-C9A
2	D	284	H4M	CX2-CX3-CX4-OX4
2	E	284	H4M	C5J-O5J-PA-O2A
2	C	284	H4M	C5J-O5J-PA-O1A
3	B	285	F42	C2'-C1'-N10-C9A
3	A	285	F42	C2'-C1'-N10-C9A
2	C	284	H4M	C3J-C4J-C5J-O5J
2	F	284	H4M	C13-C14-N10-C10
2	B	284	H4M	C13-C14-N10-C10
2	A	284	H4M	C13-C14-N10-C10
2	B	284	H4M	CX2-CX3-CX4-OX4
2	D	284	H4M	OX3-CX3-CX4-OX4
2	D	284	H4M	C5J-O5J-PA-O1A
2	A	284	H4M	O4J-C1J-OX5-CX5
3	C	285	F42	C2'-C1'-N10-C9A
3	C	285	F42	C1'-C2'-C3'-O3'

There are no ring outliers.

12 monomers are involved in 68 short contacts:

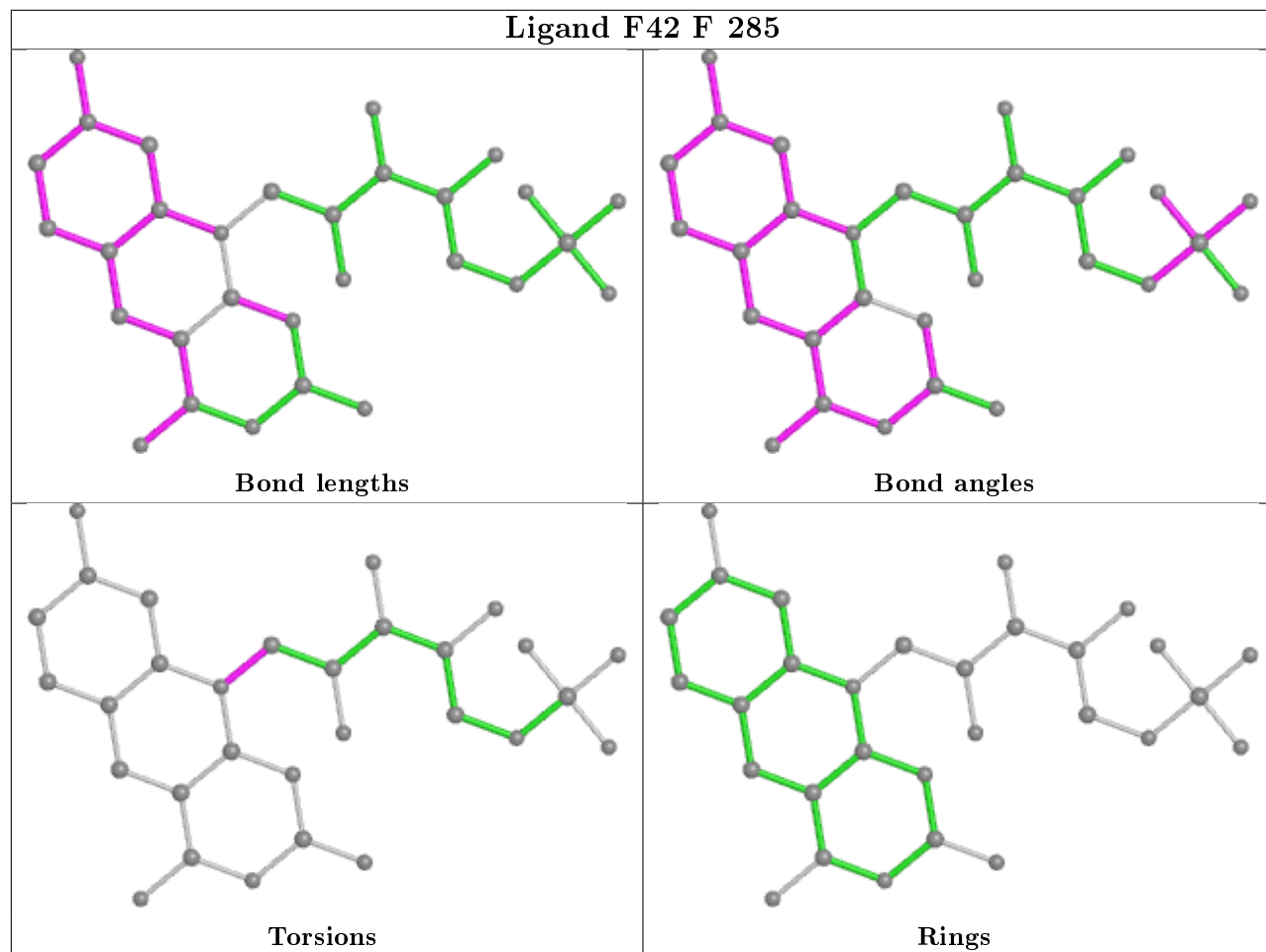
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	285	F42	9	0
3	B	285	F42	12	0
2	F	284	H4M	7	0
2	E	284	H4M	7	0
2	B	284	H4M	5	0
2	A	284	H4M	9	0

*Continued on next page...*

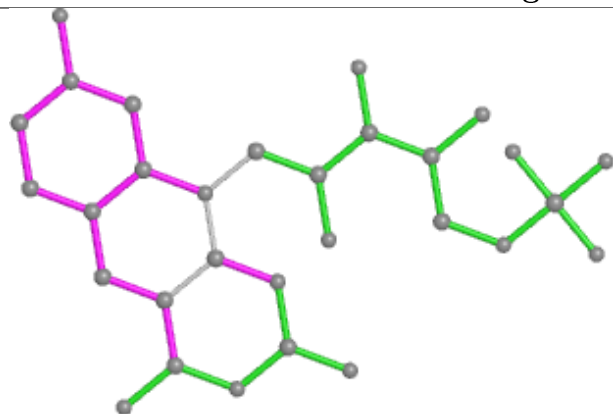
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	284	H4M	10	0
2	C	284	H4M	6	0
3	C	285	F42	10	0
3	E	285	F42	6	0
3	A	285	F42	8	0
3	D	285	F42	7	0

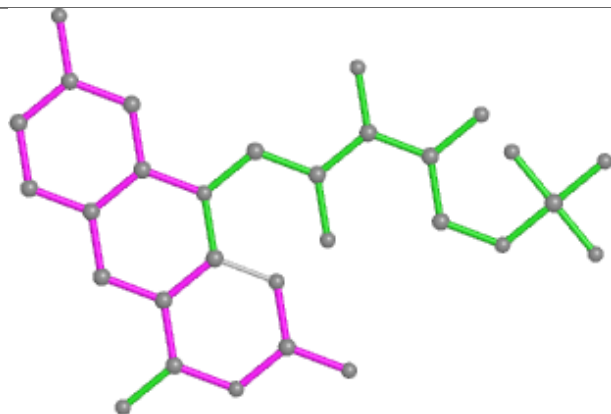
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



