Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 12:18 pm GMT

PDB ID	:	5T5M
Title	:	TUNGSTEN-CONTAINING FORMYLMETHANOFURAN DEHYDROGENASE FROM METHANOTHERMOBACTER WOLFEII, TRIGONAL FORM AT 2.5 A.
Authors	:	Wagner, T.; Ermler, U.; Shima, S.
Deposited on	:	2016-08-31
Resolution	:	2.50 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 (i) symbol.

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

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

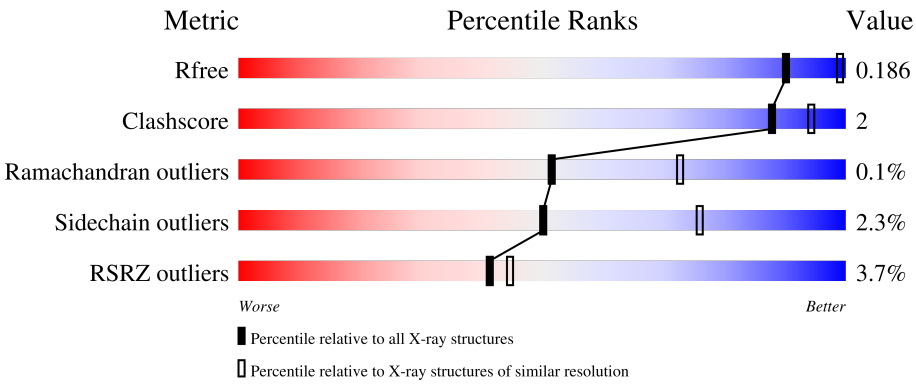
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	569	2%, 92%, 7%
2	B	432	9%, 93%, 6%
3	C	270	%, 97%
4	D	130	4%, 90%, 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	349	2% 91% 7%
6	G	82	2% 89% 7%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14415 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 Tungsten formylmethanofuran dehydrogenase subunit fwdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	569	4419	2812	735	849	23	0	0	0

- Molecule 2 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	429	3375	2122	593	629	31	0	2	0

- Molecule 3 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	269	1994	1254	336	391	13	0	0	0

- Molecule 4 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	126	977	625	158	185	9	0	0	0

- Molecule 5 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	342	2610	1611	435	523	41	0	0	0

- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	80	572	354	96	113	9	0	0	0

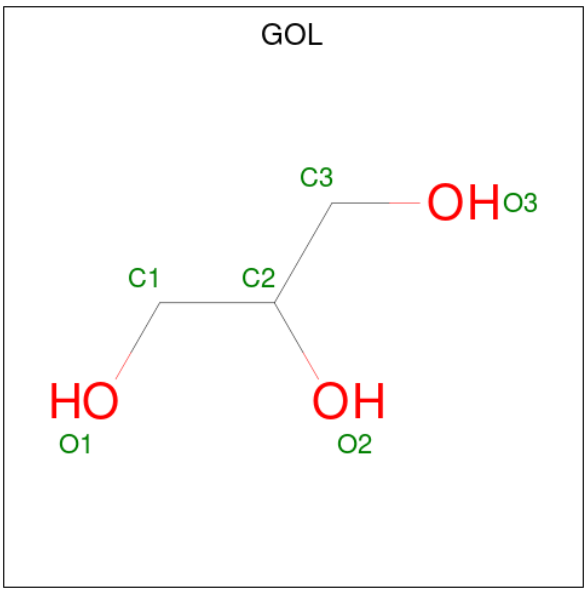
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	A	2	2	2	0	0
			Total	Mg		
7	C	1	1	1	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
8	A	2	2	2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

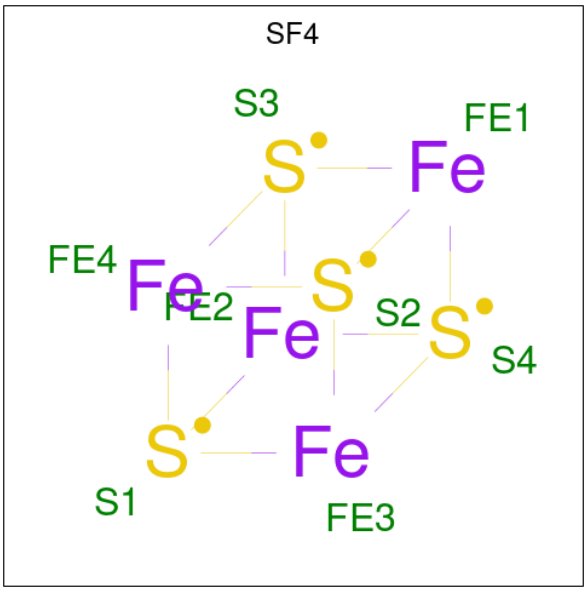


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	6	3	3	0	0
			Total	C	O		
9	A	1	6	3	3	0	0
			Total	C	O		
9	D	1	6	3	3	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
10	B	1	1	1	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	F	1	Total 8	Fe 4	S 4	0	0
11	G	1	Total 8	Fe 4	S 4	0	0

Continued on next page...

