



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 AM UTC

PDB ID : 3NVW / pdb_00003nvw
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Guanine
Authors : Cao, H.; Hille, R.
Deposited on : 2010-07-08
Resolution : 1.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

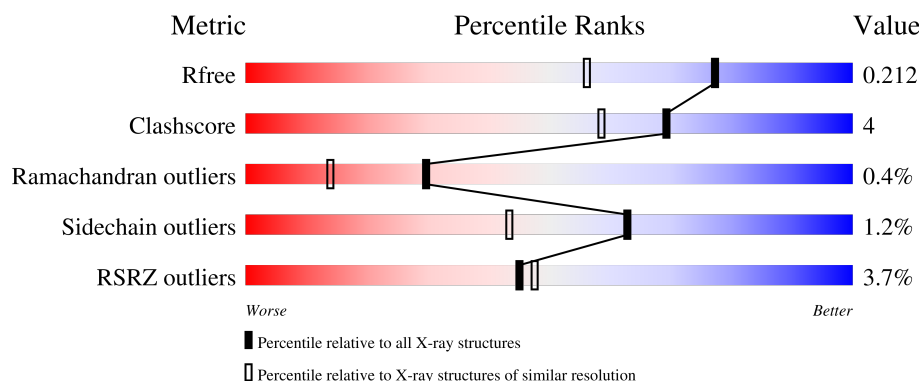
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	164	3% 96% ..
1	J	164	9% 95% 5%
2	B	334	6% 93% 7%
2	K	334	8% 84% 7% 9%
3	C	756	% 90% 9%

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Mol	Chain	Length	Quality of chain
3	L	756	3% 91% 7% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21495 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			

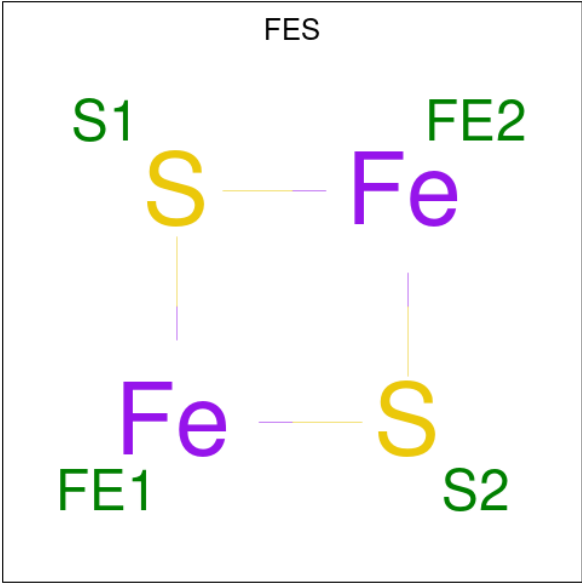
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	334	Total	C	N	O	S	0	0	0
			2630	1700	437	479	14			
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.

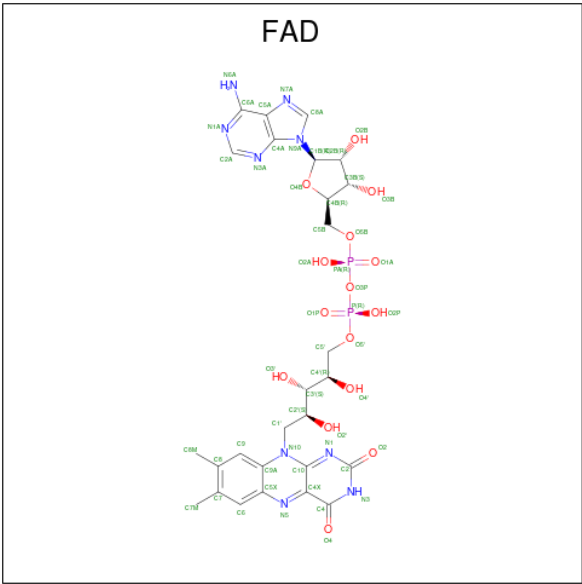
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



