



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:41 PM UTC

PDB ID : 3UNC / pdb_00003unc
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase to 1.65Å Resolution
Authors : Eger, B.T.; Okamoto, K.; Nishino, T.; Pai, E.F.
Deposited on : 2011-11-15
Resolution : 1.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

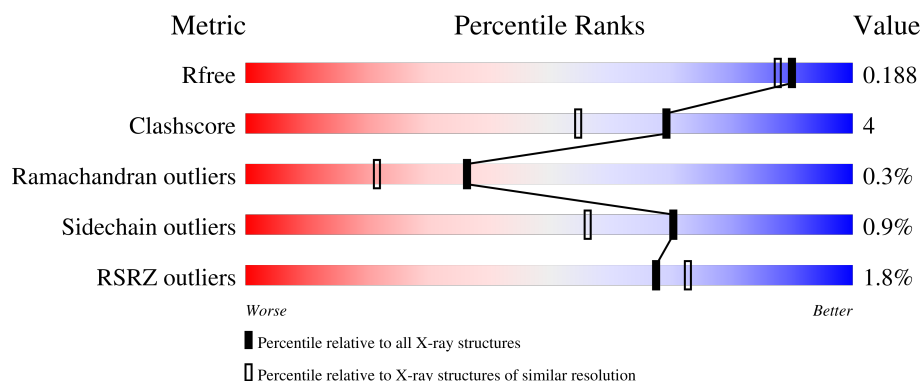
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

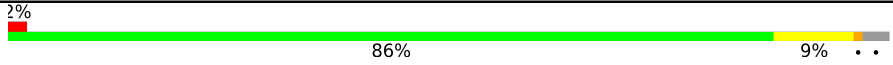
The reported resolution of this entry is 1.65 Å.

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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1332	
1	B	1332	

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
4	MOS	B	1336	-	-	X	-

2 Entry composition [i](#)

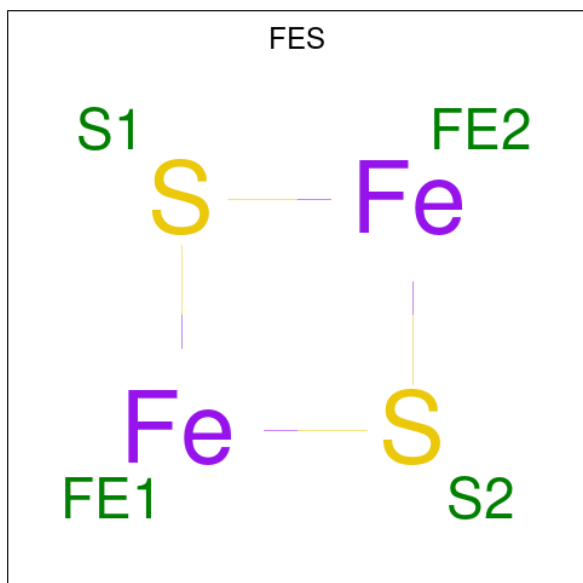
There are 10 unique types of molecules in this entry. The entry contains 22475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

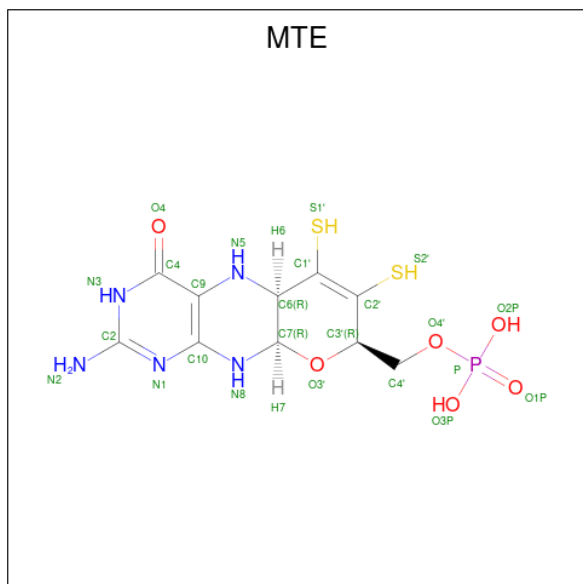
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1286	Total	C	N	O	S	0	13	0
			10084	6408	1726	1884	66			
1	B	1289	Total	C	N	O	S	0	9	0
			10073	6400	1723	1883	67			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



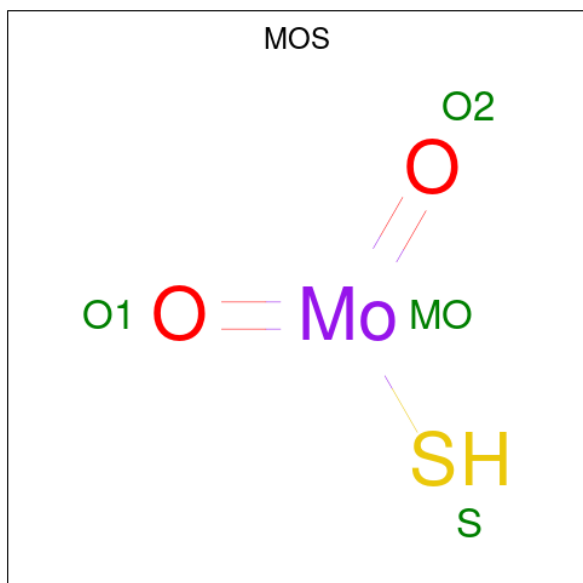
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



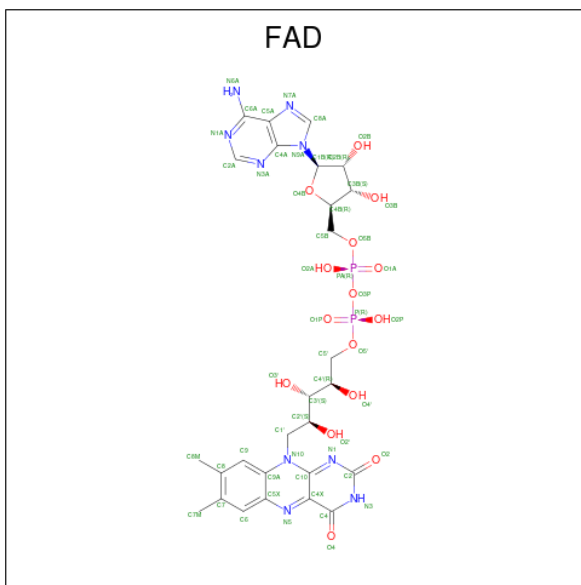
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is DIOXOTHIO MOLYBDENUM(VI) ION (CCD ID: MOS) (formula: $HMoO_2S$).



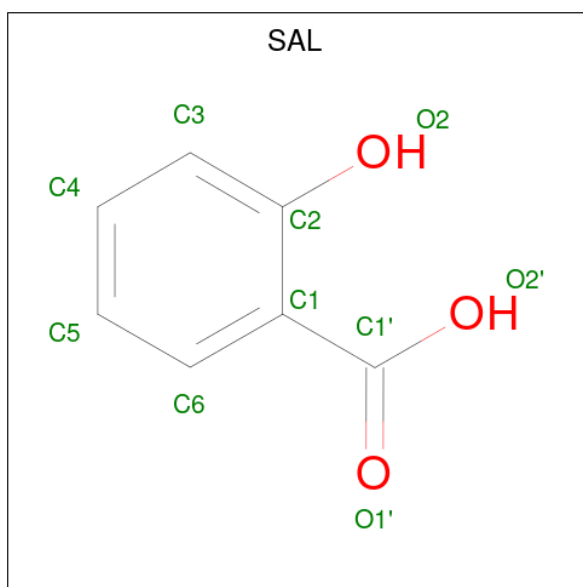
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	Mo 1	O 2	S 1	0	0
4	B	1	Total 4	Mo 1	O 2	S 1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



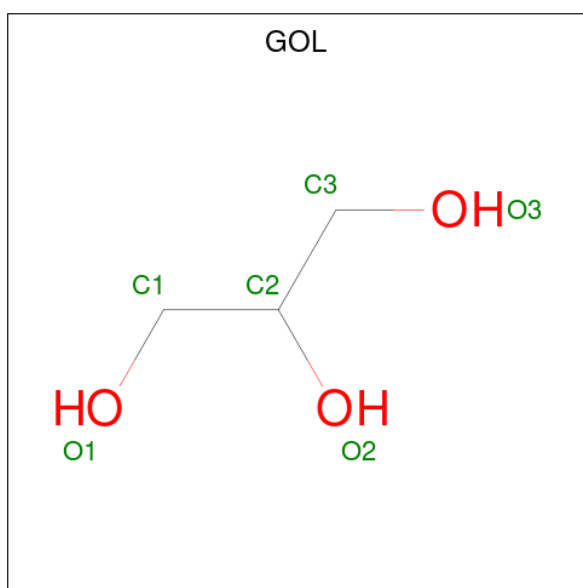
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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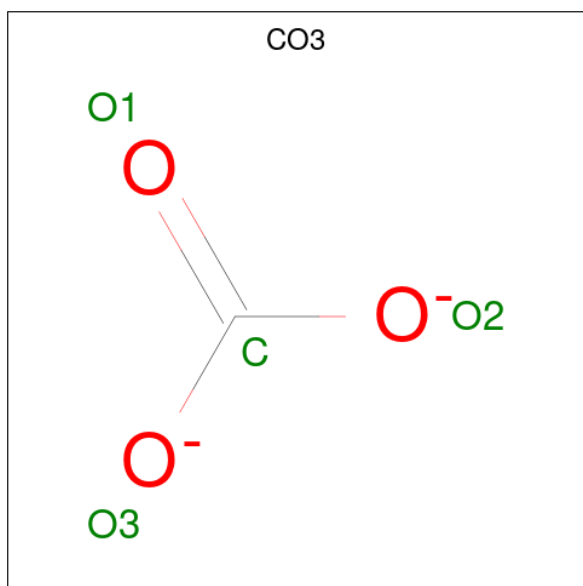
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0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