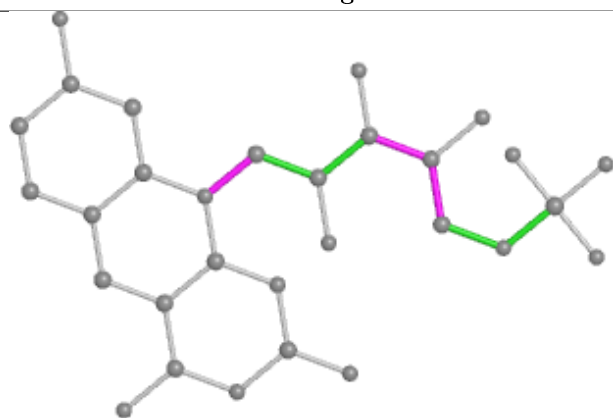
## Ligand F42 B 285



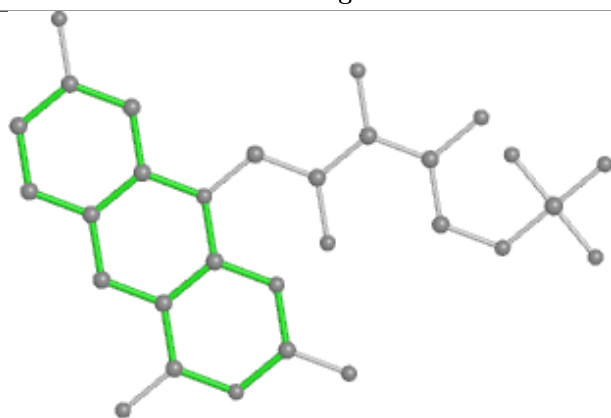
Bond lengths



Bond angles

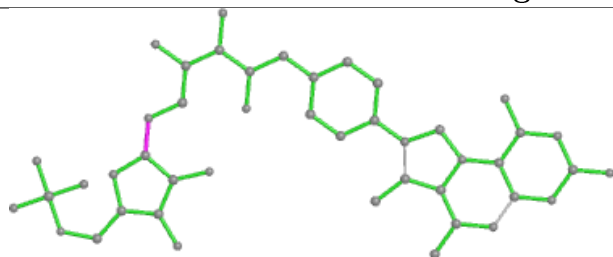


Torsions

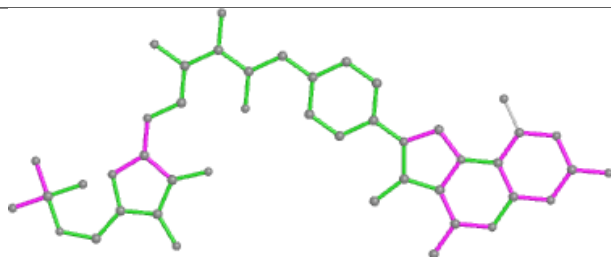


Rings

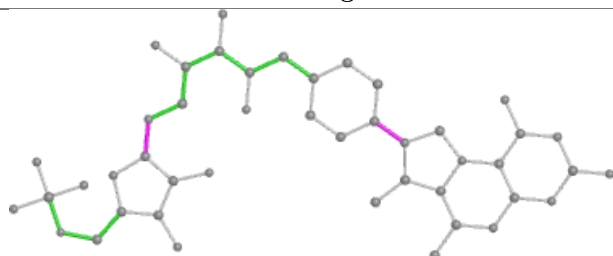