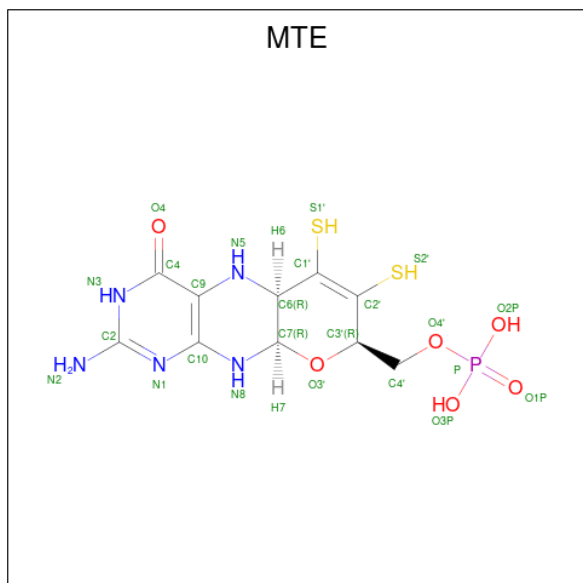
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

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



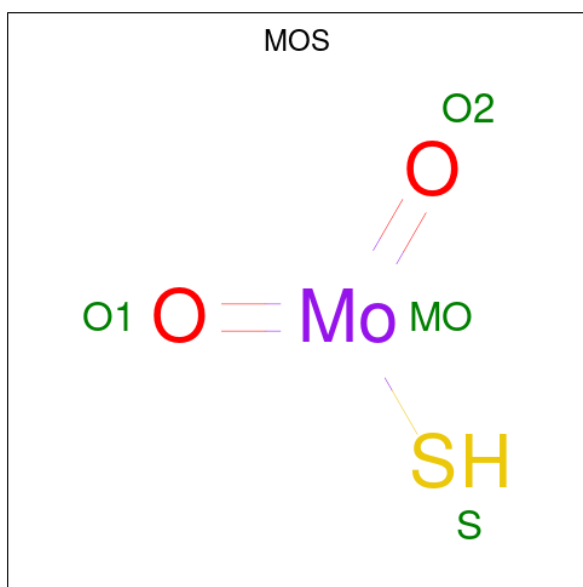
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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 (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



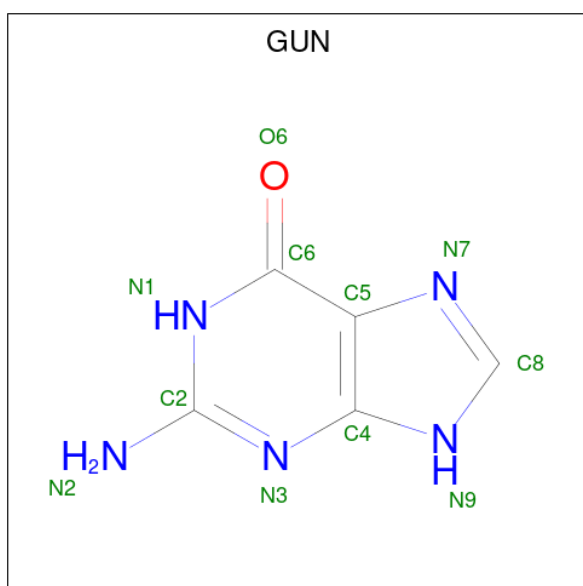
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	L	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: $HMoO_2S$).



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 GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	5	5	1		
8	L	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	149	Total 149	O 149	0	0
9	B	273	Total 273	O 273	0	0
9	C	724	Total 724	O 724	0	0
9	J	134	Total 134	O 134	0	0
9	K	219	Total 219	O 219	0	0
9	L	674	Total 674	O 674	0	0

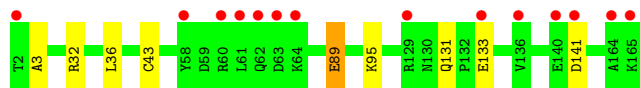
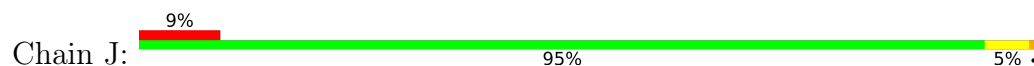
3 Residue-property plots

