Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:39 am BST

PDB ID	:	4GVS
Title	:	X-ray structure of the Archaeoglobus fulgidus methenyl-tetrahydromethanopterin cyclohydrolase in complex with N5-formyl-tetrahydromethanopterin
Authors	:	Upadhyay, V.; Demmer, U.; Warkentin, E.; Moll, J.; Shima, S.; Ermler, U.
Deposited on	:	2012-08-31
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

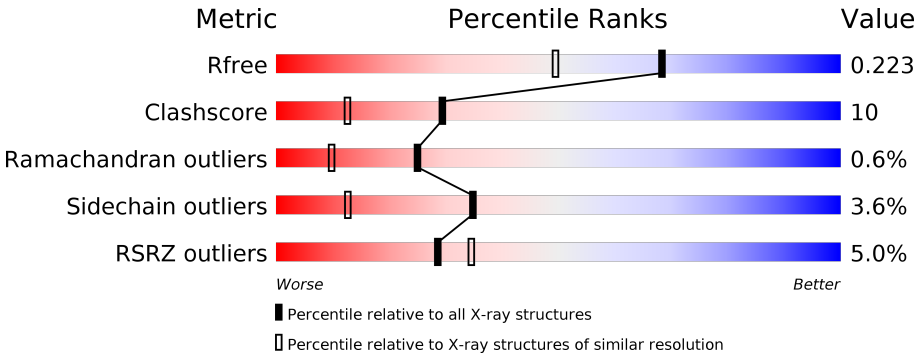
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	8% 80% 17%
1	B	316	3% 80% 18%
1	C	316	5% 82% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8065 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.

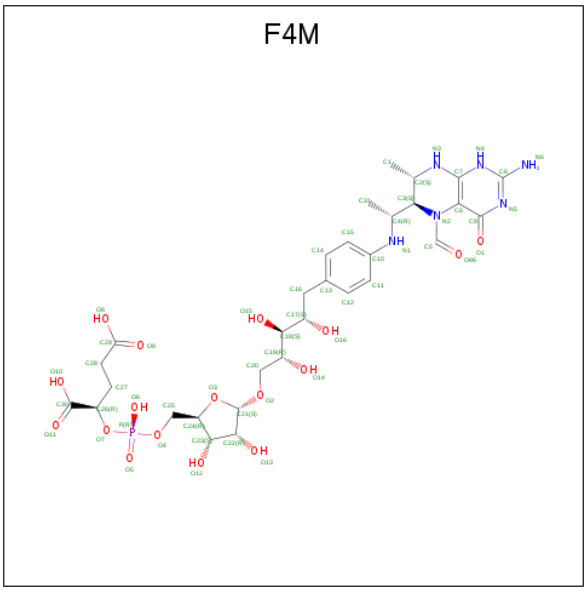
- Molecule 1 is a protein called Methenyltetrahydromethanopterin cyclohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	7	0
			2479	1585	388	489	17			
1	B	315	Total	C	N	O	S	0	9	0
			2507	1598	396	497	16			
1	C	315	Total	C	N	O	S	0	11	0
			2514	1604	393	499	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLN	GLU	ENGINEERED MUTATION	UNP O28344
B	186	GLN	GLU	ENGINEERED MUTATION	UNP O28344
C	186	GLN	GLU	ENGINEERED MUTATION	UNP O28344

- Molecule 2 is 1-[4-({(1R)-1-[(6S,7R)-2-amino-5-formyl-7-methyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]ethyl}amino)phenyl]-1-deoxy-5-O-{5-O-[(R)-{[(1R)-1,3-dicarboxypropyl]oxy}(hydroxy)phosphoryl]-alpha-D-ribofuranosyl}-D-ribitol (three-letter code: F4M) (formula: $C_{31}H_{45}N_6O_{17}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	30	0
			55	31	6	17	1		

- Molecule 3 is water.

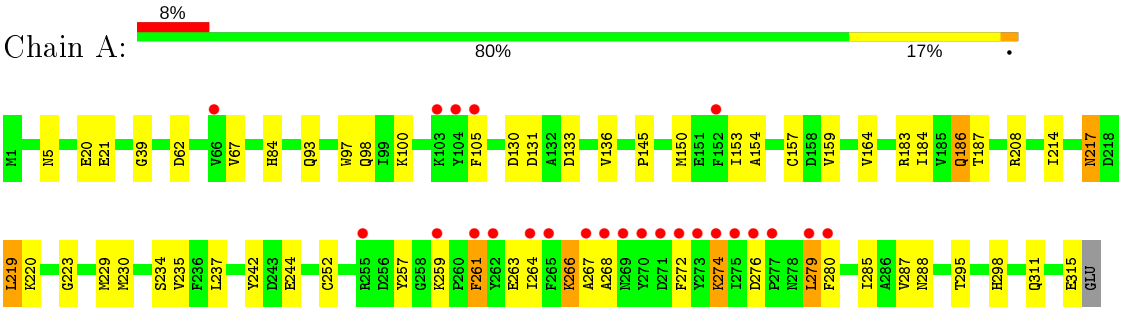
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	182	Total	O	0	0
			182	182		
3	C	178	Total	O	0	0
			178	178		

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.