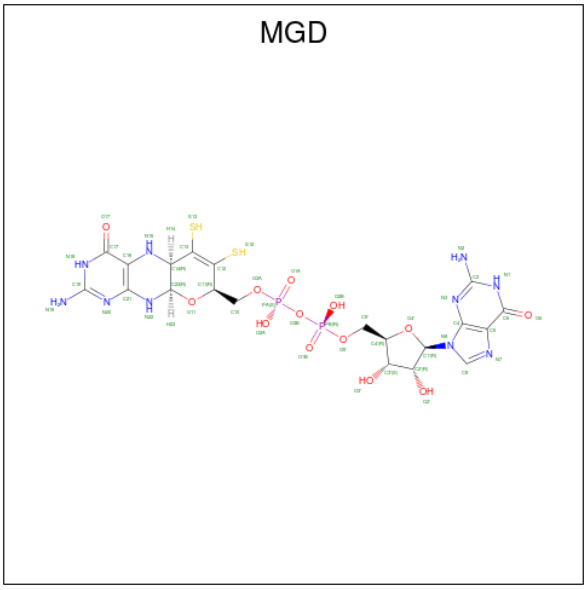
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	G	1	8	4	4	0	0

- Molecule 12 is TUNGSTEN ION (three-letter code: W) (formula: W).

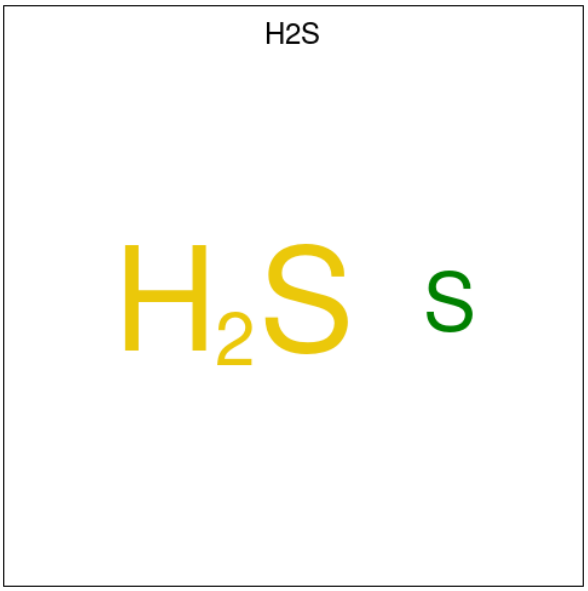
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	W		
12	B	1	1	1	0	0

- Molecule 13 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
13	B	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
13	B	1	47	20	10	13	2	2	0	0

- Molecule 14 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	S		
14	B	1	1	1	0	0

- Molecule 15 is water.

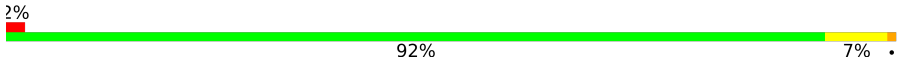
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	97	97	97	0	0
			Total	O		
15	B	69	69	69	0	0
			Total	O		
15	C	38	38	38	0	0
			Total	O		
15	D	10	10	10	0	0
			Total	O		
15	F	39	39	39	0	0
			Total	O		
15	G	7	7	7	0	0

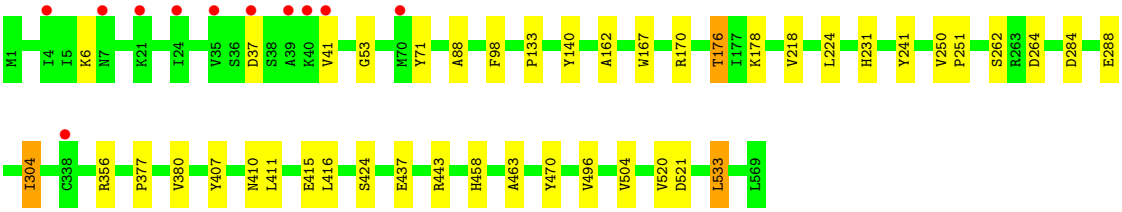
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Tungsten formylmethanofuran dehydrogenase subunit fwdA

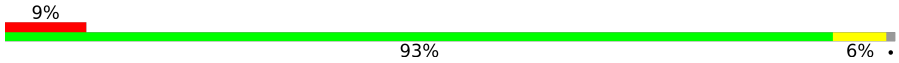
Chain A:

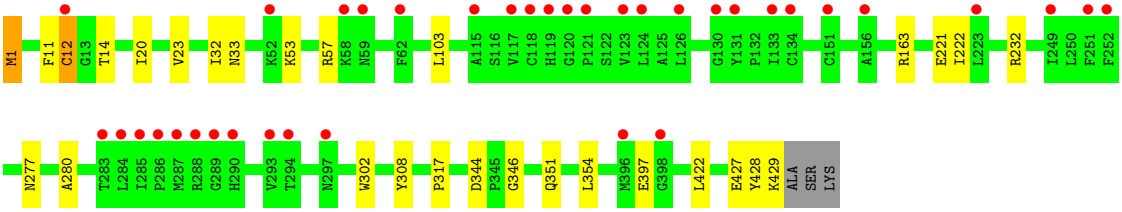




• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit fwdB

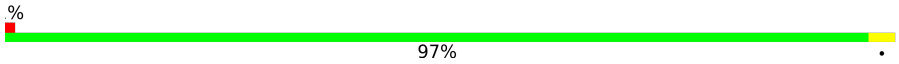
Chain B:

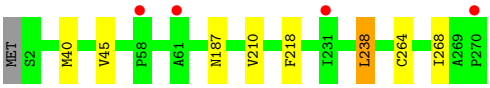




• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

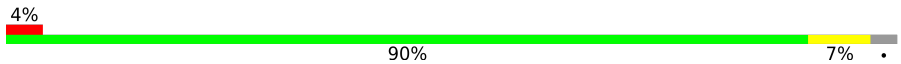
Chain C:

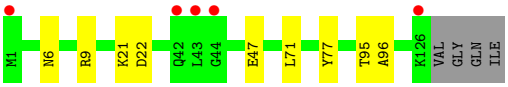




• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

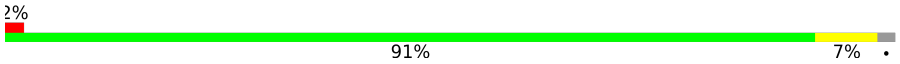
Chain D:

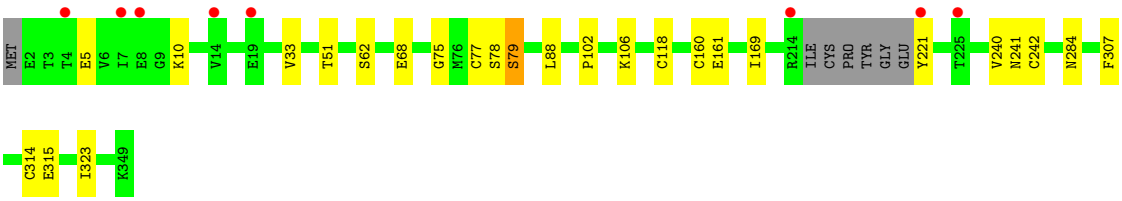




• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdF

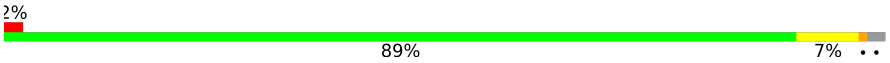
Chain F:

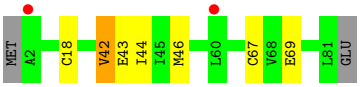




- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.54Å 105.54Å 340.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.22 – 2.50 48.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.22-2.50) 99.9 (48.22-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.158 , 0.182 0.162 , 0.186	Depositor DCC
R_{free} test set	3638 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14415	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, SF4, H2S, MGD, W, KCX, MG, ZN

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	0.33	0/4523	0.50	0/6161
2	B	0.37	0/3451	0.52	0/4669
3	C	0.33	0/2027	0.54	0/2729
4	D	0.32	0/996	0.52	0/1352
5	F	0.34	0/2646	0.52	0/3586
6	G	0.35	0/579	0.48	0/787
All	All	0.34	0/14222	0.51	0/19284

There are no bond length outliers.

There are no bond angle outliers.

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	4419	0	4272	21	0
2	B	3375	0	3325	13	0
3	C	1994	0	1962	3	0
4	D	977	0	1002	5	0
5	F	2610	0	2567	13	0
6	G	572	0	567	2	0
7	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	1	0	0	0	0
8	A	2	0	0	0	0
9	A	12	0	16	0	0
9	D	6	0	8	0	0
10	B	1	0	0	0	0
11	B	8	0	0	0	0
11	F	64	0	0	0	0
11	G	16	0	0	0	0
12	B	1	0	0	0	0
13	B	94	0	44	0	0
14	B	1	0	0	0	0
15	A	97	0	0	2	0
15	B	69	0	0	0	0
15	C	38	0	0	0	0
15	D	10	0	0	0	0
15	F	39	0	0	0	0
15	G	7	0	0	0	0
All	All	14415	0	13763	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (55) 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:A:284:ASP:O	15:A:701:HOH:O	2.11	0.68
1:A:264:ASP:O	15:A:702:HOH:O	2.12	0.66
1:A:224:LEU:HD22	1:A:520:VAL:HG11	1.81	0.61
1:A:411:LEU:HG	1:A:416:LEU:HG	1.86	0.58
3:C:210:VAL:HG11	3:C:238:LEU:HD13	1.88	0.55
2:B:20:ILE:HB	2:B:32:ILE:HB	1.87	0.55
5:F:10:LYS:O	5:F:62:SER:OG	2.16	0.54
1:A:88:ALA:HB1	2:B:317:PRO:HD3	1.91	0.53
1:A:356:ARG:NH2	1:A:415:GLU:OE2	2.42	0.53
2:B:427:GLU:O	2:B:429:LYS:N	2.42	0.52
6:G:42:VAL:HG22	6:G:44:ILE:HG23	1.92	0.51
2:B:344:ASP:OD2	4:D:21:LYS:NZ	2.42	0.49
6:G:18:CYS:HB2	6:G:67:CYS:HB2	1.95	0.48
1:A:167:TRP:CD1	1:A:533:LEU:HD11	2.50	0.47
2:B:103:LEU:HD13	2:B:422:LEU:HA	1.97	0.46
2:B:427:GLU:C	2:B:429:LYS:H	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLY:HA2	1:A:443:ARG:HG3	1.98	0.46
4:D:22:ASP:OD1	4:D:22:ASP:N	2.42	0.46
2:B:1:MET:HA	2:B:23:VAL:O	2.16	0.45
1:A:496:VAL:HB	1:A:504:VAL:HB	1.98	0.45
5:F:106:LYS:HD3	5:F:241:ASN:OD1	2.17	0.45
2:B:346:GLY:HA2	2:B:354:LEU:HD11	1.99	0.45
4:D:71:LEU:HD21	4:D:77:TYR:HB2	1.99	0.44
5:F:77:CYS:SG	5:F:78:SER:N	2.91	0.44
3:C:40:MET:SD	3:C:45:VAL:HG22	2.58	0.44
1:A:458:HIS:CE1	1:A:463:ALA:HB2	2.52	0.44
5:F:160:CYS:SG	5:F:161:GLU:N	2.91	0.44
5:F:5:GLU:CB	5:F:68:GLU:HG2	2.48	0.44
2:B:277:ASN:HA	2:B:280:ALA:O	2.18	0.43
1:A:140:TYR:CE1	1:A:176:THR:HG23	2.53	0.43
1:A:140:TYR:CD1	1:A:176:THR:HG23	2.54	0.43
4:D:6:ASN:O	4:D:77:TYR:HA	2.17	0.43
5:F:68:GLU:CD	5:F:68:GLU:H	2.21	0.43
2:B:32:ILE:O	2:B:33:ASN:HB2	2.19	0.42
5:F:75:GLY:HA3	5:F:88:LEU:HD22	2.01	0.42
5:F:314:CYS:SG	5:F:315:GLU:N	2.92	0.42
1:A:162:ALA:HA	1:A:218:VAL:HG13	2.02	0.42
2:B:222:ILE:O	2:B:232:ARG:NH1	2.37	0.42
4:D:95:THR:O	4:D:96:ALA:HB3	2.20	0.42
5:F:242:CYS:O	5:F:307:PHE:HA	2.20	0.42
1:A:6:LYS:HG3	1:A:41:VAL:HG13	2.02	0.41
1:A:377:PRO:HG3	1:A:437:GLU:HG2	2.02	0.41
1:A:98:PHE:HA	1:A:133:PRO:HD3	2.02	0.41
5:F:160:CYS:SG	5:F:169:ILE:HG21	2.61	0.41
1:A:170:ARG:NH2	1:A:521:ASP:OD1	2.37	0.41
1:A:304:ILE:O	1:A:380:VAL:HA	2.20	0.41
5:F:79:SER:OG	5:F:102:PRO:O	2.38	0.41
2:B:14:THR:HG22	2:B:163[A]:ARG:NH1	2.36	0.41
3:C:218:PHE:HB2	3:C:268:ILE:HD12	2.03	0.41
5:F:5:GLU:HB3	5:F:68:GLU:HG2	2.02	0.41
1:A:241:TYR:CD1	1:A:288:GLU:HG3	2.55	0.40
1:A:443:ARG:NH2	1:A:470:TYR:OH	2.50	0.40
5:F:33:VAL:HB	5:F:51:THR:HG23	2.02	0.40
1:A:250:VAL:HB	1:A:251:PRO:HD3	2.03	0.40
2:B:11:PHE:HD2	2:B:12:CYS:HB3	1.86	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	566/569 (100%)	543 (96%)	23 (4%)	0	100	100
2	B	429/432 (99%)	412 (96%)	16 (4%)	1 (0%)	47	68
3	C	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
4	D	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
5	F	338/349 (97%)	333 (98%)	5 (2%)	0	100	100
6	G	78/82 (95%)	78 (100%)	0	0	100	100
All	All	1802/1832 (98%)	1742 (97%)	59 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	428	TYR