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

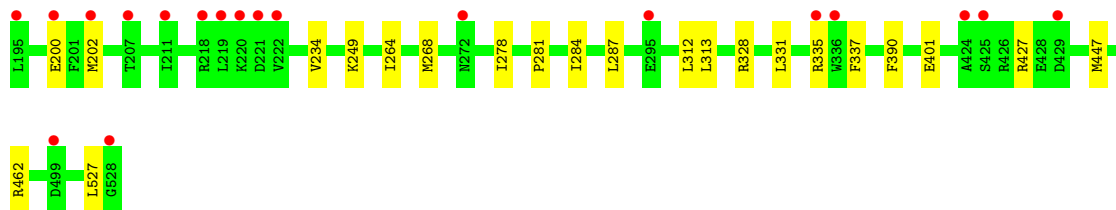
- Molecule 1: Xanthine dehydrogenase/oxidase



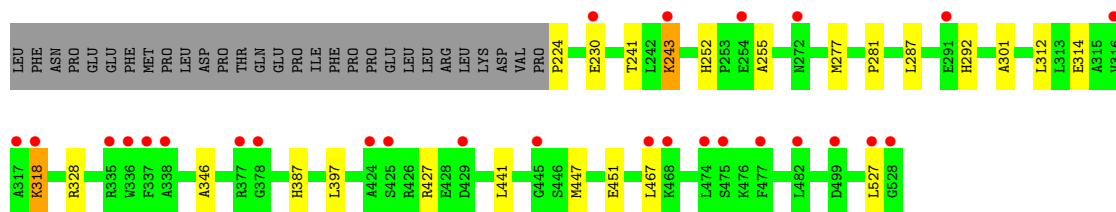
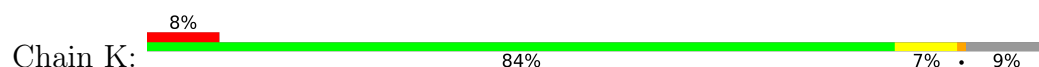
- Molecule 1: Xanthine dehydrogenase/oxidase



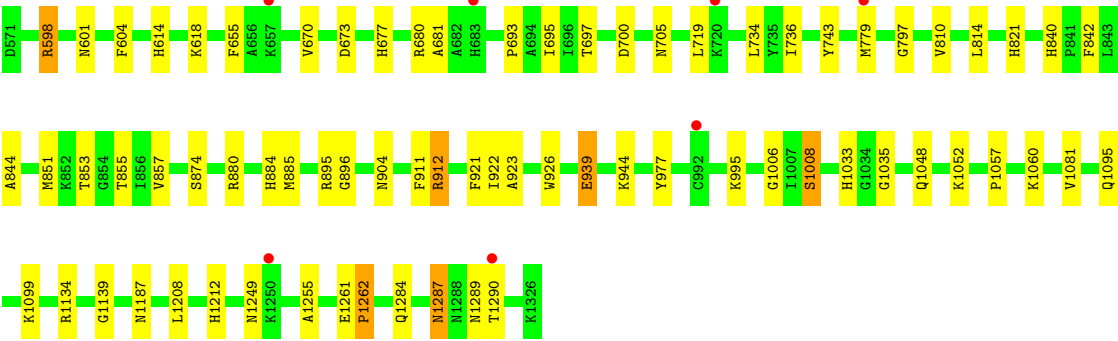
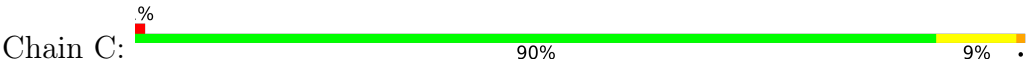
- Molecule 2: Xanthine dehydrogenase/oxidase



