



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:33 pm BST

PDB ID : 3AM9  
Title : Complex of bovine xanthine dehydrogenase and trihydroxy FYX-051  
Authors : Matsumoto, K.; Okamoto, K.; Ashizawa, N.; Matsumura, T.; Kusano, T.; Nishino, T.  
Deposited on : 2010-08-18  
Resolution : 2.17 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

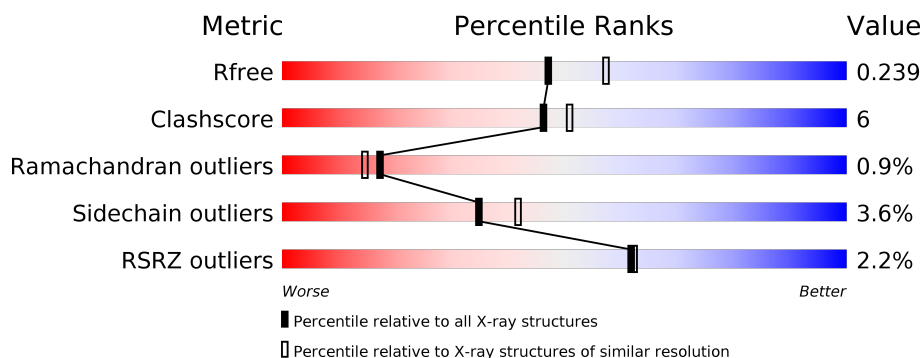
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1332	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	1332	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>

## 2 Entry composition [i](#)

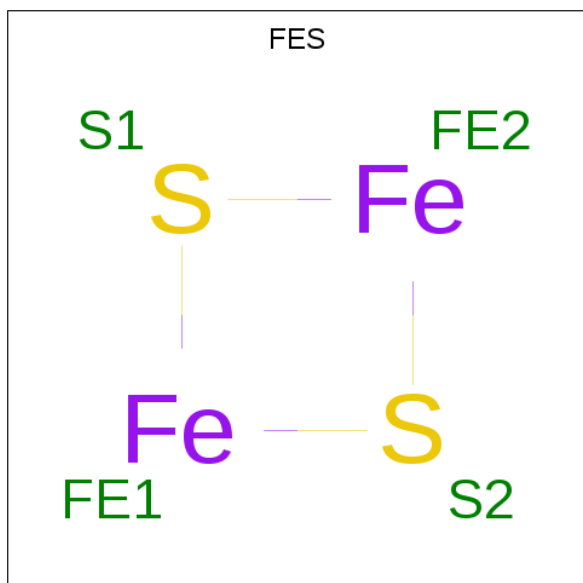
There are 10 unique types of molecules in this entry. The entry contains 22226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1293	Total	C	N	O	S	0	0	0
			10041	6384	1721	1876	60			
1	B	1291	Total	C	N	O	S	0	0	0
			10027	6375	1719	1872	61			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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		

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | B     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 3   | A     | 2        | Total Ca<br>2 2 | 0       | 0       |

- # FAD
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- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. It is composed of three main parts: an adenine base, a ribitol linker, and an isoalloxazine ring system.
- Adenine Base:** A purine ring system (fused pyrimidine and imidazole rings) at the top, colored blue. It is labeled with N1A, N3A, C2A, C4A, C6A, and N7A.
  - Ribitol Linker:** A five-carbon chain (C3B, C4B, C5B, C6B, C7B) connecting the adenine base to the isoalloxazine ring. It is shown in red and black.
  - Isoalloxazine Ring System:** A complex ring system at the bottom, colored blue and green. It includes atoms N1, N3, C2, C4, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, and C16. It is labeled with C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, and C16.
- The structure is highly detailed, showing various functional groups and bonds, including a phosphate group (HO-P(=O)(OH)-O-) and a ribitol chain (C3B, C4B, C5B, C6B, C7B).

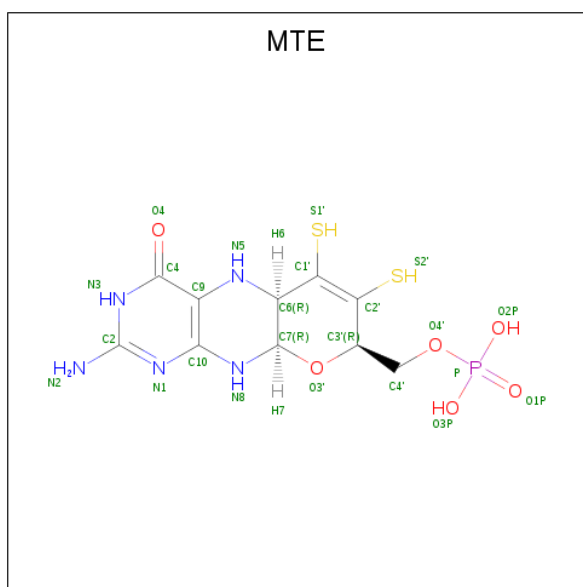
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 6 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 (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6P_2S_2$ ).



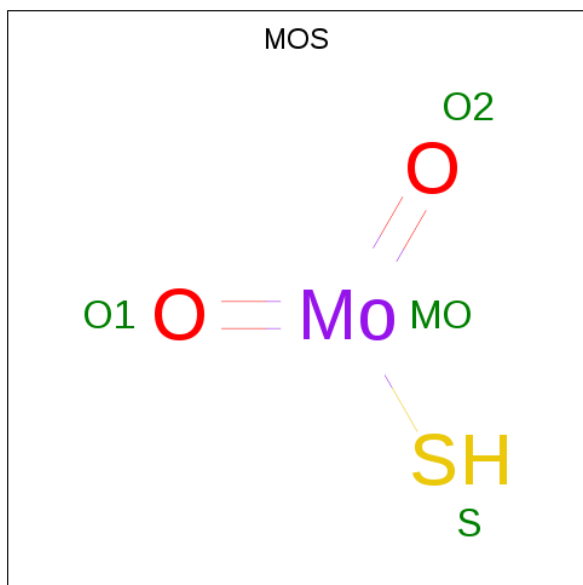
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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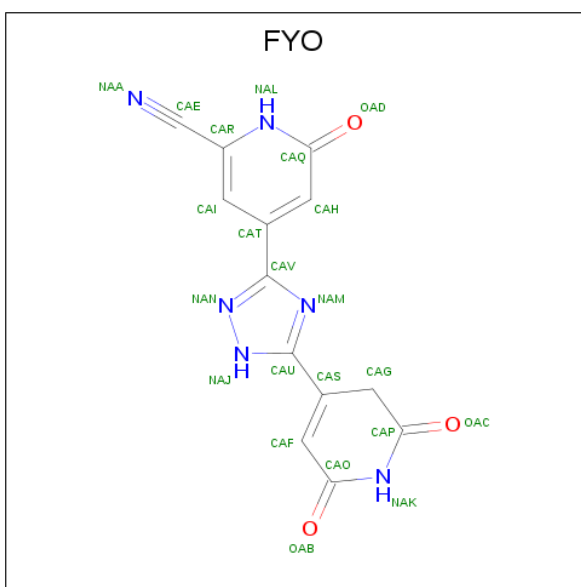
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $\text{HMoO}_2\text{S}$ ).



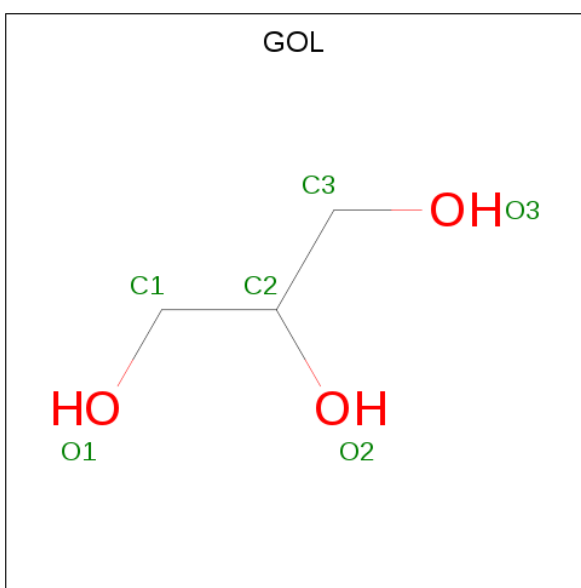
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Mo	O	S	0	0
			3	1	1	1		
7	B	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 8 is 4-[5-(2,6-dioxo-1,2,3,6-tetrahydropyridin-4-yl)-1H-1,2,4-triazol-3-yl]-6-oxo-1,6-dihydropyridine-2-carbonitrile (three-letter code: FYO) (formula:  $\text{C}_{13}\text{H}_8\text{N}_6\text{O}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			22	13	6	3		
8	B	1	Total	C	N	O	0	0
			22	13	6	3		

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



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

- Molecule 10 is water.

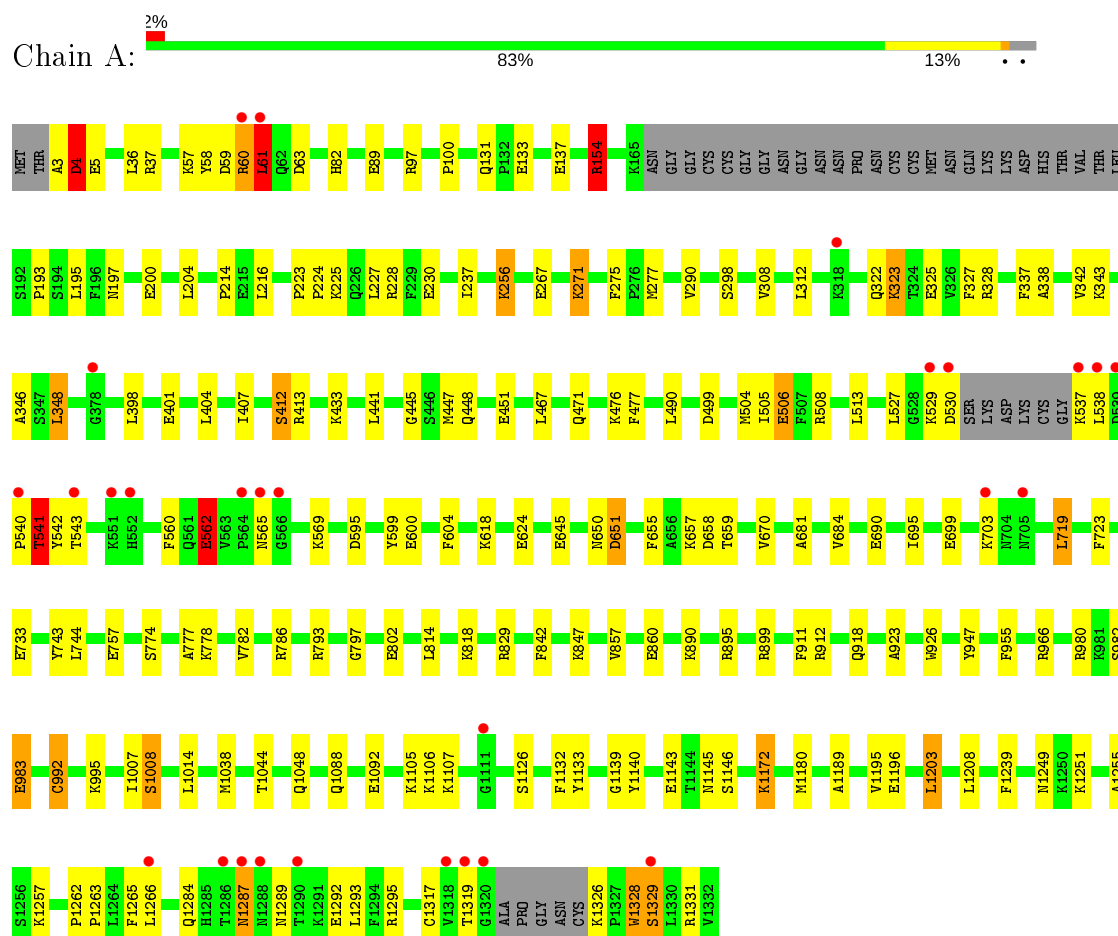
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	973	Total 973	O 973	0	0
10	B	941	Total 941	O 941	0	0