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	470/470 (100%)	460 (98%)	10 (2%)	53	78
2	B	361/361 (100%)	352 (98%)	9 (2%)	47	73
3	C	203/204 (100%)	200 (98%)	3 (2%)	65	85
4	D	108/111 (97%)	106 (98%)	2 (2%)	57	80
5	F	306/312 (98%)	300 (98%)	6 (2%)	55	79
6	G	65/67 (97%)	61 (94%)	4 (6%)	18	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1513/1525 (99%)	1479 (98%)	34 (2%)	50 77

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

Mol	Chain	Res	Type
1	A	37	ASP
1	A	71	TYR
1	A	176	THR
1	A	231	HIS
1	A	262	SER
1	A	304	ILE
1	A	407	TYR
1	A	410	ASN
1	A	424	SER
1	A	533	LEU
2	B	1	MET
2	B	12	CYS
2	B	53	LYS
2	B	57	ARG
2	B	221	GLU
2	B	302	TRP
2	B	308	TYR
2	B	351	GLN
2	B	397	GLU
3	C	187	ASN
3	C	238	LEU
3	C	264	CYS
4	D	9	ARG
4	D	47	GLU
5	F	79	SER
5	F	118	CYS
5	F	221	TYR
5	F	240	VAL
5	F	284	ASN
5	F	323	ILE
6	G	42	VAL
6	G	43	GLU
6	G	46	MET
6	G	69	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	KCX	A	178	8,1	9,11,12	0.65	0	5,12,14	1.59	1 (20%)

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
1	KCX	A	178	8,1	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	KCX	OQ1-CX-NZ	-2.40	121.24	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 7 are monoatomic and 1 is modelled with single atom - leaving 16 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	$\#\|Z\| > 2$
9	GOL	A	605	-	5,5,5	0.34	0	5,5,5	0.22	0
11	SF4	B	502	2	0,12,12	-	-	-		
11	SF4	F	502	5	0,12,12	-	-	-		
11	SF4	F	503	5	0,12,12	-	-	-		
11	SF4	F	505	5	0,12,12	-	-	-		
13	MGD	B	504	12	41,52,52	1.35	3 (7%)	40,81,81	1.53	8 (20%)
11	SF4	F	508	5	0,12,12	-	-	-		
9	GOL	A	606	-	5,5,5	0.33	0	5,5,5	0.36	0
9	GOL	D	201	-	5,5,5	0.38	0	5,5,5	0.53	0
11	SF4	F	507	5	0,12,12	-	-	-		
11	SF4	F	506	5	0,12,12	-	-	-		
11	SF4	F	504	5	0,12,12	-	-	-		
11	SF4	G	200	6	0,12,12	-	-	-		
13	MGD	B	505	12	41,52,52	1.34	5 (12%)	40,81,81	1.55	7 (17%)
11	SF4	G	201	6	0,12,12	-	-	-		
11	SF4	F	501	5	0,12,12	-	-	-		