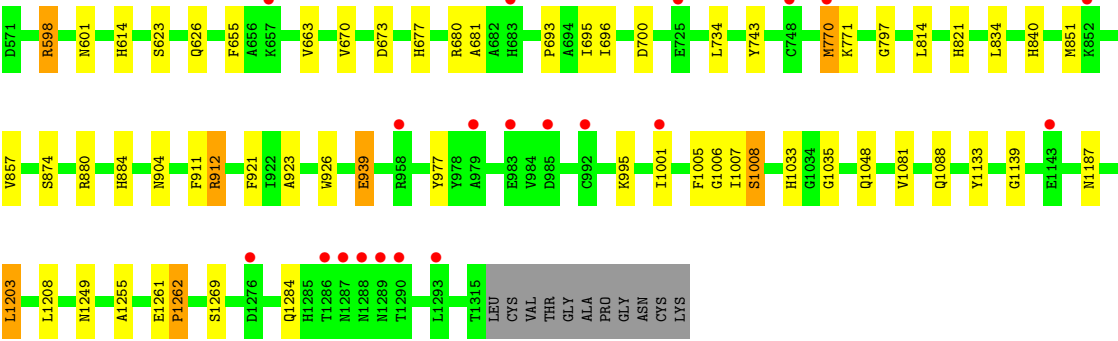
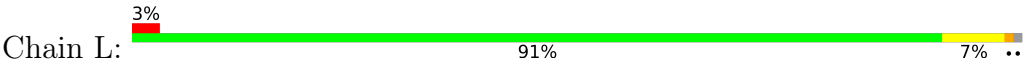
- Molecule 2: Xanthine dehydrogenase/oxidase