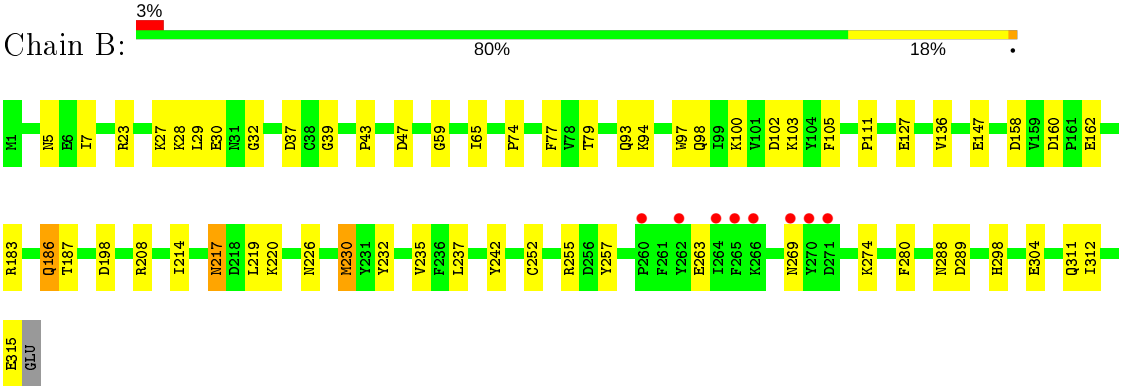
- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase

Chain A:



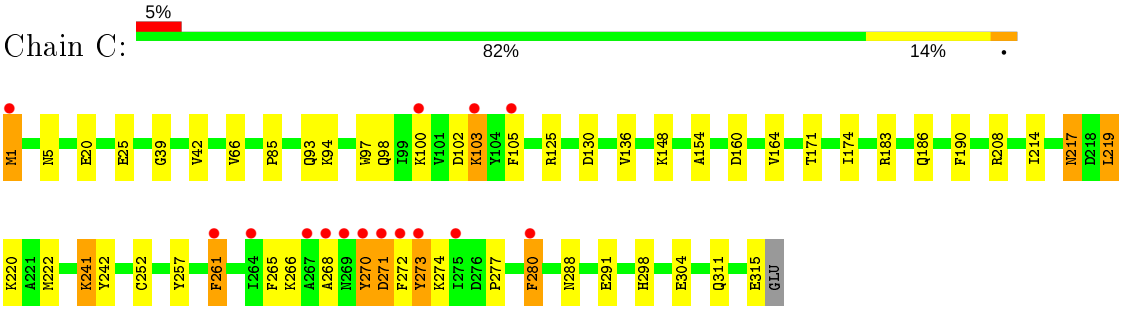
- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase

Chain B:



- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.90Å 108.99Å 114.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 1.75 43.40 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.9 (43.40-1.75) 93.0 (43.40-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.224 0.186 , 0.223	Depositor DCC
R_{free} test set	5423 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8065	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: F4M