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
9	GOL	A	605	-	-	0/4/4/4	-
11	SF4	B	502	2	-	-	0/6/5/5
11	SF4	F	502	5	-	-	0/6/5/5
11	SF4	F	503	5	-	-	0/6/5/5
13	MGD	B	504	12	-	8/18/66/66	0/6/6/6
11	SF4	F	505	5	-	-	0/6/5/5
11	SF4	F	508	5	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MGD	B	505	12	-	0/18/66/66	0/6/6/6
9	GOL	D	201	-	-	2/4/4/4	-
9	GOL	A	606	-	-	2/4/4/4	-
11	SF4	F	506	5	-	-	0/6/5/5
11	SF4	F	504	5	-	-	0/6/5/5
11	SF4	F	507	5	-	-	0/6/5/5
11	SF4	G	200	6	-	-	0/6/5/5
11	SF4	G	201	6	-	-	0/6/5/5
11	SF4	F	501	5	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	504	MGD	C16-C21	5.11	1.47	1.38
13	B	505	MGD	C16-C21	5.02	1.47	1.38
13	B	505	MGD	C21-N22	-3.06	1.32	1.35
13	B	504	MGD	C6-N1	-3.03	1.33	1.37
13	B	504	MGD	C17-N18	-3.01	1.33	1.38
13	B	505	MGD	C17-N18	-2.63	1.33	1.38
13	B	505	MGD	C16-C17	2.10	1.47	1.42
13	B	505	MGD	C6-N1	-2.09	1.34	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	504	MGD	C19-N20-C21	4.18	120.98	113.43
13	B	505	MGD	C19-N20-C21	3.90	120.47	113.43
13	B	504	MGD	O11-C23-C14	-3.58	106.58	108.96
13	B	505	MGD	O11-C23-C14	3.38	111.22	108.96
13	B	505	MGD	O17-C17-C16	-3.32	119.63	127.24
13	B	504	MGD	O11-C23-N22	3.29	111.94	108.57
13	B	505	MGD	C17-C16-N15	2.88	124.48	116.76
13	B	504	MGD	C8-N7-C5	2.77	108.27	102.99
13	B	504	MGD	O17-C17-C16	-2.52	121.47	127.24
13	B	504	MGD	C17-C16-N15	2.51	123.49	116.76
13	B	505	MGD	O11-C23-N22	-2.48	106.02	108.57
13	B	505	MGD	C8-N7-C5	2.42	107.60	102.99
13	B	505	MGD	C16-C17-N18	2.17	118.76	112.31
13	B	504	MGD	C16-C17-N18	2.10	118.57	112.31
13	B	504	MGD	PA-O3B-PB	-2.04	125.83	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

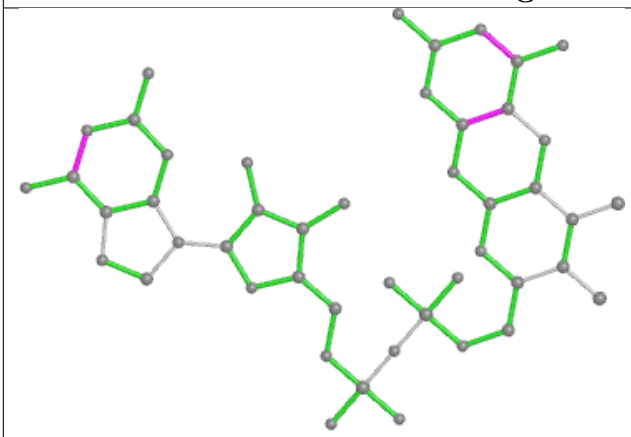
Mol	Chain	Res	Type	Atoms
9	D	201	GOL	C1-C2-C3-O3
13	B	504	MGD	C5'-O5'-PB-O1B
13	B	504	MGD	C5'-O5'-PB-O2B
13	B	504	MGD	O3A-C10-C11-C12
9	A	606	GOL	O1-C1-C2-C3
9	A	606	GOL	O1-C1-C2-O2
9	D	201	GOL	O2-C2-C3-O3
13	B	504	MGD	O3A-C10-C11-O11
13	B	504	MGD	PA-O3B-PB-O5'
13	B	504	MGD	O4'-C4'-C5'-O5'
13	B	504	MGD	C3'-C4'-C5'-O5'
13	B	504	MGD	C5'-O5'-PB-O3B

There are no ring outliers.

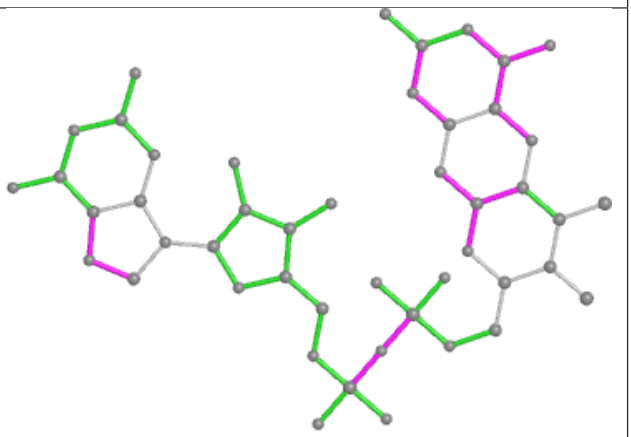
No monomer is involved in short contacts.

