



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:00 pm BST

PDB ID : 3NS1  
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with 6-Mercaptopurine  
Authors : Cao, H.; Paufl, J.M.; Hille, R.  
Deposited on : 2010-07-01  
Resolution : 2.60 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.

---

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

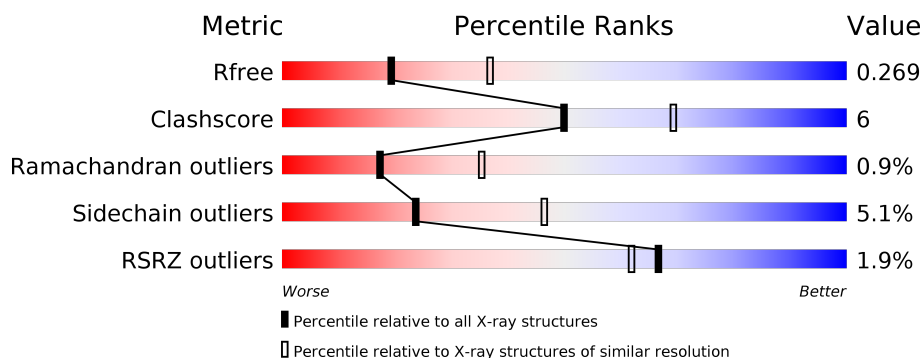
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	164	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	J	164	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	305	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
2	K	305	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>.</div> </div> </div>
3	C	755	<div> <div></div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
3	L	755	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>

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
7	MOS	C	1327	-	-	X	-
7	MOS	L	1327	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19357 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	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			
1	J	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

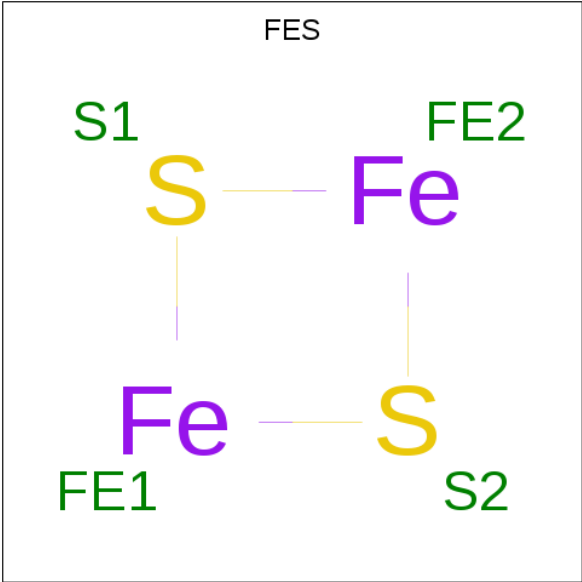
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	K	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called Xanthine dehydrogenase/oxidase.

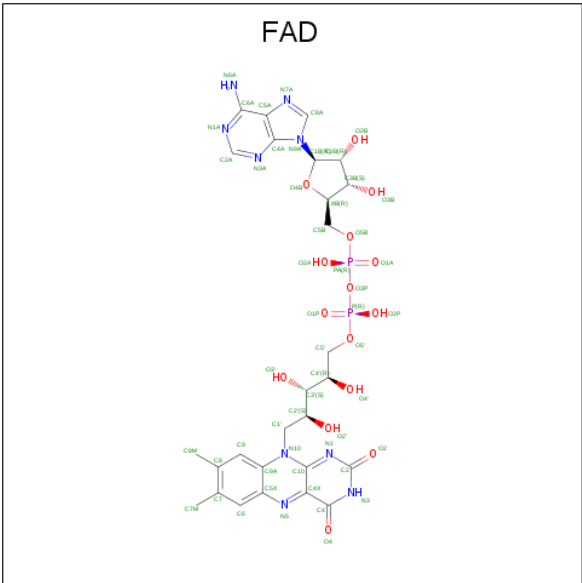
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



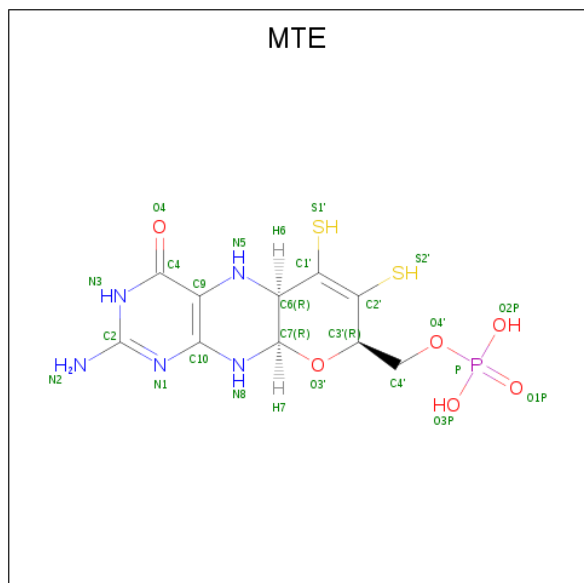
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

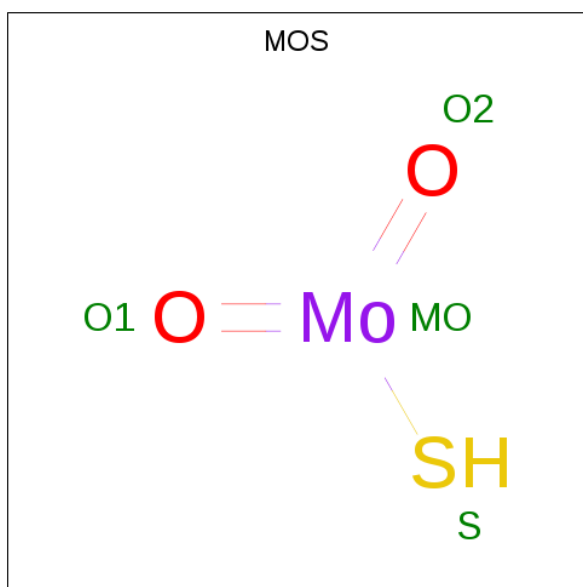
- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

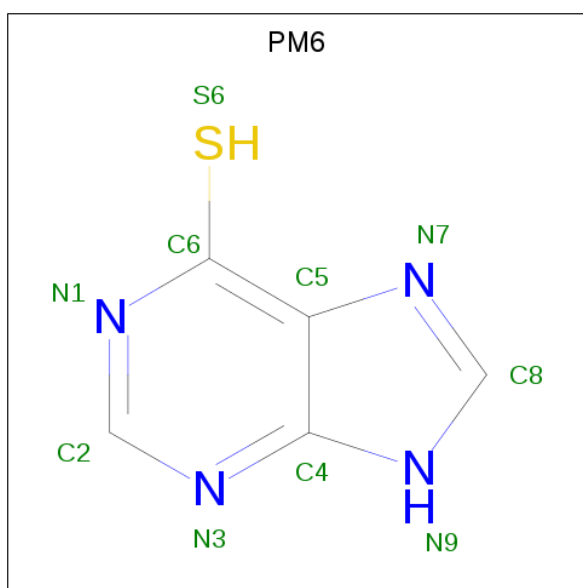
- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P S<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
7	L	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is 9H-purine-6-thiol (three-letter code: PM6) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	S	0	0
			10	5	4	1		
8	L	1	Total	C	N	S	0	0
			10	5	4	1		

- Molecule 9 is water.

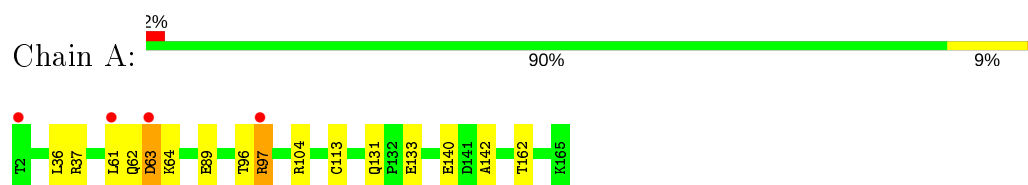
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total 24	O 24	0	0
9	B	15	Total 15	O 15	0	0
9	C	120	Total 120	O 120	0	0
9	J	14	Total 14	O 14	0	0
9	K	21	Total 21	O 21	0	0
9	L	93	Total 93	O 93	0	0



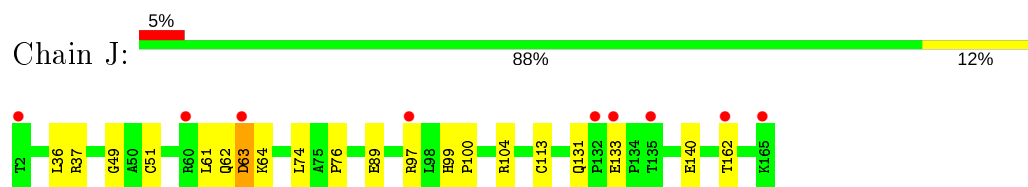
### 3 Residue-property plots [i](#)