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

- Molecule 8 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



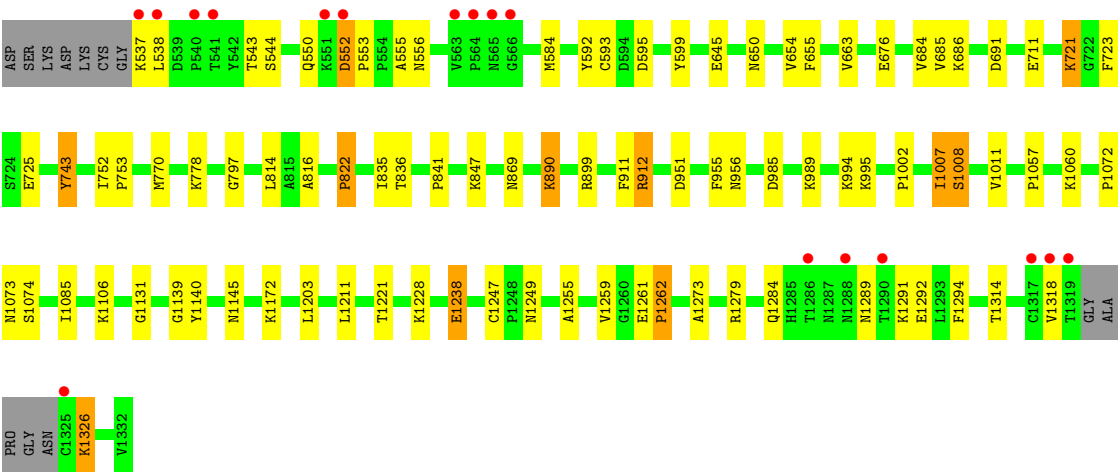
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	1	3		
8	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	B	1	Total	Ca	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	990	Total	O	0	0
			990	990		
10	B	976	Total	O	0	0
			976	976		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.57Å 124.37Å 148.18Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.65) 93.1 (20.00-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.196 0.166 , 0.188	Depositor DCC
R_{free} test set	4755 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22475	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, MTE, MOS, FAD, FES, CO3, SAL

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	0/10302	0.98	38/13941 (0.3%)
1	B	0.57	0/10291	0.98	41/13927 (0.3%)
All	All	0.56	0/20593	0.98	79/27868 (0.3%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	835	ILE	N-CA-C	9.00	121.12	111.58
1	A	835	ILE	N-CA-C	8.93	121.04	111.58
1	A	1011	VAL	N-CA-C	-8.81	98.83	107.55
1	B	836	THR	N-CA-C	8.51	123.49	113.20
1	B	869	ASN	N-CA-C	8.47	123.23	113.15
1	A	1262	PRO	N-CA-C	8.25	120.76	110.70
1	B	1011	VAL	N-CA-C	-8.24	99.40	107.55
1	B	1262	PRO	N-CA-C	8.08	120.56	110.70
1	B	433	LYS	N-CA-C	-8.00	100.51	112.04
1	A	836	THR	N-CA-C	8.00	122.88	113.20
1	A	654	VAL	N-CA-C	-7.82	103.24	110.82
1	A	433	LYS	N-CA-C	-7.57	101.14	112.04
1	A	869	ASN	N-CA-C	7.41	121.92	113.02
1	B	654	VAL	N-CA-C	-7.13	103.23	111.00
1	B	663	VAL	N-CA-C	-6.98	100.57	109.30
1	B	956	ASN	N-CA-C	6.87	121.04	112.24
1	B	131	GLN	CA-C-N	6.83	126.79	119.28
1	B	131	GLN	C-N-CA	6.83	126.79	119.28
1	A	956	ASN	N-CA-C	6.77	120.90	112.24
1	B	151	THR	N-CA-C	6.43	121.21	113.23
1	B	467	LEU	N-CA-C	6.38	118.23	111.28
1	A	552	ASP	N-CA-C	-6.36	101.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	PRO	N-CA-C	6.32	121.43	111.38
1	B	1085	ILE	N-CA-C	6.29	117.85	111.00
1	A	685	VAL	N-CA-C	-6.27	101.46	109.30
1	A	663	VAL	N-CA-C	-6.24	101.50	109.30
1	B	376	SER	N-CA-C	-6.22	99.87	109.14
1	A	151	THR	N-CA-C	6.22	120.94	113.23
1	B	150	CYS	N-CA-C	6.22	120.89	113.12
1	A	543	THR	N-CA-C	6.21	118.56	111.11
1	A	841	PRO	N-CA-C	-6.15	101.61	111.38
1	A	197	ASN	CA-C-N	6.13	125.81	119.56
1	A	197	ASN	C-N-CA	6.13	125.81	119.56
1	B	743	TYR	N-CA-C	-6.11	101.37	110.23
1	A	80	LEU	N-CA-C	6.10	119.67	112.72
1	A	743	TYR	N-CA-C	-6.07	101.43	110.23
1	B	841	PRO	N-CA-C	-6.07	101.73	111.38
1	B	300	GLY	N-CA-C	-6.03	104.99	111.93
1	A	822	PRO	N-CA-C	-6.03	101.62	111.21
1	B	410	PRO	N-CA-C	6.03	121.74	111.68
1	B	505	ILE	N-CA-C	6.03	116.21	110.42
1	B	822	PRO	N-CA-C	-6.02	101.81	111.38
1	B	257	LEU	N-CA-C	-5.88	101.78	110.48
1	B	411	TYR	N-CA-C	-5.87	102.23	110.50
1	A	828	ASP	N-CA-C	-5.87	102.79	110.53
1	A	411	TYR	N-CA-C	-5.86	101.81	110.48
1	B	263	GLU	N-CA-C	-5.85	105.15	112.93
1	A	1174	LEU	N-CA-C	5.78	117.38	111.14
1	B	685	VAL	N-CA-C	-5.72	102.15	109.30
1	A	1007	ILE	N-CA-C	5.67	116.27	107.99
1	B	1131	GLY	N-CA-C	-5.65	102.25	110.90
1	A	1273	ALA	N-CA-C	-5.64	105.22	111.36
1	B	593	CYS	N-CA-C	5.62	117.86	111.11
1	A	443	GLN	N-CA-C	-5.58	102.08	109.84
1	A	150	CYS	N-CA-C	5.58	120.09	113.12
1	A	1085	ILE	N-CA-C	5.56	117.06	111.00
1	B	1273	ALA	N-CA-C	-5.55	105.31	111.36
1	B	543	THR	N-CA-C	5.54	117.75	111.11
1	A	131	GLN	CA-C-N	5.47	125.14	119.56
1	A	131	GLN	C-N-CA	5.47	125.14	119.56
1	A	1238	GLU	N-CA-C	-5.43	99.67	108.52
1	A	447	MET	N-CA-C	-5.42	105.98	112.59
1	A	467	LEU	N-CA-C	5.41	117.18	111.28
1	B	691	ASP	N-CA-C	5.38	117.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	ALA	N-CA-C	5.34	117.98	110.23
1	B	1007	ILE	N-CA-C	5.32	115.44	107.51
1	A	300	GLY	N-CA-C	-5.26	105.88	111.93
1	B	1238	GLU	N-CA-C	-5.23	100.00	108.52
1	A	1228	LYS	N-CA-C	5.21	117.44	107.75
1	B	80	LEU	N-CA-C	5.21	119.33	112.92
1	B	282	ALA	N-CA-C	5.20	118.41	111.75
1	B	40	LYS	N-CA-C	5.16	118.14	110.14
1	A	592	TYR	N-CA-C	-5.16	102.82	110.46
1	B	1228	LYS	N-CA-C	5.15	117.33	107.75
1	A	750	ILE	N-CA-C	-5.14	100.91	108.11
1	B	152	GLY	N-CA-C	-5.11	108.20	115.30
1	B	592	TYR	N-CA-C	-5.08	102.67	110.14
1	B	414	GLU	N-CA-C	-5.03	103.41	110.50
1	B	37	ARG	N-CA-C	5.01	119.03	113.02

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	10084	0	10078	73	0
1	B	10073	0	10064	67	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	1	0
4	A	4	0	0	1	0
4	B	4	0	0	4	0
5	A	53	0	31	1	0
5	B	53	0	31	1	0
6	A	10	0	4	0	0
6	B	10	0	4	0	0
7	A	66	0	88	3	0
7	B	78	0	104	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	0	0	0
8	B	4	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	990	0	0	8	0
10	B	976	0	0	5	0
All	All	22475	0	20424	144	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 4.

