Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 04:19 AM EDT

PDB ID	:	6BFG
Title	:	Crystal structure of monotopic membrane protein (S)-mandelate dehydrogenase
Authors	:	Sukumar, N.
Deposited on	:	2017-10-26
Resolution	:	2.20 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:

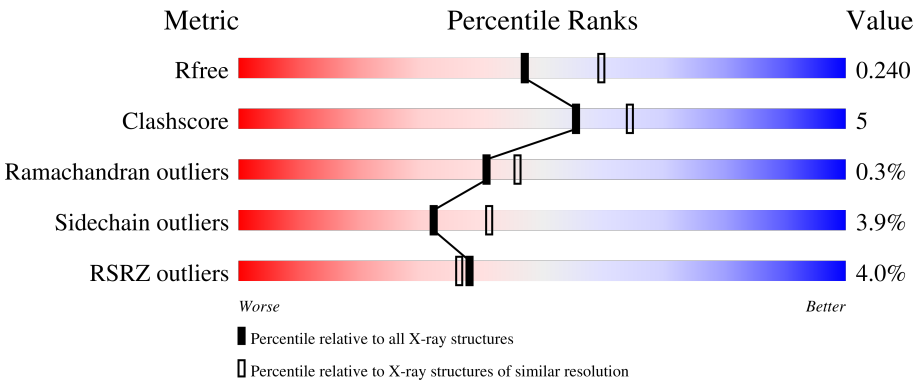
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	399	5% 83% 10% • 7%
1	B	399	3% 83% 9% • 7%

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
5	EDO	A	407	-	-	-	X
6	CIT	A	410	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11991 atoms, of which 5727 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.

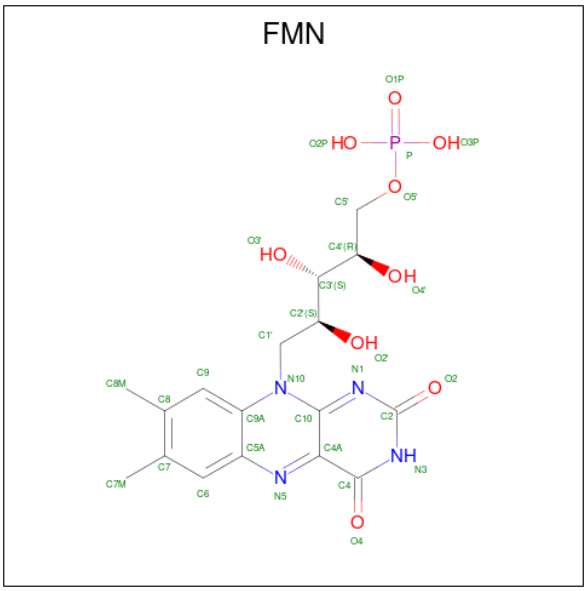
- Molecule 1 is a protein called (S)-mandelate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	373	5705	1840	2792	523	535	15	69	0	0
1	B	373	5771	1840	2858	523	535	15	37	0	0

There are 12 discrepancies between the modelled and reference sequences:

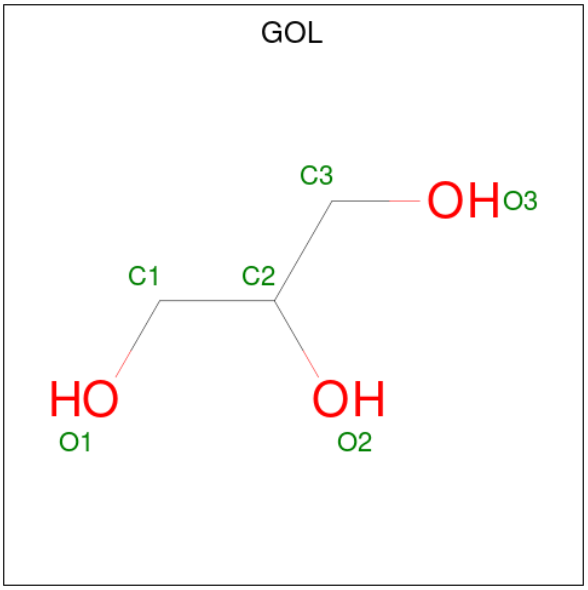
Chain	Residue	Modelled	Actual	Comment	Reference
A	394	HIS	-	expression tag	UNP P20932
A	395	HIS	-	expression tag	UNP P20932
A	396	HIS	-	expression tag	UNP P20932
A	397	HIS	-	expression tag	UNP P20932
A	398	HIS	-	expression tag	UNP P20932
A	399	HIS	-	expression tag	UNP P20932
B	394	HIS	-	expression tag	UNP P20932
B	395	HIS	-	expression tag	UNP P20932
B	396	HIS	-	expression tag	UNP P20932
B	397	HIS	-	expression tag	UNP P20932
B	398	HIS	-	expression tag	UNP P20932
B	399	HIS	-	expression tag	UNP P20932