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	0.92	2/2538 (0.1%)	0.94	3/3445 (0.1%)
1	B	1.04	1/2554 (0.0%)	1.04	5/3466 (0.1%)
1	C	0.99	2/2570 (0.1%)	1.01	2/3487 (0.1%)
All	All	0.98	5/7662 (0.1%)	1.00	10/10398 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	TRP	CD2-CE2	6.68	1.49	1.41
1	C	20	GLU	CD-OE2	-6.50	1.18	1.25
1	A	97	TRP	CD2-CE2	6.44	1.49	1.41
1	B	97	TRP	CD2-CE2	5.78	1.48	1.41
1	A	21	GLU	CD-OE1	5.08	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	MET	CG-SD-CE	-7.78	87.75	100.20
1	B	208	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	130	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	37	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	208	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	198	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	62[A]	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	62[B]	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	B	47	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	125	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2479	0	2457	54	0
1	B	2507	0	2468	53	0
1	C	2514	0	2478	51	0
2	B	55	0	41	14	0
3	A	150	0	0	0	0
3	B	182	0	0	6	0
3	C	178	0	0	1	0
All	All	8065	0	7444	143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (143) 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:B:226:ASN:HD21	2:B:401:F4M:H3	0.99	0.97
1:B:158:ASP:HB3	3:B:614:HOH:O	1.70	0.91
1:A:263:GLU:O	1:A:266:LYS:HE2	1.71	0.90
1:C:103:LYS:H	1:C:103:LYS:HD3	1.38	0.88
1:A:315:GLU:OE2	1:C:298:HIS:HD2	1.58	0.86
1:C:160:ASP:HB2	3:C:455:HOH:O	1.79	0.82
1:A:288:ASN:HD21	1:B:214:ILE:H	1.23	0.81
1:C:222[B]:MET:HA	1:C:222[B]:MET:CE	2.11	0.80
1:B:186:GLN:OE1	2:B:401:F4M:H12	1.82	0.79
1:A:98:GLN:HE21	1:A:100:LYS:HD2	1.48	0.79
1:B:288:ASN:HD21	1:C:214:ILE:H	1.31	0.78
1:B:30:GLU:HG2	1:B:147:GLU:HG2	1.65	0.77
1:B:183:ARG:HH11	2:B:401:F4M:H2	1.49	0.76
1:B:220:LYS:NZ	1:B:311:GLN:HE22	1.87	0.73
1:A:20:GLU:OE1	1:C:1:MET:HB3	1.90	0.72
1:B:226:ASN:ND2	2:B:401:F4M:H3	1.84	0.69
1:C:222[B]:MET:HE2	1:C:222[B]:MET:HA	1.73	0.68
2:B:401:F4M:H13	2:B:401:F4M:H7	1.76	0.68
1:A:214:ILE:H	1:C:288:ASN:HD21	1.41	0.67
1:A:315:GLU:OE2	1:C:298:HIS:CD2	2.46	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:NE2	1:A:100:LYS:HD2	2.09	0.66
1:B:187[A]:THR:HG22	2:B:401:F4M:H7	1.77	0.66
1:C:277:PRO:O	1:C:280:PHE:CD2	2.48	0.66
1:A:263:GLU:N	1:A:263:GLU:OE1	2.29	0.65
1:B:94:LYS:HG3	2:B:401:F4M:H15	1.77	0.65
1:C:261:PHE:HD2	1:C:261:PHE:C	2.00	0.65
1:A:187[B]:THR:HG21	1:A:229:MET:SD	2.37	0.65
1:A:276:ASP:OD2	1:A:279:LEU:HD21	1.97	0.65
1:C:171:THR:HG21	1:C:222[B]:MET:HE3	1.79	0.64
1:B:160:ASP:OD2	1:B:162:GLU:HG2	1.98	0.64
1:B:220:LYS:HZ2	1:B:311:GLN:HE22	1.46	0.64
1:B:298:HIS:HD2	1:C:315:GLU:OE2	1.80	0.63
1:C:220:LYS:NZ	1:C:311:GLN:HE22	1.96	0.63
1:C:261:PHE:C	1:C:261:PHE:CD2	2.71	0.63
1:A:298:HIS:HD2	1:B:315:GLU:OE2	1.83	0.62