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

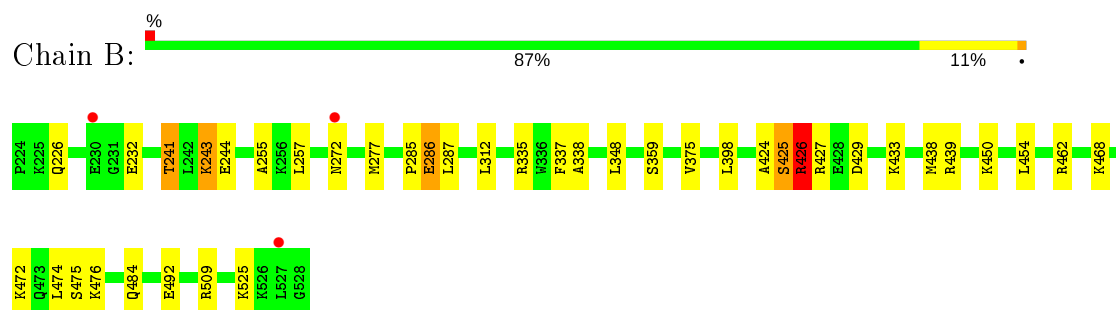
- Molecule 1: Xanthine dehydrogenase/oxidase



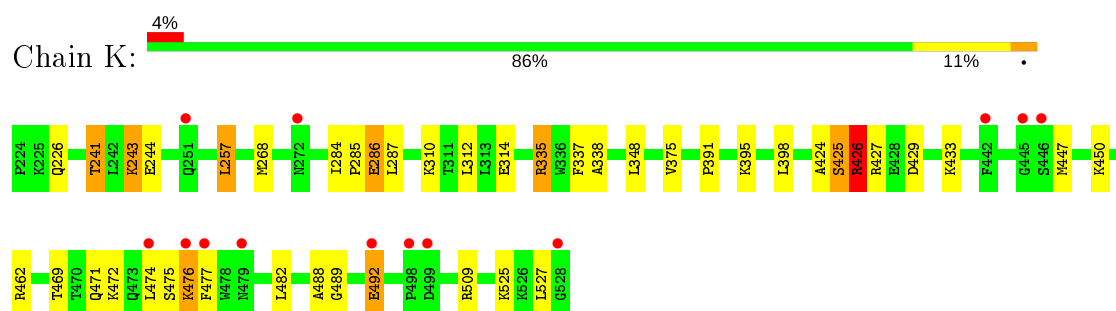
- Molecule 1: Xanthine dehydrogenase/oxidase



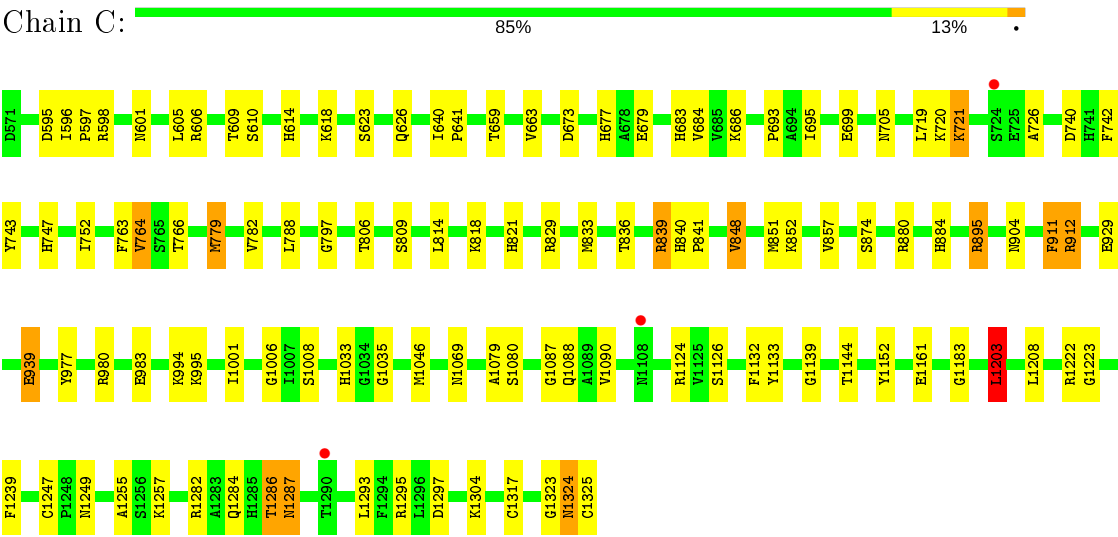
- Molecule 2: Xanthine dehydrogenase/oxidase



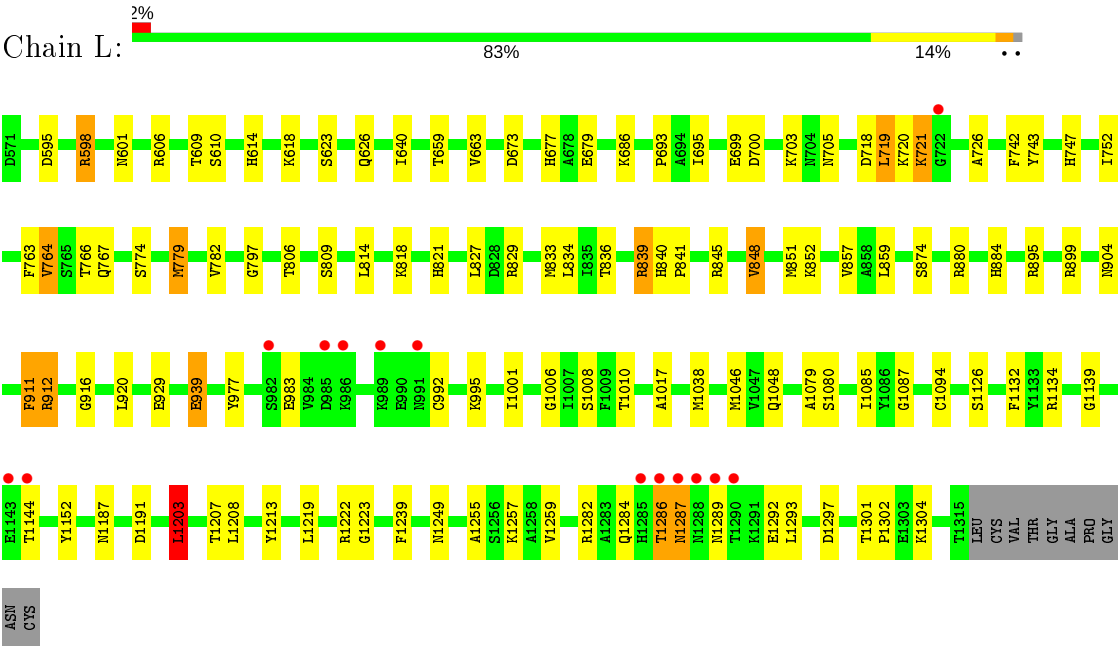
- Molecule 2: Xanthine dehydrogenase/oxidase



- Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.64Å 73.93Å 140.35Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	45.50 – 2.60 45.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.4 (45.50-2.60) 92.4 (45.52-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.217 , 0.269 0.218 , 0.269	Depositor DCC
$R_{free}$ test set	3922 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: MOS, PM6, FES, 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	0.80	0/1277	0.82	2/1723 (0.1%)
1	J	0.81	0/1277	0.82	1/1723 (0.1%)
2	B	0.69	0/2438	0.77	3/3290 (0.1%)
2	K	0.74	0/2438	0.75	2/3290 (0.1%)
3	C	0.80	1/5951 (0.0%)	0.83	6/8061 (0.1%)
3	L	0.81	3/5888 (0.1%)	0.80	5/7974 (0.1%)
All	All	0.79	4/19269 (0.0%)	0.80	19/26061 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	992	CYS	CB-SG	-6.02	1.72	1.82
3	C	699	GLU	CG-CD	5.88	1.60	1.51
3	L	699	GLU	CG-CD	5.87	1.60	1.51
3	L	1094	CYS	CB-SG	5.63	1.91	1.82

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	839	ARG	NE-CZ-NH2	-7.82	116.39	120.30
3	C	839	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	104	ARG	NE-CZ-NH2	-7.24	116.68	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	848	VAL	CB-CA-C	-6.99	98.13	111.40
3	L	839	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	104	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	C	1203	LEU	CA-CB-CG	6.37	129.95	115.30
2	K	398	LEU	CA-CB-CG	6.32	129.83	115.30
2	B	286	GLU	N-CA-C	-6.32	93.94	111.00
2	B	398	LEU	CA-CB-CG	6.02	129.16	115.30
1	J	104	ARG	NE-CZ-NH2	-5.93	117.33	120.30
3	C	1325	CYS	N-CA-C	5.72	126.43	111.00
2	K	286	GLU	N-CA-C	-5.57	95.98	111.00
3	L	718	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	439	ARG	NE-CZ-NH2	-5.14	117.73	120.30
3	L	719	LEU	CA-CB-CG	-5.14	103.47	115.30
3	C	895	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	L	1203	LEU	CA-CB-CG	5.10	127.04	115.30
3	C	1295	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1324	ASN	Peptide