All (144) 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:1211:LEU:HA	1:A:1221[B]:THR:HG21	1.47	0.95
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.33	0.93
1:B:1211:LEU:HA	1:B:1221[B]:THR:HG21	1.54	0.89
1:A:131:GLN:HE21	1:A:133:GLU:H	1.26	0.82
1:B:131:GLN:HE21	1:B:133:GLU:H	1.28	0.81
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.46	0.81
1:A:584[B]:MET:SD	10:A:1397:HOH:O	2.37	0.80
1:A:433:LYS:HE2	1:A:504:MET:SD	2.23	0.78
1:A:137:GLU:HG3	1:A:551:LYS:NZ	2.01	0.75
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.51	0.74
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.53	0.73
1:B:584[A]:MET:SD	10:B:2259:HOH:O	2.46	0.73
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.53	0.73
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.56	0.71
1:B:552:ASP:OD2	1:B:553:PRO:HD2	1.91	0.70
1:B:525:LYS:HA	1:B:537:LYS:HE3	1.75	0.67
1:B:537:LYS:N	1:B:537:LYS:HD3	2.09	0.66
1:A:137:GLU:HG3	1:A:551:LYS:HZ2	1.61	0.66
4:B:1336:MOS:O2	4:B:1336:MOS:MO	1.67	0.65
1:A:271:LYS:NZ	7:A:1345:GOL:H11	2.12	0.64
1:B:684:VAL:O	1:B:686:LYS:HD2	1.98	0.64
1:A:269:LYS:HE3	10:A:1717:HOH:O	1.96	0.63
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.97	0.63
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.64	0.63
4:B:1336:MOS:MO	4:B:1336:MOS:S	2.11	0.62
1:B:217:LEU:O	1:B:220:LYS:HG2	2.00	0.62
4:A:1336:MOS:O2	4:A:1336:MOS:MO	1.71	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:HE3	10:B:2138:HOH:O	2.01	0.60
1:B:1326:LYS:HD3	1:B:1326:LYS:H	1.67	0.59
1:A:264:ILE:O	1:A:268[B]:MET:HG3	2.06	0.56
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.07	0.55
1:A:32[A]:ARG:HH12	1:A:676:GLU:CD	2.14	0.54
1:B:994:LYS:HD3	7:B:1349:GOL:O1	2.07	0.54
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.73	0.54
1:B:770[B]:MET:HE3	1:B:1074:SER:O	2.07	0.54
1:B:770[B]:MET:HE2	1:B:1073:ASN:HA	1.91	0.53
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.55	0.53
1:A:268[B]:MET:HE1	10:A:1710:HOH:O	2.09	0.52
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	2.07	0.52
1:A:474:LEU:O	1:A:475[A]:SER:HB2	2.09	0.52
1:A:570:GLU:OE2	1:A:1057:PRO:HG3	2.10	0.51
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.74	0.51
1:B:890:LYS:HE3	1:B:951:ASP:OD2	2.10	0.51
1:A:955:PHE:HA	1:A:1145:ASN:ND2	2.16	0.51
1:A:271:LYS:HZ1	7:A:1345:GOL:H11	1.74	0.51
1:A:217:LEU:O	1:A:220:LYS:HG2	2.11	0.51
1:B:348:LEU:HD13	1:B:407:ILE:CD1	2.41	0.51
1:A:502:GLY:HA3	10:A:1868:HOH:O	2.10	0.51
1:B:371:LYS:HE3	10:B:1993:HOH:O	2.11	0.51
1:A:137:GLU:HG3	1:A:551:LYS:HZ1	1.75	0.50
1:A:263:GLU:HB2	5:A:1337:FAD:H52A	1.94	0.50
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.22	0.50
1:A:1212:HIS:H	1:A:1221[B]:THR:HG22	1.77	0.50
1:A:593:CYS:HB3	1:A:748[A]:CYS:SG	2.51	0.50
1:B:544:SER:O	1:B:994:LYS:HE2	2.12	0.49
1:A:459:MET:HE2	1:A:512:THR:HG21	1.93	0.49
1:A:264:ILE:O	1:A:268[B]:MET:CG	2.60	0.49
1:A:645:GLU:CG	1:A:650:ASN:HD22	2.22	0.49
1:A:911:PHE:O	1:A:912:ARG:C	2.55	0.49
1:A:32[A]:ARG:NH1	1:A:676:GLU:OE2	2.40	0.48
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.79	0.48
1:B:1221[B]:THR:HG23	1:B:1221[B]:THR:O	2.14	0.48
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.14	0.47
1:B:550:GLN:O	1:B:1172:LYS:NZ	2.37	0.47
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.14	0.47
1:B:467:LEU:O	1:B:471:GLN:HG2	2.15	0.47
1:B:459:MET:HE2	1:B:512:THR:HG21	1.95	0.47
1:A:618:LYS:HA	1:A:618:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:LYS:N	1:A:1327:PRO:HD2	2.30	0.47
1:B:161:ARG:HB2	10:B:1791:HOH:O	2.15	0.47
4:B:1336:MOS:S	4:B:1336:MOS:O1	2.73	0.47
1:B:985:ASP:O	1:B:989:LYS:HG3	2.16	0.46
1:A:318:LYS:HG3	1:A:319:LEU:HG	1.97	0.46
1:B:911:PHE:O	1:B:912:ARG:C	2.58	0.46
1:B:1279:ARG:HG2	1:B:1294:PHE:CE2	2.41	0.46
1:A:659[A]:THR:HG21	10:A:1845:HOH:O	2.15	0.46
1:A:555:ALA:O	1:A:1238:GLU:HA	2.16	0.46
1:A:866:ASN:C	1:A:866:ASN:HD22	2.23	0.46
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.46
1:A:271:LYS:HZ3	7:A:1345:GOL:H11	1.81	0.45
1:B:1289:ASN:ND2	1:B:1291:LYS:H	2.14	0.45
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.52	0.45
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.99	0.45
3:B:1335:MTE:S1'	4:B:1336:MOS:S	3.15	0.45
1:A:225:LYS:HE3	1:A:226:GLN:O	2.17	0.45
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.16	0.45
1:A:407[A]:ILE:HD12	1:A:407[A]:ILE:N	2.32	0.45
1:B:711:GLU:HA	1:B:899:ARG:HD2	1.98	0.45
1:A:480:GLU:O	1:A:484:GLN:HG3	2.17	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.98	0.45
1:A:1212:HIS:H	1:A:1221[B]:THR:CG2	2.30	0.45
1:B:37:ARG:HD3	1:B:595:ASP:O	2.16	0.45
1:A:348:LEU:HD13	1:A:407[B]:ILE:CD1	2.47	0.45
1:B:770[B]:MET:HG3	1:B:1073:ASN:HA	1.99	0.44
1:A:308:VAL:HG21	1:A:348:LEU:HG	2.00	0.43
1:B:407:ILE:O	1:B:407:ILE:HG13	2.16	0.43
1:A:753:PRO:HD3	1:A:816:ALA:HB1	2.00	0.43
1:A:695:ILE:HG23	1:A:700:ASP:HB3	2.00	0.43
1:B:63:ASP:CG	1:B:63:ASP:O	2.62	0.43
1:B:723:PHE:CZ	1:B:847:LYS:HE2	2.54	0.43
1:A:406:SER:C	1:A:407[A]:ILE:HD12	2.44	0.43
1:B:255:ALA:HB2	1:B:277:MET:HG2	2.01	0.43
1:A:1312:LYS:HG2	10:A:1880:HOH:O	2.19	0.43
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.34	0.42
1:A:284:ILE:CG2	1:A:287[A]:LEU:HD23	2.49	0.42
1:A:1259:VAL:O	1:A:1259:VAL:HG22	2.19	0.42
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.29	0.42
1:B:1007:ILE:O	1:B:1008:SER:CB	2.67	0.42
1:B:1057:PRO:HD2	1:B:1060:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.27	0.42
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.83	0.42
1:B:556:ASN:ND2	10:B:1792:HOH:O	2.45	0.42
1:A:718:ASP:HB3	1:A:721:LYS:HE3	2.01	0.42
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.82	0.42
1:B:1259:VAL:HG22	1:B:1259:VAL:O	2.19	0.42
1:A:1183:GLY:HA2	1:A:1247[A]:CYS:O	2.20	0.42
1:A:899:ARG:HD3	10:A:2207:HOH:O	2.19	0.41
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.45	0.41
1:A:1102:GLU:OE2	1:A:1106:LYS:HE3	2.20	0.41
1:B:270:PHE:CD2	7:B:1345:GOL:H32	2.55	0.41
1:B:721:LYS:O	1:B:725:GLU:HG3	2.20	0.41
1:B:525:LYS:HG3	1:B:537:LYS:CE	2.50	0.41
1:A:310:LYS:O	1:A:314:GLU:HG3	2.20	0.41
1:B:555:ALA:O	1:B:1238:GLU:HA	2.20	0.41
1:A:734:LEU:HD21	1:A:921:PHE:CE2	2.56	0.41
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.45	0.41
1:A:994:LYS:HE3	10:A:1886:HOH:O	2.20	0.41
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.49	0.41
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.54	0.41
1:A:615:ALA:O	1:A:659[A]:THR:HG23	2.20	0.41
1:B:263:GLU:HB2	5:B:1337:FAD:H52A	2.02	0.41
1:A:770[A]:MET:HG3	1:A:1073:ASN:HA	2.03	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.93	0.41
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.85	0.41
1:A:100:PRO:O	1:A:104:ARG:HG3	2.21	0.41
1:A:315:ALA:HA	1:A:318:LYS:HG2	2.03	0.41
1:A:975:SER:O	1:A:980:ARG:HD3	2.21	0.40
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.56	0.40
1:B:1326:LYS:HD3	1:B:1326:LYS:N	2.34	0.40
1:A:154:ARG:C	1:A:154:ARG:HD2	2.47	0.40
1:A:318:LYS:HG3	1:A:319:LEU:N	2.34	0.40
1:B:441:LEU:HB3	1:B:451:GLU:HB2	2.03	0.40
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.97	0.40
1:B:333[B]:GLN:HE21	1:B:333[B]:GLN:HA	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	1291/1332 (97%)	1254 (97%)	34 (3%)	3 (0%)	43	27
1	B	1290/1332 (97%)	1259 (98%)	27 (2%)	4 (0%)	36	21
All	All	2581/2664 (97%)	2513 (97%)	61 (2%)	7 (0%)	36	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY

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	1104/1128 (98%)	1096 (99%)	8 (1%)	76	64
1	B	1103/1128 (98%)	1090 (99%)	13 (1%)	63	45
All	All	2207/2256 (98%)	2186 (99%)	21 (1%)	70	52

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	281	PRO
1	A	348	LEU
1	A	569	LYS
1	A	743	TYR
1	A	866	ASN
1	A	1002	PRO
1	A	1072	PRO
1	B	100	PRO
1	B	538	LEU
1	B	552	ASP
1	B	721	LYS
1	B	743	TYR
1	B	890	LYS
1	B	1002	PRO
1	B	1072	PRO
1	B	1106	LYS
1	B	1247[A]	CYS
1	B	1247[B]	CYS
1	B	1292	GLU
1	B	1326	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	131	GLN
1	A	226	GLN
1	A	261	ASN
1	A	272	ASN
1	A	556	ASN
1	A	650	ASN
1	A	683	HIS
1	A	866	ASN
1	A	1145	ASN
1	A	1220	HIS
1	A	1284	GLN
1	B	131	GLN
1	B	226	GLN
1	B	251	GLN
1	B	252	HIS
1	B	556	ASN
1	B	565	ASN

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Mol	Chain	Res	Type
1	B	626	GLN
1	B	650	ASN
1	B	869	ASN
1	B	1088	GLN
1	B	1145	ASN
1	B	1220	HIS
1	B	1284	GLN
1	B	1288	ASN
1	B	1289	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	$\# Z > 2$
6	SAL	B	1338	-	10,10,10	2.15	5 (50%)	13,13,13	2.00	3 (23%)
7	GOL	B	1348	-	5,5,5	0.59	0	5,5,5	0.33	0
7	GOL	B	1339	-	5,5,5	0.31	0	5,5,5	0.18	0
7	GOL	A	1343	-	5,5,5	0.30	0	5,5,5	0.15	0
7	GOL	A	1347	-	5,5,5	0.47	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	B	1337	-	58,58,58	1.97	16 (27%)	85,89,89	1.95	18 (21%)
7	GOL	A	1340	-	5,5,5	0.30	0	5,5,5	0.19	0
7	GOL	B	1344	-	5,5,5	0.48	0	5,5,5	0.39	0
7	GOL	B	1340	-	5,5,5	0.37	0	5,5,5	0.24	0
7	GOL	A	1346	-	5,5,5	0.46	0	5,5,5	0.28	0
7	GOL	A	1341	-	5,5,5	0.41	0	5,5,5	0.37	0
7	GOL	A	1344	-	5,5,5	0.44	0	5,5,5	0.44	0
2	FES	B	1333	1	0,4,4	-	-	-	-	-
7	GOL	A	1345	-	5,5,5	0.50	0	5,5,5	0.43	0
7	GOL	A	1348	-	5,5,5	0.53	0	5,5,5	0.24	0
7	GOL	B	1350	-	5,5,5	0.56	0	5,5,5	0.53	0
2	FES	A	1334	1	0,4,4	-	-	-	-	-
7	GOL	B	1342	-	5,5,5	0.46	0	5,5,5	0.31	0
7	GOL	B	1349	-	5,5,5	0.24	0	5,5,5	0.27	0
7	GOL	B	1345	-	5,5,5	0.39	0	5,5,5	0.29	0
7	GOL	A	1339	-	5,5,5	0.34	0	5,5,5	0.22	0
8	CO3	A	1350	-	3,3,3	0.32	0	2,3,3	0.26	0
7	GOL	B	1347	-	5,5,5	0.45	0	5,5,5	0.28	0
3	MTE	B	1335	4	21,26,26	2.90	7 (33%)	19,40,40	3.09	9 (47%)
4	MOS	A	1336	3	0,3,3	-	-	-	-	-
7	GOL	B	1341	-	5,5,5	0.42	0	5,5,5	0.35	0
7	GOL	B	1343	-	5,5,5	0.28	0	5,5,5	0.21	0
6	SAL	A	1338	-	10,10,10	2.05	5 (50%)	13,13,13	2.02	4 (30%)
2	FES	A	1333	1	0,4,4	-	-	-	-	-
7	GOL	A	1349	-	5,5,5	0.46	0	5,5,5	0.32	0
5	FAD	A	1337	-	58,58,58	2.00	17 (29%)	85,89,89	1.94	20 (23%)
2	FES	B	1334	1	0,4,4	-	-	-	-	-
7	GOL	B	1351	-	5,5,5	0.52	0	5,5,5	0.21	0
8	CO3	B	1352	-	3,3,3	0.42	0	2,3,3	0.11	0
7	GOL	B	1346	-	5,5,5	0.40	0	5,5,5	0.30	0
4	MOS	B	1336	3	0,3,3	-	-	-	-	-
3	MTE	A	1335	4	21,26,26	2.82	7 (33%)	19,40,40	3.16	9 (47%)
7	GOL	A	1342	-	5,5,5	0.46	0	5,5,5	0.30	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
6	SAL	B	1338	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	1348	-	-	0/4/4/4	-
7	GOL	B	1339	-	-	0/4/4/4	-
7	GOL	A	1343	-	-	0/4/4/4	-
7	GOL	A	1347	-	-	0/4/4/4	-
5	FAD	B	1337	-	-	6/34/50/50	0/6/6/6
7	GOL	A	1340	-	-	0/4/4/4	-
7	GOL	B	1344	-	-	2/4/4/4	-
7	GOL	B	1340	-	-	0/4/4/4	-
7	GOL	A	1346	-	-	0/4/4/4	-
7	GOL	A	1341	-	-	0/4/4/4	-
7	GOL	A	1344	-	-	3/4/4/4	-
2	FES	B	1333	1	-	-	0/1/1/1
7	GOL	A	1345	-	-	1/4/4/4	-
7	GOL	A	1348	-	-	0/4/4/4	-
7	GOL	B	1350	-	-	3/4/4/4	-
2	FES	A	1334	1	-	-	0/1/1/1
7	GOL	B	1342	-	-	0/4/4/4	-
7	GOL	B	1349	-	-	2/4/4/4	-
7	GOL	B	1345	-	-	4/4/4/4	-
7	GOL	A	1339	-	-	0/4/4/4	-
7	GOL	B	1347	-	-	0/4/4/4	-
3	MTE	B	1335	4	-	1/6/34/34	0/3/3/3
7	GOL	B	1341	-	-	0/4/4/4	-
7	GOL	B	1343	-	-	0/4/4/4	-
6	SAL	A	1338	-	-	0/4/4/4	0/1/1/1
2	FES	A	1333	1	-	-	0/1/1/1
7	GOL	A	1349	-	-	4/4/4/4	-
5	FAD	A	1337	-	-	6/34/50/50	0/6/6/6
2	FES	B	1334	1	-	-	0/1/1/1
7	GOL	B	1351	-	-	0/4/4/4	-
7	GOL	B	1346	-	-	0/4/4/4	-
3	MTE	A	1335	4	-	1/6/34/34	0/3/3/3
7	GOL	A	1342	-	-	1/4/4/4	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1335	MTE	C10-N8	8.71	1.44	1.35
3	A	1335	MTE	C10-N8	8.59	1.44	1.35
5	B	1337	FAD	C9A-C5X	5.39	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1335	MTE	C9-C10	5.12	1.47	1.38
3	A	1335	MTE	O4-C4	5.08	1.33	1.23
3	A	1335	MTE	C9-C10	4.92	1.47	1.38
5	A	1337	FAD	C9A-C5X	4.92	1.49	1.41
3	B	1335	MTE	O4-C4	4.60	1.32	1.23
5	B	1337	FAD	C9A-N10	4.52	1.49	1.41
5	A	1337	FAD	C9A-N10	4.17	1.48	1.41
5	B	1337	FAD	O4B-C1B	4.05	1.51	1.42
5	A	1337	FAD	O4B-C1B	4.04	1.51	1.42
5	A	1337	FAD	C4A-N3A	3.97	1.41	1.34
3	B	1335	MTE	C9-N5	3.95	1.47	1.37
5	B	1337	FAD	C2A-N1A	3.94	1.40	1.33
5	B	1337	FAD	C4A-N3A	3.93	1.41	1.34
5	A	1337	FAD	C5A-C4A	3.85	1.46	1.39
5	A	1337	FAD	C9-C9A	3.82	1.45	1.39
5	A	1337	FAD	C2A-N1A	3.78	1.40	1.33
3	A	1335	MTE	C9-N5	3.77	1.46	1.37
5	B	1337	FAD	O4B-C4B	3.72	1.53	1.45
5	A	1337	FAD	O4B-C4B	3.55	1.52	1.45
5	B	1337	FAD	C5A-C4A	3.42	1.45	1.39
5	A	1337	FAD	C6-C5X	3.33	1.45	1.40
5	A	1337	FAD	C8-C7	3.30	1.48	1.40
6	A	1338	SAL	C1-C1'	-3.26	1.42	1.49
6	B	1338	SAL	C1-C1'	-3.25	1.42	1.49
3	B	1335	MTE	O3'-C3'	3.23	1.49	1.43
5	B	1337	FAD	C4X-N5	3.22	1.37	1.30
5	B	1337	FAD	C5A-C6A	3.18	1.49	1.41
5	B	1337	FAD	C9-C9A	3.13	1.44	1.39
5	A	1337	FAD	C5A-C6A	3.10	1.49	1.41
6	B	1338	SAL	C6-C1	2.99	1.44	1.39
5	B	1337	FAD	C8-C7	2.98	1.48	1.40
6	B	1338	SAL	C5-C6	2.96	1.44	1.38
3	A	1335	MTE	O3'-C3'	2.88	1.49	1.43
6	A	1338	SAL	C5-C6	2.87	1.43	1.38
5	B	1337	FAD	C6-C5X	2.86	1.44	1.40
5	B	1337	FAD	C2-N3	2.78	1.45	1.39
5	A	1337	FAD	C4X-N5	2.76	1.36	1.30
5	A	1337	FAD	C10-N1	2.74	1.38	1.33
5	A	1337	FAD	C2-N3	2.73	1.45	1.39
6	A	1338	SAL	C6-C1	2.72	1.44	1.39
3	B	1335	MTE	O3'-C7	2.67	1.47	1.43
3	B	1335	MTE	C2-N3	-2.56	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1337	FAD	C2A-N3A	2.49	1.38	1.33
6	A	1338	SAL	O2'-C1'	-2.46	1.23	1.30
6	B	1338	SAL	O2'-C1'	-2.43	1.23	1.30
6	B	1338	SAL	C3-C2	2.36	1.43	1.39
5	A	1337	FAD	C4X-C10	2.33	1.51	1.44
5	A	1337	FAD	C6A-N1A	2.32	1.42	1.35
3	A	1335	MTE	O3'-C7	2.32	1.47	1.43
5	B	1337	FAD	C2A-N3A	2.24	1.37	1.33
3	A	1335	MTE	C2-N1	2.20	1.38	1.33
6	A	1338	SAL	C3-C2	2.18	1.43	1.39
5	B	1337	FAD	C10-N1	2.13	1.37	1.33
5	B	1337	FAD	C4X-C10	2.08	1.50	1.44