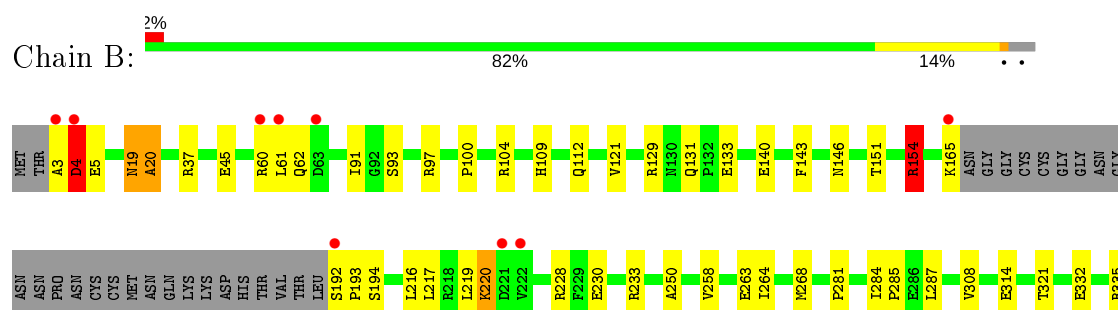
### 3 Residue-property plots

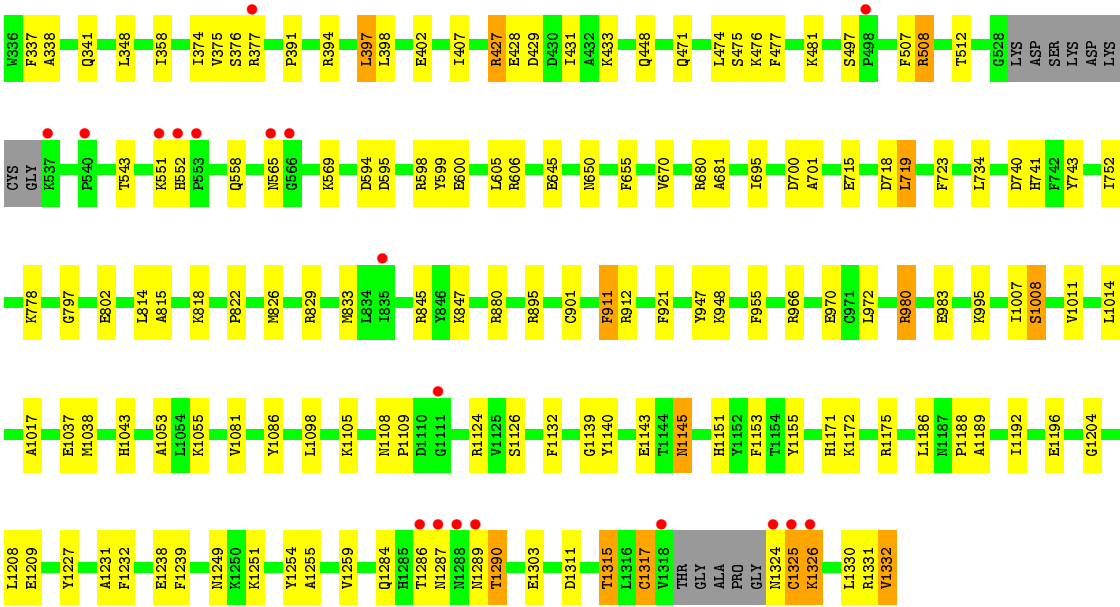
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Xanthine dehydrogenase/oxidase



#### • Molecule 1: Xanthine dehydrogenase/oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.92Å 124.72Å 146.19Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	33.44 – 2.17 33.44 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.5 (33.44-2.17) 95.5 (33.44-2.17)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.243 0.171 , 0.239	Depositor DCC
$R_{free}$ test set	7582 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.09	11/10260 (0.1%)	0.96	21/13885 (0.2%)
1	B	1.06	8/10246 (0.1%)	0.94	21/13867 (0.2%)
All	All	1.07	19/20506 (0.1%)	0.95	42/27752 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	CYS	CB-SG	-9.31	1.66	1.82
1	A	983	GLU	CG-CD	7.29	1.62	1.51
1	B	45	GLU	CB-CG	-6.59	1.39	1.52
1	A	137	GLU	CG-CD	6.55	1.61	1.51
1	A	506	GLU	CG-CD	6.26	1.61	1.51
1	B	1227	TYR	CD1-CE1	-6.12	1.30	1.39
1	A	774	SER	CB-OG	-6.08	1.34	1.42
1	A	604	PHE	CE1-CZ	5.98	1.48	1.37
1	A	562	GLU	CG-CD	5.86	1.60	1.51
1	B	4	ASP	N-CA	5.69	1.57	1.46
1	A	230	GLU	CG-CD	5.63	1.60	1.51
1	A	327	PHE	CE2-CZ	5.45	1.47	1.37
1	B	983	GLU	CG-CD	5.44	1.60	1.51
1	A	137	GLU	CB-CG	5.32	1.62	1.52
1	B	263	GLU	CD-OE2	5.30	1.31	1.25
1	A	1092	GLU	CB-CG	5.24	1.62	1.52
1	B	4	ASP	CA-C	5.17	1.66	1.52
1	B	1231	ALA	CA-CB	5.03	1.63	1.52
1	B	1317	CYS	CB-SG	-5.03	1.73	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	B	154	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	A	829	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	154	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	154	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	B	4	ASP	CB-CG-OD1	-10.69	108.68	118.30
1	A	651	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	B	4	ASP	N-CA-C	8.73	134.58	111.00
1	A	1203	LEU	CA-CB-CG	8.34	134.49	115.30
1	B	980	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	61	LEU	CA-CB-CG	7.07	131.55	115.30
1	B	845	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	427	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	829	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	719	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	B	427	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	719	LEU	CB-CG-CD1	-6.33	100.24	111.00
1	B	980	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	793	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	412	SER	N-CA-CB	-6.13	101.30	110.50
1	A	651	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	793	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	980	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	845	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	61	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	718	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	19	ASN	CB-CA-C	5.70	121.80	110.40
1	B	606	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	1124	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	1328	TRP	C-N-CA	5.50	135.44	121.70
1	B	508	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	413	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	740	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	966	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	899	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	651	ASP	N-CA-CB	-5.29	101.08	110.60
1	B	598	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	204	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	A	508	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	1124	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	268	MET	CG-SD-CE	5.06	108.30	100.20
1	A	4	ASP	CB-CA-C	5.05	120.50	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10041	0	10044	128	0
1	B	10027	0	10027	124	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	2	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	24	0	10	1	0
6	B	24	0	10	1	0
7	A	3	0	0	1	0
7	B	3	0	0	1	0
8	A	22	0	8	2	0
8	B	22	0	8	5	0
9	B	12	0	16	2	0
10	A	973	0	0	21	0
10	B	941	0	0	13	0
All	All	22226	0	20185	253	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 6.