## 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	1255	0	1265	6	0
1	J	1255	0	1265	9	0
2	B	2389	0	2459	20	0
2	K	2389	0	2459	28	0
3	C	5823	0	5746	77	0
3	L	5761	0	5685	86	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	0	0
5	K	53	0	31	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	24	0	10	0	0
6	L	24	0	10	0	0
7	C	4	0	0	3	0
7	L	4	0	0	2	0
8	C	10	0	4	1	0
8	L	10	0	4	1	0
9	A	24	0	0	1	0
9	B	15	0	0	0	0
9	C	120	0	0	0	0
9	J	14	0	0	0	0
9	K	21	0	0	2	0
9	L	93	0	0	4	0
All	All	19357	0	18969	222	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 (222) 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)
2:K:241:THR:HG23	2:K:243:LYS:HD3	1.20	1.15
2:K:426:ARG:HH11	2:K:426:ARG:HG2	0.98	1.05
2:B:426:ARG:HG3	2:B:426:ARG:HH11	1.01	1.05
2:K:426:ARG:NH1	2:K:426:ARG:HG2	1.66	1.01
3:L:779:MET:HE1	3:L:814:LEU:HD13	1.45	0.98
3:C:995:LYS:HZ1	3:C:1284:GLN:NE2	1.60	0.98
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.62	0.98
2:B:426:ARG:HG3	2:B:426:ARG:NH1	1.71	0.93
2:B:241:THR:HG22	2:B:244:GLU:H	1.34	0.92
2:K:241:THR:HG22	2:K:244:GLU:H	1.37	0.90
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.55	0.89
2:B:243:LYS:HD3	2:B:243:LYS:H	1.37	0.88
2:B:241:THR:HG23	2:B:243:LYS:HD3	1.56	0.88
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.58	0.85
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	0.88	0.85
3:L:995:LYS:NZ	3:L:1284:GLN:NE2	2.25	0.85
3:C:726:ALA:HA	3:C:851:MET:HE2	1.60	0.84
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	1.74	0.84
3:L:779:MET:CE	3:L:814:LEU:HD13	2.08	0.84
3:L:720:LYS:O	3:L:721:LYS:CB	2.25	0.82
3:L:995:LYS:HZ3	3:L:1284:GLN:NE2	1.78	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:995:LYS:HZ3	3:L:1284:GLN:HE21	1.28	0.79
1:A:131:GLN:HE21	1:A:133:GLU:H	1.27	0.79
3:L:610:SER:O	3:L:663:VAL:O	2.02	0.78
2:K:426:ARG:HH11	2:K:426:ARG:CG	1.90	0.77
2:K:241:THR:CG2	2:K:243:LYS:HD3	2.09	0.77
3:C:695:ILE:H	3:C:904:ASN:HD22	1.32	0.76
3:L:623:SER:HA	3:L:626:GLN:HE21	1.50	0.76
2:K:286:GLU:O	2:K:287:LEU:HB2	1.86	0.75
3:C:995:LYS:NZ	3:C:1284:GLN:NE2	2.26	0.74
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.36	0.73
3:C:720:LYS:O	3:C:721:LYS:CB	2.36	0.72
3:L:695:ILE:H	3:L:904:ASN:HD22	1.38	0.71
3:C:610:SER:O	3:C:663:VAL:O	2.08	0.71
2:K:243:LYS:HD3	2:K:243:LYS:H	1.56	0.70
3:C:623:SER:HA	3:C:626:GLN:HE21	1.56	0.70
3:L:640:ILE:HG23	3:L:779:MET:HE2	1.74	0.69
2:B:426:ARG:CG	2:B:426:ARG:HH11	1.91	0.69
3:L:726:ALA:HA	3:L:851:MET:HE2	1.73	0.69
2:K:243:LYS:CD	2:K:243:LYS:H	2.06	0.69
3:C:779:MET:HE1	3:C:814:LEU:HD13	1.74	0.69
3:C:779:MET:CE	3:C:814:LEU:HD13	2.22	0.69
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.75	0.69
3:L:829:ARG:HG3	3:L:833:MET:HE2	1.75	0.69
2:B:285:PRO:O	2:B:286:GLU:HB2	1.94	0.67
3:L:829:ARG:CG	3:L:833:MET:HE2	2.25	0.67
3:L:833:MET:HE3	3:L:1222:ARG:O	1.95	0.66
2:B:243:LYS:CD	2:B:243:LYS:H	2.08	0.66
1:J:131:GLN:HE21	1:J:133:GLU:H	1.43	0.65
3:L:720:LYS:O	3:L:721:LYS:HB2	1.98	0.64
2:B:286:GLU:O	2:B:287:LEU:HB2	1.98	0.64
3:C:1046:MET:HE1	3:C:1087:GLY:CA	2.28	0.62
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.48	0.62
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.17	0.62
3:C:880:ARG:O	3:C:884:HIS:HD2	1.81	0.62
3:L:1152:TYR:CE1	3:L:1257:LYS:HG2	2.34	0.62
3:L:720:LYS:O	3:L:721:LYS:HB3	1.98	0.62
7:C:1327:MOS:O2	7:C:1327:MOS:MO	1.72	0.61
2:B:285:PRO:O	2:B:286:GLU:CB	2.48	0.61
3:L:995:LYS:HZ1	3:L:1284:GLN:NE2	1.99	0.61
7:L:1327:MOS:MO	7:L:1327:MOS:O2	1.72	0.60
2:B:272:ASN:ND2	3:C:683:HIS:CE1	2.69	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:764:VAL:HG22	3:L:766:THR:HG22	1.82	0.60
3:L:1287:ASN:C	3:L:1287:ASN:HD22	2.05	0.60
3:L:833:MET:HE3	3:L:1222:ARG:C	2.21	0.60
3:L:880:ARG:O	3:L:884:HIS:HD2	1.84	0.60
3:L:623:SER:HA	3:L:626:GLN:NE2	2.16	0.60
2:B:474:LEU:O	2:B:475:SER:HB2	2.01	0.59
3:C:829:ARG:CG	3:C:833:MET:HE2	2.32	0.59
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.84	0.59
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.85	0.59
3:L:1079:ALA:O	3:L:1080:SER:HB2	2.03	0.58
3:C:764:VAL:HG22	3:C:766:THR:HG22	1.85	0.58
3:L:1046:MET:HE1	3:L:1087:GLY:CA	2.32	0.58
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.38	0.58
3:L:840:HIS:HE1	3:L:874:SER:OG	1.86	0.57
3:L:1191:ASP:OD2	9:L:168:HOH:O	2.17	0.57
3:L:1282:ARG:O	3:L:1286:THR:HG23	2.03	0.57
3:L:747:HIS:CD2	3:L:836:THR:HG21	2.39	0.56
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.41	0.56
1:A:37:ARG:HD3	3:C:595:ASP:O	2.06	0.56
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.19	0.56
3:L:851:MET:HE3	3:L:857:VAL:HG21	1.87	0.56
3:C:833:MET:HE3	3:C:1222:ARG:O	2.05	0.56
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.88	0.55
2:K:285:PRO:O	2:K:286:GLU:CB	2.54	0.55
3:L:598:ARG:NH2	9:L:509:HOH:O	2.41	0.54
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.21	0.54
3:L:848:VAL:HG13	3:L:859:LEU:HD13	1.90	0.54
3:C:1126:SER:HB2	3:L:1132:PHE:CD1	2.42	0.54
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.44	0.53
3:L:767:GLN:HG2	3:L:1038:MET:HE2	1.91	0.53
3:C:833:MET:HE3	3:C:1222:ARG:C	2.29	0.52
3:C:840:HIS:HE1	3:C:874:SER:OG	1.92	0.52
2:B:285:PRO:C	2:B:286:GLU:O	2.43	0.52
7:C:1327:MOS:O1	8:C:1:PM6:H8	2.08	0.52
3:C:720:LYS:O	3:C:721:LYS:HB2	2.08	0.52
2:K:476:LYS:HG2	2:K:477:PHE:H	1.75	0.52
3:C:640:ILE:HG12	3:C:779:MET:HE3	1.91	0.52
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.58	0.51
3:C:614:HIS:HD2	3:C:693:PRO:O	1.93	0.51
2:K:450:LYS:O	2:K:474:LEU:HD22	2.11	0.51
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1297:ASP:HB2	3:C:1304:LYS:HE2	1.93	0.51
2:K:474:LEU:O	2:K:475:SER:HB2	2.10	0.51
3:L:806:THR:HA	3:L:809:SER:HB2	1.92	0.51
3:C:640:ILE:HG23	3:C:779:MET:HE2	1.92	0.51
2:K:426:ARG:CG	2:K:426:ARG:NH1	2.52	0.51
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.36	0.51
3:C:720:LYS:O	3:C:721:LYS:HB3	2.09	0.51
3:L:614:HIS:HD2	3:L:693:PRO:O	1.93	0.50
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.28	0.50
3:L:833:MET:CE	3:L:1222:ARG:C	2.80	0.50
3:L:833:MET:HE1	3:L:1223:GLY:HA2	1.93	0.50
3:L:1297:ASP:HB2	3:L:1304:LYS:HE2	1.94	0.50
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.77	0.50
2:B:438:MET:HG2	2:B:454:LEU:HD22	1.94	0.49
1:J:99:HIS:CG	1:J:100:PRO:HD2	2.47	0.49
2:K:285:PRO:O	2:K:286:GLU:HB2	2.11	0.49
2:K:425:SER:O	2:K:426:ARG:CB	2.60	0.49
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.60	0.49
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.96	0.49
2:B:232:GLU:OE2	3:C:677:HIS:HE1	1.96	0.49
3:L:1282:ARG:HA	3:L:1286:THR:HG23	1.94	0.49
3:L:829:ARG:HG2	3:L:833:MET:HE2	1.95	0.49
3:C:684:VAL:O	3:C:684:VAL:HG13	2.13	0.48
3:C:641:PRO:HD2	3:C:779:MET:HE1	1.95	0.48
3:L:911:PHE:HD2	3:L:912:ARG:N	2.11	0.48
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.14	0.48
3:C:1124:ARG:HB3	3:L:1134:ARG:HG3	1.96	0.48
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.48	0.48
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.49	0.48
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.14	0.48
3:C:851:MET:HE3	3:C:857:VAL:HG21	1.95	0.48
3:C:1046:MET:HE3	3:C:1090:VAL:HG21	1.96	0.47
3:C:839:ARG:O	3:C:841:PRO:HD3	2.14	0.47
3:C:779:MET:HE3	3:C:814:LEU:HD13	1.95	0.47
1:J:74:LEU:O	1:J:76:PRO:HD3	2.15	0.47
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.14	0.47
2:B:272:ASN:CG	3:C:683:HIS:NE2	2.68	0.47
3:C:1079:ALA:O	3:C:1080:SER:HB2	2.14	0.47
1:J:62:GLN:O	1:J:63:ASP:HB3	2.13	0.47
2:K:469:THR:HG23	2:K:489:GLY:HA3	1.97	0.47
3:L:839:ARG:O	3:L:841:PRO:HD3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:SER:O	2:B:426:ARG:HB2	2.13	0.47
3:C:806:THR:HA	3:C:809:SER:HB2	1.96	0.47
3:C:623:SER:HA	3:C:626:GLN:NE2	2.28	0.47
3:C:719:LEU:CD1	3:C:895:ARG:HB2	2.45	0.46
3:L:1213:TYR:CE2	3:L:1219:LEU:HD13	2.50	0.46
3:C:1152:TYR:CE1	3:C:1257:LYS:HG2	2.50	0.46
2:K:257:LEU:O	5:K:606:FAD:H2B	2.16	0.46
3:L:695:ILE:H	3:L:904:ASN:ND2	2.10	0.46
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.56	0.46
3:C:719:LEU:HD11	3:C:895:ARG:HB2	1.97	0.46
3:C:1126:SER:HB2	3:L:1132:PHE:CE1	2.51	0.45
3:L:1203:LEU:O	3:L:1207:THR:OG1	2.32	0.45
3:L:606:ARG:HD3	3:L:679:GLU:HA	1.98	0.45
2:B:474:LEU:O	2:B:475:SER:CB	2.65	0.45
1:A:142:ALA:HB1	9:A:174:HOH:O	2.15	0.45
2:K:268:MET:HE1	9:K:536:HOH:O	2.15	0.45
3:L:601:ASN:HB2	3:L:821:HIS:HD2	1.80	0.45
3:C:740:ASP:OD2	3:C:833:MET:HG2	2.17	0.45
2:K:471:GLN:NE2	2:K:474:LEU:HD12	2.31	0.45
3:C:1282:ARG:O	3:C:1286:THR:HG23	2.17	0.45
3:C:911:PHE:HD2	3:C:912:ARG:N	2.15	0.45
2:K:310:LYS:HE3	2:K:314:GLU:OE2	2.17	0.45
3:L:833:MET:CE	3:L:1222:ARG:O	2.63	0.45
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	1.99	0.45
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.38	0.45
2:K:391:PRO:HD2	2:K:395:LYS:O	2.17	0.44
3:L:1301:THR:HB	3:L:1302:PRO:HD2	1.98	0.44
3:C:1132:PHE:CD1	3:L:1126:SER:HB2	2.53	0.44
3:L:845:ARG:HD2	9:L:1347:HOH:O	2.17	0.44
3:C:1282:ARG:HA	3:C:1286:THR:CG2	2.47	0.44
3:L:840:HIS:CE1	3:L:874:SER:OG	2.70	0.44
3:C:1287:ASN:HD22	3:C:1287:ASN:C	2.21	0.44
3:C:726:ALA:HA	3:C:851:MET:CE	2.37	0.44
3:L:726:ALA:HA	3:L:851:MET:CE	2.43	0.44
2:K:447:MET:HG2	2:K:527:LEU:HD13	2.00	0.43
1:J:63:ASP:OD1	1:J:63:ASP:C	2.57	0.43
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.53	0.43
3:C:880:ARG:O	3:C:884:HIS:CD2	2.68	0.43
2:K:268:MET:CE	9:K:536:HOH:O	2.67	0.43
3:L:719:LEU:CD1	3:L:895:ARG:HB2	2.48	0.43
3:L:1287:ASN:ND2	3:L:1289:ASN:H	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:980:ARG:NH1	3:C:1161:GLU:OE1	2.52	0.43
3:C:1203:LEU:HD12	3:C:1203:LEU:C	2.38	0.43
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.99	0.43
1:A:62:GLN:O	1:A:63:ASP:HB3	2.18	0.43
3:L:880:ARG:O	3:L:884:HIS:CD2	2.69	0.43
3:L:601:ASN:O	3:L:821:HIS:HD2	2.02	0.43
7:L:1327:MOS:S	7:L:1327:MOS:O2	2.77	0.42
3:L:829:ARG:HG2	3:L:833:MET:CE	2.50	0.42
3:L:827:LEU:HA	9:L:1338:HOH:O	2.19	0.42
3:C:605:LEU:C	3:C:605:LEU:HD23	2.39	0.42
3:L:929:GLU:HG2	3:L:1293:LEU:HD22	2.01	0.42
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.85	0.42
3:L:1010:THR:HG23	8:L:1:PM6:S6	2.59	0.42
3:L:700:ASP:HA	3:L:703:LYS:HE3	2.01	0.42
1:A:96:THR:OG1	1:A:97:ARG:N	2.52	0.42
3:L:1191:ASP:OD1	3:L:1259:VAL:HG11	2.20	0.42
2:B:255:ALA:HB2	2:B:277:MET:HG2	2.02	0.41
3:C:596:ILE:HA	3:C:597:PRO:HD3	1.95	0.41
2:K:243:LYS:CD	2:K:243:LYS:N	2.80	0.41
2:K:284:ILE:HB	2:K:287:LEU:HD12	2.02	0.41
1:J:37:ARG:HD3	3:L:595:ASP:O	2.20	0.41
1:J:49:GLY:C	1:J:51:CYS:H	2.22	0.41
3:C:994:LYS:O	3:C:995:LYS:HD3	2.20	0.41
1:J:49:GLY:C	1:J:51:CYS:N	2.74	0.41
2:B:450:LYS:O	2:B:474:LEU:HD22	2.20	0.41
3:L:719:LEU:HD11	3:L:895:ARG:HB2	2.03	0.41
3:L:752:ILE:HD12	3:L:763:PHE:CE1	2.56	0.41
3:L:663:VAL:HG12	3:L:834:LEU:HD11	2.03	0.41
3:L:764:VAL:HG22	3:L:766:THR:CG2	2.50	0.41
3:L:916:GLY:O	3:L:920:LEU:HG	2.19	0.41
3:L:1017:ALA:HB2	3:L:1085:ILE:HD12	2.03	0.41
3:C:929:GLU:HG2	3:C:1293:LEU:HD22	2.03	0.40
7:C:1327:MOS:S	7:C:1327:MOS:O2	2.79	0.40
3:C:684:VAL:O	3:C:684:VAL:CG1	2.69	0.40
3:C:606:ARG:HD3	3:C:679:GLU:HA	2.03	0.40
2:K:476:LYS:HG2	2:K:477:PHE:N	2.36	0.40
2:K:488:ALA:O	2:K:492:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	47
1	J	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	47
2	B	303/305 (99%)	280 (92%)	19 (6%)	4 (1%)	12	24
2	K	303/305 (99%)	279 (92%)	19 (6%)	5 (2%)	9	18
3	C	753/755 (100%)	723 (96%)	25 (3%)	5 (1%)	22	43
3	L	743/755 (98%)	705 (95%)	33 (4%)	5 (1%)	22	43
All	All	2426/2448 (99%)	2291 (94%)	114 (5%)	21 (1%)	17	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	721	LYS
3	C	1008	SER
2	K	426	ARG
3	L	721	LYS
3	L	1008	SER
2	B	338	ALA
2	B	426	ARG
3	L	1139	GLY
3	C	912	ARG
2	K	424	ALA
2	K	425	SER
2	B	424	ALA
2	B	425	SER
2	K	338	ALA
3	L	797	GLY
3	L	912	ARG
1	A	61	LEU
3	C	797	GLY
1	J	61	LEU
2	K	335	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	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	137/137 (100%)	131 (96%)	6 (4%)	28	53
1	J	137/137 (100%)	131 (96%)	6 (4%)	28	53
2	B	261/261 (100%)	239 (92%)	22 (8%)	11	21
2	K	261/261 (100%)	241 (92%)	20 (8%)	13	25
3	C	631/631 (100%)	606 (96%)	25 (4%)	31	57
3	L	624/631 (99%)	598 (96%)	26 (4%)	30	55
All	All	2051/2058 (100%)	1946 (95%)	105 (5%)	24	46