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.

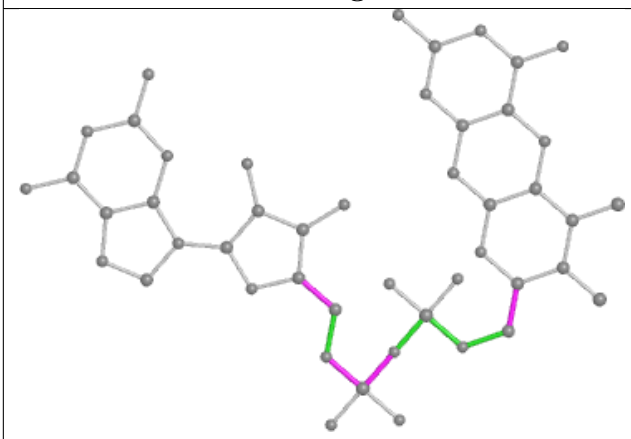
Ligand MGD B 504



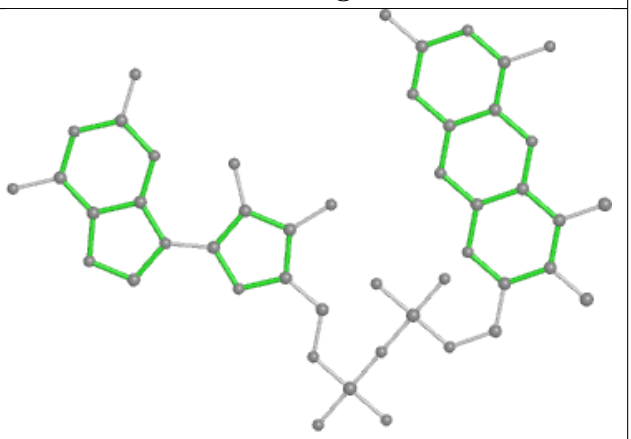
Bond lengths



Bond angles

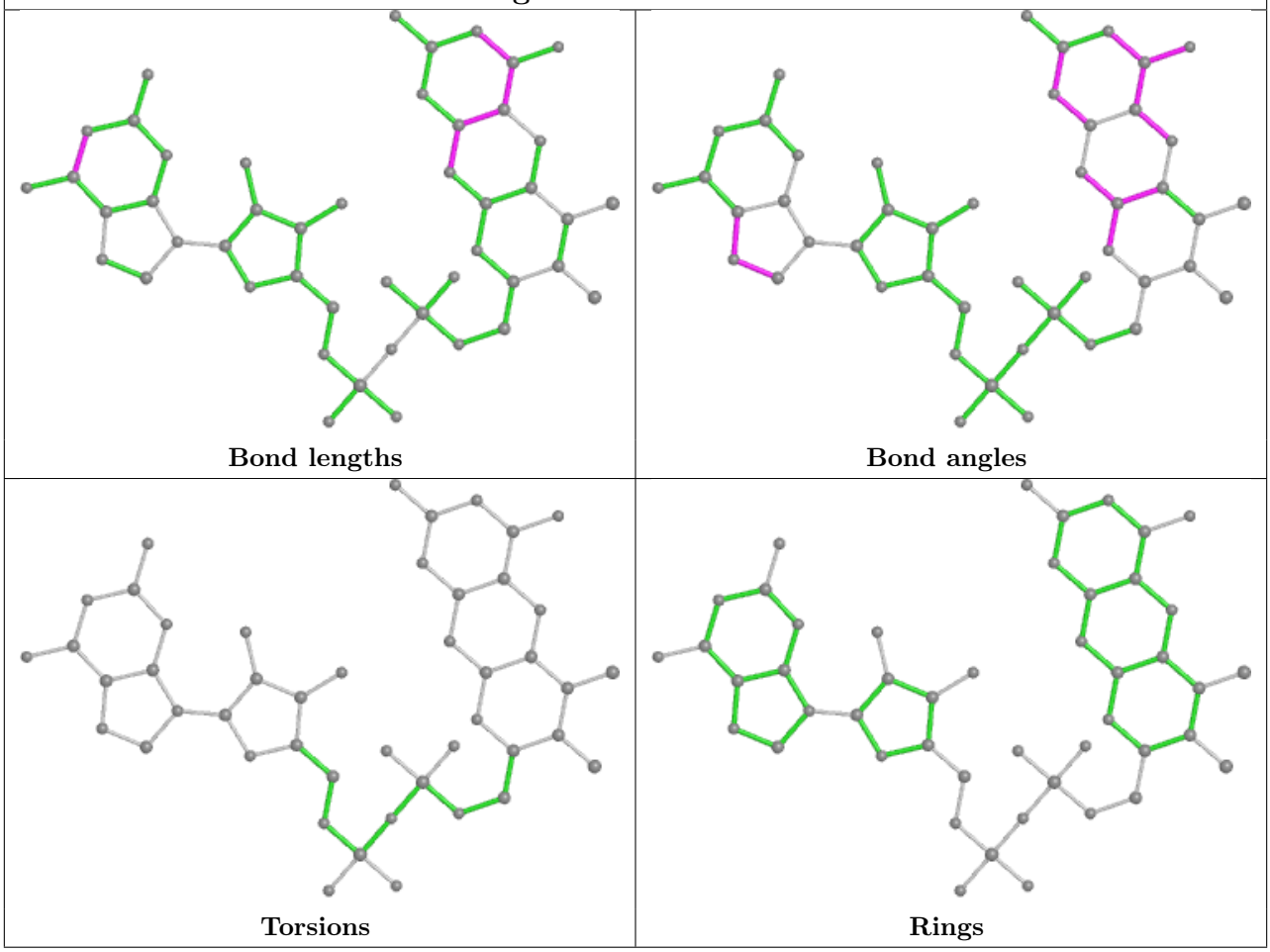


Torsions



Rings

Ligand MGD B 505



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	568/569 (99%)	-0.03	11 (1%)	66	69	41, 64, 94, 128	0
2	B	429/432 (99%)	0.49	37 (8%)	10	10	40, 62, 101, 143	0
3	C	269/270 (99%)	-0.17	4 (1%)	73	75	43, 60, 90, 122	0
4	D	126/130 (96%)	0.10	5 (3%)	38	41	52, 71, 96, 106	0
5	F	342/349 (97%)	0.15	8 (2%)	60	63	51, 68, 103, 131	0
6	G	80/82 (97%)	0.19	2 (2%)	57	61	59, 72, 97, 111	0
All	All	1814/1832 (99%)	0.13	67 (3%)	41	45	40, 65, 98, 143	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	221	TYR	5.3
6	G	2	ALA	5.2
3	C	270	PRO	4.7
5	F	14	VAL	4.0
2	B	12	CYS	3.9
2	B	294	THR	3.4
2	B	285	ILE	3.3
2	B	62	PHE	3.3
2	B	52	LYS	3.3
5	F	7	ILE	3.3
2	B	59	ASN	3.2
2	B	288	ARG	3.2
5	F	8	GLU	3.0
1	A	39	ALA	3.0
2	B	286	PRO	2.9
2	B	289	GLY	2.9
2	B	284	LEU	2.8
2	B	287	MET	2.8
2	B	58	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	1	MET	2.8
2	B	118[A]	CYS	2.8
1	A	35	VAL	2.7
2	B	156	ALA	2.7
2	B	223	LEU	2.7
1	A	37	ASP	2.7
2	B	119	HIS	2.6
2	B	134	CYS	2.6
1	A	41	VAL	2.6
2	B	131	TYR	2.6
2	B	115	ALA	2.5
2	B	251	PHE	2.5