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	50	17	19	4	9	1	0	0
			Total	C	H	N	O	P		
2	B	1	50	17	19	4	9	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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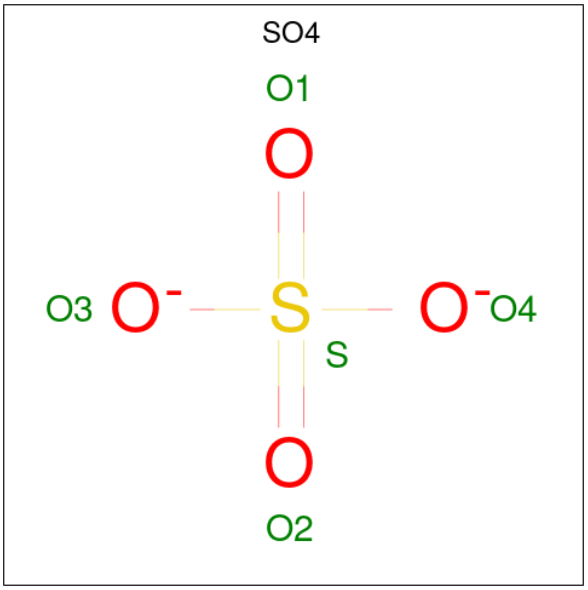
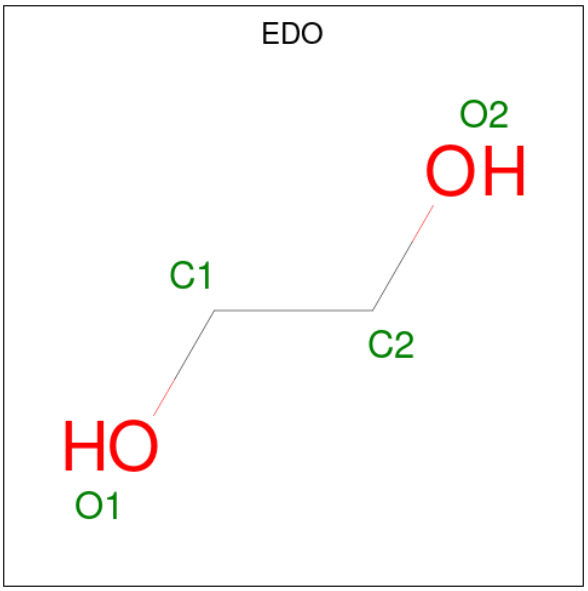
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



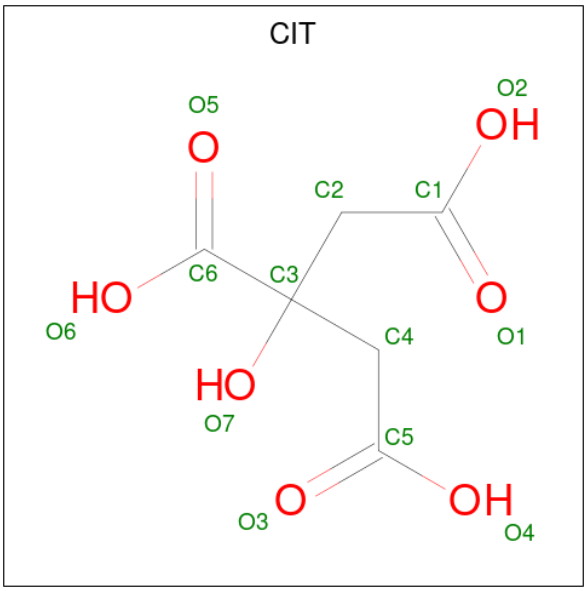
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



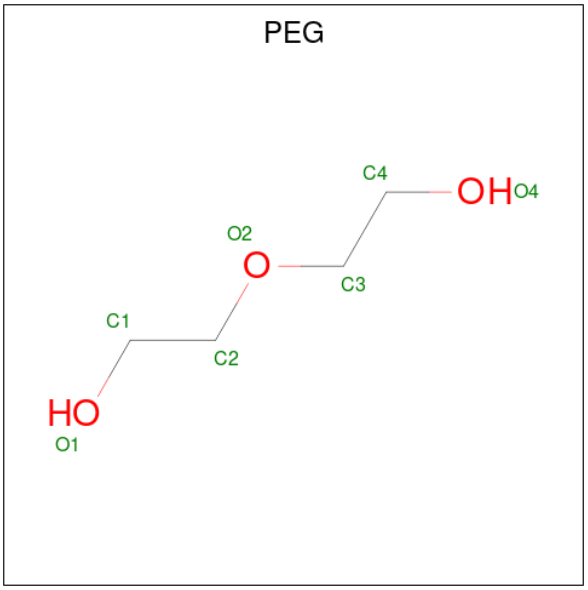
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	B	1	4	2	2	0	0

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



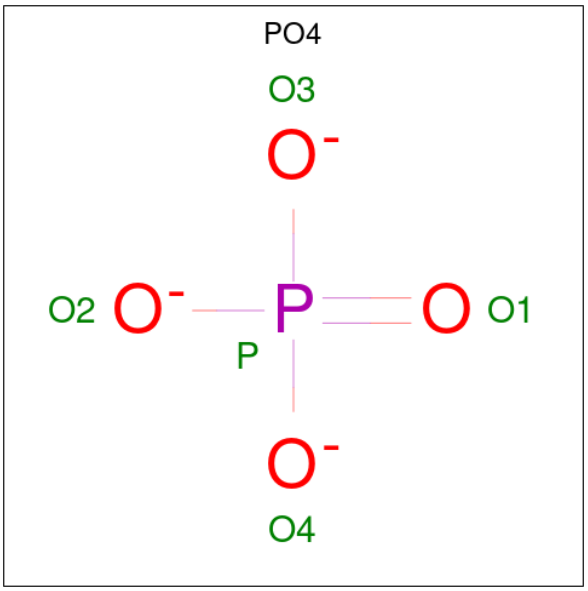
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 5 3 2	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

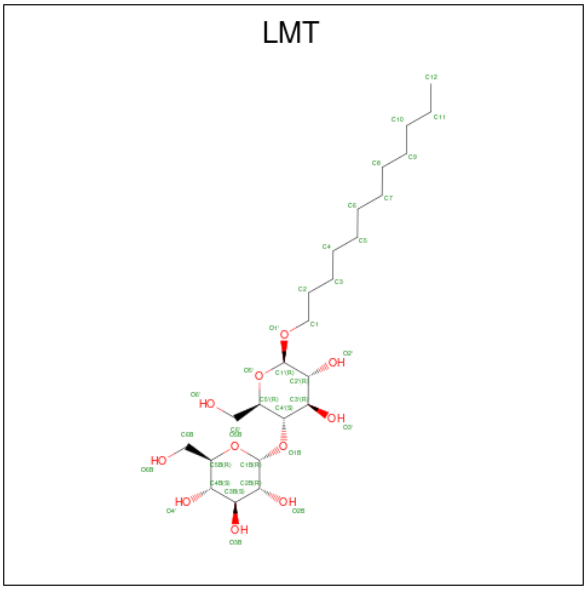


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O P 5 4 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	B	1	74	24	39	11	9	0

- Molecule 11 is water.