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	64	LYS
1	A	97	ARG
1	A	113	CYS
1	A	140	GLU
1	A	162	THR
2	B	226	GLN
2	B	241	THR
2	B	243	LYS
2	B	257	LEU
2	B	312	LEU
2	B	335	ARG
2	B	337	PHE
2	B	348	LEU
2	B	359	SER
2	B	375	VAL
2	B	426	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	427	ARG
2	B	429	ASP
2	B	433	LYS
2	B	462	ARG
2	B	468	LYS
2	B	472	LYS
2	B	476	LYS
2	B	484	GLN
2	B	492	GLU
2	B	509	ARG
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	618	LYS
3	C	659	THR
3	C	686	LYS
3	C	705	ASN
3	C	742	PHE
3	C	743	TYR
3	C	764	VAL
3	C	779	MET
3	C	782	VAL
3	C	818	LYS
3	C	848	VAL
3	C	852	LYS
3	C	911	PHE
3	C	939	GLU
3	C	983	GLU
3	C	1001	ILE
3	C	1144	THR
3	C	1203	LEU
3	C	1208	LEU
3	C	1239	PHE
3	C	1286	THR
3	C	1287	ASN
3	C	1324	ASN
1	J	63	ASP
1	J	64	LYS
1	J	97	ARG
1	J	113	CYS
1	J	140	GLU
1	J	162	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	226	GLN
2	K	241	THR
2	K	243	LYS
2	K	257	LEU
2	K	312	LEU
2	K	335	ARG
2	K	337	PHE
2	K	348	LEU
2	K	375	VAL
2	K	426	ARG
2	K	427	ARG
2	K	429	ASP
2	K	433	LYS
2	K	462	ARG
2	K	472	LYS
2	K	476	LYS
2	K	482	LEU
2	K	492	GLU
2	K	509	ARG
2	K	525	LYS
3	L	598	ARG
3	L	609	THR
3	L	618	LYS
3	L	659	THR
3	L	686	LYS
3	L	705	ASN
3	L	742	PHE
3	L	743	TYR
3	L	764	VAL
3	L	774	SER
3	L	779	MET
3	L	782	VAL
3	L	818	LYS
3	L	848	VAL
3	L	852	LYS
3	L	899	ARG
3	L	911	PHE
3	L	939	GLU
3	L	983	GLU
3	L	1001	ILE
3	L	1144	THR
3	L	1203	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	L	1208	LEU
3	L	1239	PHE
3	L	1286	THR
3	L	1287	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	ASN
2	B	272	ASN
2	B	351	ASN
2	B	471	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	728	ASN
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1033	HIS
3	C	1048	GLN
3	C	1284	GLN
3	C	1287	ASN
1	J	131	GLN
2	K	351	ASN
2	K	471	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	728	ASN
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1033	HIS
3	L	1048	GLN
3	L	1122	GLN
3	L	1284	GLN
3	L	1285	HIS
3	L	1287	ASN