## Ligand H4M F 284



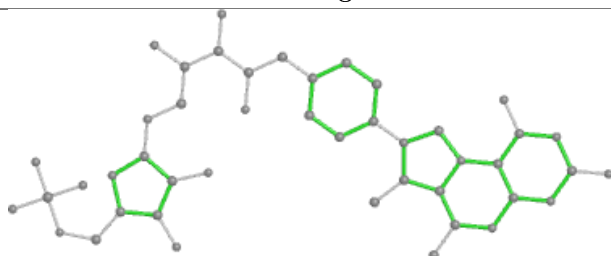
Bond lengths



Bond angles

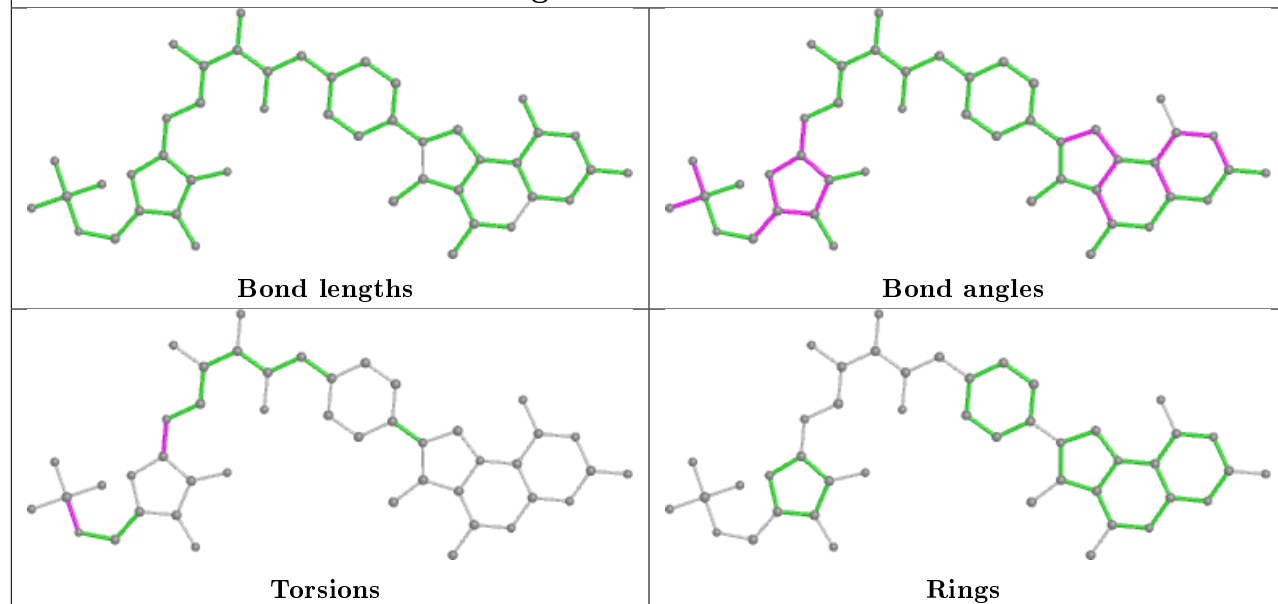


Torsions

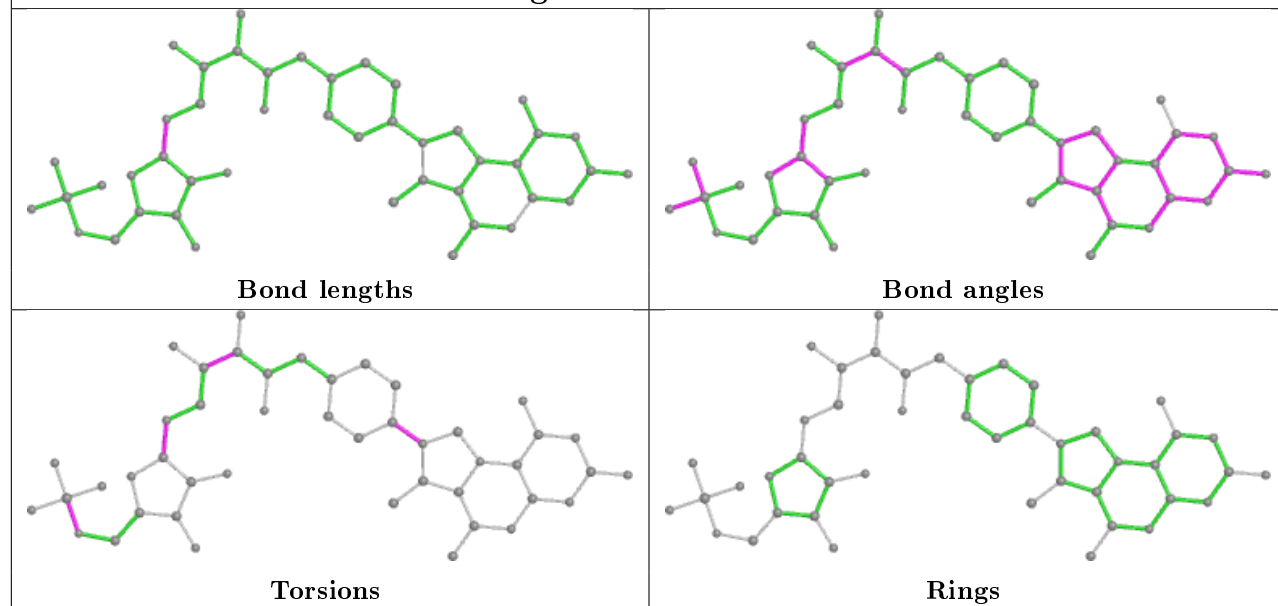


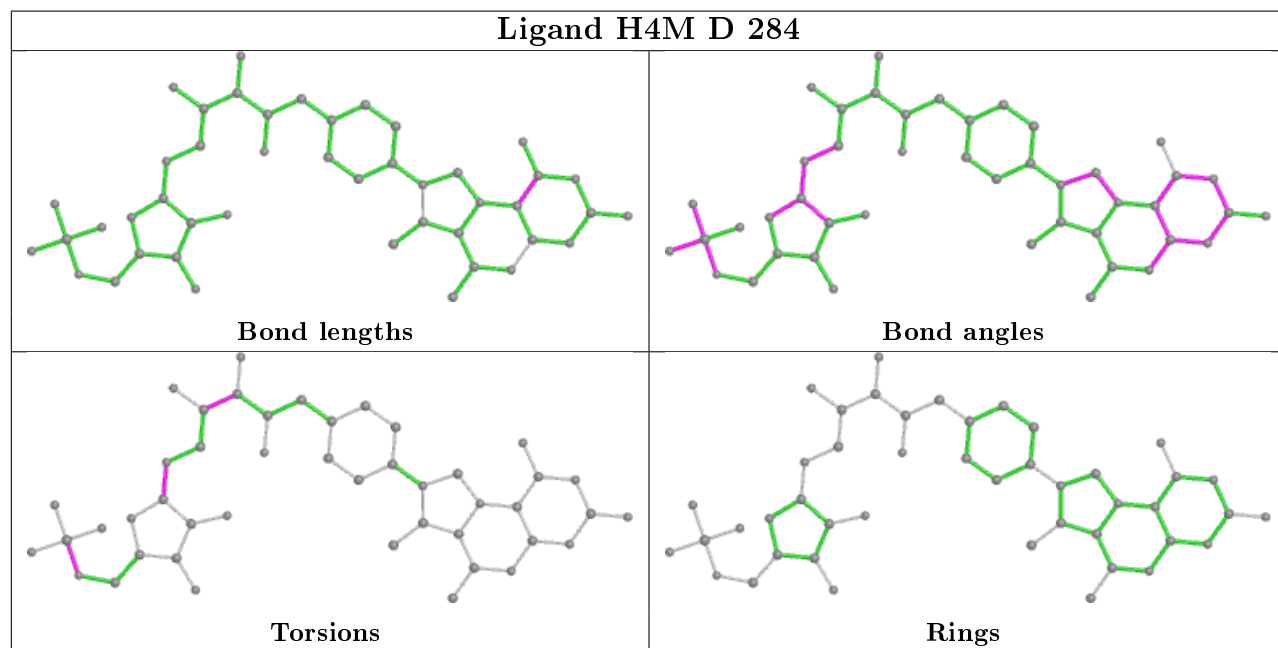
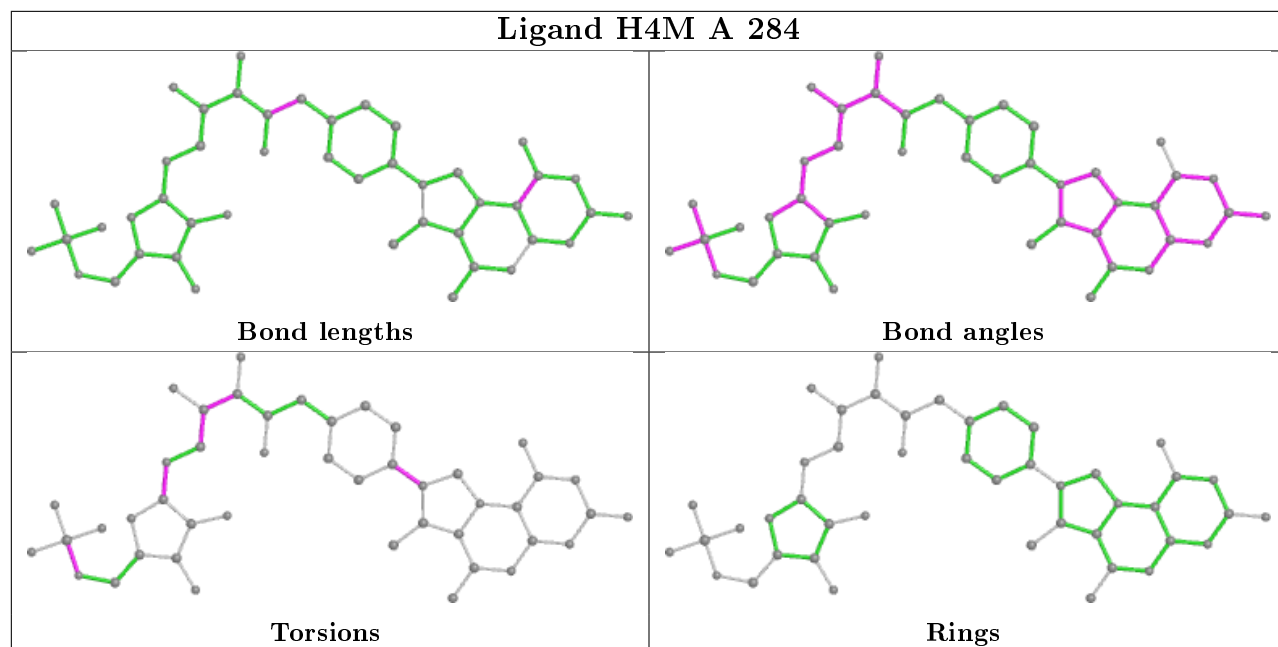
Rings