1:A:220:LYS:NZ	1:A:311:GLN:HE22	1.98	0.61
1:A:234:SER:HB3	1:B:74:PRO:HB3	1.82	0.61
1:A:145:PRO:CG	1:A:150[B]:MET:HE3	2.30	0.61
1:B:183:ARG:NH1	2:B:401:F4M:H2	2.14	0.61
1:A:214:ILE:H	1:C:288:ASN:ND2	1.98	0.61
1:C:183:ARG:HH11	1:C:186:GLN:HE22	1.49	0.60
1:B:288:ASN:ND2	1:C:214:ILE:H	1.96	0.60
1:A:288:ASN:ND2	1:B:214:ILE:H	1.97	0.59
1:A:268:ALA:HB1	1:A:274:LYS:HB3	1.83	0.59
1:C:242:TYR:OH	1:C:298:HIS:HE1	1.84	0.59
1:C:268:ALA:O	1:C:271:ASP:HB2	2.01	0.59
1:C:93:GLN:HG2	1:C:186:GLN:HE21	1.68	0.59
1:C:222[B]:MET:HA	1:C:222[B]:MET:HE3	1.85	0.59
1:C:217:ASN:HD22	1:C:219:LEU:H	1.50	0.58
1:B:183:ARG:HD3	2:B:401:F4M:H2	1.84	0.58
1:B:28:LYS:NZ	3:B:638:HOH:O	2.36	0.58
1:C:265:PHE:CE2	1:C:270:TYR:HA	2.39	0.58
1:A:220:LYS:HZ3	1:A:311:GLN:HE22	1.51	0.57
1:B:94:LYS:HG3	2:B:401:F4M:C11	2.35	0.57
1:C:241:LYS:HE2	1:C:291:GLU:OE2	2.05	0.56
1:C:270:TYR:N	1:C:270:TYR:HD2	2.05	0.55
1:B:187[A]:THR:HG22	2:B:401:F4M:C1	2.34	0.55
1:C:261:PHE:HD2	1:C:261:PHE:O	1.89	0.55
1:C:94:LYS:HD3	1:C:190:PHE:CD1	2.42	0.54
1:B:186:GLN:HE22	2:B:401:F4M:H2	1.72	0.54
1:C:25:GLU:HG3	1:C:42:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:HG2	1:A:186:GLN:HE21	1.73	0.53
1:A:145:PRO:HG3	1:A:150[B]:MET:HE3	1.90	0.53
1:C:270:TYR:N	1:C:270:TYR:CD2	2.77	0.53
1:C:5:ASN:HD22	1:C:136:VAL:H	1.56	0.53
1:B:269:ASN:HD22	1:B:274:LYS:NZ	2.07	0.52
1:A:184:ILE:O	1:A:187[A]:THR:HG22	2.09	0.52
1:C:103:LYS:HD3	1:C:103:LYS:N	2.17	0.52
1:B:217:ASN:ND2	1:B:220:LYS:H	2.07	0.52
1:B:94:LYS:CG	2:B:401:F4M:H15	2.39	0.52
1:A:67:VAL:O	1:C:208[B]:ARG:HD2	2.10	0.52
1:B:304:GLU:CD	1:B:304:GLU:H	2.13	0.52
1:B:28:LYS:HE3	1:B:32:GLY:HA2	1.91	0.51
1:A:259:LYS:HE3	1:A:264:ILE:HD11	1.91	0.51
1:C:242:TYR:OH	1:C:298:HIS:CE1	2.63	0.51
1:B:79:THR:HG21	1:C:66[B]:VAL:HG13	1.93	0.51
1:B:183:ARG:HH11	1:B:186:GLN:HE22	1.60	0.50
1:B:27[A]:LYS:NZ	3:B:565:HOH:O	2.43	0.50
1:A:230:MET:HE2	1:A:280:PHE:HA	1.94	0.50
1:C:154:ALA:HB2	1:C:164:VAL:HG21	1.94	0.50
1:A:217:ASN:ND2	1:A:220:LYS:H	2.09	0.49
1:C:265:PHE:CZ	1:C:270:TYR:HA	2.47	0.49
1:A:276:ASP:HB3	1:A:279:LEU:HD11	1.93	0.49
1:B:5:ASN:ND2	1:B:136:VAL:H	2.11	0.49
1:A:223:GLY:HA2	1:A:261:PHE:HD2	1.78	0.48
1:C:277:PRO:O	1:C:280:PHE:CE2	2.66	0.48
1:B:5:ASN:HD22	1:B:136:VAL:H	1.60	0.48
1:C:171:THR:CG2	1:C:222[B]:MET:HE3	2.42	0.48
1:A:298:HIS:CD2	1:B:315:GLU:OE2	2.66	0.48
1:C:273:TYR:HB3	1:C:274:LYS:HD2	1.95	0.48
1:B:235:VAL:HG12	1:B:237:LEU:HG	1.96	0.47
1:A:263:GLU:O	1:A:266:LYS:HG3	2.13	0.47
1:B:127:GLU:HG2	3:B:621:HOH:O	2.14	0.47
1:A:217:ASN:HD22	1:A:219:LEU:H	1.63	0.46
1:B:252:CYS:HA	1:B:257:TYR:CG	2.50	0.46
1:C:98:GLN:HG3	1:C:105:PHE:HE1	1.80	0.46
1:A:187[B]:THR:CG2	1:A:229:MET:SD	3.03	0.46
1:C:217:ASN:HD22	1:C:219:LEU:N	2.13	0.46
1:A:285:ILE:HD12	1:A:287:VAL:CG2	2.46	0.46
1:A:266:LYS:C	1:A:268:ALA:H	2.20	0.45
1:B:5:ASN:ND2	1:B:111:PRO:HB2	2.31	0.45