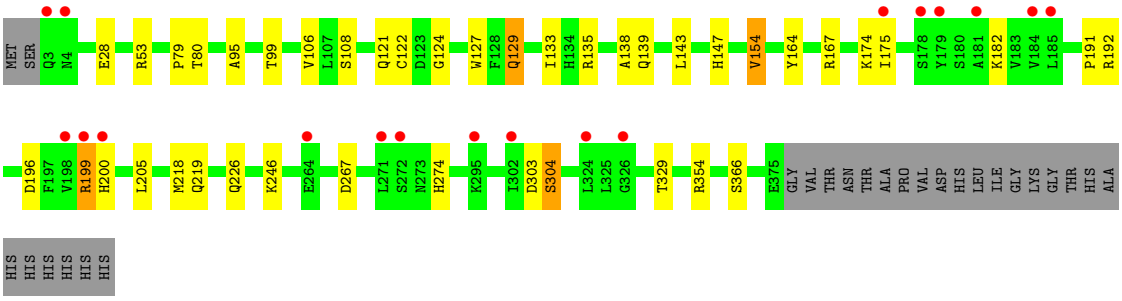
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	145	145	145	0	0
11	B	115	115	115	0	0

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.

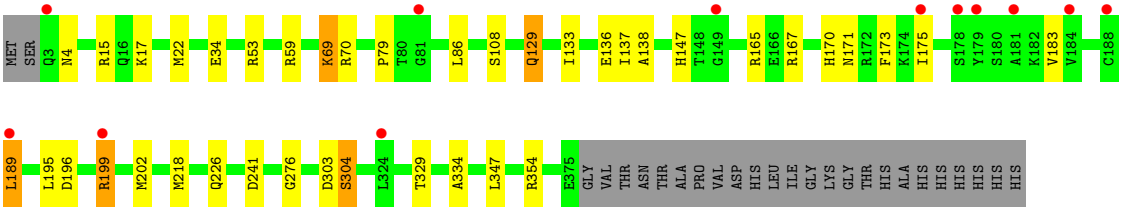
• Molecule 1: (S)-mandelate dehydrogenase

Chain A:



• Molecule 1: (S)-mandelate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.36Å 129.88Å 143.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.40 – 2.20 41.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.40-2.20) 81.9 (41.44-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.197 , 0.240 0.198 , 0.240	Depositor DCC
R_{free} test set	1995 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.922	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11991	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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

[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: PO4, NA, GOL, LMT, CIT, EDO, FMN, SO4, PEG

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	0.56	0/2968	0.69	1/4016 (0.0%)
1	B	0.56	0/2968	0.72	3/4016 (0.1%)
All	All	0.56	0/5936	0.71	4/8032 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	354	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	354	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	354	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	165	ARG	NE-CZ-NH2	-5.08	117.76	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	2913	2792	2942	30	0
1	B	2913	2858	2942	26	0
2	A	31	19	19	1	0
2	B	31	19	19	2	0
3	A	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	2	0
4	A	5	0	0	0	0
5	A	20	0	30	3	0
5	B	8	0	12	3	0
6	A	13	0	5	6	0
7	B	5	0	5	0	0
8	B	5	0	0	0	0
9	B	1	0	0	0	0
10	B	35	39	44	6	0
11	A	145	0	0	3	0
11	B	115	0	0	4	0
All	All	6264	5727	6050	60	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 5.

All (60) 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:191:PRO:HG2	6:A:410:CIT:H22	1.67	0.74
1:A:191:PRO:CG	6:A:410:CIT:H22	2.18	0.73
1:A:164:TYR:CZ	5:B:406:EDO:H21	2.28	0.69
1:A:95:ALA:O	1:A:99:THR:HG23	1.94	0.68
1:B:347:LEU:HD22	5:B:406:EDO:H22	1.74	0.68
1:B:53:ARG:HH11	5:B:408:EDO:H21	1.60	0.66
1:A:191:PRO:HD2	6:A:410:CIT:H22	1.76	0.66
1:A:147:HIS:ND1	11:A:502:HOH:O	2.30	0.65
1:A:28:GLU:OE1	5:A:408:EDO:H12	1.97	0.65
1:B:79:PRO:CB	1:B:129:GLN:HG2	2.29	0.62
3:A:402:GOL:O1	3:A:403:GOL:H31	2.00	0.62
1:A:191:PRO:CD	6:A:410:CIT:H22	2.30	0.61
1:A:121:GLN:NE2	11:A:501:HOH:O	2.20	0.59
1:A:79:PRO:CB	1:A:129:GLN:HG2	2.34	0.58
1:A:191:PRO:HD2	6:A:410:CIT:C2	2.34	0.58
1:B:183:VAL:HG13	10:B:407:LMT:H4B	1.85	0.57
2:B:401:FMN:H6	3:B:403:GOL:H31	1.87	0.56
1:B:175:ILE:HD12	10:B:407:LMT:C3	2.36	0.56
2:B:401:FMN:C6	3:B:403:GOL:H31	2.35	0.56
1:B:175:ILE:HD12	10:B:407:LMT:H32	1.89	0.54
1:A:99:THR:HG22	1:A:124:GLY:HA3	1.90	0.53
1:A:192:ARG:HD3	6:A:410:CIT:O2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:HG13	1:B:138:ALA:HB2	1.90	0.52
1:A:99:THR:CG2	1:A:124:GLY:HA3	2.41	0.51
1:B:79:PRO:HB2	1:B:129:GLN:HG2	1.92	0.49
1:A:53:ARG:HH11	5:A:409:EDO:H22	1.78	0.48
1:A:199:ARG:HG2	1:A:200:HIS:ND1	2.28	0.48
1:B:22:MET:HG3	1:B:171:ASN:HB3	1.94	0.48
1:A:303:ASP:O	1:A:304:SER:HB2	2.14	0.47
1:A:99:THR:HG21	1:A:122:CYS:SG	2.54	0.47
1:B:303:ASP:O	1:B:304:SER:HB2	2.15	0.46
1:B:108:SER:HA	1:B:129:GLN:HG3	1.98	0.46
1:B:69:LYS:NZ	11:B:510:HOH:O	2.47	0.45
1:B:303:ASP:OD1	1:B:303:ASP:C	2.54	0.45
1:A:79:PRO:HB2	1:A:129:GLN:HG2	1.98	0.45
1:A:167:ARG:HH22	5:A:408:EDO:H21	1.81	0.44
1:B:276:GLY:HA2	11:B:594:HOH:O	2.16	0.44
1:A:129:GLN:CB	1:A:154:VAL:HG22	2.47	0.44
1:B:147:HIS:ND1	11:B:503:HOH:O	2.36	0.44
1:A:133:ILE:HG13	1:A:138:ALA:HB2	1.99	0.44
1:A:205:LEU:HB2	1:A:219:GLN:HB3	2.01	0.43
1:B:170:HIS:CE1	11:B:527:HOH:O	2.71	0.43
1:A:274:HIS:NE2	3:A:404:GOL:C1	2.82	0.43
1:A:106:VAL:HG22	1:A:127:TRP:HB2	2.01	0.43
1:B:86:LEU:HB3	1:B:334:ALA:HB2	2.01	0.43
1:A:366:SER:HB3	11:A:631:HOH:O	2.18	0.43
1:B:173:PHE:CE2	10:B:407:LMT:H21	2.54	0.43
1:B:4:ASN:OD1	1:B:4:ASN:N	2.48	0.42
1:B:136:GLU:H	1:B:136:GLU:CD	2.23	0.42
1:B:34:GLU:OE2	1:B:167:ARG:HD2	2.20	0.42
1:B:195:LEU:HD23	1:B:199:ARG:HD3	2.02	0.41
1:A:80:THR:HA	2:A:401:FMN:N5	2.35	0.41
1:A:139:GLN:O	1:A:143:LEU:HG	2.20	0.41
1:B:175:ILE:HD12	10:B:407:LMT:H31	2.02	0.41
1:A:108:SER:HA	1:A:129:GLN:HG3	2.02	0.41
1:B:137:ILE:CD1	1:B:226:GLN:HG3	2.50	0.41
1:B:303:ASP:O	1:B:304:SER:CB	2.69	0.41
1:B:189:LEU:HD13	1:B:189:LEU:N	2.36	0.41
10:B:407:LMT:O1B	10:B:407:LMT:O2'	2.39	0.40
1:A:246:LYS:HA	1:A:267:ASP:OD2	2.22	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	371/399 (93%)	357 (96%)	13 (4%)	1 (0%)	41	46
1	B	371/399 (93%)	357 (96%)	13 (4%)	1 (0%)	41	46
All	All	742/798 (93%)	714 (96%)	26 (4%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	SER
1	A	304	SER