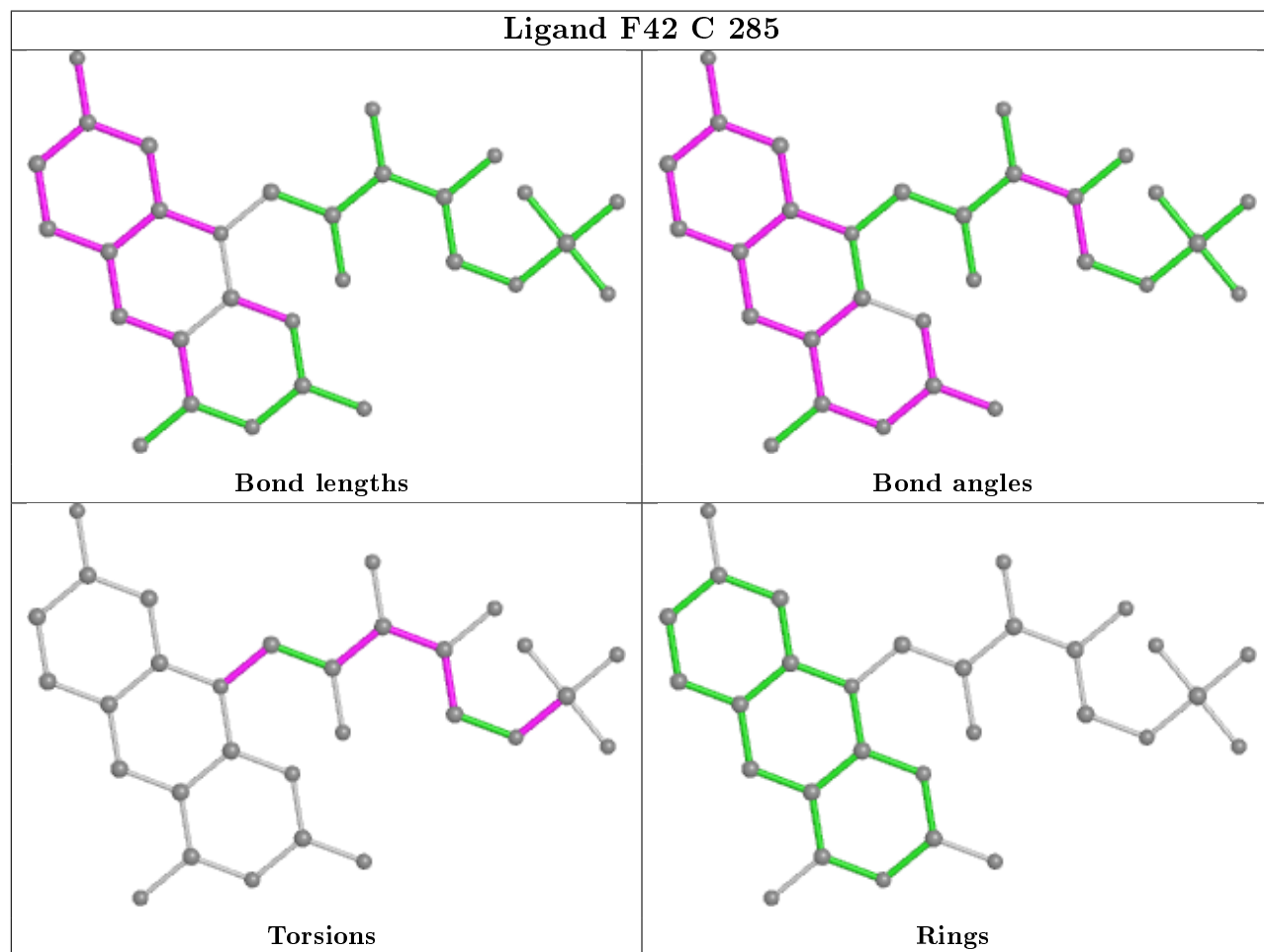
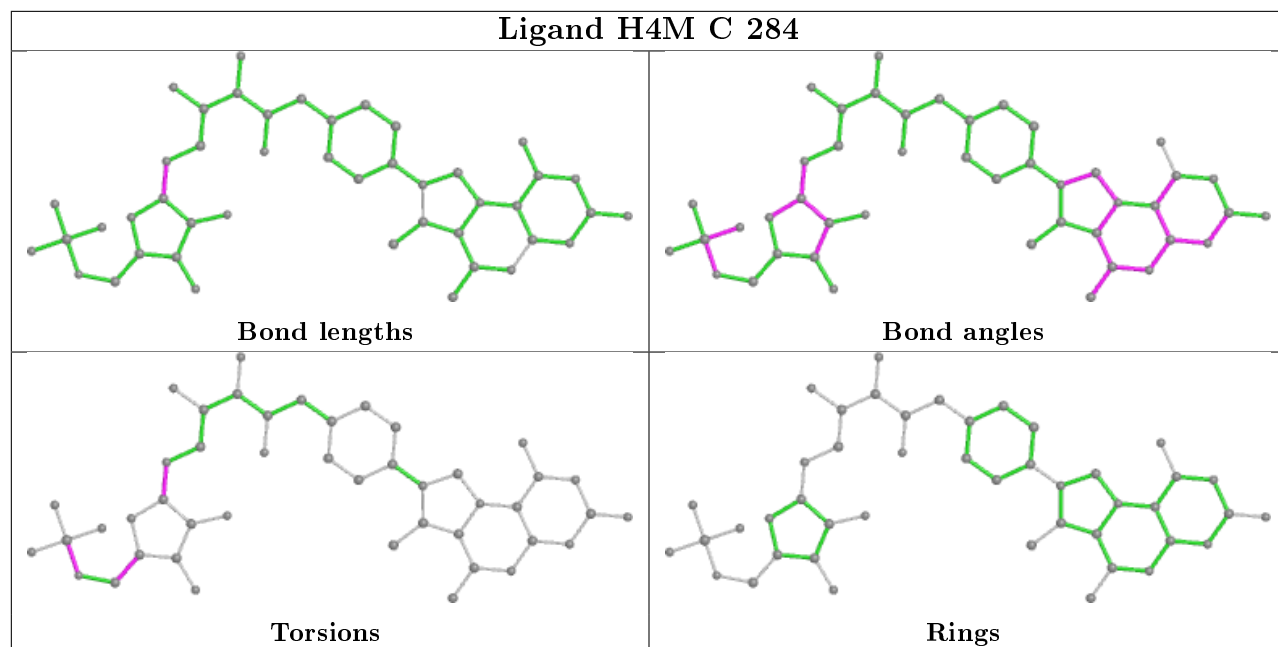
## Ligand H4M E 284