1:A:252:CYS:HA	1:A:257:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HG	1:A:219:LEU:H	1.65	0.45
1:A:150[B]:MET:HE1	1:A:153:ILE:HD12	1.98	0.45
1:B:93:GLN:HG2	1:B:186:GLN:HE21	1.81	0.45
1:A:276:ASP:OD2	1:A:279:LEU:CD2	2.65	0.45
1:C:5:ASN:ND2	1:C:136:VAL:H	2.14	0.45
1:A:84:HIS:HD2	3:B:659:HOH:O	2.00	0.44
1:A:157:CYS:HB2	1:A:159:VAL:HG22	1.99	0.44
1:C:252:CYS:HA	1:C:257:TYR:CG	2.52	0.44
1:A:183:ARG:HH11	1:A:186:GLN:HE22	1.65	0.44
1:B:280:PHE:CD2	2:B:401:F4M:H17	2.53	0.44
1:C:102:ASP:OD1	1:C:148:LYS:NZ	2.36	0.44
1:B:217:ASN:HD22	1:B:219:LEU:H	1.66	0.44
1:B:23[A]:ARG:HD2	1:B:43:PRO:HG2	1.98	0.44
1:C:252:CYS:HA	1:C:257:TYR:CD1	2.53	0.43
3:B:633:HOH:O	1:C:174:ILE:HG12	2.19	0.43
1:A:100:LYS:HG2	1:A:105:PHE:CD1	2.54	0.43
1:A:5:ASN:ND2	1:A:136:VAL:H	2.16	0.43
1:A:268:ALA:HA	1:A:274:LYS:HD2	2.00	0.43
1:B:217:ASN:HD22	1:B:219:LEU:N	2.16	0.43
1:C:94:LYS:HD3	1:C:190:PHE:CE1	2.54	0.42
1:A:150[B]:MET:CE	1:A:153:ILE:HD12	2.49	0.42
1:B:242:TYR:HB2	1:B:289:ASP:HB2	2.00	0.42
1:B:7:ILE:HG22	1:B:59:GLY:HA3	2.01	0.42
1:A:154:ALA:HB2	1:A:164:VAL:HG21	2.01	0.42
1:B:242:TYR:OH	1:B:298:HIS:HE1	2.02	0.41
1:C:217:ASN:HD21	1:C:220:LYS:H	1.68	0.41
1:A:252:CYS:HA	1:A:257:TYR:CD1	2.55	0.41
1:A:272:PHE:CE1	1:A:280:PHE:HZ	2.38	0.41
1:B:100:LYS:HA	1:B:100:LYS:HD3	1.78	0.41
1:B:29:LEU:HB3	1:B:147:GLU:HG3	2.02	0.41
1:B:65:ILE:HA	1:B:77:PHE:O	2.20	0.41
1:B:304:GLU:N	1:B:304:GLU:CD	2.74	0.41
1:A:295:THR:HB	1:B:312:ILE:HD13	2.03	0.41
1:A:130:ASP:OD1	1:A:131:ASP:N	2.54	0.41
1:C:304:GLU:H	1:C:304:GLU:CD	2.23	0.41
1:A:145:PRO:CB	1:A:150[B]:MET:HE3	2.51	0.41
1:A:183:ARG:O	1:A:187[B]:THR:HG23	2.21	0.40
1:A:242:TYR:OH	1:A:298:HIS:HE1	2.04	0.40
1:B:98:GLN:HG3	1:B:105:PHE:CE1	2.56	0.40
1:C:217:ASN:ND2	1:C:220:LYS:H	2.19	0.40
1:A:235:VAL:HG12	1:A:237:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	320/316 (101%)	308 (96%)	9 (3%)	3 (1%)	17 5
1	B	322/316 (102%)	313 (97%)	7 (2%)	2 (1%)	25 10
1	C	324/316 (102%)	309 (95%)	14 (4%)	1 (0%)	41 22
All	All	966/948 (102%)	930 (96%)	30 (3%)	6 (1%)	25 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PHE
1	C	39	GLY
1	A	39	GLY
1	A	267	ALA
1	B	39	GLY
1	B	102	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	272/266 (102%)	264 (97%)	8 (3%)	42 19
1	B	274/266 (103%)	267 (97%)	7 (3%)	46 23
1	C	276/266 (104%)	262 (95%)	14 (5%)	24 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	822/798 (103%)	793 (96%)	29 (4%)	35 13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASP
1	A	186	GLN
1	A	217	ASN
1	A	219	LEU
1	A	244	GLU
1	A	266	LYS
1	A	274	LYS
1	A	279	LEU
1	B	103	LYS
1	B	186	GLN
1	B	217	ASN
1	B	230	MET
1	B	232	TYR
1	B	255	ARG
1	B	263	GLU
1	C	1	MET
1	C	85	PRO
1	C	100	LYS
1	C	103	LYS
1	C	217	ASN
1	C	219	LEU
1	C	241	LYS
1	C	261	PHE
1	C	266	LYS
1	C	270	TYR
1	C	271	ASP
1	C	272	PHE
1	C	273	TYR
1	C	280	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	98	GLN
1	A	186	GLN