All (253) 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:506:GLU:HG2	10:A:2141:HOH:O	1.40	1.17
1:A:504:MET:SD	10:A:1779:HOH:O	2.09	1.09
1:A:540:PRO:O	1:A:541:THR:HB	1.52	1.08
1:A:3:ALA:HB2	10:A:2268:HOH:O	1.52	1.07
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.22	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HD13	1:B:431:ILE:HG23	1.50	0.94
1:A:1180:MET:CE	1:A:1263:PRO:HB3	1.97	0.94
1:B:4:ASP:HB3	1:B:228:ARG:O	1.68	0.92
1:A:131:GLN:HE21	1:A:133:GLU:H	1.16	0.91
1:A:3:ALA:HB1	1:A:228:ARG:H	1.32	0.91
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.72	0.90
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.39	0.87
1:B:129:ARG:NH1	10:B:1669:HOH:O	2.09	0.85
1:A:818:LYS:HE2	10:A:2283:HOH:O	1.77	0.83
1:A:1180:MET:HE1	1:A:1263:PRO:HB3	1.59	0.83
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.45	0.82
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.43	0.81
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.45	0.81
1:A:154:ARG:CD	1:A:1196:GLU:OE2	2.28	0.81
1:B:217:LEU:O	1:B:220:LYS:HE2	1.79	0.81
1:A:1180:MET:HE3	1:A:1263:PRO:HB3	1.63	0.81
1:A:467:LEU:O	1:A:471:GLN:HG2	1.81	0.79
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.80	0.79
1:B:966:ARG:O	1:B:970:GLU:HG3	1.83	0.78
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.47	0.78
1:A:562:GLU:HB2	10:A:1573:HOH:O	1.84	0.76
1:A:802:GLU:OE1	8:A:1335:FYO:NAN	2.19	0.76
1:A:3:ALA:HB1	1:A:228:ARG:N	2.02	0.73
1:B:3:ALA:HA	1:B:230:GLU:HB2	1.73	0.71
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.73	0.71
1:A:3:ALA:O	1:A:4:ASP:C	2.28	0.70
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.74	0.70
1:B:1331:ARG:O	1:B:1332:VAL:HG23	1.91	0.70
1:A:1257:LYS:HE3	10:A:1807:HOH:O	1.92	0.70
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.74	0.69
1:A:541:THR:HG22	1:A:542:TYR:HD1	1.57	0.68
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.59	0.68
1:A:323:LYS:NZ	10:A:1707:HOH:O	2.25	0.68
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.59	0.68
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.29	0.67
1:B:474:LEU:O	1:B:475:SER:HB2	1.95	0.66
1:B:594:ASP:OD1	9:B:1338:GOL:H32	1.96	0.66
1:B:1287:ASN:HB3	1:B:1289:ASN:HB3	1.77	0.66
1:A:1328:TRP:HB3	1:A:1329:SER:HB2	1.76	0.66
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.01	0.66
1:A:3:ALA:O	1:A:5:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1334:MOS:MO	7:A:1334:MOS:O1	1.66	0.64
1:B:19:ASN:O	1:B:20:ALA:CB	2.46	0.63
7:B:1334:MOS:O1	7:B:1334:MOS:MO	1.69	0.63
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.80	0.63
1:A:540:PRO:O	1:A:541:THR:CB	2.39	0.62
1:B:1007:ILE:O	1:B:1008:SER:HB3	1.99	0.62
1:B:19:ASN:O	1:B:20:ALA:HB3	1.99	0.62
1:A:58:TYR:OH	1:A:63:ASP:OD1	2.16	0.62
1:B:802:GLU:OE1	8:B:1335:FYO:NAN	2.32	0.62
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.00	0.62
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.14	0.61
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.65	0.61
1:B:715:GLU:HG3	1:B:895:ARG:HB2	1.82	0.61
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.15	0.61
1:B:1175:ARG:HG3	1:B:1238:GLU:HB3	1.83	0.61
1:B:826:MET:H	9:B:1338:GOL:H12	1.67	0.60
1:B:4:ASP:CB	1:B:228:ARG:O	2.46	0.60
1:A:1287:ASN:HD22	1:A:1289:ASN:H	1.48	0.60
1:B:140:GLU:OE2	1:B:551:LYS:HE3	2.02	0.59
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.49	0.59
1:A:1287:ASN:ND2	1:A:1289:ASN:HB3	2.17	0.59
1:A:1146:SER:HB3	10:A:1909:HOH:O	2.03	0.58
1:B:1105:LYS:HD2	10:B:1837:HOH:O	2.03	0.58
1:A:154:ARG:HD2	1:A:1196:GLU:OE2	2.02	0.58
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.84	0.58
1:A:59:ASP:OD2	1:A:61:LEU:HB3	2.05	0.57
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.51	0.57
1:A:1038:MET:HG3	6:A:1333:MTE:C4	2.35	0.56
1:A:346:ALA:HB1	4:A:3005:FAD:H4'	1.87	0.56
1:A:1292:GLU:HG2	1:A:1293:LEU:N	2.20	0.56
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	2.02	0.56
1:A:719:LEU:HD11	1:A:895:ARG:HB3	1.88	0.56
8:A:1335:FYO:HAH	10:A:2289:HOH:O	2.04	0.56
1:A:237:ILE:CD1	1:A:277:MET:CE	2.83	0.56
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.52	0.55
1:B:1324:ASN:O	1:B:1325:CYS:HB2	2.05	0.55
1:A:447:MET:HG2	1:A:527:LEU:HD13	1.87	0.55
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.06	0.55
1:B:818:LYS:HE2	10:B:1609:HOH:O	2.06	0.55
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.40	0.55
1:A:504:MET:HE3	10:A:2264:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.43	0.54
1:A:1105:LYS:HE2	10:A:1942:HOH:O	2.07	0.54
1:A:237:ILE:HD13	1:A:277:MET:CE	2.37	0.54
1:A:529:LYS:O	1:A:530:ASP:HB2	2.06	0.54
1:B:471:GLN:HG3	10:B:2245:HOH:O	2.07	0.54
1:A:197:ASN:O	1:A:200:GLU:HG2	2.08	0.53
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.56	0.53
1:B:348:LEU:HD13	1:B:407:ILE:HD13	1.90	0.53
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.90	0.53
1:B:3:ALA:HB3	1:B:19:ASN:OD1	2.09	0.52
1:A:131:GLN:HE21	1:A:133:GLU:N	1.97	0.52
1:A:237:ILE:CD1	1:A:277:MET:HE2	2.39	0.52
1:B:995:LYS:HZ3	1:B:1284:GLN:NE2	2.07	0.52
1:A:995:LYS:HZ3	1:A:1284:GLN:NE2	2.08	0.52
1:A:338:ALA:HB1	1:A:342:VAL:HB	1.92	0.52
1:B:217:LEU:O	1:B:220:LYS:CE	2.53	0.52
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.09	0.52
1:A:695:ILE:HD11	10:A:1836:HOH:O	2.10	0.52
1:B:284:ILE:HB	1:B:287:LEU:HD12	1.92	0.51
1:B:605:LEU:HD12	1:B:815:ALA:HB2	1.92	0.51
1:A:343:LYS:HE3	10:A:2055:HOH:O	2.09	0.51
1:A:703:LYS:O	1:A:703:LYS:HG3	2.09	0.51
1:B:1324:ASN:HA	1:B:1326:LYS:HB3	1.91	0.51
1:A:1140:TYR:OH	1:A:1145:ASN:ND2	2.36	0.51
1:A:1180:MET:HE3	1:A:1195:VAL:HG22	1.92	0.51
1:B:146:ASN:ND2	1:B:341:GLN:HE22	2.08	0.51
1:A:154:ARG:HD2	10:A:1458:HOH:O	2.10	0.51
1:A:195:LEU:HD22	1:A:1189:ALA:HA	1.92	0.51
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.45	0.51
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.46	0.50
1:A:645:GLU:CG	1:A:650:ASN:HD22	2.19	0.50
1:B:1287:ASN:HB3	1:B:1289:ASN:CB	2.41	0.50
1:B:376:SER:HB3	1:B:402:GLU:HG2	1.93	0.50
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	2.11	0.50
1:A:57:LYS:NZ	10:A:1872:HOH:O	2.45	0.50
1:B:1289:ASN:O	1:B:1290:THR:HB	2.12	0.50
1:B:37:ARG:CD	1:B:595:ASP:O	2.59	0.49
1:A:670:VAL:HG11	1:A:681:ALA:HB3	1.94	0.49
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.42	0.49
1:B:1289:ASN:C	1:B:1289:ASN:OD1	2.50	0.49
1:A:58:TYR:CE2	1:A:60:ARG:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.47	0.49
1:A:657:LYS:O	1:A:658:ASP:HB2	2.12	0.49
1:B:131:GLN:HE21	1:B:133:GLU:H	1.61	0.49
1:B:250:ALA:HB2	1:B:377:ARG:HB2	1.94	0.49
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.48	0.49
1:B:1315:THR:O	1:B:1315:THR:CG2	2.59	0.49
1:B:1311:ASP:O	1:B:1315:THR:HB	2.13	0.49
1:A:308:VAL:HG21	1:A:348:LEU:HG	1.93	0.49
1:B:308:VAL:HG21	1:B:348:LEU:HG	1.95	0.49
1:B:217:LEU:O	1:B:220:LYS:HG3	2.13	0.48
1:B:995:LYS:NZ	1:B:1284:GLN:NE2	2.60	0.48
1:B:655:PHE:HE1	1:B:814:LEU:CD2	2.24	0.48
1:A:540:PRO:HA	1:A:543:THR:HG23	1.95	0.48
1:A:1007:ILE:O	1:A:1008:SER:HB3	2.13	0.48
1:B:143:PHE:HB3	1:B:1232:PHE:CE1	2.49	0.48
1:A:82:HIS:HA	1:A:216:LEU:HD21	1.96	0.47
1:B:507:PHE:HB2	1:B:1303:GLU:HG3	1.96	0.47
1:A:624:GLU:HG3	10:A:2285:HOH:O	2.13	0.47
1:B:980:ARG:HD2	10:B:1687:HOH:O	2.13	0.47
1:A:1044:THR:O	1:A:1048:GLN:HG3	2.13	0.47
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.49	0.47
1:B:165:LYS:HG3	1:B:165:LYS:O	2.14	0.47
1:B:391:PRO:HG3	1:B:397:LEU:HD23	1.97	0.47
1:B:358:ILE:CD1	1:B:431:ILE:HG23	2.32	0.47
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.96	0.47
1:B:192:SER:N	1:B:193:PRO:CD	2.78	0.47
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.96	0.47
1:A:267:GLU:HA	1:A:271:LYS:HG2	1.97	0.47
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.48	0.47
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.25	0.47
1:A:322:GLN:O	1:A:412:SER:HB3	2.15	0.47
1:B:680:ARG:HD2	10:B:1560:HOH:O	2.14	0.47
1:A:61:LEU:H	1:A:63:ASP:H	1.63	0.47
1:B:569:LYS:HE3	10:B:1473:HOH:O	2.15	0.46
1:A:506:GLU:CD	1:A:506:GLU:H	2.18	0.46
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.97	0.46
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.23	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.16	0.46
1:B:154:ARG:HD2	1:B:1196:GLU:OE2	2.14	0.46
1:A:154:ARG:HD3	1:A:1196:GLU:CD	2.35	0.46
1:B:216:LEU:HA	1:B:219:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:LYS:HE2	1:A:1172:LYS:HB2	1.57	0.46
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.58	0.46
1:B:802:GLU:OE1	8:B:1335:FYO:HA1	2.15	0.46
1:B:258:VAL:HG22	1:B:264:ILE:HG13	1.97	0.45
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.45
1:A:58:TYR:HE2	1:A:60:ARG:HB2	1.82	0.45
1:B:192:SER:HB2	10:B:1938:HOH:O	2.17	0.45
1:B:192:SER:HA	10:B:1712:HOH:O	2.16	0.45
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.44	0.45
1:B:4:ASP:CG	1:B:5:GLU:H	2.20	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.52	0.45
1:B:394:ARG:HD3	10:B:1527:HOH:O	2.16	0.45
1:B:146:ASN:HD21	1:B:341:GLN:HE22	1.65	0.45
1:A:1287:ASN:ND2	1:A:1289:ASN:CB	2.80	0.44
1:A:723:PHE:CZ	1:A:847:LYS:HE2	2.52	0.44
1:B:428:GLU:HG2	10:B:1742:HOH:O	2.17	0.44
1:A:599:TYR:HA	1:B:599:TYR:HA	2.00	0.44
1:B:552:HIS:HE1	1:B:1172:LYS:HD2	1.82	0.44
1:B:1325:CYS:N	1:B:1326:LYS:CB	2.80	0.44
8:B:1335:FYO:HAH	10:B:2247:HOH:O	2.18	0.43
1:A:1014:LEU:HD23	1:A:1014:LEU:HA	1.86	0.43
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.34	0.43
1:B:701:ALA:CB	1:B:901:CYS:HB3	2.48	0.43
1:A:777:ALA:HB1	1:A:782:VAL:O	2.19	0.43
1:A:256:LYS:HE2	10:A:2057:HOH:O	2.19	0.43
1:A:490:LEU:HB2	1:A:513:LEU:HD22	2.00	0.43
1:A:37:ARG:HD3	1:A:595:ASP:O	2.19	0.43
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.33	0.43
1:A:1251:LYS:HE2	10:A:1924:HOH:O	2.19	0.43
1:B:281:PRO:HB2	1:B:287:LEU:HD13	2.00	0.43
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.54	0.43
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.83	0.43
1:A:325:GLU:HB2	1:A:412:SER:OG	2.19	0.43
1:B:1315:THR:O	1:B:1315:THR:HG23	2.17	0.43
1:B:880:ARG:NH2	8:B:1335:FYO:OAD	2.50	0.43
1:B:508:ARG:O	1:B:512:THR:HG23	2.19	0.43
1:A:441:LEU:HB3	1:A:451:GLU:HB2	2.01	0.42
1:A:97:ARG:NH1	10:A:2131:HOH:O	2.51	0.42
1:B:1011:VAL:CG2	1:B:1014:LEU:HD12	2.48	0.42
1:B:1038:MET:HG3	6:B:1333:MTE:C4	2.49	0.42
1:B:3:ALA:N	10:B:2169:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:TRP:CA	1:A:1329:SER:HB2	2.49	0.42
1:B:112:GLN:HG3	1:B:151:THR:HG22	2.01	0.42
1:B:37:ARG:HD3	1:B:595:ASP:O	2.19	0.42
1:A:541:THR:HG22	1:A:542:TYR:CD1	2.46	0.42
1:A:36:LEU:HD22	1:A:89:GLU:CG	2.47	0.42
1:A:1180:MET:HE3	1:A:1263:PRO:CB	2.42	0.42
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.55	0.42
1:A:337:PHE:O	1:A:338:ALA:C	2.58	0.42
1:B:972:LEU:HA	1:B:972:LEU:HD23	1.81	0.42
1:B:129:ARG:HH11	1:B:129:ARG:HD2	1.67	0.42
1:A:1328:TRP:CB	1:A:1329:SER:HB2	2.46	0.41
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.55	0.41
1:B:337:PHE:CE1	4:B:4005:FAD:C2	3.04	0.41
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.01	0.41
1:B:1151:HIS:CE1	1:B:1251:LYS:HD2	2.55	0.41
1:B:448:GLN:HB2	1:B:477:PHE:CE2	2.54	0.41
1:A:733:GLU:O	1:A:1295:ARG:HD2	2.20	0.41
1:A:1265:PHE:O	1:A:1265:PHE:CG	2.74	0.41
1:A:448:GLN:HB2	1:A:477:PHE:CE2	2.55	0.41
1:B:1186:LEU:HD21	1:B:1254:TYR:HB2	2.02	0.41
1:A:842:PHE:CD2	1:A:918:GLN:HG2	2.54	0.41
1:A:719:LEU:CD1	1:A:860:GLU:HG2	2.51	0.41
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.36	0.41
1:B:109:HIS:CE1	1:B:1189:ALA:HB1	2.56	0.41
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.21	0.41
1:B:752:ILE:HD13	1:B:822:PRO:HB3	2.03	0.41
1:B:91:ILE:HD11	1:B:121:VAL:CG1	2.51	0.41
1:A:290:VAL:HA	1:A:298:SER:O	2.21	0.41
1:A:723:PHE:CE2	1:A:847:LYS:HE2	2.56	0.41
1:B:1204:GLY:HA3	1:B:1209:GLU:OE2	2.21	0.41
1:B:233:ARG:NH1	1:B:680:ARG:HD3	2.36	0.41
1:B:723:PHE:CZ	1:B:847:LYS:HE3	2.56	0.41
1:A:328:ARG:HD2	10:A:1713:HOH:O	2.22	0.40
1:B:100:PRO:O	1:B:104:ARG:HG3	2.21	0.40
1:B:829:ARG:O	1:B:833:MET:HG3	2.21	0.40
1:A:618:LYS:HD3	1:A:690:GLU:HB2	2.03	0.40
1:B:1014:LEU:HD11	8:B:1335:FYO:HAGA	2.03	0.40
1:B:284:ILE:HA	1:B:285:PRO:HD3	1.99	0.40
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.22	0.40
1:B:374:ILE:HG21	1:B:398:LEU:HD13	2.03	0.40
1:B:741:HIS:HA	1:B:911:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:HD2	10:A:2013:HOH:O	2.21	0.40
1:B:734:LEU:HD21	1:B:921:PHE:CE2	2.57	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	1285/1332 (96%)	1220 (95%)	53 (4%)	12 (1%)	17	15
1	B	1283/1332 (96%)	1227 (96%)	45 (4%)	11 (1%)	17	15
All	All	2568/2664 (96%)	2447 (95%)	98 (4%)	23 (1%)	17	15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	1319	THR
1	A	1329	SER
1	B	4	ASP
1	B	20	ALA
1	A	4	ASP
1	A	61	LEU
1	A	541	THR
1	B	62	GLN
1	B	1008	SER
1	B	1290	THR
1	B	1325	CYS
1	A	445	GLY
1	A	912	ARG
1	A	1008	SER
1	B	912	ARG