### 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 ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	FAD	K	606	-	51,58,58	1.45	7 (13%)	60,89,89	1.80	9 (15%)
6	MTE	L	1326	7	21,26,26	2.22	3 (14%)	21,40,40	2.76	12 (57%)
4	FES	J	602	1	0,4,4	0.00	-	-		
8	PM6	C	1	-	8,11,11	2.39	4 (50%)	4,15,15	2.37	3 (75%)
7	MOS	L	1327	6	0,3,3	0.00	-	-		
6	MTE	C	1326	7	21,26,26	2.03	2 (9%)	21,40,40	2.26	10 (47%)
4	FES	A	602	1	0,4,4	0.00	-	-		
5	FAD	B	606	-	51,58,58	1.55	8 (15%)	60,89,89	1.92	11 (18%)
7	MOS	C	1327	6	0,3,3	0.00	-	-		
4	FES	A	601	1	0,4,4	0.00	-	-		
4	FES	J	601	1	0,4,4	0.00	-	-		
8	PM6	L	1	-	8,11,11	2.12	4 (50%)	4,15,15	2.75	3 (75%)

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
5	FAD	K	606	-	-	8/30/50/50	0/6/6/6
6	MTE	L	1326	7	-	1/6/34/34	0/3/3/3
4	FES	J	602	1	-	-	0/1/1/1
8	PM6	C	1	-	-	-	0/2/2/2
6	MTE	C	1326	7	-	1/6/34/34	0/3/3/3
4	FES	A	602	1	-	-	0/1/1/1
5	FAD	B	606	-	-	4/30/50/50	0/6/6/6
4	FES	A	601	1	-	-	0/1/1/1
4	FES	J	601	1	-	-	0/1/1/1
8	PM6	L	1	-	-	-	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1326	MTE	C4-C9	7.76	1.52	1.41
6	C	1326	MTE	C4-C9	6.88	1.50	1.41
6	C	1326	MTE	C9-C10	5.59	1.52	1.41
5	B	606	FAD	C4X-N5	4.46	1.39	1.33
6	L	1326	MTE	C9-C10	4.31	1.49	1.41
5	K	606	FAD	C10-N1	4.09	1.38	1.33
5	B	606	FAD	C10-N1	4.08	1.38	1.33
5	K	606	FAD	C2A-N3A	3.96	1.38	1.32
5	B	606	FAD	C1'-N10	3.71	1.52	1.48
8	C	1	PM6	C6-N1	3.65	1.37	1.33
5	K	606	FAD	C4X-N5	3.62	1.38	1.33
5	B	606	FAD	C2A-N3A	3.60	1.37	1.32
8	C	1	PM6	C2-N3	3.39	1.37	1.32
8	L	1	PM6	C6-N1	3.32	1.37	1.33
5	K	606	FAD	C4-N3	3.17	1.38	1.33
5	K	606	FAD	C2A-N1A	3.00	1.39	1.33
6	L	1326	MTE	C4-N3	2.99	1.38	1.33
5	B	606	FAD	C2A-N1A	2.99	1.39	1.33
8	C	1	PM6	C6-C5	2.96	1.49	1.43
8	L	1	PM6	C2-N3	2.92	1.36	1.32
8	L	1	PM6	C5-C4	2.69	1.48	1.40
8	L	1	PM6	C6-C5	2.51	1.48	1.43
8	C	1	PM6	C5-C4	2.50	1.47	1.40
5	B	606	FAD	C9A-N10	2.50	1.41	1.38
5	K	606	FAD	C1'-N10	2.42	1.50	1.48
5	B	606	FAD	C2B-C1B	-2.41	1.50	1.53
5	B	606	FAD	C4-N3	2.22	1.36	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	606	FAD	C5X-N5	2.08	1.38	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1326	MTE	C4-C9-N5	7.27	125.22	119.12
5	B	606	FAD	N3A-C2A-N1A	-7.14	117.52	128.68
5	K	606	FAD	C1'-N10-C9A	6.54	123.44	118.29
5	K	606	FAD	N3A-C2A-N1A	-5.93	119.41	128.68
5	B	606	FAD	C5X-C9A-N10	5.51	121.71	117.72
5	B	606	FAD	C1'-N10-C9A	5.18	122.37	118.29
6	C	1326	MTE	C4-C9-N5	5.08	123.39	119.12
5	B	606	FAD	C4-N3-C2	4.71	119.12	115.14
6	L	1326	MTE	C4-N3-C2	4.05	122.36	115.93
8	L	1	PM6	N3-C2-N1	-3.95	122.50	128.68
6	C	1326	MTE	C4-N3-C2	3.88	122.09	115.93
6	C	1326	MTE	O3'-C7-N8	3.77	112.44	108.57
5	K	606	FAD	C4X-N5-C5X	3.76	120.53	116.77
6	L	1326	MTE	C2-N1-C10	3.73	122.89	114.54
6	L	1326	MTE	O3'-C7-N8	3.40	112.06	108.57
5	B	606	FAD	C4X-N5-C5X	3.40	120.16	116.77
5	K	606	FAD	O4'-C4'-C3'	3.20	116.89	109.10
5	K	606	FAD	C4-N3-C2	3.20	117.85	115.14
6	C	1326	MTE	C10-N8-C7	-3.06	117.67	123.67
5	B	606	FAD	C6-C5X-C9A	3.05	123.05	119.05
6	L	1326	MTE	N2-C2-N3	2.98	121.88	117.25
5	K	606	FAD	O3'-C3'-C2'	-2.97	101.64	108.81
5	B	606	FAD	C9A-N10-C10	-2.89	118.12	121.91
8	C	1	PM6	N3-C2-N1	-2.89	124.17	128.68
6	C	1326	MTE	O2P-P-O4'	-2.78	99.35	106.73
5	K	606	FAD	C5X-C9A-N10	2.72	119.69	117.72
6	C	1326	MTE	C4-C9-C10	2.67	116.94	114.57
6	L	1326	MTE	C9-C10-N8	2.62	120.52	118.13
8	L	1	PM6	C2-N3-C4	2.61	119.56	113.45
8	L	1	PM6	C2-N1-C6	2.59	122.14	116.32
6	L	1326	MTE	O2P-P-O4'	-2.55	99.95	106.73
8	C	1	PM6	C2-N3-C4	2.53	119.38	113.45
5	B	606	FAD	C8M-C8-C9	-2.50	114.35	120.34
6	C	1326	MTE	O3'-C7-C6	-2.43	107.34	108.96
5	K	606	FAD	O5'-C5'-C4'	-2.39	102.98	109.36
6	L	1326	MTE	C10-N8-C7	-2.38	119.02	123.67
6	C	1326	MTE	C9-C4-N3	-2.34	117.35	124.01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1326	MTE	O3'-C7-C6	-2.34	107.40	108.96
5	B	606	FAD	C2A-N1A-C6A	2.27	122.64	118.75
8	C	1	PM6	C4-C5-N7	-2.25	107.06	109.40
6	L	1326	MTE	N3-C2-N1	-2.25	121.89	125.42
6	L	1326	MTE	C9-C4-N3	-2.20	117.75	124.01
5	B	606	FAD	C4X-C4-N3	-2.16	120.47	123.43
6	C	1326	MTE	C2-N1-C10	2.12	119.30	114.54
5	K	606	FAD	P-O3P-PA	-2.10	125.61	132.83
5	B	606	FAD	C9A-C5X-N5	-2.08	119.10	122.36
6	L	1326	MTE	C4-C9-C10	2.03	116.38	114.57
6	C	1326	MTE	O2P-P-O1P	2.02	118.57	110.68