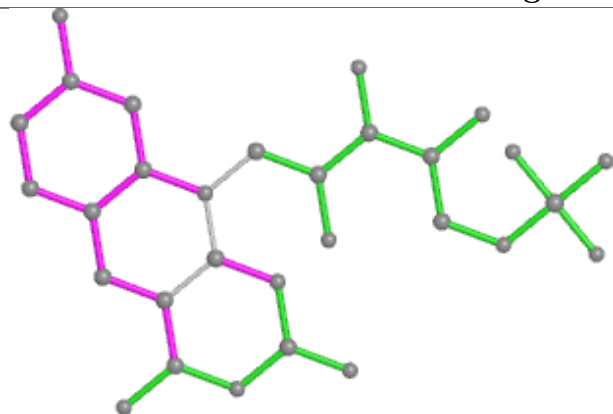
## Ligand H4M B 284



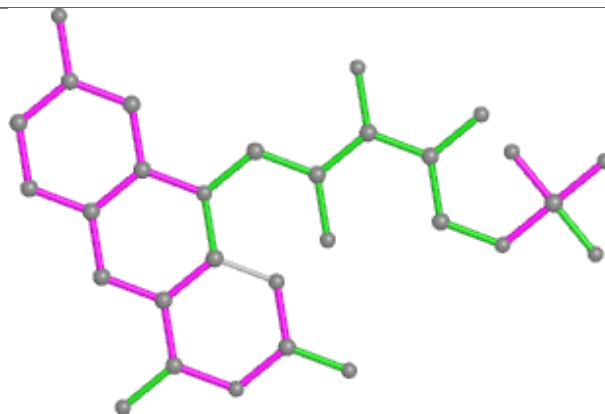




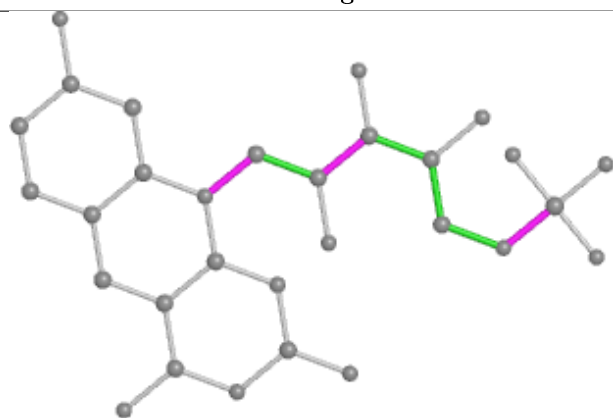
## Ligand F42 E 285



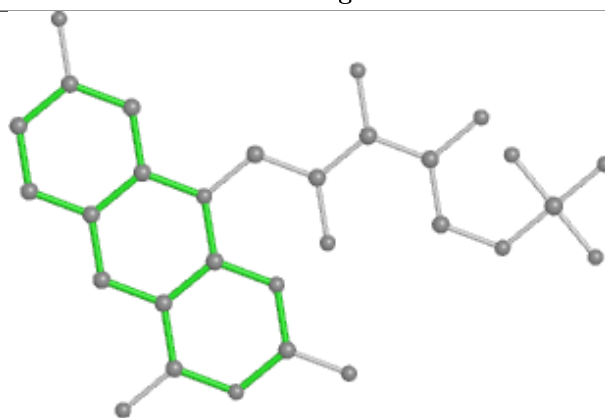
Bond lengths



Bond angles



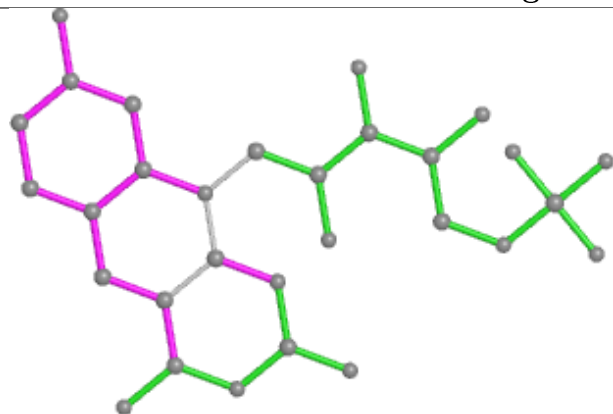
Torsions



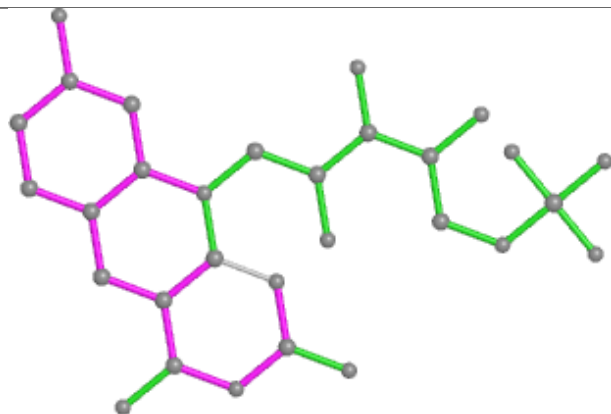
Rings



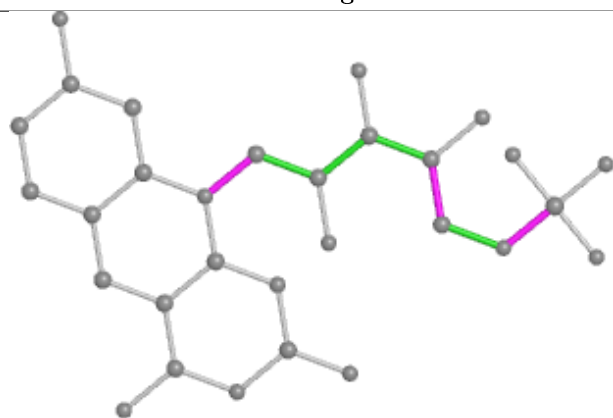
## Ligand F42 A 285



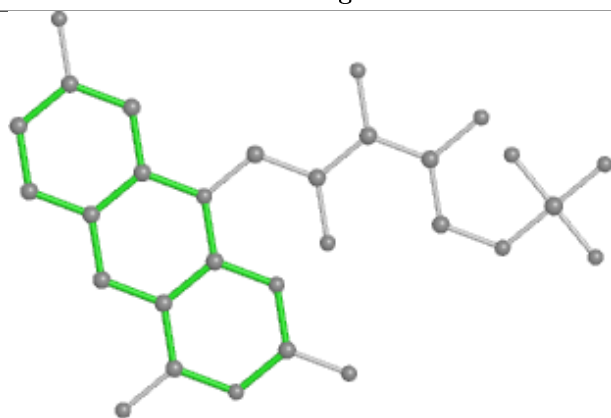
Bond lengths



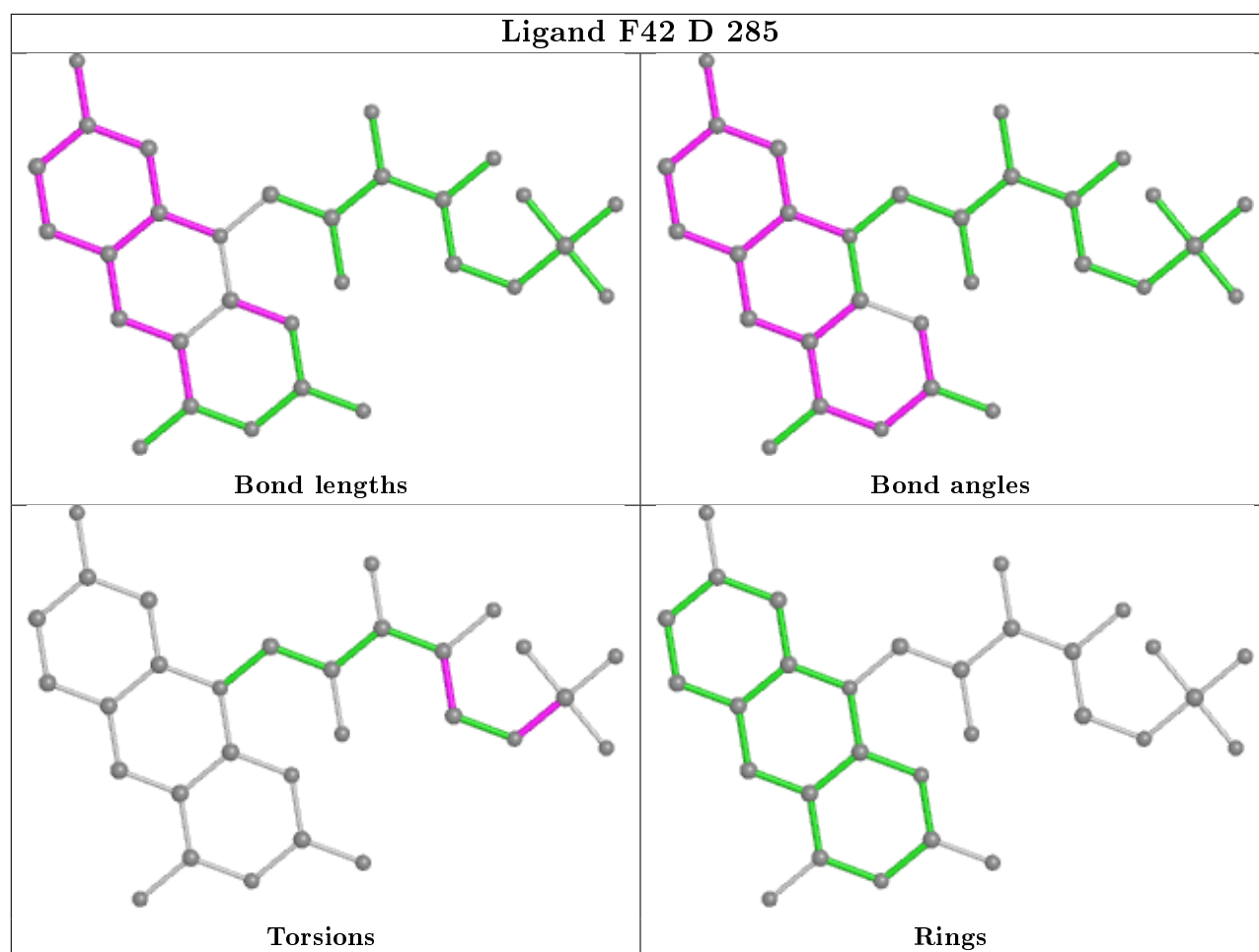
Bond angles



Torsions



Rings



## 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%)	0.05	5 (1%) 68 64	14, 21, 32, 53	0
1	B	282/283 (99%)	-0.13	4 (1%) 75 72	14, 21, 31, 53	1 (0%)
1	C	282/283 (99%)	-0.05	8 (2%) 53 47	13, 20, 30, 53	1 (0%)
1	D	282/283 (99%)	0.02	7 (2%) 57 52	14, 21, 30, 53	0
1	E	282/283 (99%)	-0.06	3 (1%) 80 78	13, 20, 29, 53	1 (0%)
1	F	282/283 (99%)	-0.10	4 (1%) 75 72	13, 21, 31, 53	1 (0%)
All	All	1692/1698 (99%)	-0.05	31 (1%) 68 64	13, 21, 31, 53	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	ASP	6.4
1	B	2	THR	5.5
1	B	171	ASP	5.3
1	C	172	GLU	4.9
1	B	172	GLU	4.6
1	C	171	ASP	4.3
1	A	171	ASP	3.7
1	C	173	ILE	3.4
1	F	171	ASP	3.4
1	B	170	GLU	3.3
1	E	171	ASP	3.3
1	A	2	THR	3.2
1	F	172	GLU	3.0
1	D	172	GLU	3.0
1	D	283	GLU	2.8
1	E	172	GLU	2.7
1	C	58	ASP	2.5
1	A	176	ASN	2.5
1	C	170	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	89	ASP	2.5
1	D	175	GLU	2.4
1	C	91	GLU	2.2
1	E	91	GLU	2.2
1	A	172	GLU	2.1
1	A	283	GLU	2.1
1	C	176	ASN	2.1
1	D	111	GLU	2.1
1	F	175	GLU	2.1
1	C	111	GLU	2.1