5	F	214	ARG	2.5
4	D	44	GLY	2.5
2	B	151	CYS	2.4
4	D	43	LEU	2.4
1	A	4	ILE	2.4
1	A	338	CYS	2.4
1	A	21	LYS	2.4
2	B	121	PRO	2.4
2	B	398	GLY	2.3
2	B	283	THR	2.3
2	B	396	MET	2.3
5	F	225	THR	2.3
2	B	133	ILE	2.3
2	B	252	PHE	2.3
2	B	126	LEU	2.3
1	A	70	MET	2.3
2	B	120	GLY	2.3
5	F	4	THR	2.3
6	G	60	LEU	2.2
3	C	58	PRO	2.2
3	C	61	ALA	2.2
3	C	231	ILE	2.2
2	B	297	ASN	2.2
1	A	40	LYS	2.1
1	A	7	ASN	2.1
1	A	24	ILE	2.1
2	B	293	VAL	2.1
2	B	290	HIS	2.1
4	D	42	GLN	2.1
2	B	249	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	19	GLU	2.0
2	B	117	VAL	2.0
2	B	123	VAL	2.0
4	D	126	LYS	2.0
2	B	130	GLY	2.0
2	B	124	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	A	178	12/13	0.99	0.18	48,50,56,57	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	K	B	501	1/1	0.73	0.29	133,133,133,133	0
9	GOL	A	606	6/6	0.82	0.38	57,59,61,66	0
9	GOL	D	201	6/6	0.86	0.17	53,54,57,59	0
9	GOL	A	605	6/6	0.90	0.15	52,53,56,64	0
7	MG	C	301	1/1	0.95	0.11	62,62,62,62	0
7	MG	A	604	1/1	0.96	0.16	42,42,42,42	0
7	MG	A	601	1/1	0.97	0.20	65,65,65,65	0
13	MGD	B	505	47/47	0.97	0.20	50,54,58,61	0
11	SF4	F	505	8/8	0.98	0.08	64,70,80,85	0
13	MGD	B	504	47/47	0.98	0.20	49,62,71,83	0
11	SF4	B	502	8/8	0.98	0.17	50,59,63,67	0

Continued on next page...

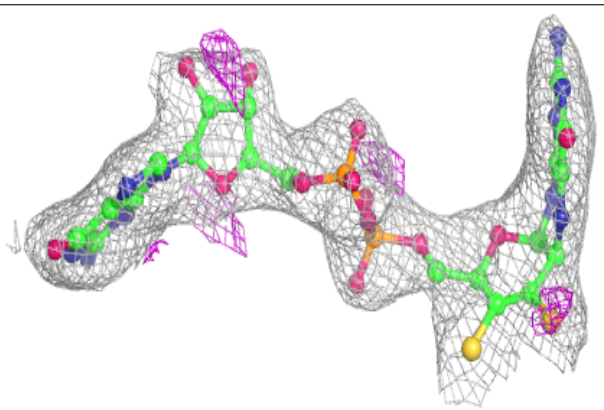
Continued from previous page...