There are no chirality outliers.

All (14) torsion outliers are listed below:

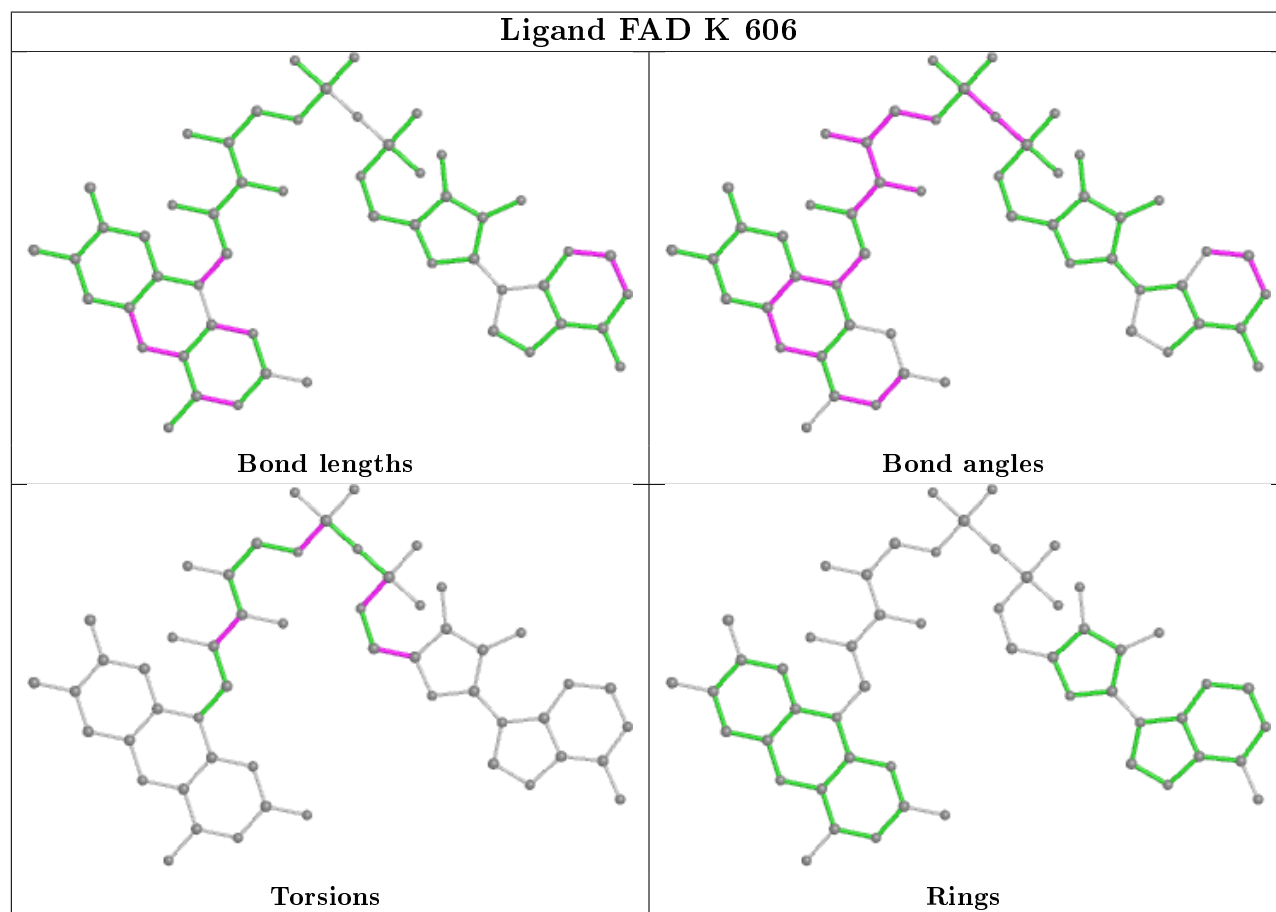
Mol	Chain	Res	Type	Atoms
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O3P
5	K	606	FAD	C1'-C2'-C3'-O3'
5	B	606	FAD	C5B-O5B-PA-O1A
6	L	1326	MTE	C3'-C4'-O4'-P
5	K	606	FAD	O2'-C2'-C3'-O3'
5	K	606	FAD	O4B-C4B-C5B-O5B
5	B	606	FAD	O4B-C4B-C5B-O5B
5	B	606	FAD	C3B-C4B-C5B-O5B
5	K	606	FAD	C5'-O5'-P-O3P
6	C	1326	MTE	C3'-C4'-O4'-P
5	K	606	FAD	C3B-C4B-C5B-O5B
5	K	606	FAD	O2'-C2'-C3'-C4'
5	B	606	FAD	C5B-O5B-PA-O3P

There are no ring outliers.

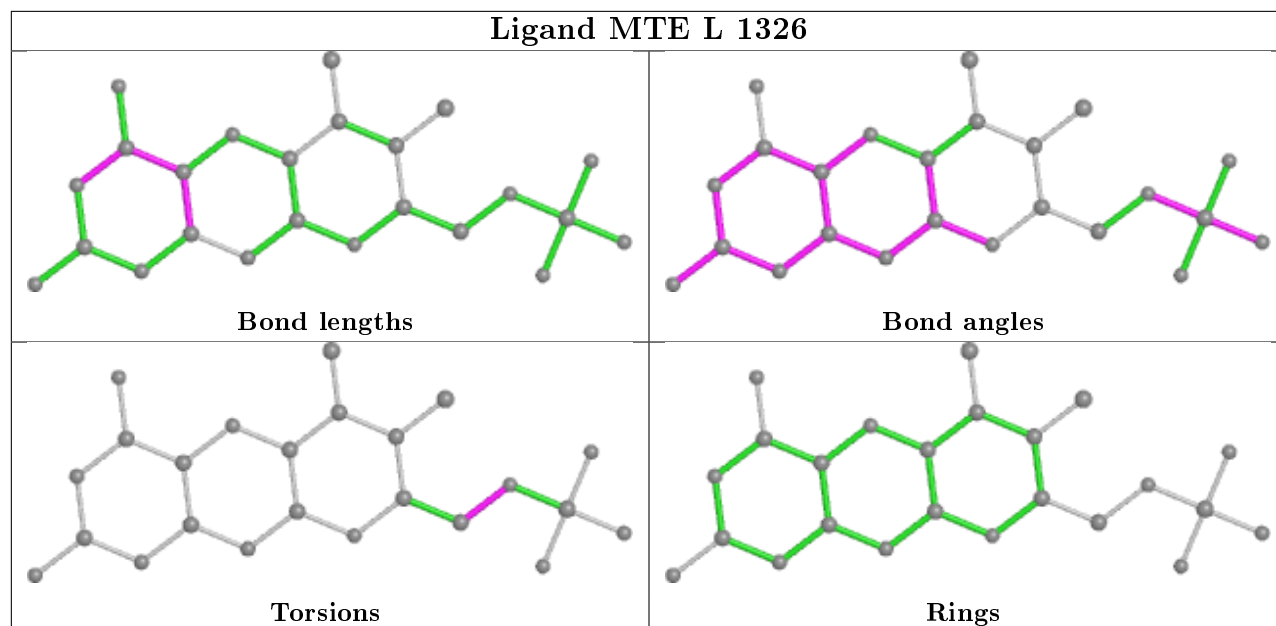
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	606	FAD	1	0
8	C	1	PM6	1	0
7	L	1327	MOS	2	0
7	C	1327	MOS	3	0
8	L	1	PM6	1	0