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	226	ASN
1	A	288	ASN
1	A	298	HIS
1	A	311	GLN
1	B	5	ASN
1	B	217	ASN
1	B	226	ASN
1	B	269	ASN
1	B	288	ASN
1	B	298	HIS
1	B	311	GLN
1	C	5	ASN
1	C	186	GLN
1	C	217	ASN
1	C	288	ASN
1	C	298	HIS
1	C	311	GLN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	F4M	B	401	-	51,58,58	2.11	10 (19%)	59,84,84	2.80	17 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F4M	B	401	-	-	18/41/79/79	0/3/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	F4M	C16-C17	9.94	1.62	1.53
2	B	401	F4M	C9-C6	6.01	1.49	1.41
2	B	401	F4M	C4-C3	3.93	1.60	1.53
2	B	401	F4M	O2-C21	3.57	1.46	1.40
2	B	401	F4M	C3-N2	2.97	1.50	1.47
2	B	401	F4M	C9-N5	2.78	1.37	1.33
2	B	401	F4M	C6-C7	2.76	1.46	1.41
2	B	401	F4M	C6-N2	2.43	1.44	1.41
2	B	401	F4M	O3-C21	2.28	1.45	1.41
2	B	401	F4M	O7-C26	-2.11	1.43	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	F4M	O16-C17-C16	11.85	131.67	109.57
2	B	401	F4M	O96-C5-N2	-9.02	112.30	125.36
2	B	401	F4M	C4-C3-N2	5.71	119.08	110.93
2	B	401	F4M	C13-C16-C17	5.53	123.50	113.61
2	B	401	F4M	O3-C21-O2	4.99	117.44	111.95
2	B	401	F4M	C8-N4-C7	4.53	124.70	114.54
2	B	401	F4M	C10-N1-C4	3.58	130.89	121.60
2	B	401	F4M	C6-N2-C3	3.42	125.36	119.32
2	B	401	F4M	N5-C8-N4	-3.24	120.33	125.42
2	B	401	F4M	C20-O2-C21	3.02	119.63	113.74
2	B	401	F4M	C9-N5-C8	2.89	120.52	115.93
2	B	401	F4M	O2-C21-C22	2.61	112.02	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	F4M	P-O7-C26	-2.43	117.45	123.04
2	B	401	F4M	C12-C11-C10	2.32	122.98	120.30
2	B	401	F4M	C21-C22-C23	2.14	105.02	102.30
2	B	401	F4M	O2-C20-C19	2.13	114.23	109.27
2	B	401	F4M	C1-C2-N3	2.07	111.90	109.55