- 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, α , β , γ	132.68Å 73.40Å 138.11Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	131.70 – 1.60 131.70 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (131.70-1.60) 96.5 (131.70-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.212 0.184 , 0.212	Depositor DCC
R_{free} test set	16908 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21495	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/1277	0.74	0/1723
1	J	0.52	0/1277	0.73	0/1723
2	B	0.48	0/2689	0.75	0/3637
2	K	0.47	0/2438	0.75	0/3290
3	C	0.53	0/5960	0.75	1/8072 (0.0%)
3	L	0.51	0/5888	0.75	1/7974 (0.0%)
All	All	0.51	0/19529	0.75	2/26419 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1262	PRO	N-CA-C	6.55	118.69	110.70
3	L	1262	PRO	N-CA-C	6.39	118.50	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1255	0	1265	3	0
1	J	1255	0	1265	9	0
2	B	2630	0	2697	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	2389	0	2459	19	0
3	C	5832	0	5759	55	0
3	L	5761	0	5685	39	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
6	C	24	0	10	0	0
6	L	24	0	10	0	0
7	C	4	0	0	1	0
7	L	4	0	0	1	0
8	C	11	0	5	0	0
8	L	11	0	5	0	0
9	A	149	0	0	0	0
9	B	273	0	0	2	0
9	C	724	0	0	7	0
9	J	134	0	0	2	0
9	K	219	0	0	4	0
9	L	674	0	0	4	0
All	All	21495	0	19222	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (136) 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)
3:C:1052:LYS:HE3	9:C:475:HOH:O	1.20	1.27
2:K:255:ALA:HB2	2:K:277:MET:CE	1.94	0.95
3:L:851:MET:HE2	3:L:857:VAL:HG11	1.48	0.95
3:L:770:MET:HG3	3:L:771:LYS:N	1.84	0.93
2:K:252:HIS:HB2	2:K:277:MET:HE1	1.53	0.88
2:K:252:HIS:CB	2:K:277:MET:HE1	2.07	0.84
3:L:1001:ILE:HD12	3:L:1269:SER:HA	1.63	0.81
3:L:695:ILE:H	3:L:904:ASN:HD22	1.32	0.77
1:A:131:GLN:HE21	1:A:133:GLU:H	1.30	0.76
3:C:695:ILE:H	3:C:904:ASN:HD22	1.32	0.76
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.32	0.75
2:K:255:ALA:HB2	2:K:277:MET:HE3	1.69	0.74
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.22	0.73
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:ALA:HB2	2:K:230:GLU:HG2	1.69	0.72
2:K:314:GLU:O	2:K:318:LYS:HD2	1.88	0.72
2:K:427:ARG:HD2	9:K:537:HOH:O	1.92	0.70
1:J:141:ASP:O	9:J:956:HOH:O	2.08	0.70
3:C:680:ARG:NH2	9:C:1817:HOH:O	2.20	0.70
1:J:95:LYS:HE3	9:L:1408:HOH:O	1.92	0.69
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.75	0.68
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.13	0.67
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.79	0.65
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.43	0.65
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.15	0.65
3:C:614:HIS:HD2	3:C:693:PRO:O	1.80	0.64
3:L:770:MET:HG3	3:L:771:LYS:H	1.62	0.64
1:J:95:LYS:NZ	9:J:850:HOH:O	2.24	0.63
3:C:705:ASN:HB2	9:C:44:HOH:O	1.99	0.62
7:C:1328:MOS:O2	7:C:1328:MOS:MO	1.71	0.62
3:C:840:HIS:HE1	3:C:874:SER:OG	1.82	0.61
7:L:1328:MOS:O2	7:L:1328:MOS:MO	1.72	0.61
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.36	0.61
3:L:840:HIS:HE1	3:L:874:SER:OG	1.83	0.60
3:C:851:MET:HB2	3:C:853:THR:HG22	1.83	0.60
1:J:131:GLN:HE21	1:J:133:GLU:H	1.50	0.60
3:C:719:LEU:HD11	3:C:895:ARG:CB	2.32	0.59
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.84	0.59
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.51	0.59
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.21	0.58
2:B:331:LEU:O	2:B:335:ARG:HG2	2.03	0.58
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.85	0.57
3:C:601:ASN:O	3:C:821:HIS:HD2	1.86	0.57
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.87	0.57
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.23	0.57
1:J:95:LYS:CE	9:L:1408:HOH:O	2.52	0.57
1:A:139:ILE:HD12	1:A:164:ALA:HB2	1.86	0.56
3:L:601:ASN:O	3:L:821:HIS:HD2	1.89	0.55
2:K:255:ALA:CB	2:K:277:MET:HE3	2.34	0.55
2:B:427:ARG:HD2	9:B:568:HOH:O	2.07	0.55
2:K:241:THR:HB	2:K:243:LYS:HE2	1.89	0.55
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.06	0.53
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.55	0.53
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.44	0.52
2:K:287:LEU:HD22	2:K:301:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:281:PRO:HB2	2:K:287:LEU:HD12	1.91	0.52
3:L:623:SER:HA	3:L:626:GLN:HE21	1.74	0.52
2:B:390:PHE:O	2:B:462:ARG:HD2	2.10	0.51
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.58	0.51
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	2.08	0.51
3:L:880:ARG:O	3:L:884:HIS:HD2	1.94	0.50