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Mol	Chain	Res	Type
1	B	397	LEU
1	B	797	GLY
1	A	797	GLY
1	A	947	TYR
1	A	1139	GLY
1	B	947	TYR
1	B	1139	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1097/1128 (97%)	1051 (96%)	46 (4%)	30	35
1	B	1096/1128 (97%)	1062 (97%)	34 (3%)	40	48
All	All	2193/2256 (97%)	2113 (96%)	80 (4%)	35	42

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	61	LEU
1	A	100	PRO
1	A	154	ARG
1	A	225	LYS
1	A	256	LYS
1	A	271	LYS
1	A	312	LEU
1	A	323	LYS
1	A	348	LEU
1	A	398	LEU
1	A	401	GLU
1	A	433	LYS
1	A	476	LYS
1	A	499	ASP
1	A	505	ILE

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Mol	Chain	Res	Type
1	A	537	LYS
1	A	538	LEU
1	A	541	THR
1	A	562	GLU
1	A	569	LYS
1	A	600	GLU
1	A	651	ASP
1	A	659	THR
1	A	684	VAL
1	A	699	GLU
1	A	743	TYR
1	A	744	LEU
1	A	857	VAL
1	A	890	LYS
1	A	911	PHE
1	A	982	SER
1	A	983	GLU
1	A	992	CYS
1	A	1106	LYS
1	A	1107	LYS
1	A	1143	GLU
1	A	1172	LYS
1	A	1203	LEU
1	A	1208	LEU
1	A	1239	PHE
1	A	1262	PRO
1	A	1287	ASN
1	A	1317	CYS
1	A	1326	LYS
1	A	1331	ARG
1	B	4	ASP
1	B	60	ARG
1	B	93	SER
1	B	97	ARG
1	B	154	ARG
1	B	194	SER
1	B	220	LYS
1	B	314	GLU
1	B	321	THR
1	B	332	GLU
1	B	335	ARG
1	B	375	VAL

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Mol	Chain	Res	Type
1	B	433	LYS
1	B	476	LYS
1	B	481	LYS
1	B	497	SER
1	B	543	THR
1	B	565	ASN
1	B	600	GLU
1	B	743	TYR
1	B	911	PHE
1	B	948	LYS
1	B	1055	LYS
1	B	1143	GLU
1	B	1145	ASN
1	B	1188	PRO
1	B	1208	LEU
1	B	1239	PHE
1	B	1286	THR
1	B	1315	THR
1	B	1317	CYS
1	B	1326	LYS
1	B	1330	LEU
1	B	1332	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	473	GLN
1	A	567	GLN
1	A	650	ASN
1	A	1145	ASN
1	A	1284	GLN
1	A	1285	HIS
1	A	1287	ASN
1	B	62	GLN
1	B	71	ASN
1	B	131	GLN
1	B	146	ASN
1	B	252	HIS
1	B	333	GLN
1	B	552	HIS
1	B	565	ASN

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Mol	Chain	Res	Type
1	B	626	GLN
1	B	650	ASN
1	B	976	GLN
1	B	1088	GLN
1	B	1145	ASN
1	B	1284	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - 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	$\# Z  > 2$
5	BCT	A	1904	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	A	3001	1	0,4,4	0.00	-	-		
9	GOL	B	1338	-	5,5,5	0.60	0	5,5,5	1.85	1 (20%)
6	MTE	B	1333	7	21,26,26	1.34	4 (19%)	21,40,40	3.12	11 (52%)
6	MTE	A	1333	7	21,26,26	1.14	1 (4%)	21,40,40	2.38	10 (47%)
4	FAD	A	3005	-	51,58,58	1.55	8 (15%)	60,89,89	2.23	14 (23%)
9	GOL	B	1336	-	5,5,5	0.61	0	5,5,5	1.89	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FES	B	4001	1	0,4,4	0.00	-	-		
5	BCT	B	1904	-	0,3,3	0.00	-	0,3,3	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	-		
4	FAD	B	4005	-	51,58,58	1.78	10 (19%)	60,89,89	1.64	10 (16%)
8	FYO	A	1335	7	22,24,24	4.17	10 (45%)	23,34,34	6.49	17 (73%)
7	MOS	B	1334	8,6	0,2,3	0.00	-	-		
7	MOS	A	1334	8,6	0,2,3	0.00	-	-		
8	FYO	B	1335	7	22,24,24	4.07	12 (54%)	23,34,34	6.22	15 (65%)
2	FES	A	3002	1	0,4,4	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	A	3001	1	-	-	0/1/1/1
9	GOL	B	1338	-	-	4/4/4/4	-
6	MTE	B	1333	7	-	2/6/34/34	0/3/3/3
6	MTE	A	1333	7	-	3/6/34/34	0/3/3/3
4	FAD	A	3005	-	-	6/30/50/50	0/6/6/6
9	GOL	B	1336	-	-	2/4/4/4	-
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	B	4002	1	-	-	0/1/1/1
4	FAD	B	4005	-	-	6/30/50/50	0/6/6/6
8	FYO	A	1335	7	-	0/4/22/22	0/3/3/3
8	FYO	B	1335	7	-	0/4/22/22	0/3/3/3
2	FES	A	3002	1	-	-	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1335	FYO	CAR-NAL	10.66	1.50	1.35
8	A	1335	FYO	CAR-NAL	9.74	1.49	1.35
8	A	1335	FYO	OAC-CAP	8.04	1.39	1.23
8	B	1335	FYO	OAC-CAP	7.20	1.37	1.23
8	A	1335	FYO	OAB-CAO	7.10	1.38	1.24
8	A	1335	FYO	CAG-CAS	-6.22	1.39	1.50
8	B	1335	FYO	OAB-CAO	6.14	1.36	1.24
8	B	1335	FYO	CAI-CAR	5.85	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1335	FYO	OAD-CAQ	5.78	1.39	1.24
8	A	1335	FYO	CAR-CAE	5.67	1.61	1.44
8	A	1335	FYO	OAD-CAQ	5.56	1.38	1.24
8	B	1335	FYO	CAG-CAS	-5.53	1.41	1.50
8	B	1335	FYO	CAR-CAE	5.50	1.60	1.44
4	A	3005	FAD	C1'-N10	5.13	1.53	1.48
4	B	4005	FAD	C10-N1	4.51	1.39	1.33
4	B	4005	FAD	C2A-N3A	4.45	1.39	1.32
8	A	1335	FYO	CAI-CAR	4.39	1.44	1.39
4	A	3005	FAD	C4X-N5	4.28	1.39	1.33
8	A	1335	FYO	CAQ-NAL	4.12	1.40	1.33
4	B	4005	FAD	C1'-N10	4.10	1.52	1.48
4	B	4005	FAD	C4X-N5	3.72	1.38	1.33
4	B	4005	FAD	C9A-N10	3.63	1.43	1.38
8	A	1335	FYO	CAE-NAA	-3.46	1.06	1.14
4	B	4005	FAD	C4-N3	3.43	1.39	1.33
4	B	4005	FAD	C2A-N1A	3.11	1.39	1.33
6	B	1333	MTE	C6-N5	3.08	1.49	1.45
4	A	3005	FAD	C4-N3	3.07	1.38	1.33
4	B	4005	FAD	C4X-C10	3.06	1.41	1.38
8	A	1335	FYO	NAN-NAJ	2.93	1.43	1.37
4	B	4005	FAD	C5X-N5	2.86	1.40	1.35
6	A	1333	MTE	C4-N3	2.73	1.37	1.33
4	B	4005	FAD	O4'-C4'	-2.72	1.37	1.43
4	A	3005	FAD	C2A-N3A	2.60	1.36	1.32
6	B	1333	MTE	O4-C4	2.56	1.31	1.24
4	A	3005	FAD	O3B-C3B	-2.44	1.37	1.43
8	B	1335	FYO	CAQ-NAL	2.39	1.37	1.33
8	B	1335	FYO	CAV-NAN	2.37	1.36	1.33
6	B	1333	MTE	C10-N1	2.36	1.39	1.34
8	B	1335	FYO	CAU-NAJ	2.36	1.36	1.33
8	B	1335	FYO	CAF-CAS	2.32	1.40	1.35
4	A	3005	FAD	C9A-N10	2.22	1.41	1.38
4	A	3005	FAD	C2A-N1A	2.13	1.37	1.33
8	B	1335	FYO	CAG-CAP	-2.10	1.41	1.48
4	A	3005	FAD	C4X-C10	2.06	1.40	1.38
6	B	1333	MTE	C2-N2	2.03	1.38	1.33