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1337	FAD	C5X-C9A-N10	-6.66	111.95	117.97
3	A	1335	MTE	C2-N1-C10	6.39	124.63	113.36
3	B	1335	MTE	C2-N1-C10	6.36	124.58	113.36
5	B	1337	FAD	C9-C9A-N10	6.31	130.34	121.85
3	A	1335	MTE	C7-C6-N5	6.23	113.98	107.87
5	A	1337	FAD	C5X-C9A-N10	-6.17	112.39	117.97
5	A	1337	FAD	C9-C9A-N10	5.88	129.76	121.85
3	B	1335	MTE	C7-C6-N5	5.87	113.64	107.87
3	B	1335	MTE	O3'-C7-C6	-4.88	105.71	108.96
3	A	1335	MTE	O3'-C7-C6	-4.80	105.76	108.96
5	A	1337	FAD	N3A-C2A-N1A	-4.79	121.33	128.58
3	A	1335	MTE	O4-C4-C9	-4.76	115.79	127.26
3	B	1335	MTE	O4-C4-C9	-4.61	116.15	127.26
5	B	1337	FAD	N3A-C2A-N1A	-4.42	121.89	128.58
5	A	1337	FAD	O4B-C1B-N9A	-4.42	99.60	108.09
5	A	1337	FAD	C4-C4X-N5	4.17	123.97	118.21
5	B	1337	FAD	C4-C4X-N5	4.11	123.89	118.21
5	B	1337	FAD	O4B-C1B-N9A	-3.86	100.69	108.09
3	B	1335	MTE	C4-C9-N5	3.81	126.66	116.27
6	B	1338	SAL	O2'-C1'-O1'	-3.79	115.21	123.35
6	A	1338	SAL	O2'-C1'-O1'	-3.77	115.25	123.35
6	A	1338	SAL	C3-C2-C1	3.74	123.78	119.89
6	B	1338	SAL	C3-C2-C1	3.72	123.76	119.89
3	A	1335	MTE	N2-C2-N3	3.67	124.52	116.76
3	A	1335	MTE	C4-C9-N5	3.66	126.24	116.27
5	B	1337	FAD	C8M-C8-C7	3.52	127.94	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1335	MTE	N2-C2-N3	3.45	124.05	116.76
5	B	1337	FAD	C4'-C3'-C2'	-3.45	107.83	113.57
5	B	1337	FAD	C10-N1-C2	3.39	124.19	116.85
3	A	1335	MTE	N3-C2-N1	-3.38	117.14	123.32
5	A	1337	FAD	C4'-C3'-C2'	-3.35	107.99	113.57
5	A	1337	FAD	C10-N1-C2	3.34	124.08	116.85
3	A	1335	MTE	C9-C4-N3	3.33	121.28	112.13
5	A	1337	FAD	C8M-C8-C7	3.26	127.41	120.76
5	B	1337	FAD	C9A-N10-C10	3.21	125.65	120.75
3	B	1335	MTE	C9-C4-N3	3.21	120.95	112.13
5	B	1337	FAD	C8M-C8-C9	-3.15	114.03	119.57
3	B	1335	MTE	N3-C2-N1	-3.09	117.67	123.32
5	A	1337	FAD	C9A-N10-C10	2.97	125.28	120.75
5	A	1337	FAD	C8M-C8-C9	-2.96	114.35	119.57
6	A	1338	SAL	C2-C1-C1'	2.85	122.92	120.00
5	A	1337	FAD	C2A-N3A-C4A	2.84	118.76	111.83
5	A	1337	FAD	O2'-C2'-C3'	2.80	115.79	109.25
5	A	1337	FAD	C1'-N10-C9A	-2.75	115.29	120.63
5	A	1337	FAD	O3B-C3B-C4B	-2.61	103.58	111.08
5	B	1337	FAD	O4-C4-C4X	-2.60	119.67	126.53
5	B	1337	FAD	O3B-C3B-C4B	-2.58	103.67	111.08
3	A	1335	MTE	O4'-C4'-C3'	2.58	114.95	108.58
5	A	1337	FAD	O4-C4-C4X	-2.56	119.78	126.53
5	B	1337	FAD	O3'-C3'-C4'	2.55	114.73	108.93
5	B	1337	FAD	C1'-N10-C9A	-2.54	115.70	120.63
5	B	1337	FAD	O2'-C2'-C3'	2.49	115.08	109.25
6	B	1338	SAL	O2'-C1'-C1	2.49	122.36	115.28
5	B	1337	FAD	C2A-N3A-C4A	2.47	117.87	111.83
3	B	1335	MTE	O4'-C4'-C3'	2.47	114.67	108.58
6	A	1338	SAL	O2'-C1'-C1	2.36	121.98	115.28
5	A	1337	FAD	O3'-C3'-C4'	2.29	114.14	108.93
5	A	1337	FAD	N3A-C4A-N9A	2.24	130.98	127.17
5	A	1337	FAD	C6A-C5A-C4A	-2.21	114.16	117.18
5	B	1337	FAD	C10-C4X-N5	-2.20	120.32	124.81
5	A	1337	FAD	C10-C4X-N5	-2.11	120.49	124.81
5	B	1337	FAD	C2A-N1A-C6A	2.03	122.06	118.73
5	A	1337	FAD	O4B-C4B-C5B	-2.02	102.86	109.33

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1337	FAD	N10-C1'-C2'-O2'
5	A	1337	FAD	N10-C1'-C2'-C3'
5	B	1337	FAD	N10-C1'-C2'-O2'
5	B	1337	FAD	N10-C1'-C2'-C3'
7	A	1349	GOL	O1-C1-C2-C3
7	A	1349	GOL	C1-C2-C3-O3
7	B	1345	GOL	O1-C1-C2-C3
7	B	1345	GOL	C1-C2-C3-O3
7	B	1350	GOL	O1-C1-C2-C3
5	A	1337	FAD	C2'-C3'-C4'-C5'
5	B	1337	FAD	C2'-C3'-C4'-C5'
3	B	1335	MTE	C3'-C4'-O4'-P
7	A	1349	GOL	O1-C1-C2-O2
3	A	1335	MTE	C3'-C4'-O4'-P
5	A	1337	FAD	O3'-C3'-C4'-O4'
5	B	1337	FAD	O3'-C3'-C4'-O4'
7	A	1344	GOL	O1-C1-C2-C3
7	A	1344	GOL	C1-C2-C3-O3
7	A	1345	GOL	C1-C2-C3-O3
7	B	1344	GOL	C1-C2-C3-O3
7	B	1349	GOL	C1-C2-C3-O3
7	B	1345	GOL	O1-C1-C2-O2
7	B	1345	GOL	O2-C2-C3-O3
7	B	1350	GOL	O1-C1-C2-O2
5	A	1337	FAD	O3'-C3'-C4'-C5'
5	B	1337	FAD	O3'-C3'-C4'-C5'
5	A	1337	FAD	C2'-C3'-C4'-O4'
5	B	1337	FAD	C2'-C3'-C4'-O4'
7	A	1349	GOL	O2-C2-C3-O3
7	A	1344	GOL	O1-C1-C2-O2
7	B	1344	GOL	O2-C2-C3-O3
7	B	1349	GOL	O2-C2-C3-O3
7	A	1342	GOL	C1-C2-C3-O3
7	B	1350	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 12 short contacts:

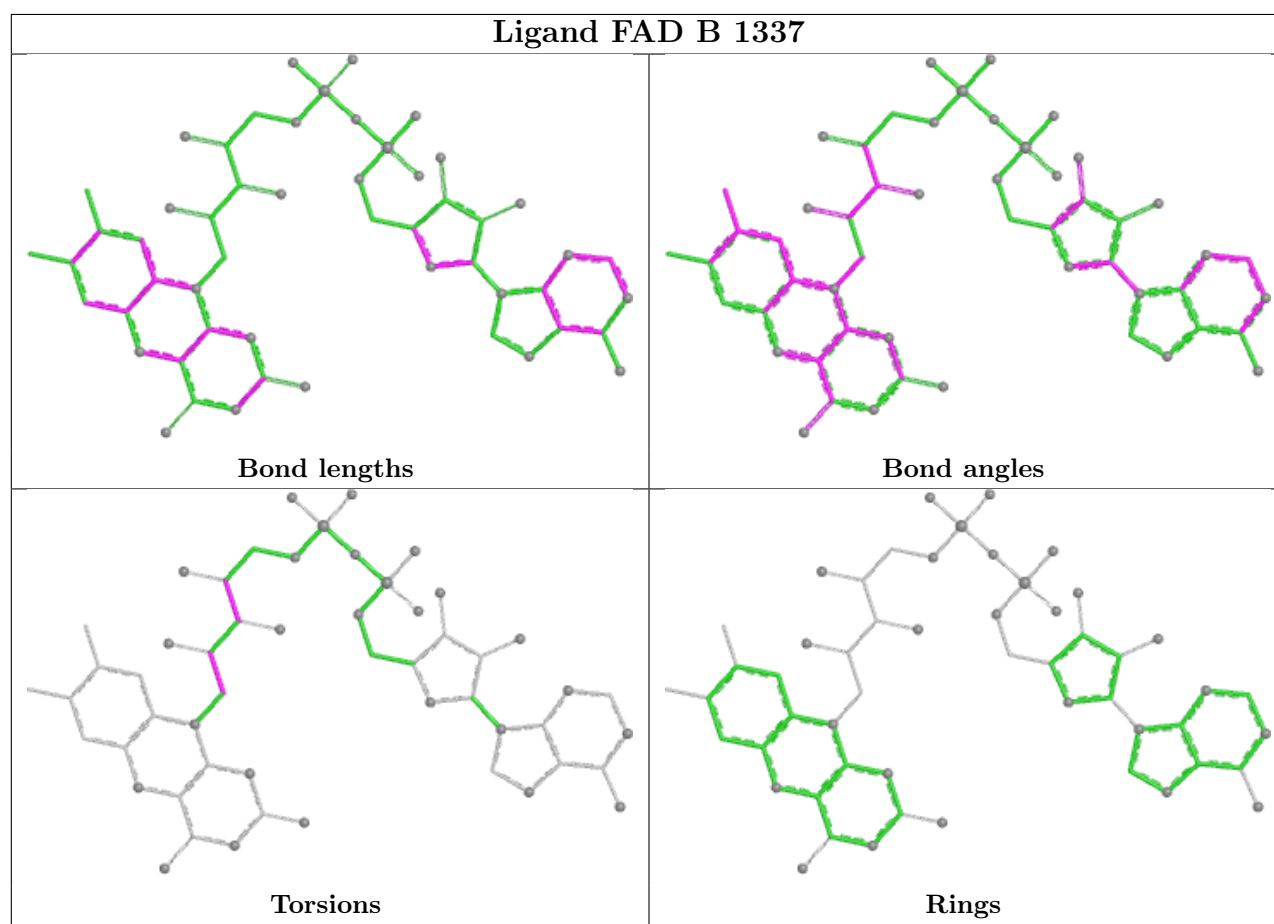
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1337	FAD	1	0
7	A	1345	GOL	3	0
7	B	1349	GOL	1	0
7	B	1345	GOL	1	0

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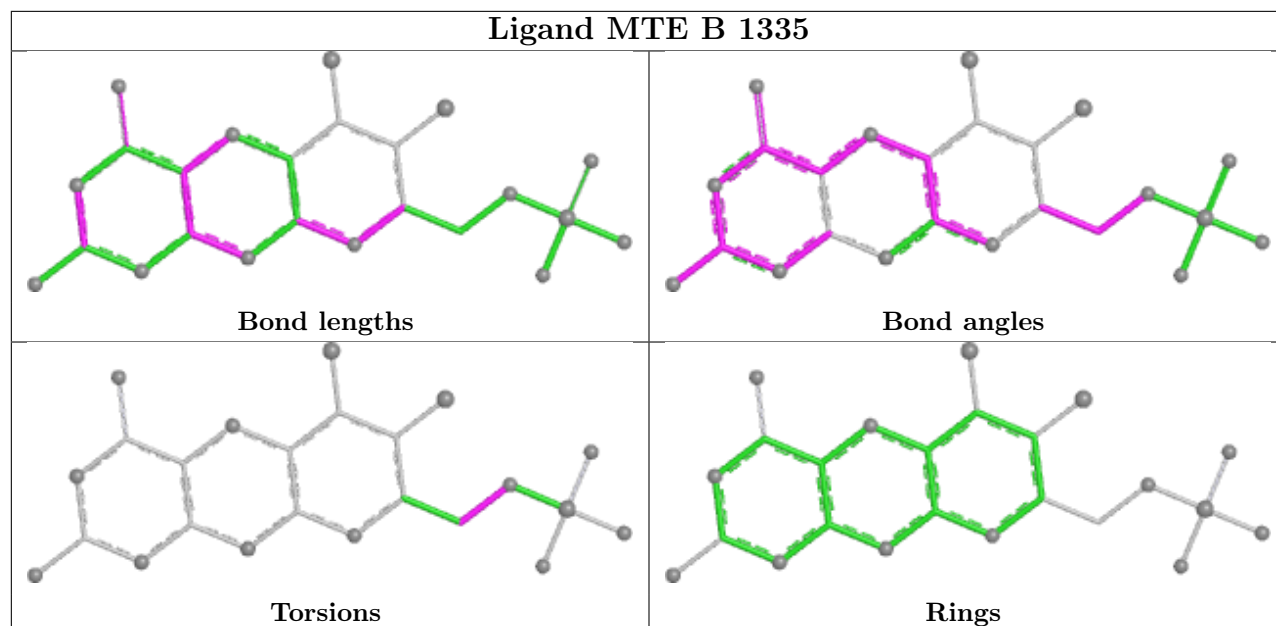
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1335	MTE	1	0
4	A	1336	MOS	1	0
5	A	1337	FAD	1	0
4	B	1336	MOS	4	0