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.94	0.49
3:C:880:ARG:O	3:C:884:HIS:HD2	1.95	0.49
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.78	0.49
2:B:249:LYS:HG2	2:B:401:GLU:O	2.13	0.49
3:C:853:THR:HG23	3:C:855:THR:H	1.76	0.49
3:C:598:ARG:HD2	3:C:604:PHE:CZ	2.48	0.49
2:B:281:PRO:HB2	2:B:287:LEU:CD1	2.43	0.49
3:C:680:ARG:HG2	9:C:1532:HOH:O	2.14	0.48
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.13	0.48
2:K:292:HIS:HE1	9:K:564:HOH:O	1.95	0.48
3:C:821:HIS:HE1	9:C:2949:HOH:O	1.96	0.48
3:C:851:MET:HE2	3:C:857:VAL:HG21	1.94	0.48
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.79	0.48
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.95	0.48
2:B:337:PHE:O	9:B:2882:HOH:O	2.20	0.47
3:L:939:GLU:CD	3:L:939:GLU:H	2.21	0.47
2:B:281:PRO:HB2	2:B:287:LEU:HD13	1.96	0.47
2:K:441:LEU:HB3	2:K:451:GLU:HB2	1.95	0.47
3:C:1287:ASN:HD22	3:C:1289:ASN:H	1.61	0.47
2:B:427:ARG:HD3	3:C:1212:HIS:CD2	2.50	0.47
3:C:779:MET:SD	3:C:810:VAL:CG1	3.02	0.47
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.96	0.47
3:L:1001:ILE:CD1	3:L:1269:SER:HA	2.38	0.47
3:L:695:ILE:HG23	3:L:700:ASP:HB3	1.97	0.46
3:C:697:THR:O	3:C:700:ASP:HB2	2.15	0.46
3:C:939:GLU:H	3:C:939:GLU:CD	2.23	0.46
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.96	0.46
3:C:1134:ARG:NE	9:C:546:HOH:O	2.48	0.46
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.61	0.46
3:C:885:MET:SD	3:C:896:GLY:HA3	2.56	0.45
2:K:255:ALA:HB2	2:K:277:MET:HE2	1.89	0.45
3:L:911:PHE:O	3:L:912:ARG:C	2.59	0.45
3:L:1007:ILE:O	3:L:1008:SER:HB3	2.17	0.45
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.99	0.45
2:B:284:ILE:HB	2:B:287:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1008:SER:HA	3:C:1081:VAL:HG11	2.00	0.45
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.16	0.44
1:J:32:ARG:HD2	3:L:598:ARG:NH2	2.32	0.44
3:C:853:THR:O	3:C:944:LYS:NZ	2.43	0.44
3:L:614:HIS:HD2	3:L:693:PRO:O	1.99	0.44
2:K:224:PRO:N	9:K:2913:HOH:O	2.50	0.44
2:B:313:LEU:HD21	2:B:335:ARG:HH12	1.83	0.44
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.33	0.44
9:K:1960:HOH:O	3:L:680:ARG:HG2	2.18	0.44
3:C:923:ALA:HA	3:C:926:TRP:NE1	2.33	0.43
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.18	0.43
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.44	0.43
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.18	0.43
3:C:844:ALA:HB2	3:C:922:ILE:HD13	2.00	0.43
3:C:911:PHE:O	3:C:912:ARG:C	2.61	0.42
3:L:696:ILE:HG12	9:L:1602:HOH:O	2.19	0.42
3:C:618:LYS:HA	3:C:618:LYS:HD3	1.88	0.42
3:L:1008:SER:HA	3:L:1081:VAL:HG11	2.02	0.42
3:C:939:GLU:HG2	3:C:977:TYR:CZ	2.55	0.42
2:K:387:HIS:CG	2:K:467:LEU:HD11	2.55	0.41
2:B:234:VAL:HG11	2:B:278:ILE:HD12	2.02	0.41
3:C:614:HIS:HE1	9:C:2711:HOH:O	2.02	0.41
2:B:264:ILE:HG22	2:B:268:MET:HE2	2.02	0.41
3:C:1287:ASN:ND2	3:C:1289:ASN:H	2.17	0.41
3:L:734:LEU:HD21	3:L:921:PHE:CE2	2.56	0.41
3:C:779:MET:HE2	3:C:779:MET:HB3	1.98	0.41
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.34	0.41
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.68	0.41
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.84	0.41
1:J:3:ALA:HB2	2:K:230:GLU:CG	2.46	0.41
3:L:884:HIS:HE1	3:L:1005:PHE:HA	1.86	0.41
3:C:779:MET:SD	3:C:810:VAL:HG12	2.60	0.40
1:A:36:LEU:HD22	1:A:89:GLU:HG3	2.02	0.40
3:L:663:VAL:HG12	3:L:834:LEU:HD11	2.04	0.40
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.85	0.40
3:C:736:ILE:CG2	3:C:842:PHE:HB2	2.52	0.40
3:C:734:LEU:HD21	3:C:921:PHE:CE2	2.56	0.40
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.86	0.40
3:C:1057:PRO:HD2	3:C:1060:LYS:HD2	2.02	0.40
3:L:770:MET:HG2	9:L:2880:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	21	7
2	B	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	K	303/334 (91%)	294 (97%)	9 (3%)	0	100	100
3	C	754/756 (100%)	734 (97%)	16 (2%)	4 (0%)	24	10
3	L	743/756 (98%)	726 (98%)	13 (2%)	4 (0%)	24	10
All	All	2456/2508 (98%)	2394 (98%)	53 (2%)	9 (0%)	30	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	912	ARG
3	C	1008	SER
3	L	1008	SER
3	L	912	ARG
3	L	1139	GLY
3	L	797	GLY
3	C	797	GLY
3	C	1139	GLY
1	J	43	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/137 (100%)	135 (98%)	2 (2%)	57	35
1	J	137/137 (100%)	136 (99%)	1 (1%)	76	63
2	B	290/290 (100%)	286 (99%)	4 (1%)	59	38
2	K	261/290 (90%)	256 (98%)	5 (2%)	50	27
3	C	632/632 (100%)	626 (99%)	6 (1%)	70	55
3	L	624/632 (99%)	618 (99%)	6 (1%)	68	50
All	All	2081/2118 (98%)	2057 (99%)	24 (1%)	63	43