1	D	61	GLU	2.0
1	F	173	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
3	F42	D	285	30/53	0.75	0.17	29,33,49,50	30
3	F42	A	285	30/53	0.77	0.20	29,32,48,49	30
3	F42	C	285	30/53	0.78	0.17	28,33,54,54	30
3	F42	E	285	30/53	0.80	0.18	27,36,55,57	30
3	F42	B	285	30/53	0.81	0.17	24,28,48,50	30
3	F42	F	285	30/53	0.82	0.15	23,29,50,51	30
4	CA	B	287	1/1	0.85	0.09	60,60,60,60	0
2	H4M	A	284	45/54	0.88	0.11	25,31,54,55	0
2	H4M	D	284	45/54	0.88	0.11	20,28,53,55	0
5	NA	C	287	1/1	0.88	0.08	42,42,42,42	0
5	NA	E	286	1/1	0.90	0.15	42,42,42,42	0

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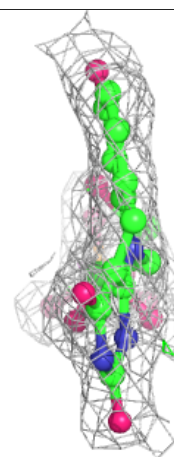
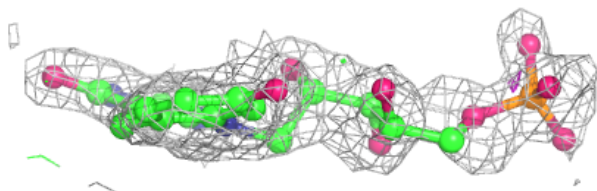
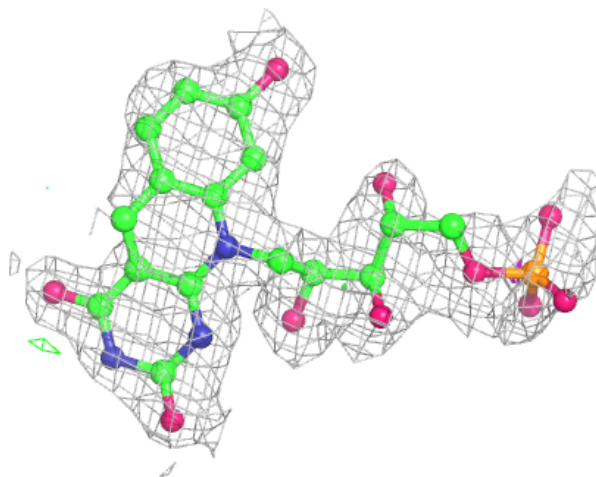
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	H4M	F	284	45/54	0.90	0.09	20,24,47,50	0
2	H4M	E	284	45/54	0.91	0.10	20,27,51,52	0
2	H4M	B	284	45/54	0.91	0.09	21,26,55,56	0
2	H4M	C	284	45/54	0.92	0.09	21,26,50,53	0
4	CA	D	286	1/1	0.96	0.04	36,36,36,36	0
5	NA	D	287	1/1	0.97	0.08	39,39,39,39	0
4	CA	B	286	1/1	1.00	0.09	23,23,23,23	0
4	CA	C	286	1/1	1.00	0.04	25,25,25,25	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.

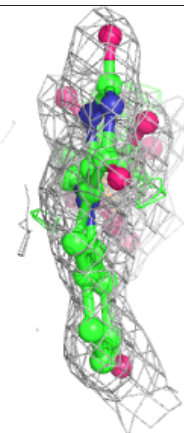
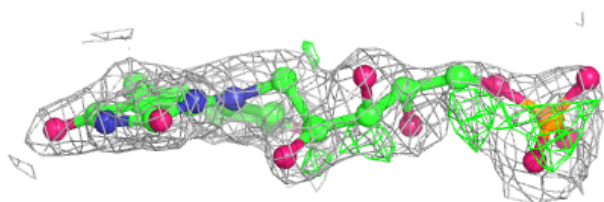
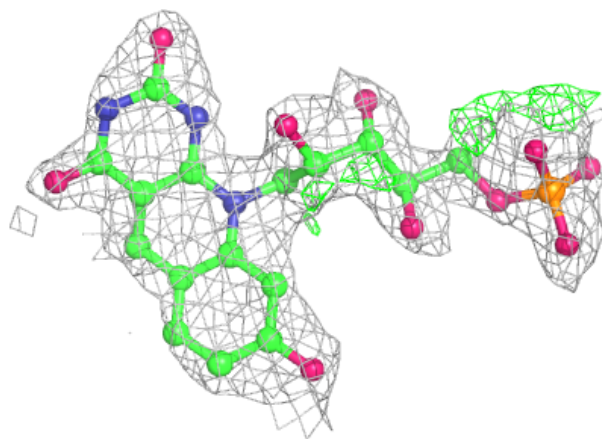
**Electron density around F42 D 285:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



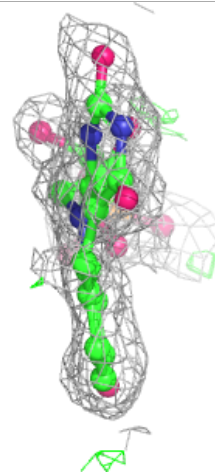
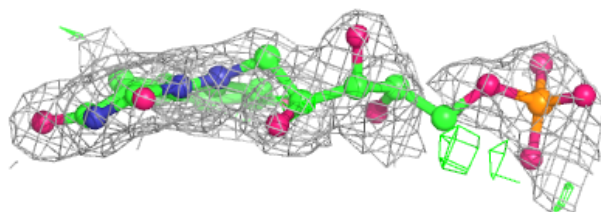
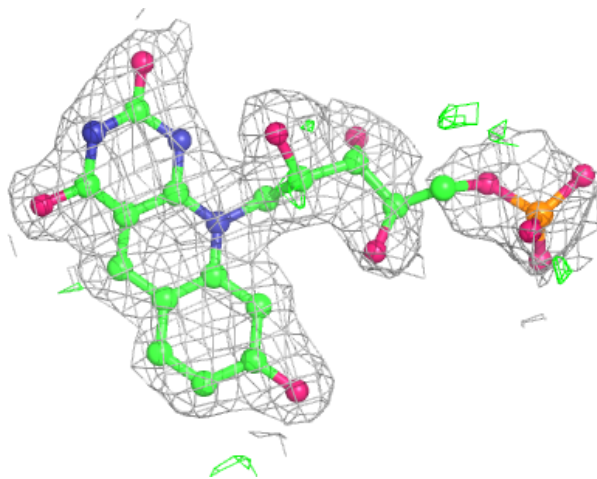
**Electron density around F42 A 285:**