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1335	FYO	CAR-CAE-NAA	-19.41	124.36	177.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1335	FYO	CAR-CAE-NAA	-18.33	127.32	177.46
8	A	1335	FYO	CAE-CAR-NAL	14.72	126.60	115.29
8	A	1335	FYO	CAV-NAM-CAU	12.46	108.02	101.04
8	B	1335	FYO	CAV-NAM-CAU	10.90	107.14	101.04
8	B	1335	FYO	CAE-CAR-NAL	8.92	122.14	115.29
8	B	1335	FYO	CAI-CAR-NAL	-8.22	115.18	123.61
4	A	3005	FAD	C1'-N10-C9A	7.79	124.42	118.29
8	A	1335	FYO	CAI-CAR-NAL	-7.38	116.05	123.61
8	B	1335	FYO	CAT-CAV-NAM	6.80	132.21	123.71
6	B	1333	MTE	O3'-C7-C6	6.49	113.29	108.96
4	A	3005	FAD	C4-N3-C2	6.46	120.60	115.14
8	B	1335	FYO	CAQ-NAL-CAR	6.33	120.42	115.79
8	A	1335	FYO	OAB-CAO-CAF	-6.21	116.77	125.47
6	B	1333	MTE	C4-N3-C2	5.77	125.09	115.93
4	B	4005	FAD	C4X-N5-C5X	5.74	122.50	116.77
8	B	1335	FYO	CAF-CAO-NAK	5.53	121.81	115.14
4	A	3005	FAD	C5X-C9A-N10	5.49	121.70	117.72
8	B	1335	FYO	CAI-CAT-CAV	-5.36	112.17	120.05
8	B	1335	FYO	CAP-NAK-CAO	-5.36	121.36	127.22
8	A	1335	FYO	CAP-NAK-CAO	-5.20	121.53	127.22
4	B	4005	FAD	N3A-C2A-N1A	-5.10	120.71	128.68
6	A	1333	MTE	P-O4'-C4'	5.07	132.25	118.30
4	A	3005	FAD	N3A-C2A-N1A	-5.05	120.79	128.68
6	B	1333	MTE	O3'-C7-N8	5.02	113.73	108.57
6	B	1333	MTE	C4-C9-C10	5.01	119.02	114.57
8	A	1335	FYO	CAV-NAN-NAJ	4.93	108.85	104.70
8	A	1335	FYO	CAT-CAV-NAM	4.92	129.85	123.71
6	A	1333	MTE	C4-N3-C2	4.74	123.47	115.93
4	A	3005	FAD	C4X-N5-C5X	4.56	121.32	116.77
6	B	1333	MTE	N3-C2-N1	-4.31	118.66	125.42
4	A	3005	FAD	C4X-C4-N3	-4.11	117.81	123.43
8	A	1335	FYO	CAI-CAT-CAV	-4.04	114.11	120.05
4	B	4005	FAD	C10-C4X-N5	-4.03	118.47	121.26
8	A	1335	FYO	CAF-CAO-NAK	4.00	119.97	115.14
6	B	1333	MTE	P-O4'-C4'	3.99	129.29	118.30
9	B	1336	GOL	O3-C3-C2	-3.97	91.19	110.20
8	B	1335	FYO	CAV-NAN-NAJ	3.60	107.73	104.70
4	A	3005	FAD	C9A-N10-C10	-3.43	117.42	121.91
6	B	1333	MTE	N2-C2-N1	3.39	122.52	117.25
8	B	1335	FYO	CAT-CAV-NAN	-3.34	118.46	124.12
8	A	1335	FYO	CAQ-NAL-CAR	3.31	118.21	115.79
8	B	1335	FYO	CAH-CAT-CAI	3.30	123.19	118.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1333	MTE	C4-C9-C10	3.18	117.39	114.57
4	A	3005	FAD	C10-C4X-N5	-3.17	119.07	121.26
6	A	1333	MTE	O3'-C7-N8	3.16	111.81	108.57
8	B	1335	FYO	CAH-CAT-CAV	3.12	124.64	120.05
8	A	1335	FYO	CAT-CAI-CAR	3.12	121.53	118.98
6	B	1333	MTE	O3P-P-O4'	-2.94	98.90	106.73
8	A	1335	FYO	CAH-CAT-CAV	2.94	124.37	120.05
6	A	1333	MTE	C10-N8-C7	-2.85	118.08	123.67
4	A	3005	FAD	O3B-C3B-C4B	-2.79	102.98	111.05
4	B	4005	FAD	C4-N3-C2	2.76	117.47	115.14
4	A	3005	FAD	C4A-C5A-N7A	-2.71	106.57	109.40
8	A	1335	FYO	OAB-CAO-NAK	2.70	123.27	119.31
4	A	3005	FAD	C6-C5X-C9A	2.68	122.57	119.05
8	B	1335	FYO	OAB-CAO-CAF	-2.67	121.73	125.47
4	A	3005	FAD	C9A-C5X-N5	-2.64	118.24	122.36
8	A	1335	FYO	CAI-CAR-CAE	-2.62	113.83	119.82
6	A	1333	MTE	O2P-P-O4'	-2.61	99.80	106.73
4	B	4005	FAD	C4'-C3'-C2'	-2.60	107.94	113.36
8	B	1335	FYO	CAG-CAP-NAK	2.49	119.19	116.82
6	B	1333	MTE	C9-C4-N3	-2.48	116.96	124.01
4	B	4005	FAD	O3'-C3'-C4'	2.39	114.58	108.81
6	A	1333	MTE	C9-C4-N3	-2.37	117.28	124.01
6	A	1333	MTE	N3-C2-N1	-2.34	121.74	125.42
4	B	4005	FAD	O4B-C1B-C2B	-2.28	103.59	106.93
4	B	4005	FAD	C1'-N10-C9A	2.28	120.08	118.29
6	A	1333	MTE	N2-C2-N1	2.27	120.79	117.25
8	A	1335	FYO	CAG-CAP-NAK	2.27	118.98	116.82
6	B	1333	MTE	C4-C9-N5	2.24	121.00	119.12
4	B	4005	FAD	C5'-C4'-C3'	2.20	116.45	112.20
8	A	1335	FYO	CAH-CAT-CAI	2.17	121.52	118.31
4	B	4005	FAD	C4X-C4-N3	-2.13	120.52	123.43
9	B	1338	GOL	C3-C2-C1	-2.12	103.47	111.70
6	A	1333	MTE	O2P-P-O1P	2.06	118.75	110.68
4	A	3005	FAD	C7-C6-C5X	-2.06	118.31	121.22
6	B	1333	MTE	C2-N1-C10	2.05	119.14	114.54
4	A	3005	FAD	P-O3P-PA	-2.03	125.85	132.83

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1333	MTE	C4'-O4'-P-O2P

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Mol	Chain	Res	Type	Atoms
6	A	1333	MTE	C4'-O4'-P-O3P
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
9	B	1336	GOL	C1-C2-C3-O3
4	B	4005	FAD	N10-C1'-C2'-O2'
4	B	4005	FAD	N10-C1'-C2'-C3'
4	B	4005	FAD	C2'-C3'-C4'-C5'
9	B	1336	GOL	O2-C2-C3-O3
4	B	4005	FAD	C2'-C3'-C4'-O4'
4	B	4005	FAD	O3'-C3'-C4'-O4'
6	B	1333	MTE	C3'-C4'-O4'-P
9	B	1338	GOL	O1-C1-C2-O2
9	B	1338	GOL	O2-C2-C3-O3
4	A	3005	FAD	C2'-C3'-C4'-O4'
6	A	1333	MTE	C3'-C4'-O4'-P
4	A	3005	FAD	C2'-C3'-C4'-C5'
6	B	1333	MTE	C4'-O4'-P-O3P
4	B	4005	FAD	O3'-C3'-C4'-C5'
9	B	1338	GOL	O1-C1-C2-C3
9	B	1338	GOL	C1-C2-C3-O3
4	A	3005	FAD	O3'-C3'-C4'-O4'