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	89	GLU
2	B	200	GLU
2	B	202	MET
2	B	312	LEU
2	B	328	ARG
3	C	598	ARG
3	C	743	TYR
3	C	939	GLU
3	C	1208	LEU
3	C	1287	ASN
3	C	1290	THR
1	J	89	GLU
2	K	243	LYS
2	K	312	LEU
2	K	318	LYS
2	K	328	ARG
2	K	397	LEU
3	L	598	ARG
3	L	743	TYR
3	L	770	MET
3	L	939	GLU
3	L	1203	LEU
3	L	1208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN

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Mol	Chain	Res	Type
2	B	261	ASN
2	B	322	GLN
2	B	333	GLN
2	B	351	ASN
2	B	471	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
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	1148	ASN
3	C	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	226	GLN
2	K	292	HIS
2	K	333	GLN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	683	HIS
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	1220	HIS
3	L	1284	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	FES	J	601	1	0,4,4	-	-	-		
6	MTE	L	1327	7	21,26,26	1.50	2 (9%)	19,40,40	1.74	5 (26%)
8	GUN	C	503	-	12,12,12	1.51	2 (16%)	15,17,17	2.04	6 (40%)
6	MTE	C	1327	7	21,26,26	1.60	2 (9%)	19,40,40	1.81	6 (31%)
4	FES	A	602	1	0,4,4	-	-	-		
7	MOS	L	1328	6	0,3,3	-	-	-		
4	FES	A	601	1	0,4,4	-	-	-		
7	MOS	C	1328	6	0,3,3	-	-	-		
5	FAD	K	606	-	58,58,58	1.11	5 (8%)	85,89,89	1.50	14 (16%)
5	FAD	B	606	-	58,58,58	1.05	5 (8%)	85,89,89	1.53	14 (16%)
8	GUN	L	503	-	12,12,12	1.39	2 (16%)	15,17,17	2.10	6 (40%)
4	FES	J	602	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MTE	L	1327	7	-	1/6/34/34	0/3/3/3
4	FES	J	601	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GUN	C	503	-	-	-	0/2/2/2
6	MTE	C	1327	7	-	1/6/34/34	0/3/3/3
4	FES	A	602	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1
5	FAD	K	606	-	-	0/34/50/50	0/6/6/6
5	FAD	B	606	-	-	0/34/50/50	0/6/6/6
8	GUN	L	503	-	-	-	0/2/2/2
4	FES	J	602	1	-	-	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1327	MTE	C9-C10	6.02	1.48	1.38
6	L	1327	MTE	C9-C10	5.62	1.48	1.38
5	K	606	FAD	C4X-N5	4.08	1.39	1.30
5	B	606	FAD	C4X-N5	3.73	1.38	1.30
5	K	606	FAD	C10-N1	3.00	1.39	1.33
5	K	606	FAD	C2A-N1A	2.84	1.39	1.33
5	B	606	FAD	C2A-N3A	2.68	1.38	1.33
5	K	606	FAD	C2A-N3A	2.61	1.38	1.33
8	C	503	GUN	C5-N7	-2.59	1.33	1.39
5	B	606	FAD	C10-N1	2.58	1.38	1.33
5	B	606	FAD	C2A-N1A	2.53	1.38	1.33
8	L	503	GUN	C5-C4	2.52	1.46	1.39
8	C	503	GUN	C5-C4	2.49	1.46	1.39
8	L	503	GUN	C5-N7	-2.28	1.34	1.39
5	K	606	FAD	C8A-N7A	2.22	1.36	1.31
5	B	606	FAD	C8A-N7A	2.11	1.35	1.31
6	C	1327	MTE	C4-N3	-2.05	1.35	1.38