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	309/330 (94%)	298 (96%)	11 (4%)	35	45
1	B	309/330 (94%)	296 (96%)	13 (4%)	30	38
All	All	618/660 (94%)	594 (96%)	24 (4%)	32	41

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	135	ARG
1	A	154	VAL
1	A	174	LYS

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Mol	Chain	Res	Type
1	A	175	ILE
1	A	182	LYS
1	A	196	ASP
1	A	199	ARG
1	A	218	MET
1	A	226	GLN
1	A	329	THR
1	B	15	ARG
1	B	17	LYS
1	B	59	ARG
1	B	69	LYS
1	B	70	ARG
1	B	129	GLN
1	B	189	LEU
1	B	196	ASP
1	B	199	ARG
1	B	202	MET
1	B	218	MET
1	B	241	ASP
1	B	329	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	GOL	A	404	-	5,5,5	0.55	0	5,5,5	0.76	0
3	GOL	B	403	-	5,5,5	0.66	0	5,5,5	0.97	0
5	EDO	B	408	-	3,3,3	0.72	0	2,2,2	0.18	0
4	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.51	0
5	EDO	A	406	-	3,3,3	0.62	0	2,2,2	0.34	0
7	PEG	B	402	-	4,4,6	0.46	0	3,3,5	0.30	0
5	EDO	A	409	-	3,3,3	0.79	0	2,2,2	0.04	0
10	LMT	B	407	-	36,36,36	1.10	4 (11%)	47,47,47	1.50	7 (14%)
2	FMN	A	401	-	33,33,33	1.32	4 (12%)	48,50,50	1.29	6 (12%)
5	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.34	0
8	PO4	B	404	-	4,4,4	0.76	0	6,6,6	0.97	0
2	FMN	B	401	-	33,33,33	1.16	3 (9%)	48,50,50	1.54	9 (18%)
5	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.47	0
3	GOL	A	403	-	5,5,5	0.29	0	5,5,5	0.50	0
5	EDO	A	408	-	3,3,3	0.54	0	2,2,2	0.46	0
6	CIT	A	410	-	12,12,12	1.20	1 (8%)	17,17,17	2.17	5 (29%)
5	EDO	A	411	-	3,3,3	0.59	0	2,2,2	0.47	0
3	GOL	A	402	-	5,5,5	0.19	0	5,5,5	0.89	0