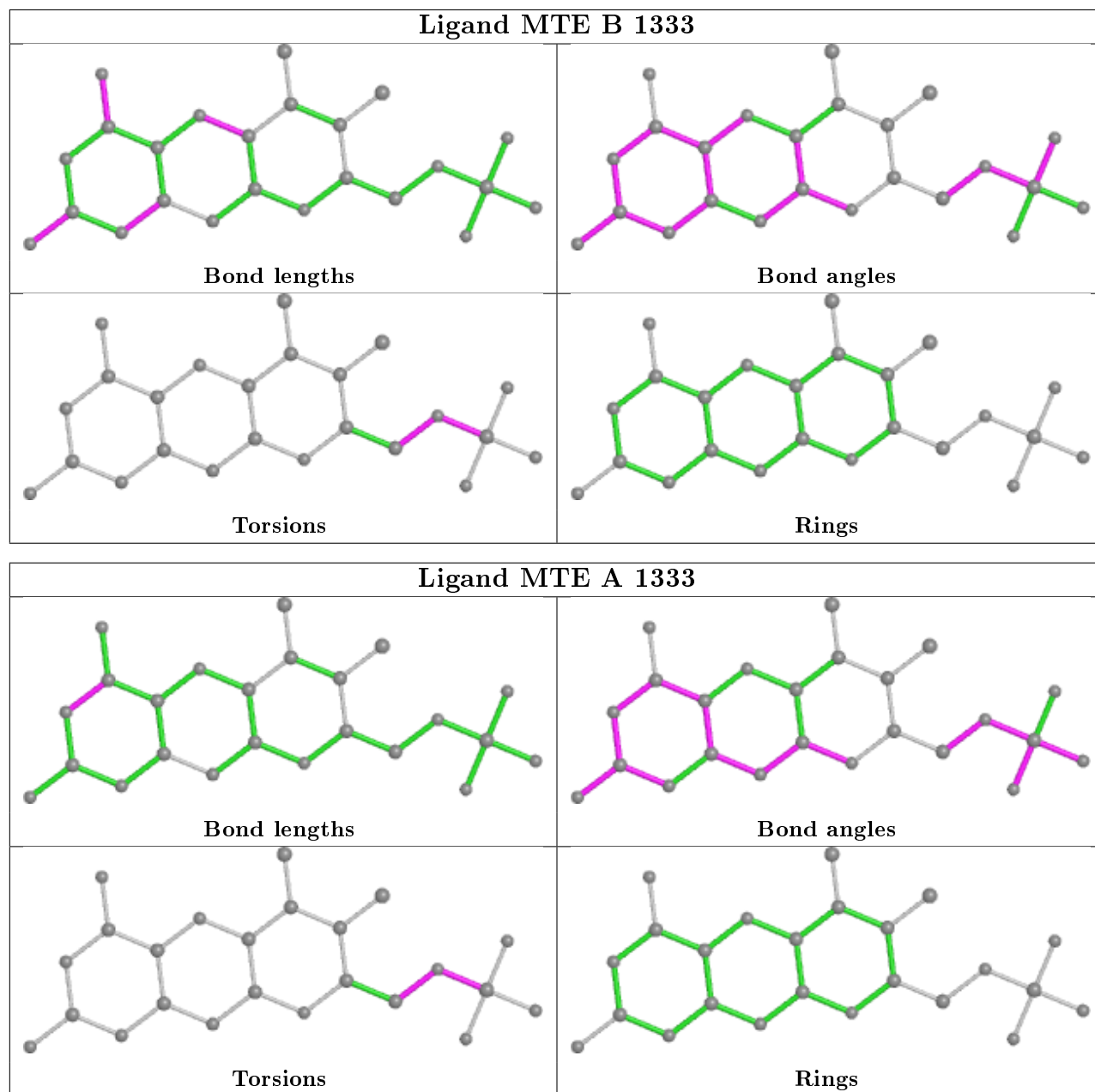
There are no ring outliers.

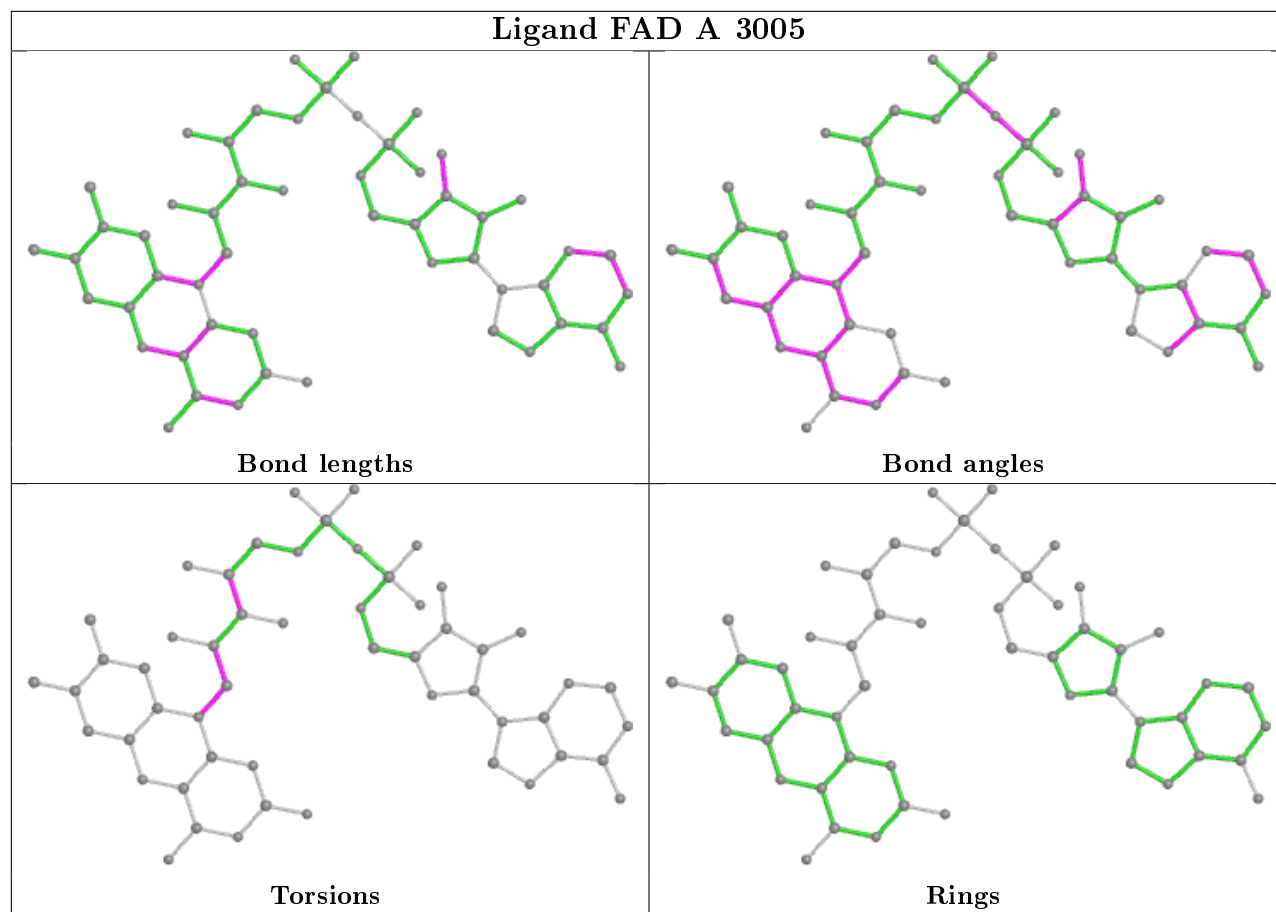
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1338	GOL	2	0
6	B	1333	MTE	1	0
6	A	1333	MTE	1	0
4	A	3005	FAD	1	0
4	B	4005	FAD	2	0
8	A	1335	FYO	2	0
7	B	1334	MOS	1	0
7	A	1334	MOS	1	0
8	B	1335	FYO	5	0