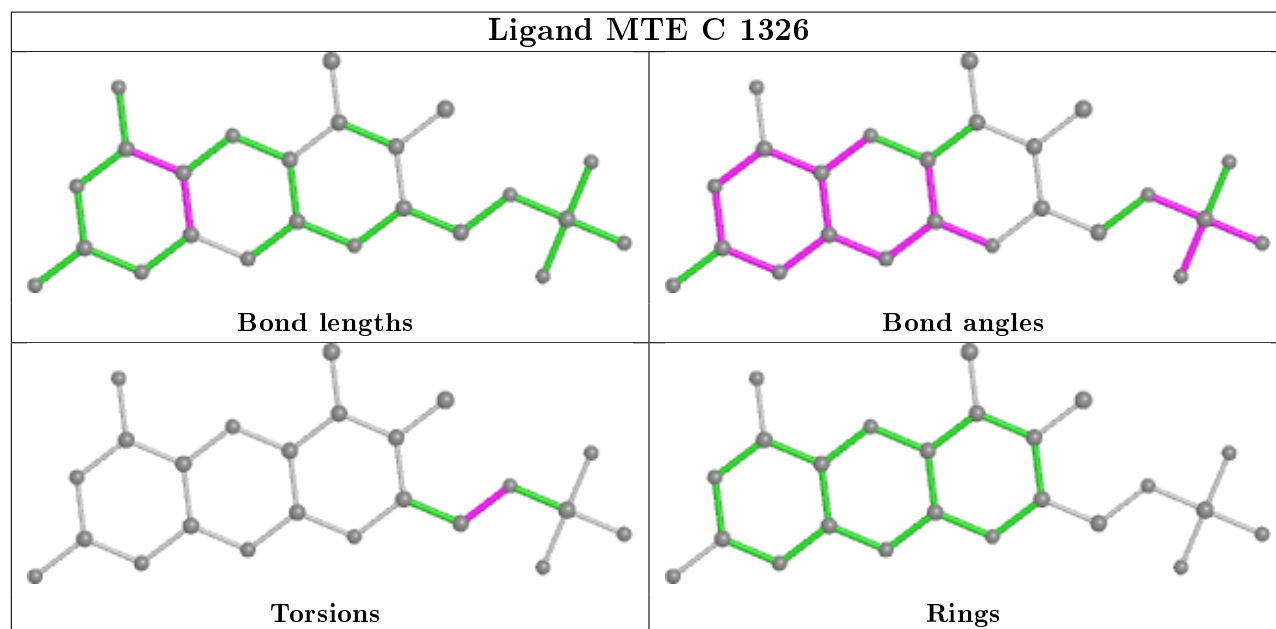
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

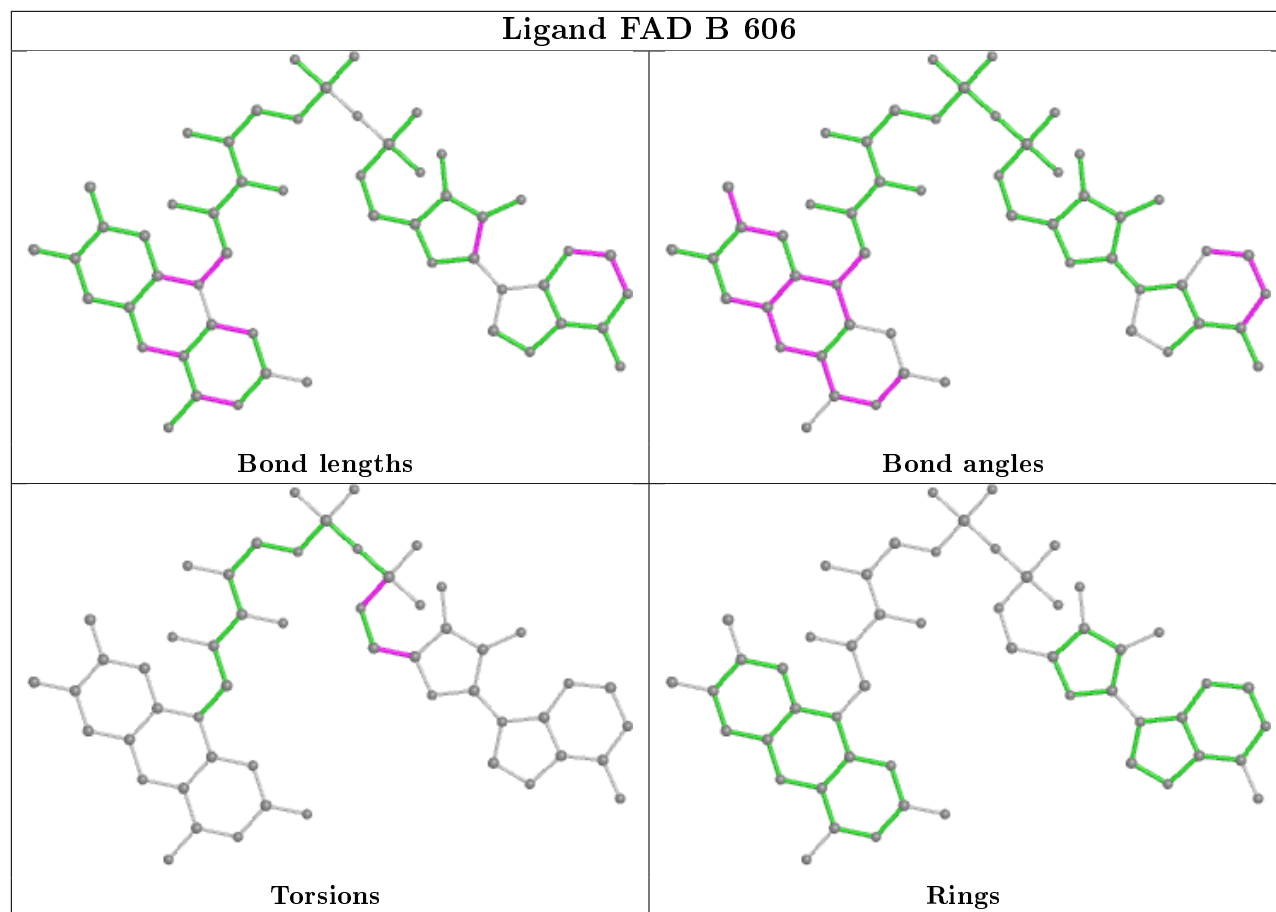


## Ligand MTE L 1326



## Ligand MTE C 1326





## 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	164/164 (100%)	-0.10	4 (2%) 59 53	14, 24, 42, 55	0
1	J	164/164 (100%)	0.02	9 (5%) 25 19	14, 24, 42, 56	0
2	B	305/305 (100%)	0.03	3 (0%) 82 80	22, 34, 47, 50	0
2	K	305/305 (100%)	0.13	13 (4%) 35 28	22, 34, 47, 51	0
3	C	755/755 (100%)	-0.23	3 (0%) 92 91	13, 22, 36, 49	0
3	L	745/755 (98%)	-0.10	14 (1%) 66 62	13, 22, 36, 49	0
All	All	2438/2448 (99%)	-0.09	46 (1%) 66 62	13, 25, 43, 56	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1288	ASN	6.4
3	L	985	ASP	4.3
2	K	528	GLY	4.1
1	J	60	ARG	3.9
3	L	1290	THR	3.9
1	J	165	LYS	3.8
2	K	477	PHE	3.4
1	J	2	THR	3.4
3	L	1289	ASN	3.3
3	L	1287	ASN	3.2
2	B	527	LEU	3.2
1	A	63	ASP	2.8
3	L	1144	THR	2.8
1	A	2	THR	2.8
1	J	162	THR	2.8
2	B	230	GLU	2.7
3	L	991	ASN	2.7
3	L	722	GLY	2.6
3	C	724	SER	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	L	1285	HIS	2.6
1	J	97	ARG	2.6
3	L	989	LYS	2.6
3	L	1286	THR	2.5
3	C	1290	THR	2.5
2	K	476	LYS	2.4
1	A	97	ARG	2.3
1	J	63	ASP	2.3
2	K	446	SER	2.3
1	J	132	PRO	2.3
2	K	474	LEU	2.2
3	C	1108	ASN	2.2
2	K	499	ASP	2.2
1	J	133	GLU	2.2
3	L	986	LYS	2.2
2	K	498	PRO	2.2
3	L	1143	GLU	2.1
2	K	251	GLN	2.1
2	K	445	GLY	2.1
1	J	135	THR	2.1
3	L	982	SER	2.1
2	B	272	ASN	2.1
2	K	272	ASN	2.1
2	K	442	PHE	2.1
1	A	61	LEU	2.0
2	K	479	ASN	2.0
2	K	492	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