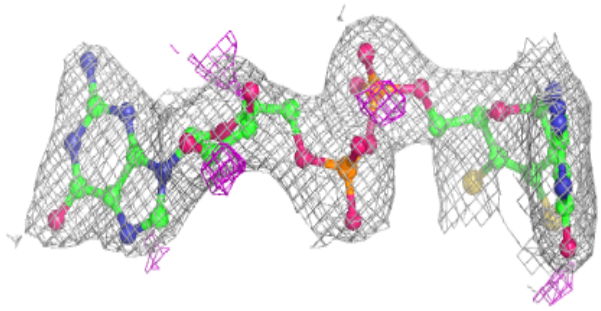
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	SF4	F	503	8/8	0.99	0.10	46,52,58,60	0
11	SF4	F	504	8/8	0.99	0.10	45,51,58,61	0
8	ZN	A	603	1/1	0.99	0.16	60,60,60,60	0
11	SF4	F	506	8/8	0.99	0.10	57,62,67,68	0
11	SF4	F	507	8/8	0.99	0.08	43,57,59,60	0
11	SF4	F	508	8/8	0.99	0.08	50,54,60,64	0
11	SF4	G	200	8/8	0.99	0.14	53,61,68,68	0
11	SF4	G	201	8/8	0.99	0.10	51,66,72,73	0
11	SF4	F	501	8/8	0.99	0.08	41,51,53,56	0
11	SF4	F	502	8/8	0.99	0.08	46,52,53,53	0
8	ZN	A	602	1/1	1.00	0.14	58,58,58,58	0
12	W	B	503	1/1	1.00	0.19	58,58,58,58	0
14	H2S	B	506	1/1	1.00	0.23	60,60,60,60	0

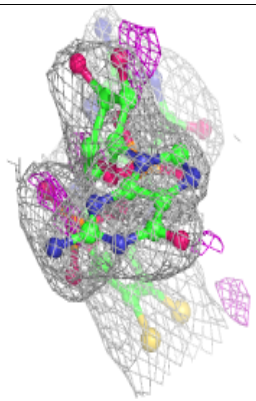
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD B 505:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

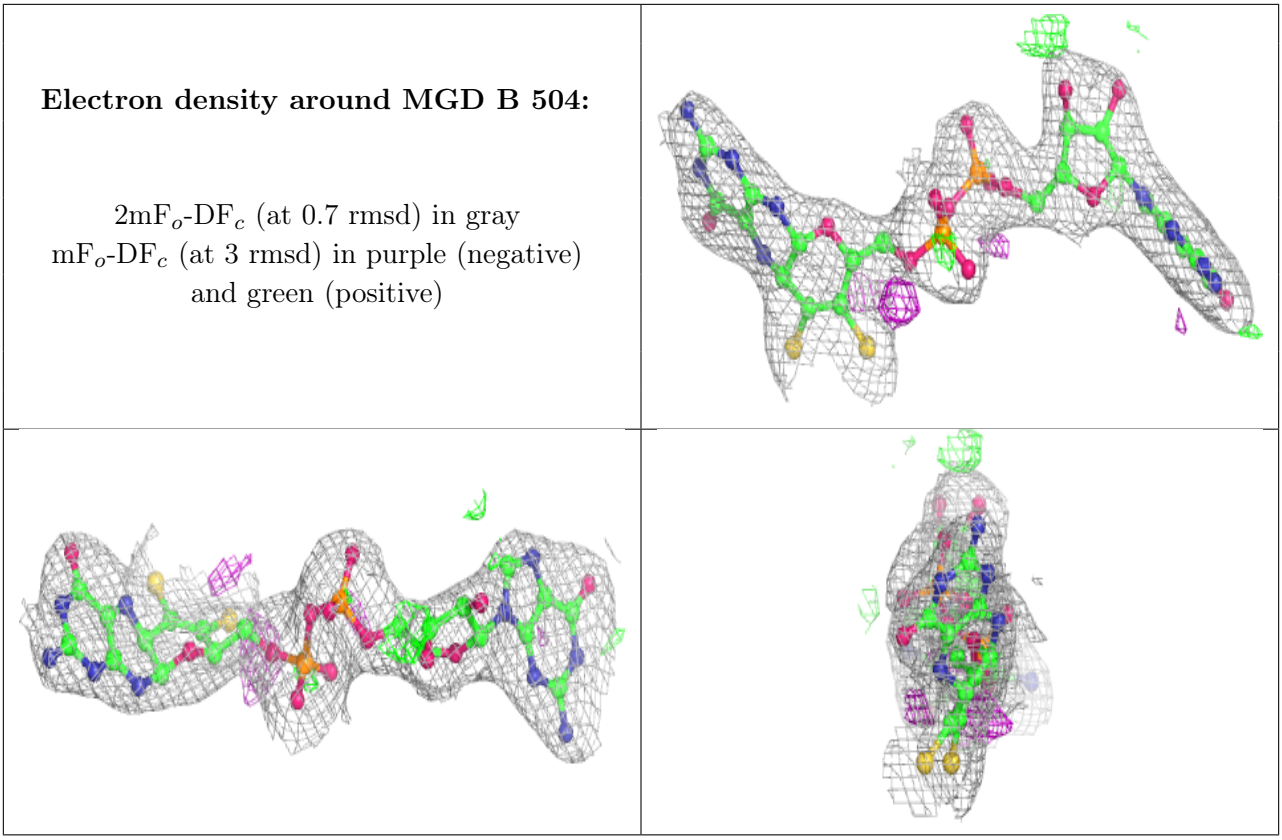






Electron density around MGD B 504:

$2mF_o$-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.