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	F4M	O96-C5-N2-C6
2	B	401	F4M	O96-C5-N2-C3
2	B	401	F4M	N2-C3-C4-N1
2	B	401	F4M	C2-C3-C4-N1
2	B	401	F4M	O16-C17-C18-O15
2	B	401	F4M	O16-C17-C18-C19
2	B	401	F4M	C22-C21-O2-C20
2	B	401	F4M	O3-C21-O2-C20
2	B	401	F4M	C30-C26-C27-C28
2	B	401	F4M	C26-C27-C28-C29
2	B	401	F4M	C13-C16-C17-O16
2	B	401	F4M	O7-C26-C27-C28
2	B	401	F4M	C25-O4-P-O7
2	B	401	F4M	C13-C16-C17-C18
2	B	401	F4M	C26-O7-P-O4
2	B	401	F4M	C24-C25-O4-P
2	B	401	F4M	C16-C17-C18-O15
2	B	401	F4M	O3-C24-C25-O4

There are no ring outliers.

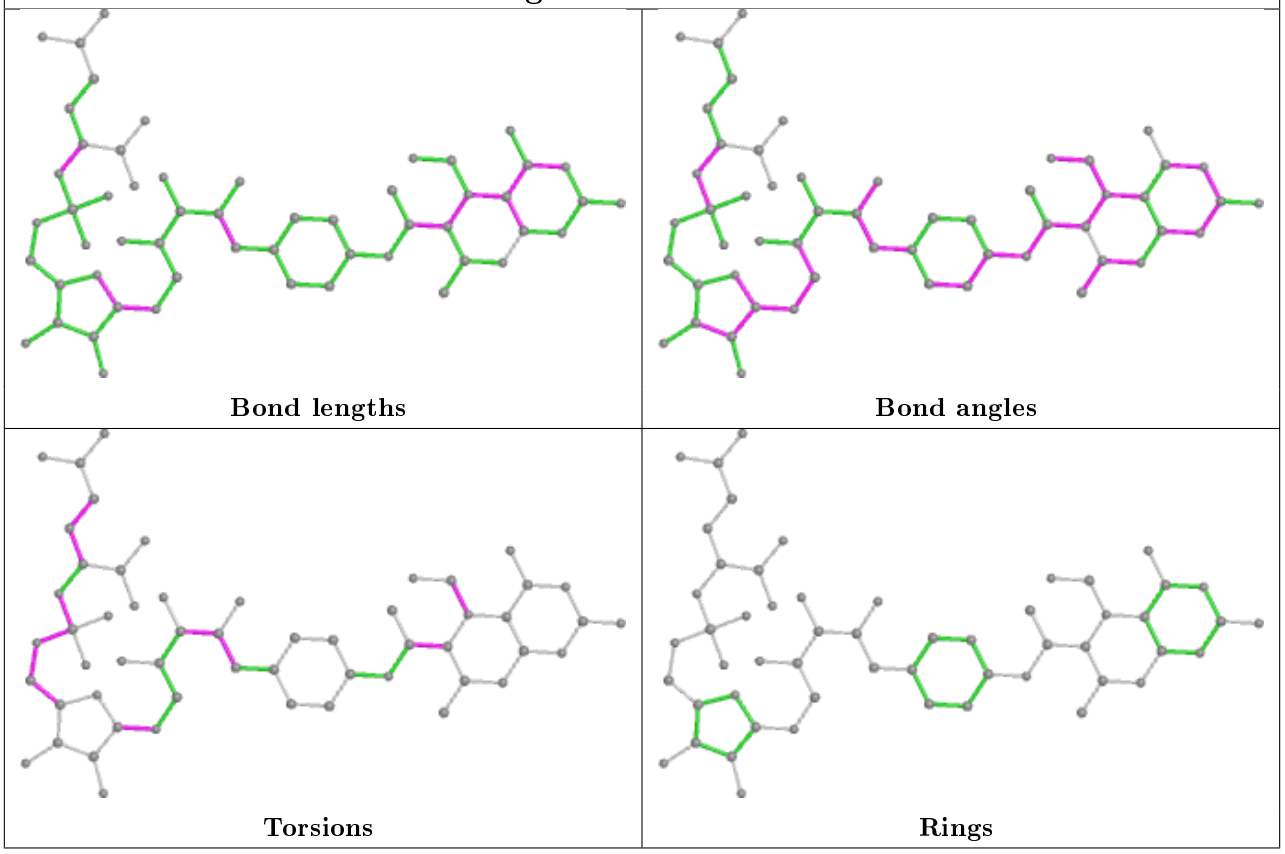
1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	F4M	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand F4M B 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	315/316 (99%)	0.51	24 (7%)	13	18	16, 29, 61, 88	0
1	B	315/316 (99%)	-0.14	8 (2%)	57	63	13, 22, 42, 52	0
1	C	315/316 (99%)	0.07	15 (4%)	30	36	13, 23, 47, 98	0
All	All	945/948 (99%)	0.15	47 (4%)	28	34	13, 24, 48, 98	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	TYR	9.6
1	A	264	ILE	9.4
1	A	270	TYR	9.1
1	C	272	PHE	6.4
1	A	265	PHE	6.3
1	C	268	ALA	5.4
1	A	277	PRO	5.4
1	A	274	LYS	5.4
1	A	275	ILE	5.1
1	C	275	ILE	5.1
1	A	267	ALA	4.8
1	B	264	ILE	4.4
1	C	280	PHE	4.3
1	B	262	TYR	4.2
1	B	270	TYR	4.2
1	A	271	ASP	4.1
1	A	269	ASN	4.0
1	A	273	TYR	4.0
1	C	264	ILE	3.9
1	C	270	TYR	3.9
1	A	262	TYR	3.7
1	B	269	ASN	3.7
1	A	261	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	265	PHE	3.5
1	A	276	ASP	3.4
1	C	267	ALA	3.4
1	A	279	LEU	3.3
1	A	66[A]	VAL	3.3
1	C	1	MET	3.1
1	A	255	ARG	3.0
1	A	152	PHE	3.0
1	C	261	PHE	3.0
1	B	271	ASP	2.9
1	A	105	PHE	2.9
1	A	268	ALA	2.8
1	A	259	LYS	2.8
1	A	272	PHE	2.7
1	A	280	PHE	2.7
1	C	105	PHE	2.5
1	A	103	LYS	2.4
1	C	271	ASP	2.3
1	C	103	LYS	2.3
1	C	269	ASN	2.2
1	C	100	LYS	2.2
1	B	266	LYS	2.1
1	B	260	PRO	2.1
1	A	104	TYR	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)