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



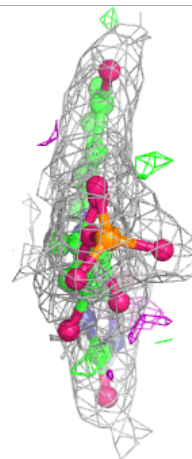
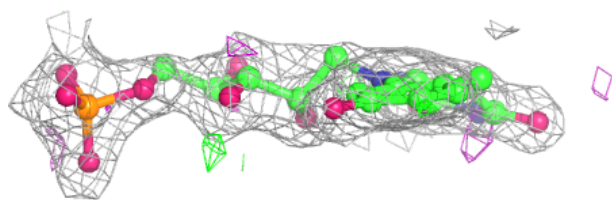
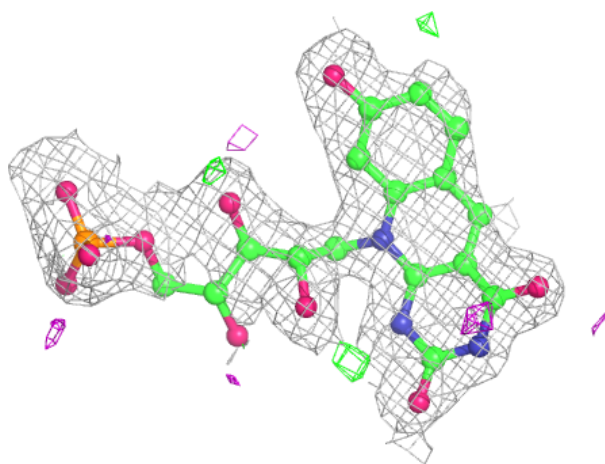
**Electron density around F42 C 285:**

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



**Electron density around F42 E 285:**

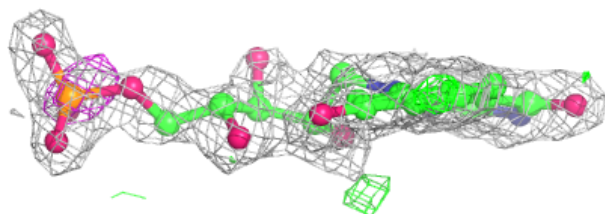
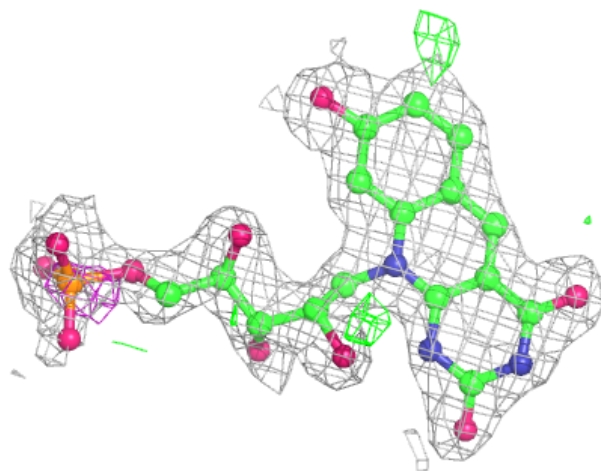
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





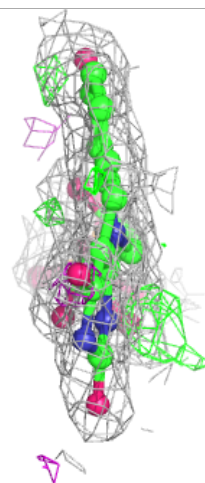
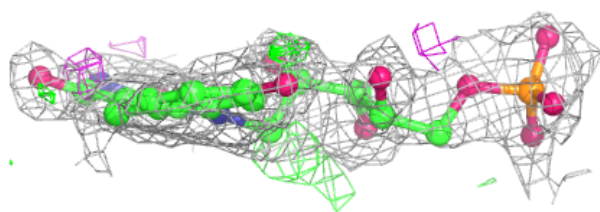
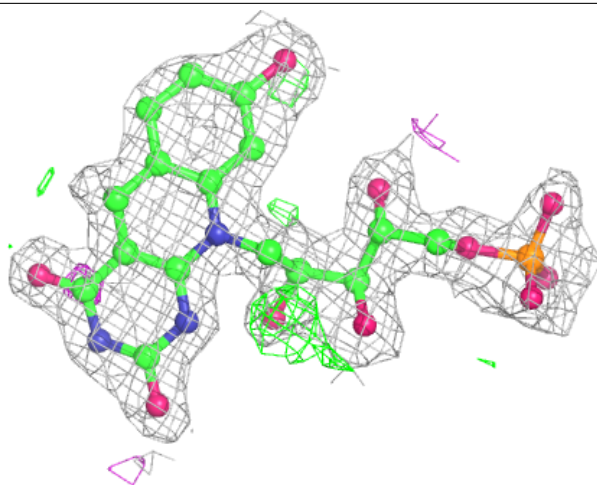
**Electron density around F42 B 285:**

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



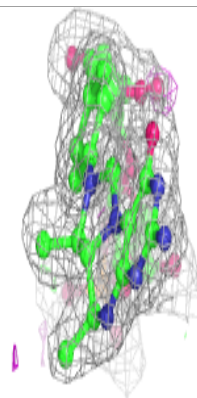
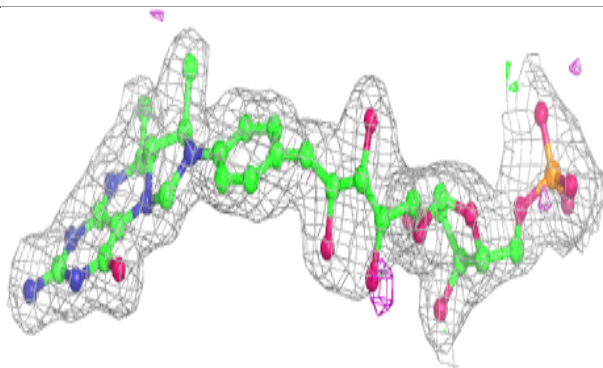
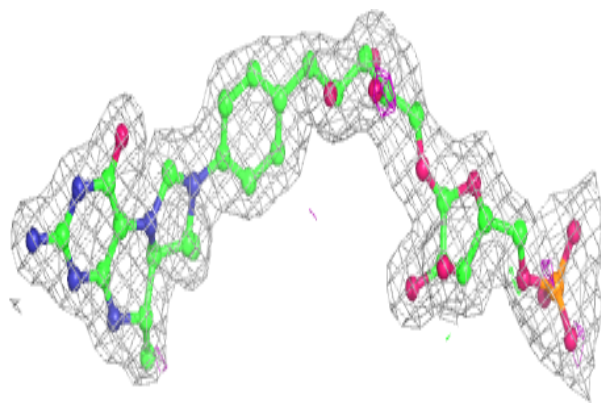
**Electron density around F42 F 285:**

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

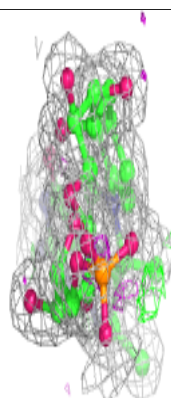
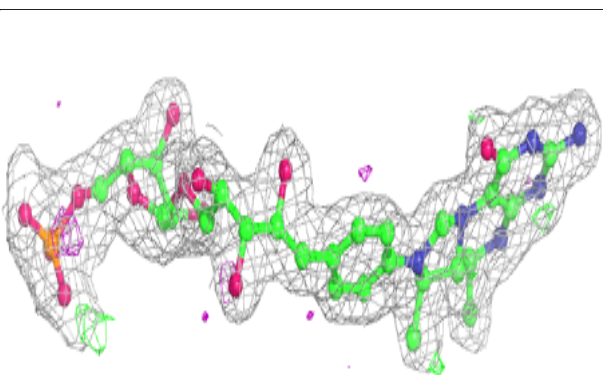
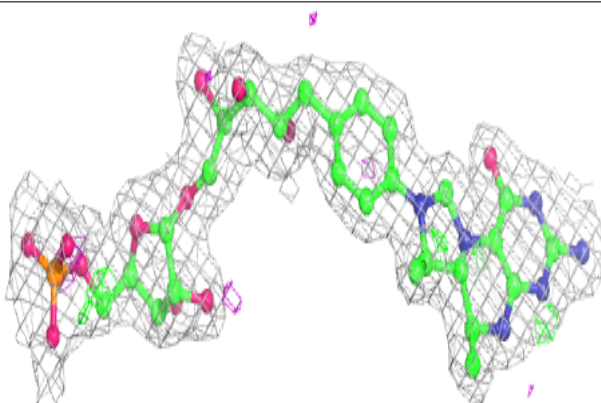