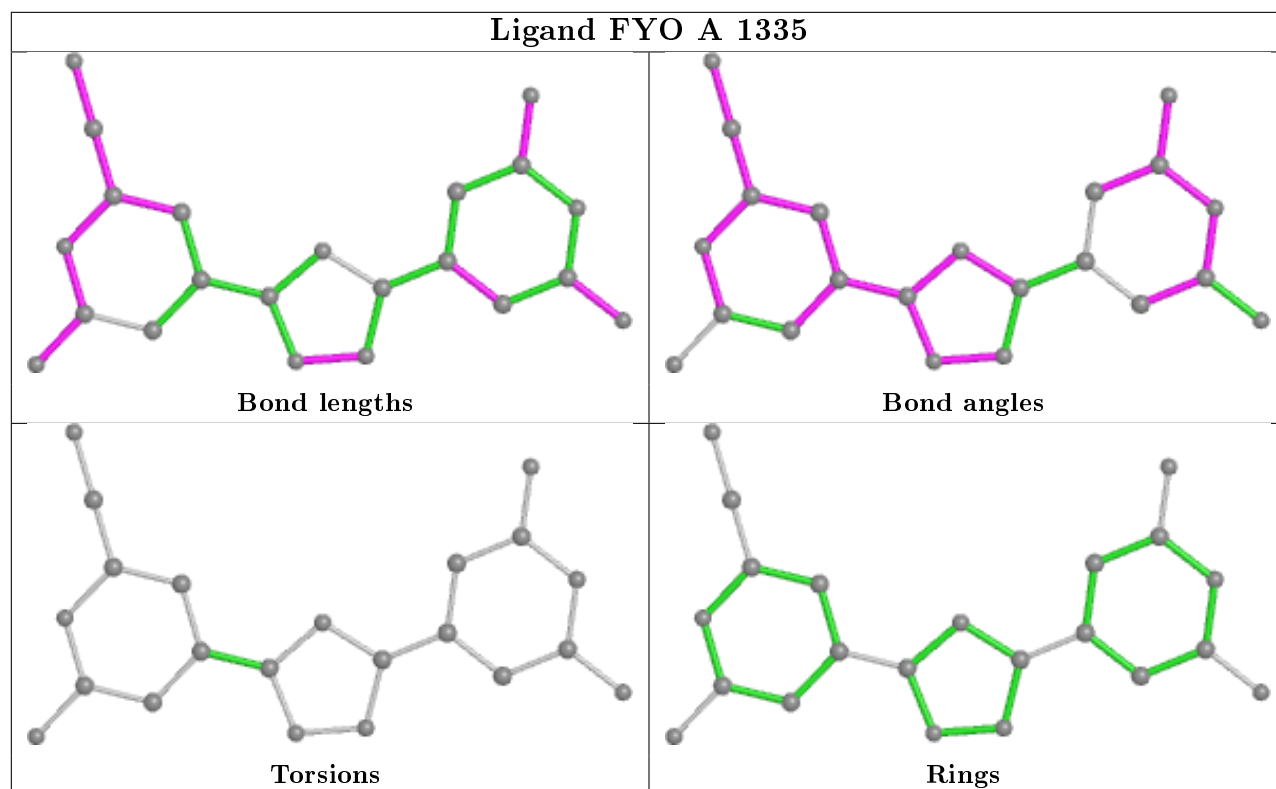
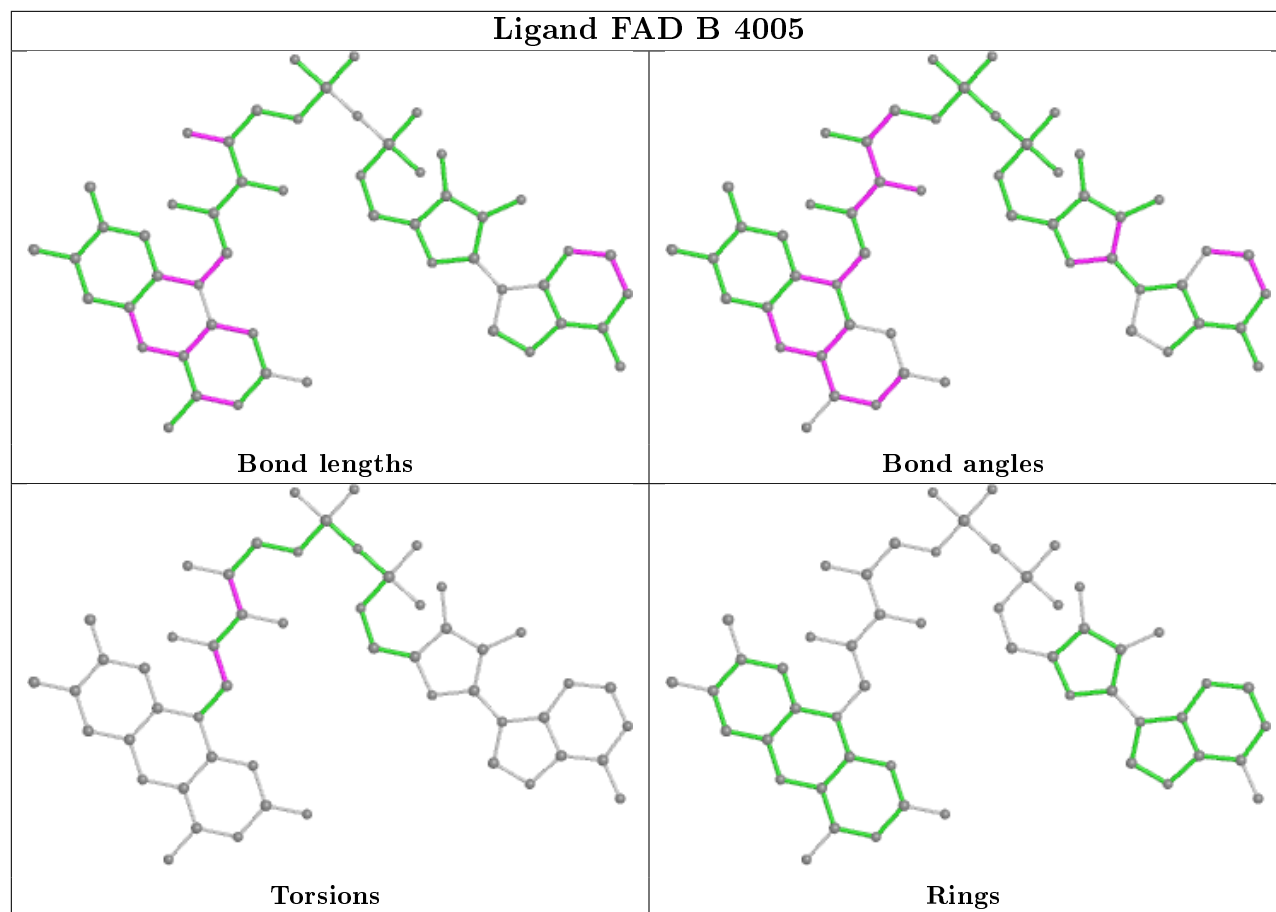
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

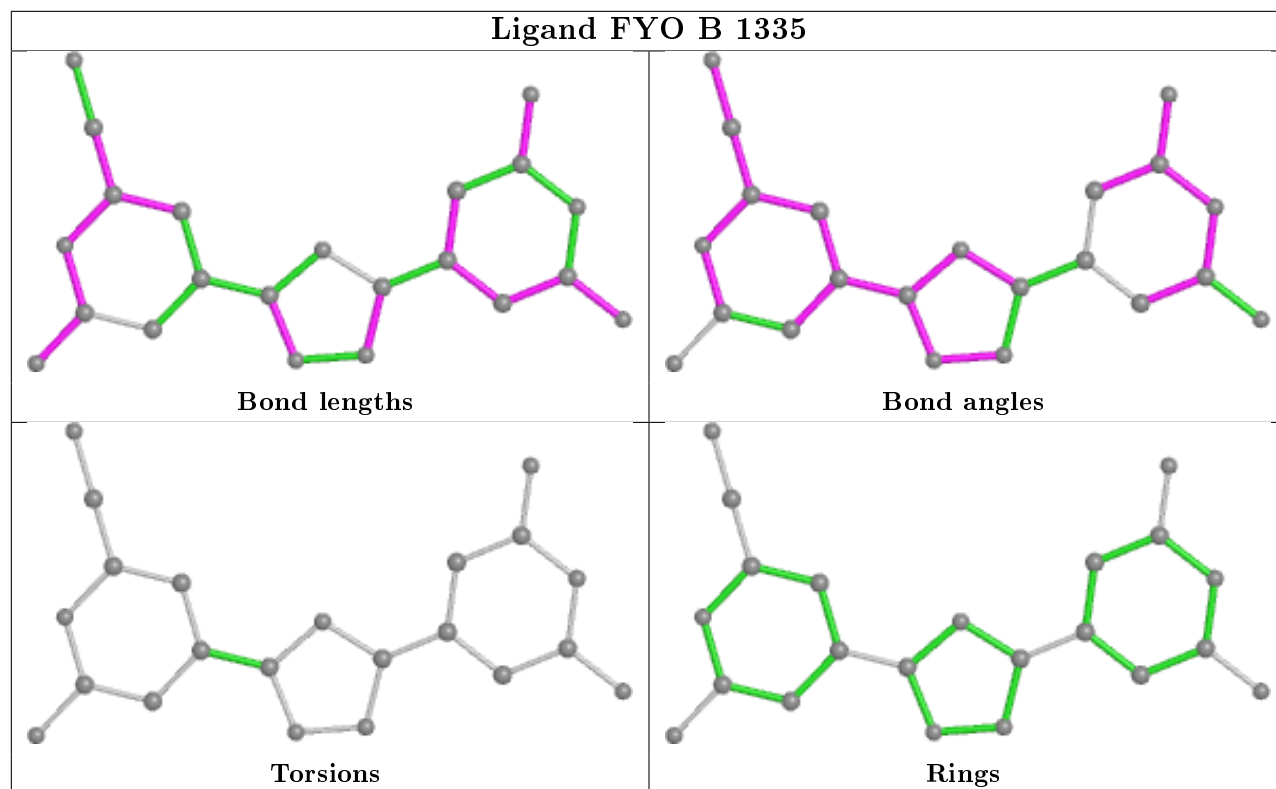
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1293/1332 (97%)	-0.18	28 (2%) 62 62	12, 25, 44, 85	0
1	B	1291/1332 (96%)	-0.20	28 (2%) 62 62	13, 25, 45, 72	0
All	All	2584/2664 (96%)	-0.19	56 (2%) 62 62	12, 25, 45, 85	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	8.9
1	B	1324	ASN	8.3
1	A	538	LEU	8.1
1	A	1320	GLY	8.0
1	B	1325	CYS	7.2
1	A	1319	THR	6.7
1	B	1286	THR	5.7
1	B	1287	ASN	5.7
1	A	530	ASP	5.7
1	A	540	PRO	5.1
1	A	1288	ASN	5.0
1	A	1287	ASN	5.0
1	B	552	HIS	4.7
1	A	1318	VAL	4.7
1	B	1288	ASN	4.7
1	A	537	LYS	4.6
1	B	1318	VAL	4.5
1	B	4	ASP	4.2
1	B	565	ASN	4.0
1	A	565	ASN	3.9
1	A	60	ARG	3.8
1	B	566	GLY	3.8
1	A	552	HIS	3.7
1	B	192	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	566	GLY	3.6
1	B	540	PRO	3.6
1	B	60	ARG	3.6
1	B	1289	ASN	3.5
1	B	221	ASP	3.5
1	A	543	THR	2.9
1	A	529	LYS	2.9
1	A	564	PRO	2.8
1	A	1329	SER	2.8
1	A	1111	GLY	2.8
1	B	1111	GLY	2.8
1	B	222	VAL	2.7
1	A	539	ASP	2.7
1	A	1286	THR	2.5
1	A	1290	THR	2.5
1	B	498	PRO	2.5
1	B	1326	LYS	2.5
1	A	551	LYS	2.4
1	B	551	LYS	2.4
1	A	61	LEU	2.3
1	B	165	LYS	2.3
1	A	703	LYS	2.3
1	A	705	ASN	2.2
1	B	835	ILE	2.2
1	B	377	ARG	2.2
1	A	1266	LEU	2.2
1	B	63	ASP	2.1
1	A	318	LYS	2.1
1	B	537	LYS	2.1
1	B	553	PRO	2.0
1	B	61	LEU	2.0
1	A	378	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

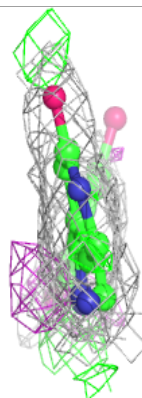
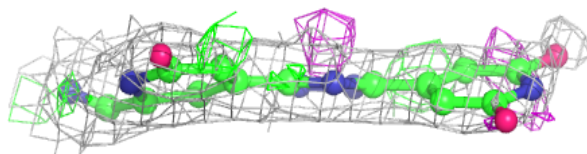
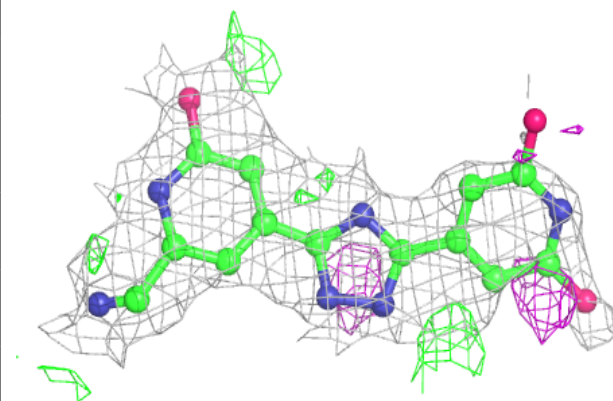
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	FYO	A	1335	22/22	0.85	0.20	25,41,59,61	0
9	GOL	B	1338	6/6	0.88	0.17	38,38,41,44	0
8	FYO	B	1335	22/22	0.89	0.16	20,37,60,65	0
9	GOL	B	1336	6/6	0.90	0.21	22,24,29,36	0
3	CA	A	1336	1/1	0.97	0.06	38,38,38,38	0
4	FAD	A	3005	53/53	0.97	0.09	15,23,26,29	0
5	BCT	A	1904	4/4	0.98	0.10	24,24,24,25	0
4	FAD	B	4005	53/53	0.98	0.09	16,22,26,31	0
5	BCT	B	1904	4/4	0.99	0.08	18,19,20,20	0
2	FES	B	4002	4/4	0.99	0.06	14,15,16,17	0
3	CA	B	4008	1/1	0.99	0.07	21,21,21,21	0
6	MTE	A	1333	24/24	0.99	0.10	12,18,20,23	0
6	MTE	B	1333	24/24	0.99	0.08	14,16,18,21	0
3	CA	A	3008	1/1	0.99	0.10	25,25,25,25	0
2	FES	A	3002	4/4	0.99	0.07	16,17,17,18	0
3	CA	B	1337	1/1	0.99	0.07	34,34,34,34	0
2	FES	B	4001	4/4	1.00	0.06	15,17,18,18	0
7	MOS	A	1334	3/4	1.00	0.07	22,22,22,24	0
7	MOS	B	1334	3/4	1.00	0.06	18,18,20,20	0
2	FES	A	3001	4/4	1.00	0.06	16,17,18,19	0