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	GOL	A	404	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
5	EDO	B	408	-	-	1/1/1/1	-
7	PEG	B	402	-	-	1/2/2/4	-
5	EDO	A	406	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	B	407	-	-	14/21/61/61	0/2/2/2
5	EDO	A	409	-	-	1/1/1/1	-
2	FMN	A	401	-	-	2/18/18/18	0/3/3/3
5	EDO	A	407	-	-	0/1/1/1	-
2	FMN	B	401	-	-	6/18/18/18	0/3/3/3
5	EDO	B	406	-	-	0/1/1/1	-
3	GOL	A	403	-	-	2/4/4/4	-
5	EDO	A	408	-	-	0/1/1/1	-
6	CIT	A	410	-	-	3/16/16/16	-
5	EDO	A	411	-	-	1/1/1/1	-
3	GOL	A	402	-	-	3/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C4A-N5	3.78	1.38	1.30
2	B	401	FMN	C4A-N5	3.15	1.36	1.30
2	B	401	FMN	C4A-C10	-2.77	1.36	1.44
10	B	407	LMT	O3'-C3'	-2.75	1.36	1.43
2	B	401	FMN	C10-N1	2.69	1.38	1.33
2	A	401	FMN	C10-N1	2.68	1.38	1.33
6	A	410	CIT	O2-C1	-2.52	1.22	1.30
10	B	407	LMT	O2B-C2B	-2.32	1.37	1.43
2	A	401	FMN	C4A-C10	-2.24	1.37	1.44
10	B	407	LMT	O3B-C3B	-2.22	1.37	1.43
2	A	401	FMN	C9A-C5A	-2.22	1.37	1.41
10	B	407	LMT	O2'-C2'	-2.16	1.37	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	410	CIT	O6-C6-C3	5.32	122.28	113.05
10	B	407	LMT	C3'-C4'-C5'	-4.77	99.99	110.93
10	B	407	LMT	O5B-C5B-C4B	4.75	118.31	109.69
6	A	410	CIT	O7-C3-C6	4.59	115.31	108.86
2	B	401	FMN	C9A-C5A-N5	-4.03	118.06	122.43
2	B	401	FMN	C4-N3-C2	-3.55	119.09	125.64
2	B	401	FMN	O4-C4-C4A	-3.37	117.66	126.60
2	B	401	FMN	C4A-C4-N3	3.14	121.17	113.19
10	B	407	LMT	C6B-C5B-C4B	-3.08	105.78	113.00
2	A	401	FMN	C4A-C4-N3	3.07	120.99	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FMN	C4-N3-C2	-2.99	120.12	125.64
2	A	401	FMN	O4-C4-C4A	-2.83	119.10	126.60
2	A	401	FMN	C9A-C5A-N5	-2.60	119.61	122.43
10	B	407	LMT	O5'-C1'-C2'	-2.54	104.96	110.35
10	B	407	LMT	C1B-O5B-C5B	2.54	118.68	113.69
6	A	410	CIT	C2-C3-C6	-2.49	104.75	110.11
2	A	401	FMN	O2P-P-O5'	2.43	113.21	106.73
2	B	401	FMN	C4A-C10-N1	-2.37	119.23	124.73
10	B	407	LMT	O1B-C1B-C2B	2.35	114.19	108.10
2	B	401	FMN	C6-C5A-C9A	2.34	122.24	118.94
10	B	407	LMT	C1'-O5'-C5'	-2.31	109.15	113.69
2	B	401	FMN	O4'-C4'-C3'	2.26	114.59	109.10
6	A	410	CIT	O6-C6-O5	-2.20	116.81	123.82
2	B	401	FMN	C5A-C9A-N10	2.18	120.21	117.95
6	A	410	CIT	O7-C3-C2	-2.14	104.39	109.40
2	A	401	FMN	C4A-C10-N1	-2.07	119.92	124.73
2	B	401	FMN	C5A-N5-C4A	2.04	121.46	118.07

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
6	A	410	CIT	C1-C2-C3-O7
6	A	410	CIT	C1-C2-C3-C4
6	A	410	CIT	C1-C2-C3-C6
10	B	407	LMT	O5'-C1'-O1'-C1
10	B	407	LMT	C2-C1-O1'-C1'
10	B	407	LMT	C3'-C4'-O1B-C1B
10	B	407	LMT	O5B-C1B-O1B-C4'
10	B	407	LMT	O5'-C5'-C6'-O6'
10	B	407	LMT	C4'-C5'-C6'-O6'
10	B	407	LMT	C11-C10-C9-C8
10	B	407	LMT	C3-C4-C5-C6
3	A	404	GOL	O2-C2-C3-O3
5	A	409	EDO	O1-C1-C2-O2
5	B	408	EDO	O1-C1-C2-O2
10	B	407	LMT	O1'-C1-C2-C3
10	B	407	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
10	B	407	LMT	C4-C5-C6-C7
3	A	402	GOL	O1-C1-C2-O2
10	B	407	LMT	C2'-C1'-O1'-C1
2	B	401	FMN	C2'-C3'-C4'-O4'
2	A	401	FMN	C4'-C5'-O5'-P
3	A	403	GOL	O1-C1-C2-O2
2	B	401	FMN	C2'-C3'-C4'-C5'
2	B	401	FMN	C4'-C5'-O5'-P
7	B	402	PEG	C4-C3-O2-C2
3	A	402	GOL	O2-C2-C3-O3
10	B	407	LMT	C7-C8-C9-C10
2	B	401	FMN	O3'-C3'-C4'-C5'
2	B	401	FMN	C5'-O5'-P-O3P
10	B	407	LMT	C2-C3-C4-C5
3	A	403	GOL	O1-C1-C2-C3
5	A	411	EDO	O1-C1-C2-O2
2	B	401	FMN	O3'-C3'-C4'-O4'
2	A	401	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

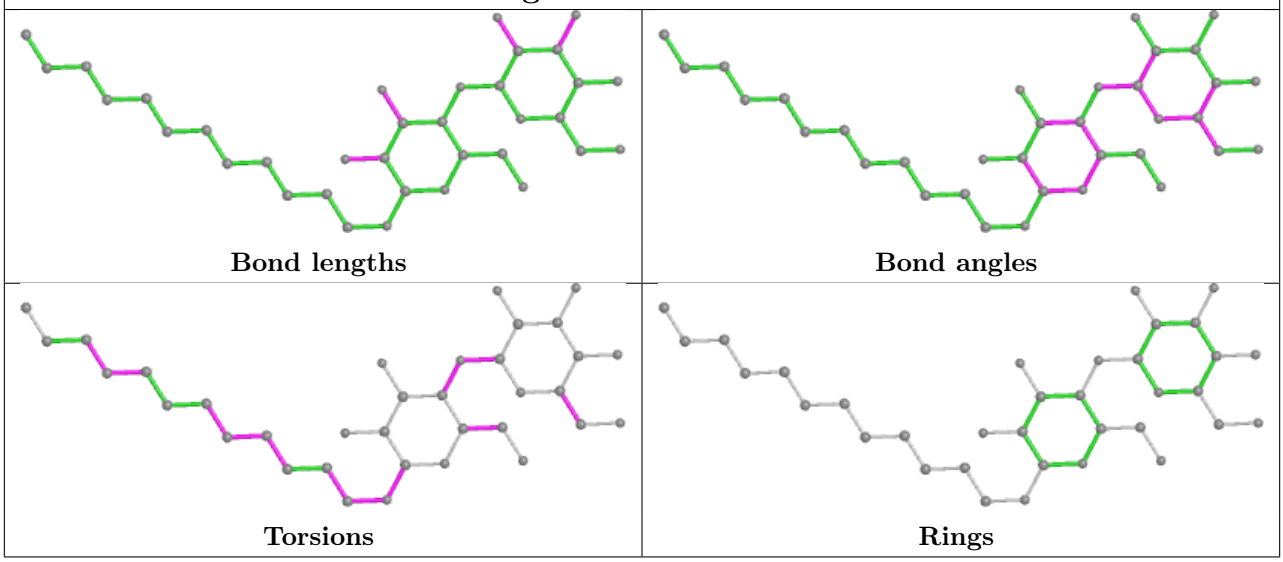
12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	GOL	1	0
3	B	403	GOL	2	0
5	B	408	EDO	1	0
5	A	409	EDO	1	0
10	B	407	LMT	6	0
2	A	401	FMN	1	0
2	B	401	FMN	2	0
5	B	406	EDO	2	0
3	A	403	GOL	1	0
5	A	408	EDO	2	0
6	A	410	CIT	6	0
3	A	402	GOL	1	0