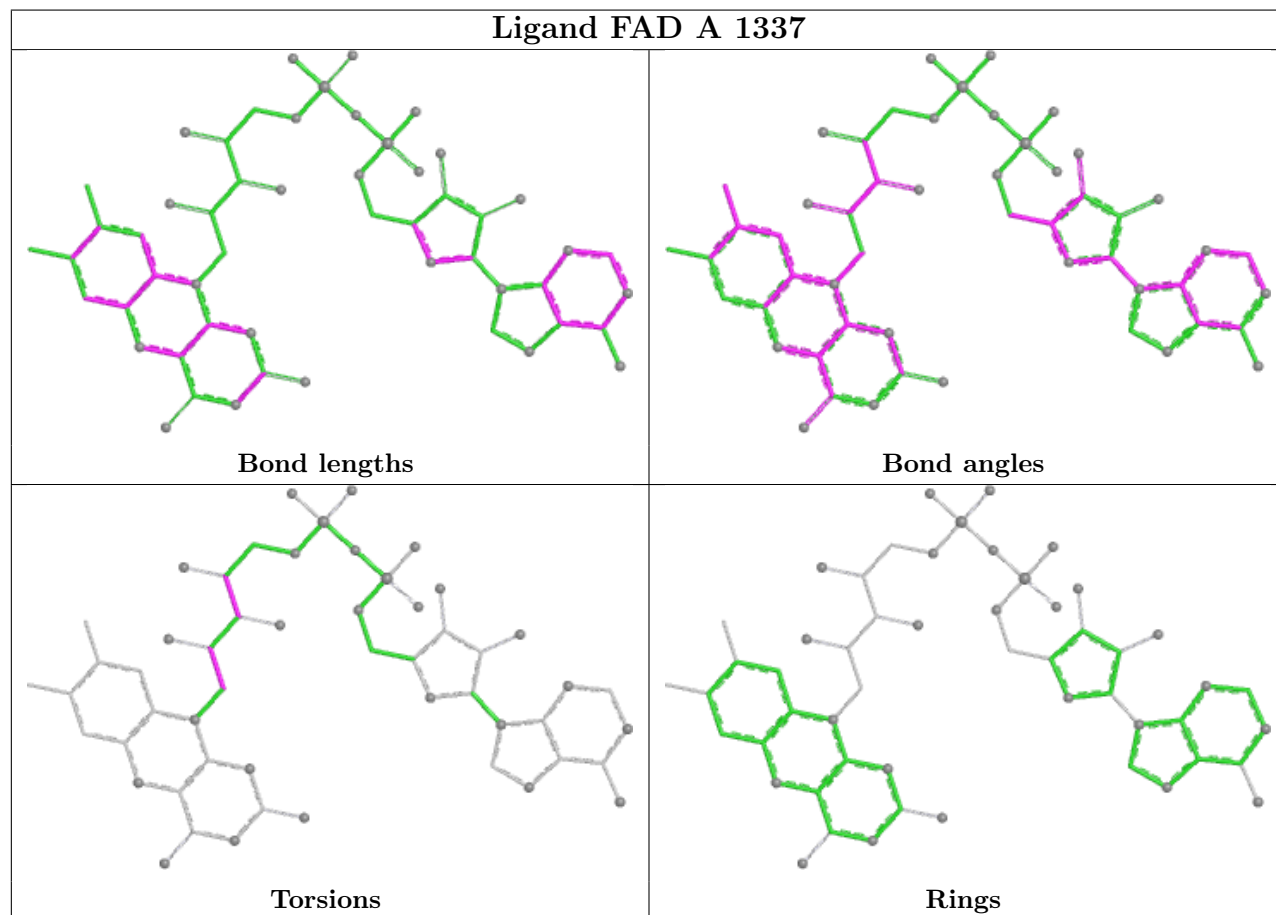
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

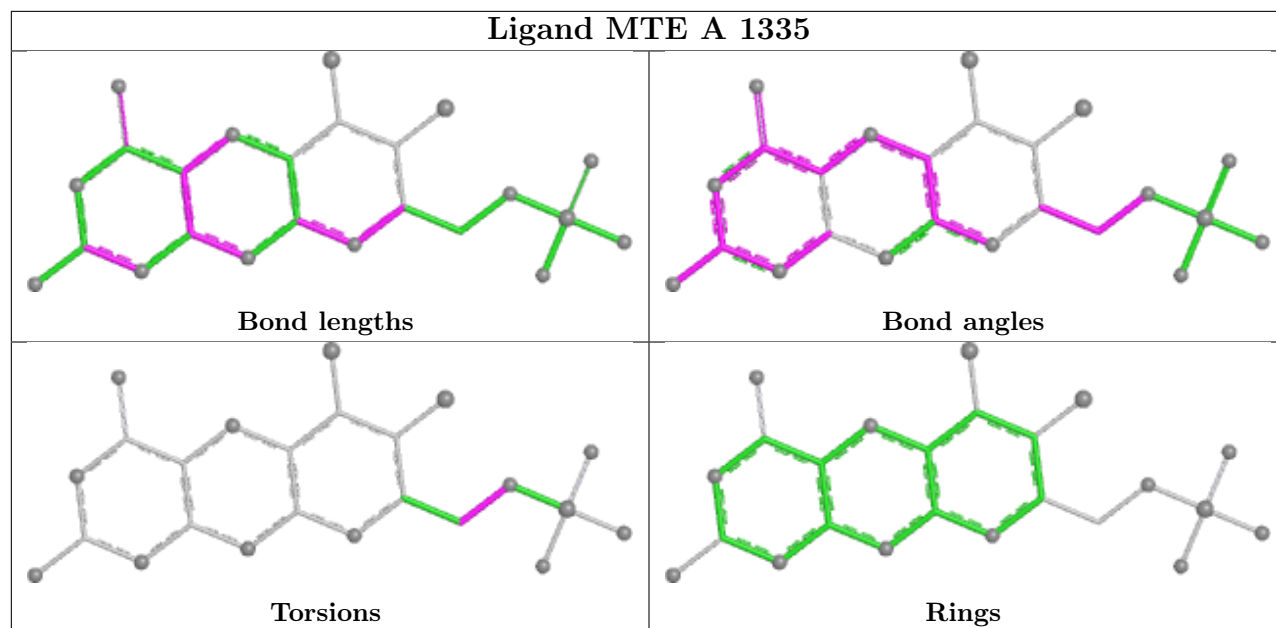


Ligand MTE B 1335



Ligand FAD A 1337





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1286/1332 (96%)	-0.14	24 (1%) 66 71	9, 21, 36, 61	13 (1%)
1	B	1289/1332 (96%)	-0.07	23 (1%) 67 73	9, 21, 36, 57	9 (0%)
All	All	2575/2664 (96%)	-0.11	47 (1%) 67 73	9, 21, 36, 61	22 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1317	CYS	5.1
1	B	528	GLY	4.2
1	A	61	LEU	3.9
1	B	61	LEU	3.7
1	A	222	VAL	3.6
1	A	1288	ASN	3.6
1	B	1319	THR	3.5
1	B	1318	VAL	3.3
1	A	1316	LEU	3.3
1	B	564	PRO	3.0
1	B	565	ASN	3.0
1	B	552	ASP	2.9
1	A	538	LEU	2.9
1	B	1325	CYS	2.9
1	A	528	GLY	2.8
1	A	219	LEU	2.8
1	B	1288	ASN	2.8
1	A	555	ALA	2.7
1	A	540	PRO	2.7
1	B	222	VAL	2.7
1	B	538	LEU	2.7
1	B	566	GLY	2.7
1	B	540	PRO	2.6
1	A	1286	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLY	2.5
1	B	1286	THR	2.5
1	A	1287	ASN	2.4
1	B	63	ASP	2.4
1	A	221	ASP	2.4
1	A	537	LYS	2.4
1	A	553	PRO	2.4
1	B	537	LYS	2.4
1	A	62	GLN	2.3
1	B	551	LYS	2.3
1	A	565	ASN	2.3
1	A	1143	GLU	2.2
1	B	272	ASN	2.2
1	A	32[A]	ARG	2.2
1	A	60	ARG	2.2
1	A	217	LEU	2.1
1	B	541	THR	2.1
1	A	566	GLY	2.1
1	A	699	GLU	2.1
1	A	724	SER	2.1
1	B	1290	THR	2.1
1	B	1317	CYS	2.0
1	B	563	VAL	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 oligosaccharides 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.