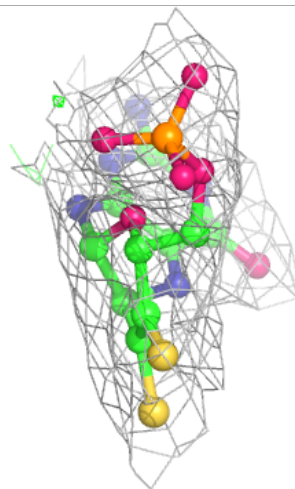
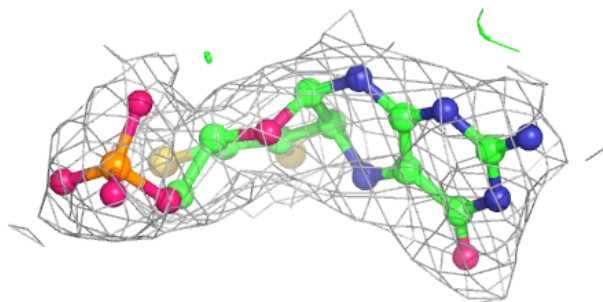
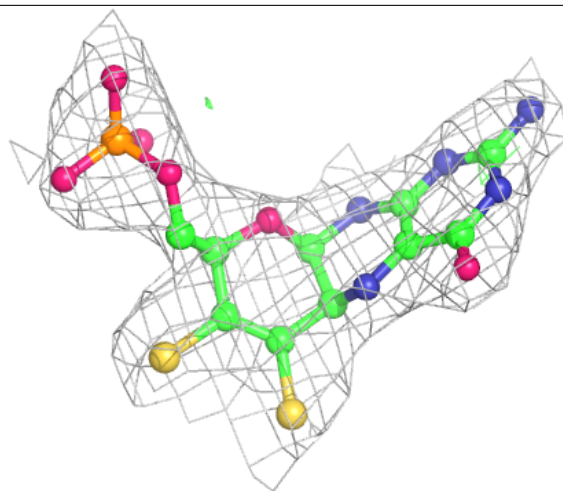
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PM6	L	1	10/10	0.91	0.21	42,43,44,44	0
8	PM6	C	1	10/10	0.93	0.18	31,32,33,33	0
6	MTE	L	1326	24/24	0.95	0.16	24,28,35,36	0
5	FAD	K	606	53/53	0.96	0.16	21,27,34,38	0
5	FAD	B	606	53/53	0.97	0.13	16,21,26,28	0
6	MTE	C	1326	24/24	0.97	0.13	18,22,26,29	0
4	FES	J	601	4/4	0.98	0.11	14,14,15,19	0
7	MOS	C	1327	4/4	0.98	0.14	34,34,36,48	0
4	FES	A	601	4/4	0.99	0.10	12,12,14,17	0
4	FES	J	602	4/4	0.99	0.10	18,19,20,21	0
4	FES	A	602	4/4	0.99	0.10	15,16,17,18	0
7	MOS	L	1327	4/4	0.99	0.11	37,39,42,45	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.

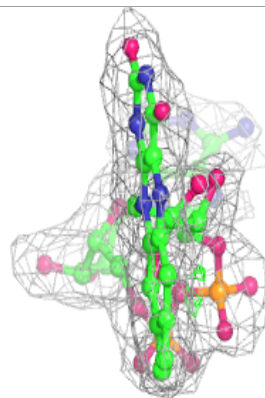
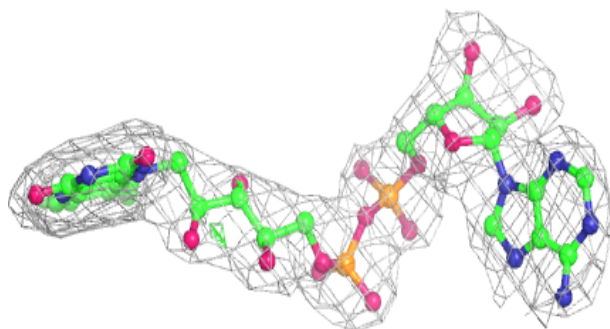
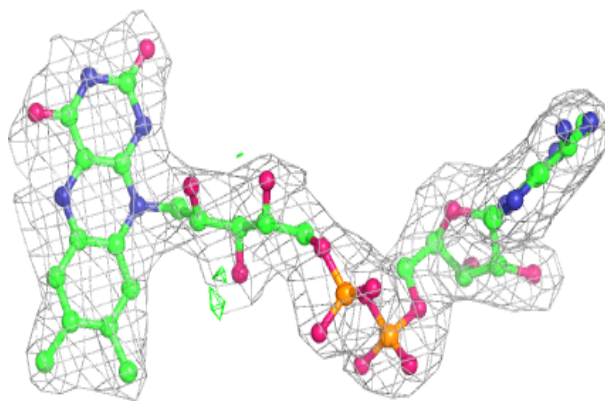
**Electron density around MTE L 1326:**

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

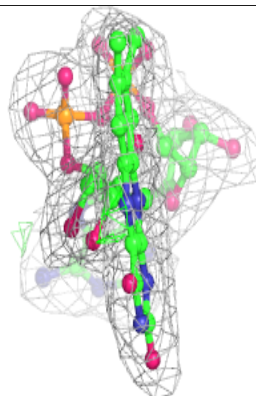
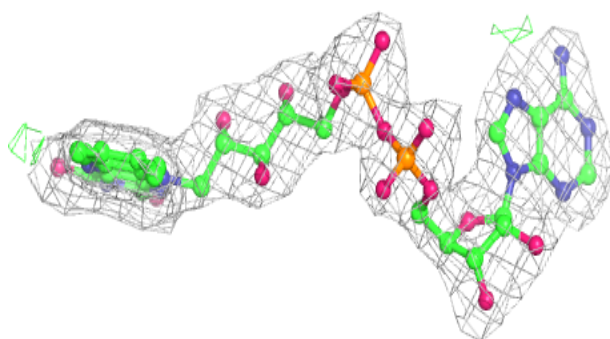
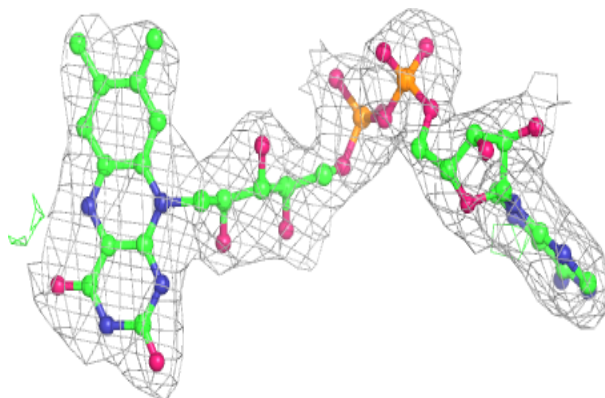


**Electron density around FAD K 606:**

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

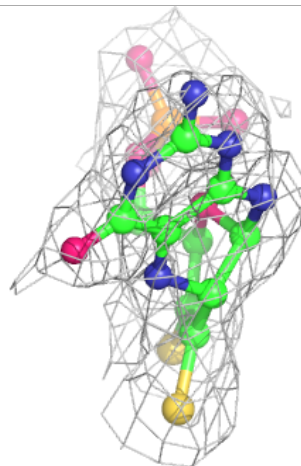
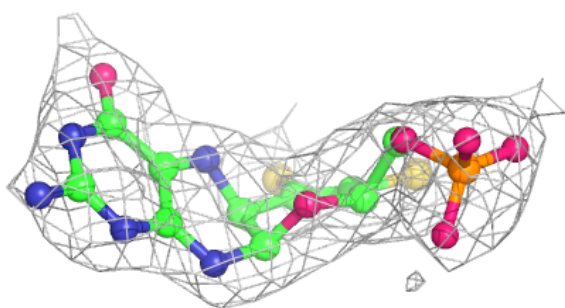
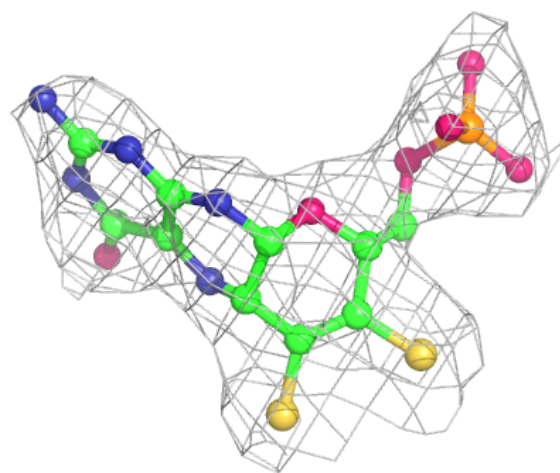
**Electron density around FAD B 606:**

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



**Electron density around MTE C 1326:**

$2mF_o-DF_c$  (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.