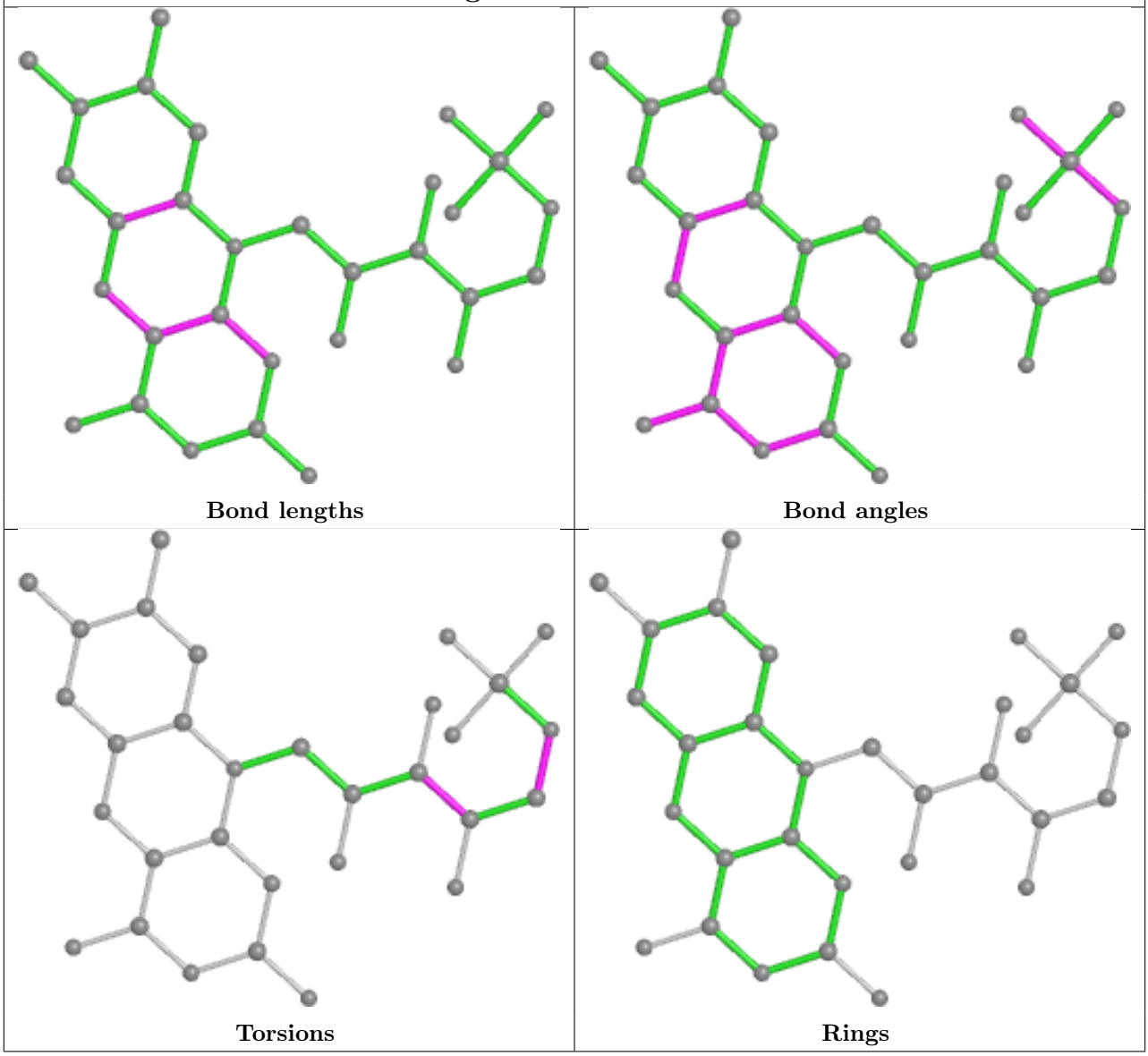
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