**Electron density around H4M A 284:**

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

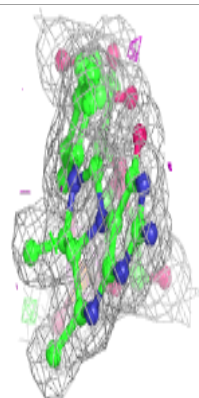
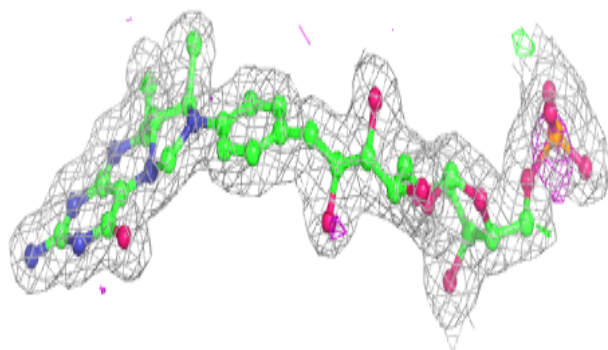
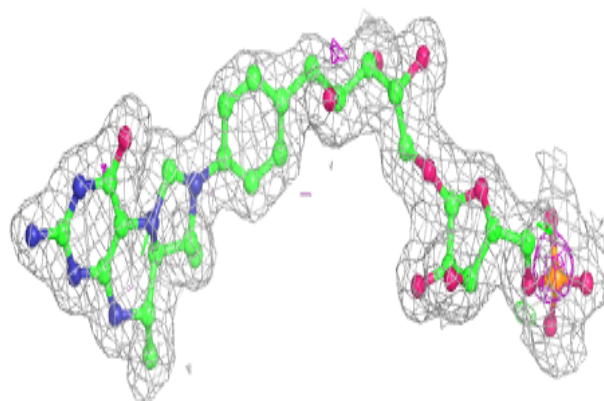
**Electron density around H4M D 284:**

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and green (positive)

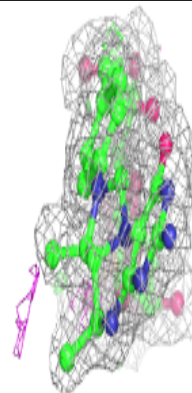
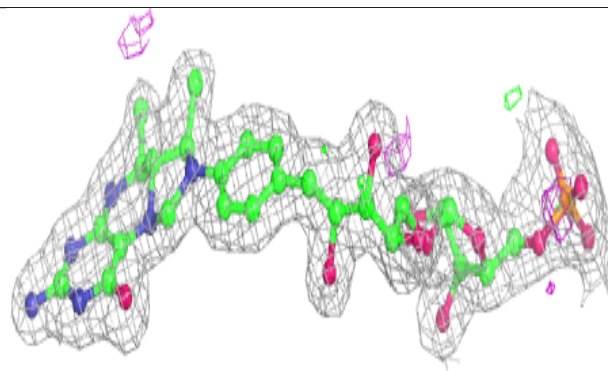
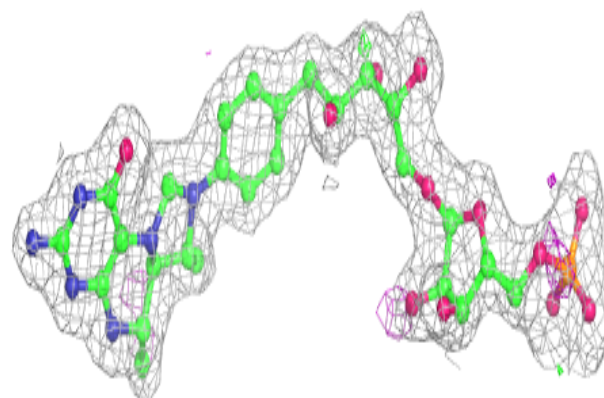


**Electron density around H4M F 284:**

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

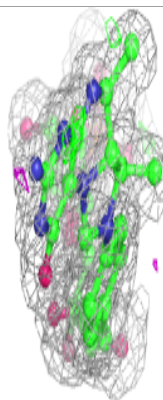
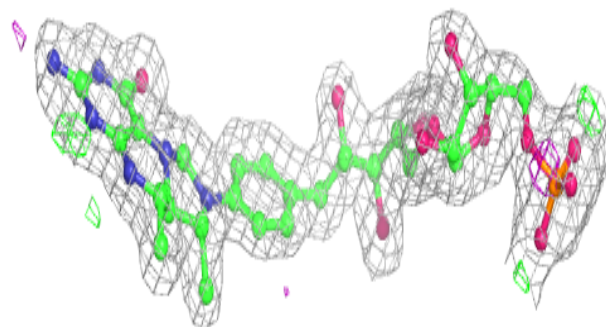
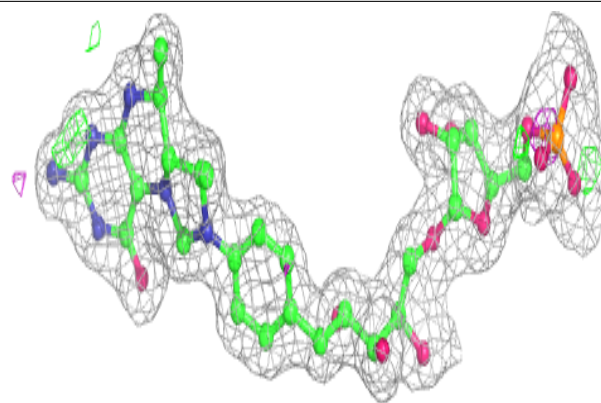
**Electron density around H4M E 284:**

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

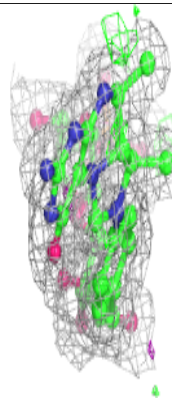
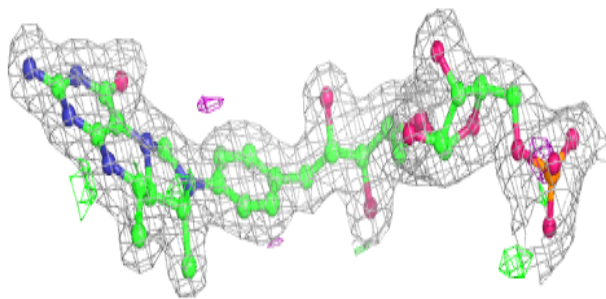
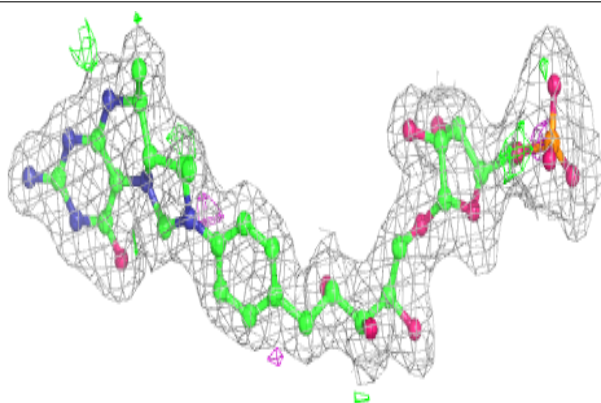


**Electron density around H4M B 284:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.