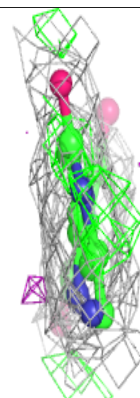
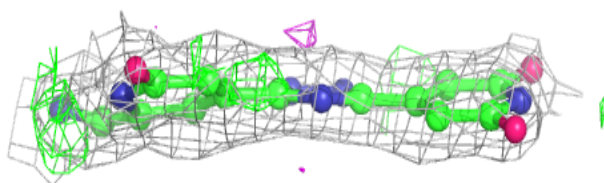
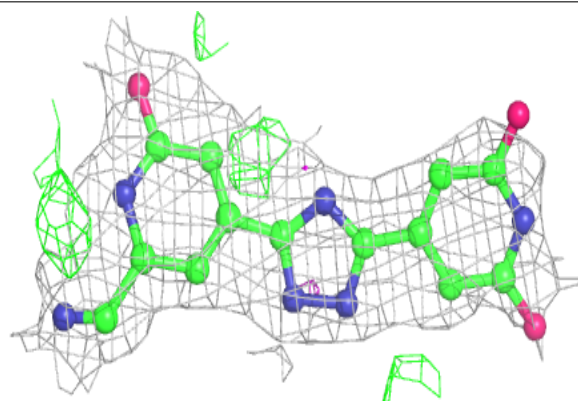
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FYO 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)

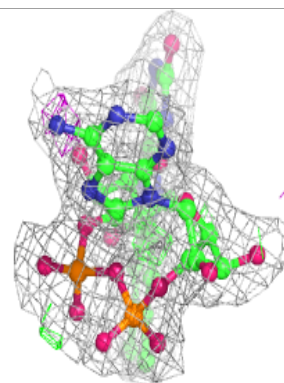
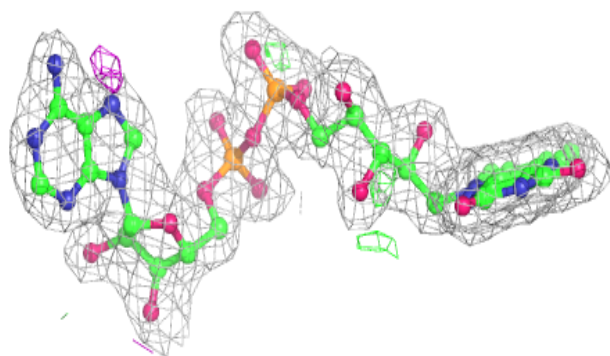
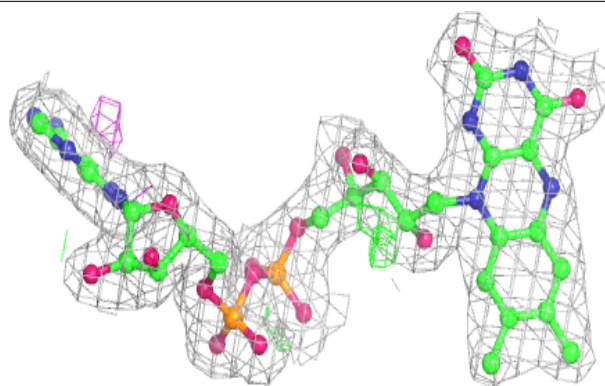
**Electron density around FYO B 1335:**

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

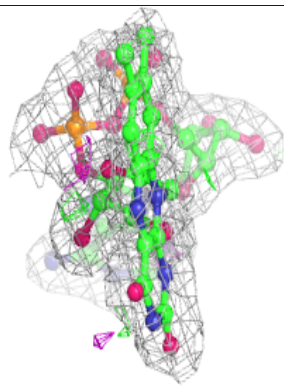
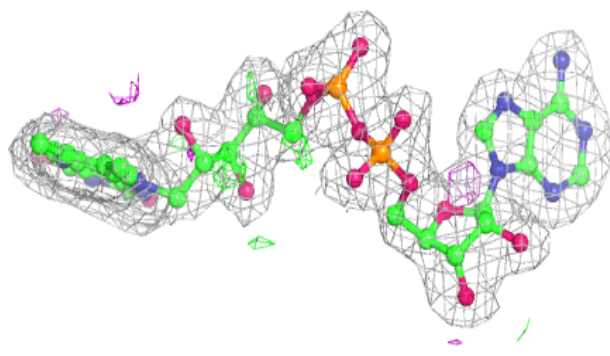
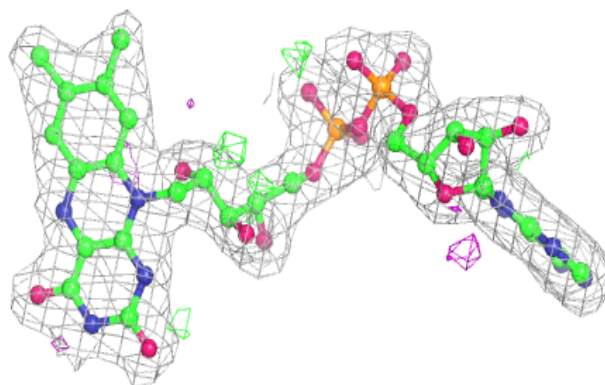


**Electron density around FAD A 3005:**

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

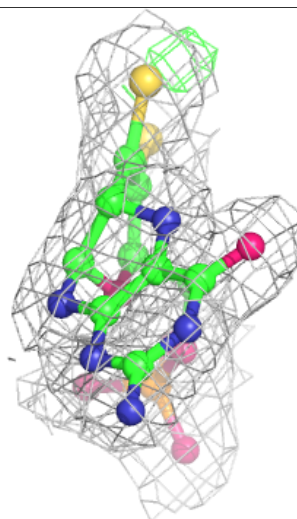
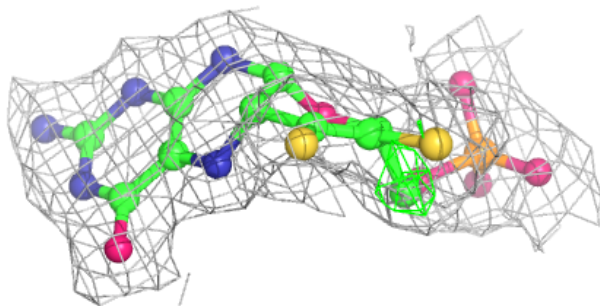
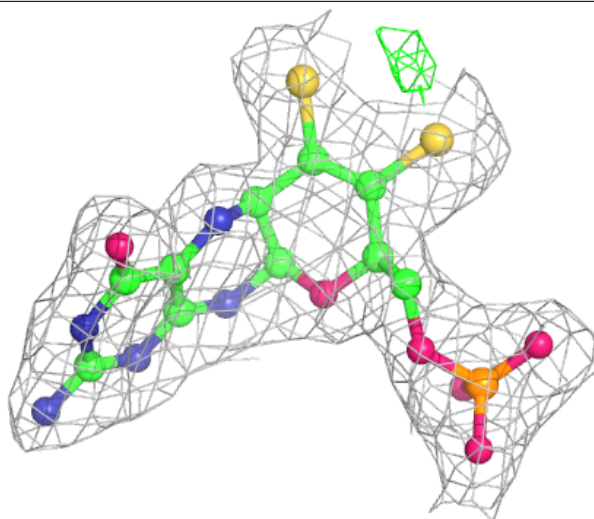
**Electron density around FAD B 4005:**

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



**Electron density around MTE A 1333:**

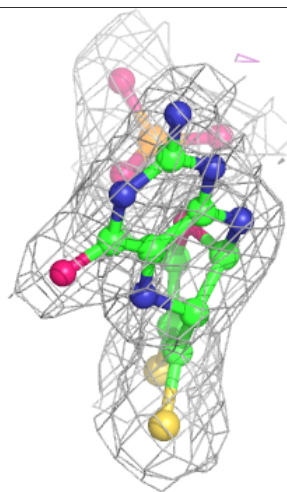
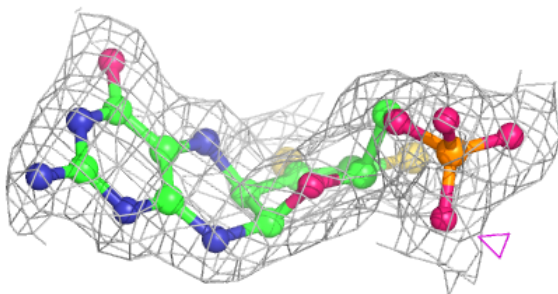
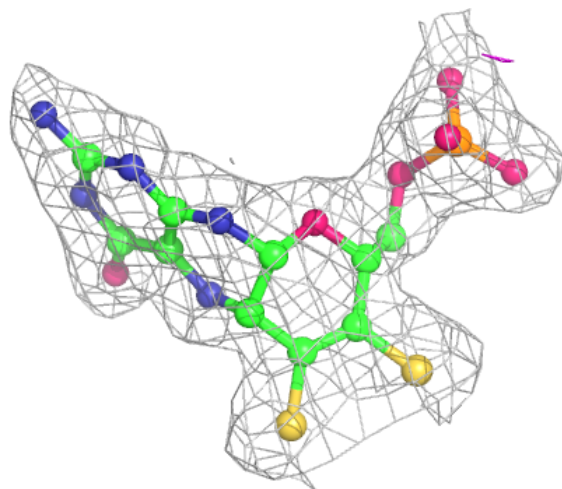
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MTE B 1333:**

$2mF_o-DF_c$  (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.