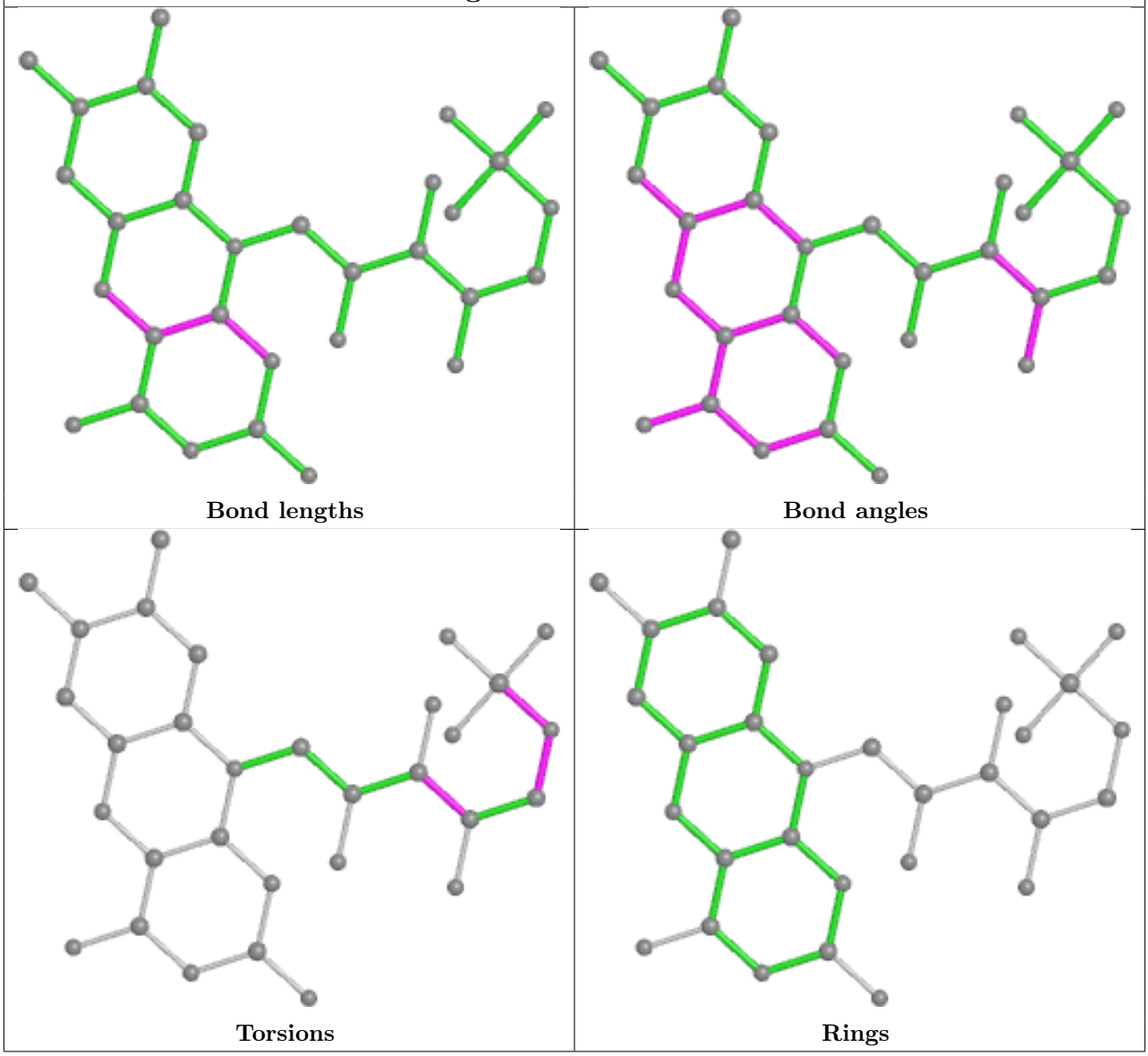
Ligand LMT B 407



Ligand FMN A 401



Ligand FMN B 401



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	373/399 (93%)	0.06	18 (4%)	30	29	26, 39, 67, 129	14 (3%)
1	B	373/399 (93%)	0.07	12 (3%)	47	45	25, 38, 65, 108	7 (1%)
All	All	746/798 (93%)	0.06	30 (4%)	38	36	25, 39, 66, 129	21 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ILE	5.9
1	B	179	TYR	5.8
1	B	178	SER	3.5
1	A	199	ARG	3.4
1	A	175	ILE	3.3
1	A	178	SER	3.2
1	A	295	LYS	3.1
1	A	184	VAL	2.9
1	A	198	VAL	2.9
1	B	184	VAL	2.8
1	B	324	LEU	2.7
1	B	181	ALA	2.7
1	B	199	ARG	2.7
1	B	81	GLY	2.5
1	A	302	ILE	2.5
1	A	3	GLN	2.5
1	A	272	SER	2.3
1	A	4	ASN	2.3
1	A	185	LEU	2.3
1	B	188	CYS	2.3
1	A	271	LEU	2.2
1	B	3	GLN	2.2
1	A	181	ALA	2.1
1	A	200	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	179	TYR	2.1
1	B	149	GLY	2.0
1	A	324	LEU	2.0
1	A	264	GLU	2.0
1	A	326	GLY	2.0
1	B	189	LEU	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 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
7	PEG	B	402	5/7	0.54	0.16	44,53,57,58	0
10	LMT	B	407	35/35	0.61	0.29	56,84,111,127	9
4	SO4	A	405	5/5	0.64	0.18	76,85,111,117	0
6	CIT	A	410	13/13	0.65	0.28	42,64,76,81	0
3	GOL	A	404	6/6	0.73	0.27	41,53,56,57	0
5	EDO	A	409	4/4	0.76	0.28	41,46,48,50	0
3	GOL	A	402	6/6	0.77	0.27	55,62,64,68	0
5	EDO	A	408	4/4	0.80	0.59	47,47,52,54	0
5	EDO	A	407	4/4	0.80	0.48	75,82,84,85	0
9	NA	B	405	1/1	0.80	0.31	46,46,46,46	0
5	EDO	B	408	4/4	0.80	0.26	44,46,46,48	0
8	PO4	B	404	5/5	0.81	0.16	71,73,75,126	0
3	GOL	A	403	6/6	0.84	0.26	51,52,54,55	0
5	EDO	B	406	4/4	0.86	0.29	32,35,37,41	0
5	EDO	A	406	4/4	0.88	0.22	57,59,62,66	0
3	GOL	B	403	6/6	0.89	0.22	40,47,51,53	0
5	EDO	A	411	4/4	0.92	0.19	46,48,48,52	0