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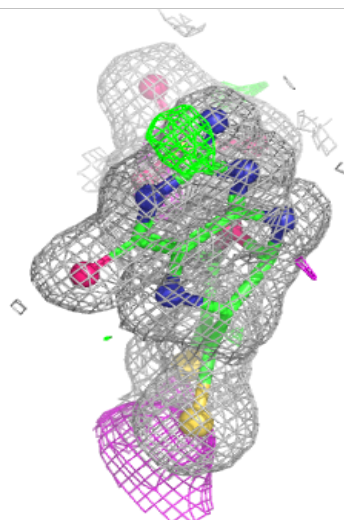
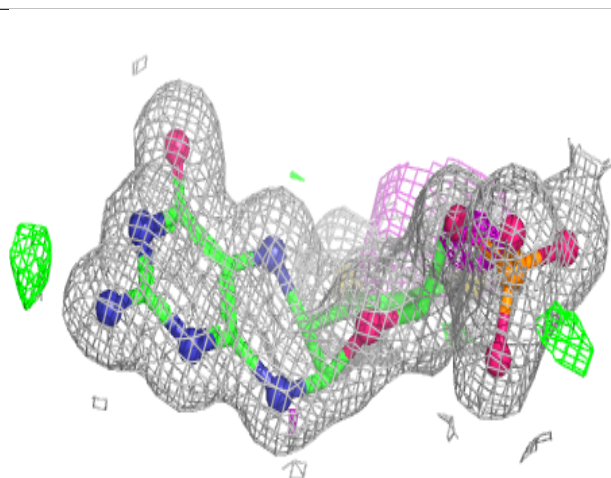
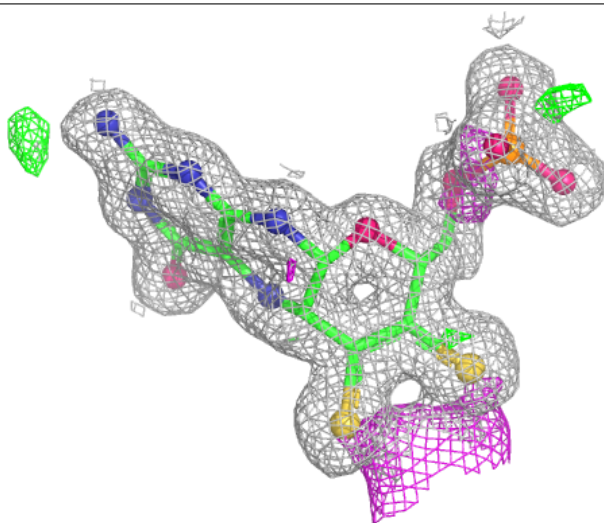
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1345	6/6	0.73	0.20	41,49,50,52	0
7	GOL	B	1351	6/6	0.75	0.14	41,45,45,46	0
7	GOL	B	1349	6/6	0.76	0.18	48,51,52,52	0
7	GOL	B	1342	6/6	0.77	0.14	54,54,54,54	0
7	GOL	B	1344	6/6	0.77	0.17	40,41,42,43	0
7	GOL	A	1344	6/6	0.79	0.15	39,40,40,42	0
7	GOL	A	1349	6/6	0.80	0.15	31,41,43,43	0
7	GOL	A	1340	6/6	0.83	0.13	31,32,33,34	0
7	GOL	B	1340	6/6	0.84	0.13	31,34,36,38	0
7	GOL	B	1350	6/6	0.85	0.15	43,44,45,46	0
7	GOL	B	1345	6/6	0.85	0.13	36,40,43,45	0
7	GOL	A	1347	6/6	0.86	0.12	36,38,40,42	0
7	GOL	A	1342	6/6	0.88	0.10	45,45,46,47	0
7	GOL	A	1348	6/6	0.89	0.10	31,34,35,38	0
7	GOL	A	1341	6/6	0.90	0.10	24,29,30,31	0
7	GOL	A	1343	6/6	0.90	0.13	20,27,29,32	0
7	GOL	B	1343	6/6	0.91	0.13	22,28,29,32	0
7	GOL	B	1348	6/6	0.92	0.09	32,35,35,36	0
7	GOL	B	1347	6/6	0.92	0.09	32,34,35,36	0
7	GOL	B	1346	6/6	0.93	0.14	23,26,26,28	0
6	SAL	B	1338	10/10	0.93	0.08	23,24,25,26	0
7	GOL	A	1346	6/6	0.94	0.11	23,25,26,29	0
7	GOL	B	1341	6/6	0.94	0.09	23,29,31,34	0
6	SAL	A	1338	10/10	0.95	0.07	22,23,24,24	0
7	GOL	A	1339	6/6	0.95	0.07	19,20,20,22	0
7	GOL	B	1339	6/6	0.97	0.05	20,21,22,22	0
8	CO3	A	1350	4/4	0.97	0.04	14,15,16,16	0
3	MTE	B	1335	24/24	0.98	0.05	15,17,20,22	0
5	FAD	A	1337	53/53	0.98	0.04	15,18,22,24	0
5	FAD	B	1337	53/53	0.98	0.05	15,17,21,23	0
8	CO3	B	1352	4/4	0.98	0.04	16,17,17,17	0
3	MTE	A	1335	24/24	0.99	0.04	16,17,20,21	0
4	MOS	A	1336	4/4	0.99	0.11	20,20,21,29	0
4	MOS	B	1336	4/4	0.99	0.09	19,20,20,28	0
9	CA	A	1351	1/1	0.99	0.02	17,17,17,17	0
9	CA	B	1353	1/1	0.99	0.04	18,18,18,18	0
2	FES	A	1333	4/4	1.00	0.02	14,14,15,15	0
2	FES	A	1334	4/4	1.00	0.02	14,14,14,15	0
2	FES	B	1333	4/4	1.00	0.03	13,14,14,14	0
2	FES	B	1334	4/4	1.00	0.03	13,14,14,15	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.

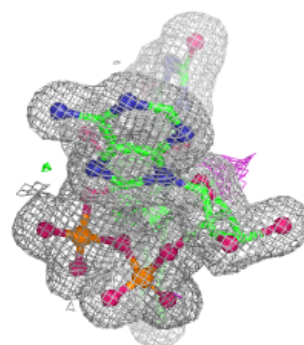
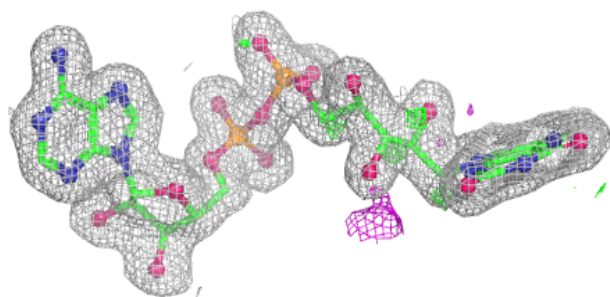
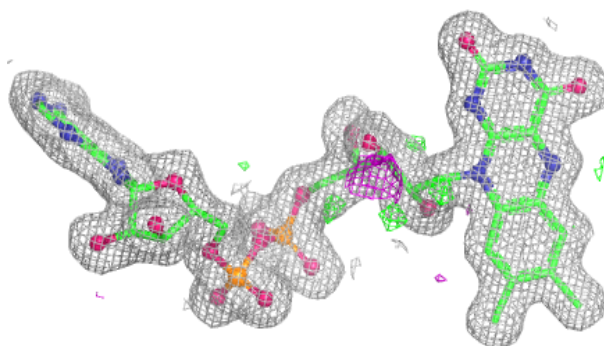
Electron density around MTE B 1335:

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

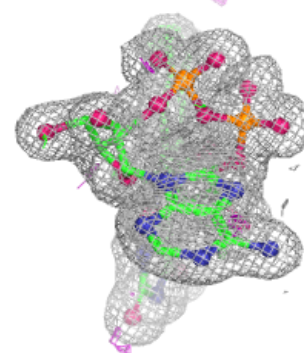
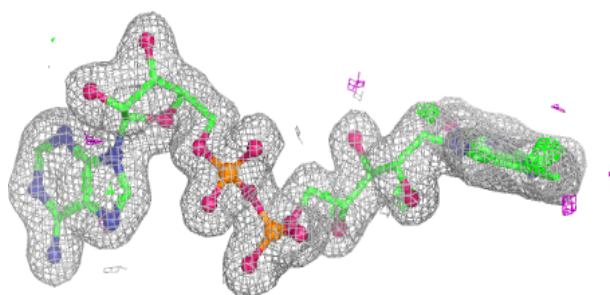
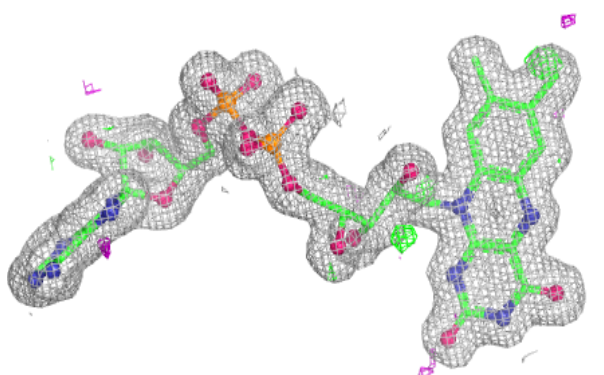


Electron density around FAD A 1337:

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

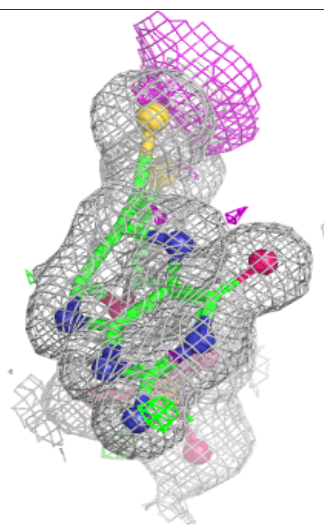
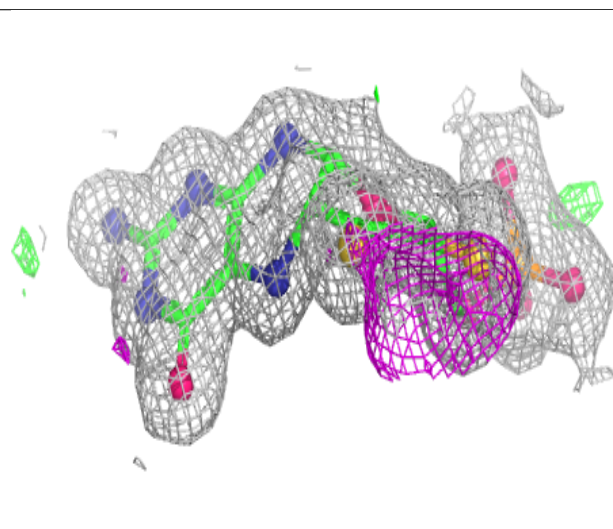
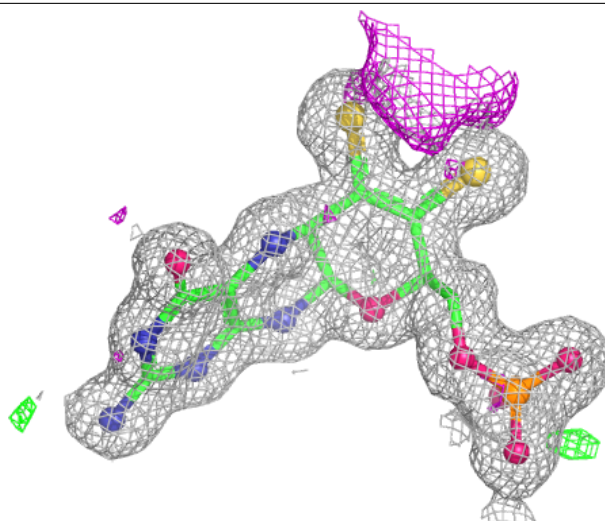
**Electron density around FAD B 1337:**

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



Electron density around MTE A 1335:

$2mF_o-DF_c$ (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.