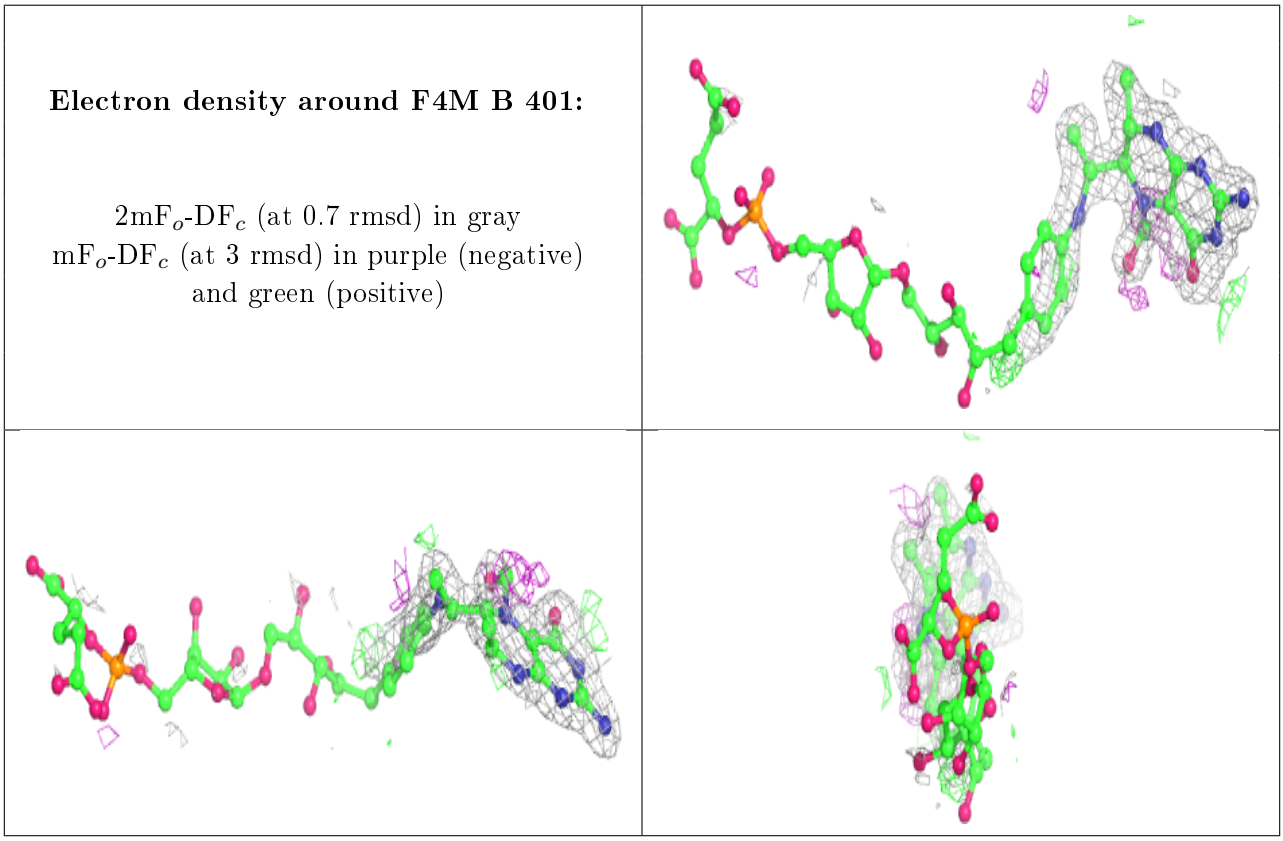
There are no carbohydrates in this entry.

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F4M	B	401	55/55	0.87	0.21	20,20,66,73	30

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.



6.5 Other polymers

There are no such residues in this entry.