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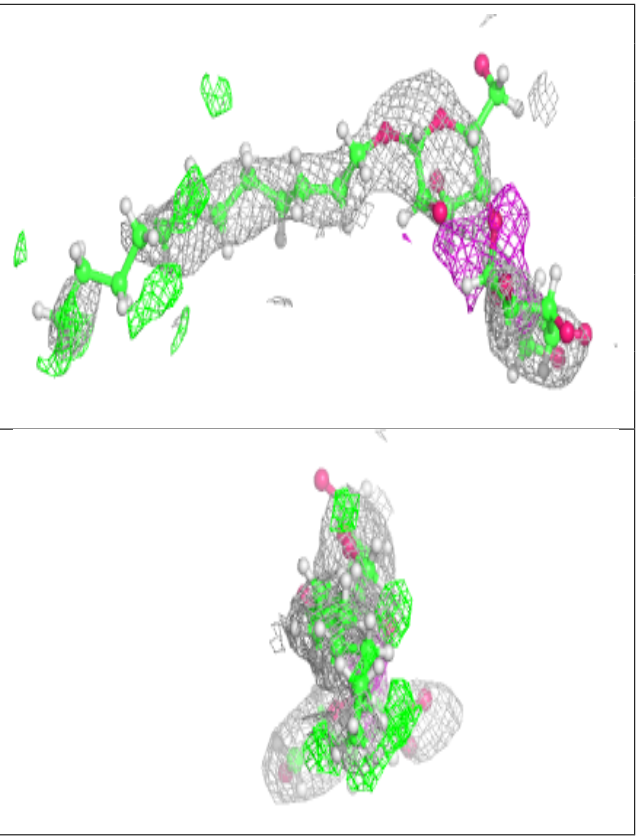
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	A	401	31/31	0.95	0.27	22,30,37,40	0
2	FMN	B	401	31/31	0.96	0.23	23,30,36,38	0

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.

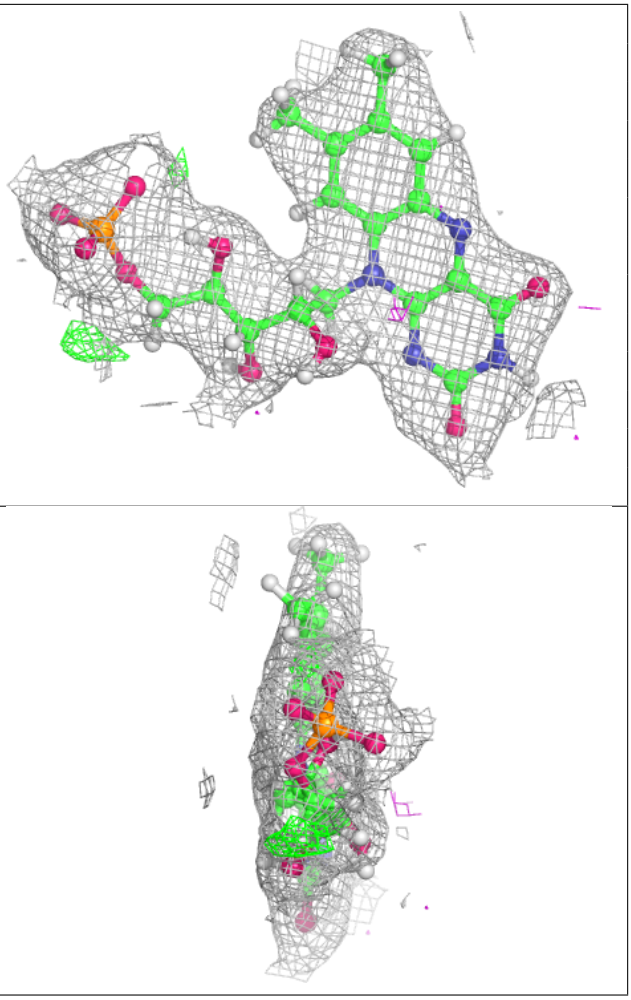
Electron density around LMT B 407:

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



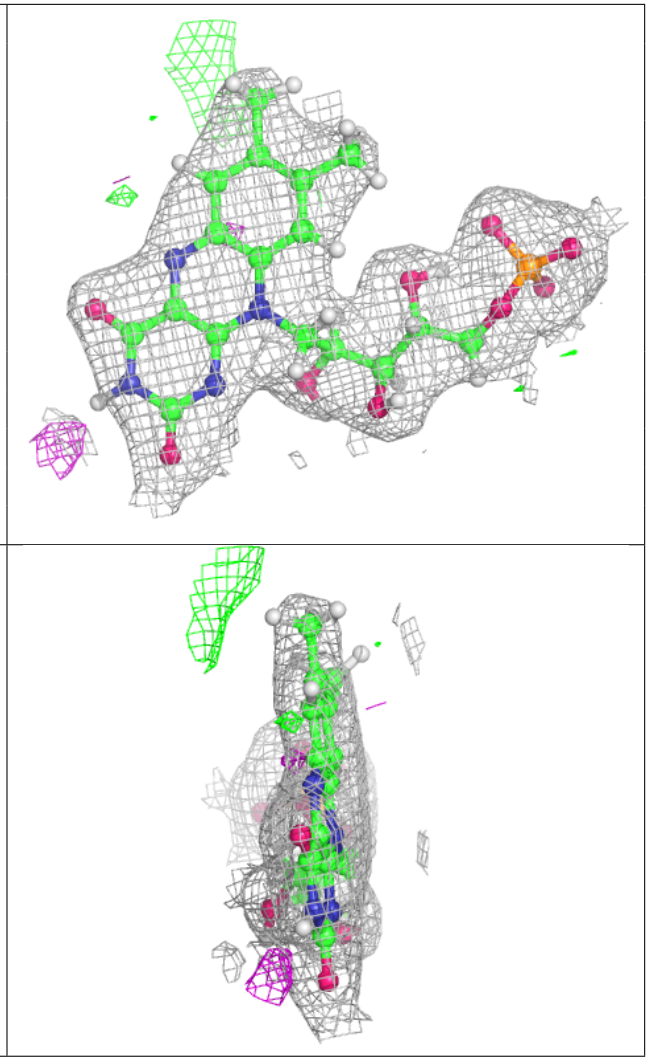
Electron density around FMN A 401:

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



Electron density around FMN B 401:

$2mF_o$-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.