6	L	1327	MTE	C9-C4	2.01	1.47	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-5.94	119.59	128.58
5	K	606	FAD	N3A-C2A-N1A	-5.49	120.28	128.58
8	L	503	GUN	C6-C5-N7	4.14	137.82	130.29
5	K	606	FAD	C5A-C4A-N3A	-4.09	121.08	126.72
5	K	606	FAD	N9A-C8A-N7A	-4.04	108.20	113.94
5	B	606	FAD	C5A-C4A-N3A	-3.87	121.39	126.72
5	B	606	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
6	L	1327	MTE	C2-N1-C10	3.78	120.03	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	GUN	C6-C5-N7	3.73	137.08	130.29
6	C	1327	MTE	C2-N1-C10	3.63	119.77	113.36
8	C	503	GUN	N9-C4-N3	3.37	130.09	125.99
8	L	503	GUN	N9-C4-N3	3.32	130.03	125.99
8	L	503	GUN	C2-N3-C4	3.22	119.05	113.36
5	K	606	FAD	C5A-N7A-C8A	3.19	108.47	103.45
5	K	606	FAD	C2A-N3A-C4A	3.16	119.54	111.83
5	B	606	FAD	C2A-N3A-C4A	3.15	119.52	111.83
5	B	606	FAD	C5A-N7A-C8A	3.13	108.37	103.45
6	L	1327	MTE	O4-C4-C9	-2.98	120.07	127.26
5	B	606	FAD	C4X-C10-N10	2.96	120.72	116.48
8	C	503	GUN	C2-N3-C4	2.94	118.55	113.36
5	K	606	FAD	C4-N3-C2	-2.91	120.48	125.64
5	K	606	FAD	N3A-C4A-N9A	2.89	132.07	127.17
6	C	1327	MTE	O4-C4-C9	-2.88	120.31	127.26
5	B	606	FAD	C4-N3-C2	-2.87	120.55	125.64
5	B	606	FAD	N3A-C4A-N9A	2.81	131.94	127.17
5	K	606	FAD	C4X-C10-N10	2.71	120.36	116.48
5	B	606	FAD	C4X-C4-N3	2.66	120.03	113.25
6	L	1327	MTE	C4-C9-N5	2.63	123.43	116.27
6	L	1327	MTE	O3'-C7-C6	-2.60	107.23	108.96
6	C	1327	MTE	C4-C9-N5	2.58	123.31	116.27
6	C	1327	MTE	O3P-P-O4'	-2.55	100.01	106.67
8	C	503	GUN	O6-C6-C5	-2.54	119.82	126.53
5	K	606	FAD	C10-C4X-N5	-2.52	119.66	124.81
5	B	606	FAD	C10-C4X-N5	-2.52	119.66	124.81
5	K	606	FAD	C4X-C4-N3	2.51	119.63	113.25
8	L	503	GUN	C4-C5-N7	-2.46	106.31	110.17
8	L	503	GUN	O6-C6-C5	-2.36	120.30	126.53
5	K	606	FAD	C4A-N9A-C8A	2.35	108.20	105.74
8	C	503	GUN	C4-C5-N7	-2.28	106.60	110.17
5	K	606	FAD	C5'-C4'-C3'	-2.24	107.99	112.22
5	B	606	FAD	C4A-N9A-C8A	2.22	108.07	105.74
8	L	503	GUN	C8-N7-C5	2.22	107.37	104.38
5	B	606	FAD	C4-C4X-N5	2.15	121.18	118.21
6	C	1327	MTE	C9-C4-N3	2.15	118.03	112.13
6	L	1327	MTE	C9-C4-N3	2.14	118.02	112.13
8	C	503	GUN	C8-N7-C5	2.10	107.22	104.38
5	K	606	FAD	O2P-P-O3P	2.09	112.93	107.27
6	C	1327	MTE	O3'-C7-N8	2.08	110.49	108.61
5	B	606	FAD	O4-C4-C4X	-2.08	121.06	126.53
5	B	606	FAD	C9A-C5X-N5	-2.04	120.29	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	606	FAD	C4A-C5A-N7A	-2.02	108.27	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1327	MTE	C3'-C4'-O4'-P
6	L	1327	MTE	C3'-C4'-O4'-P

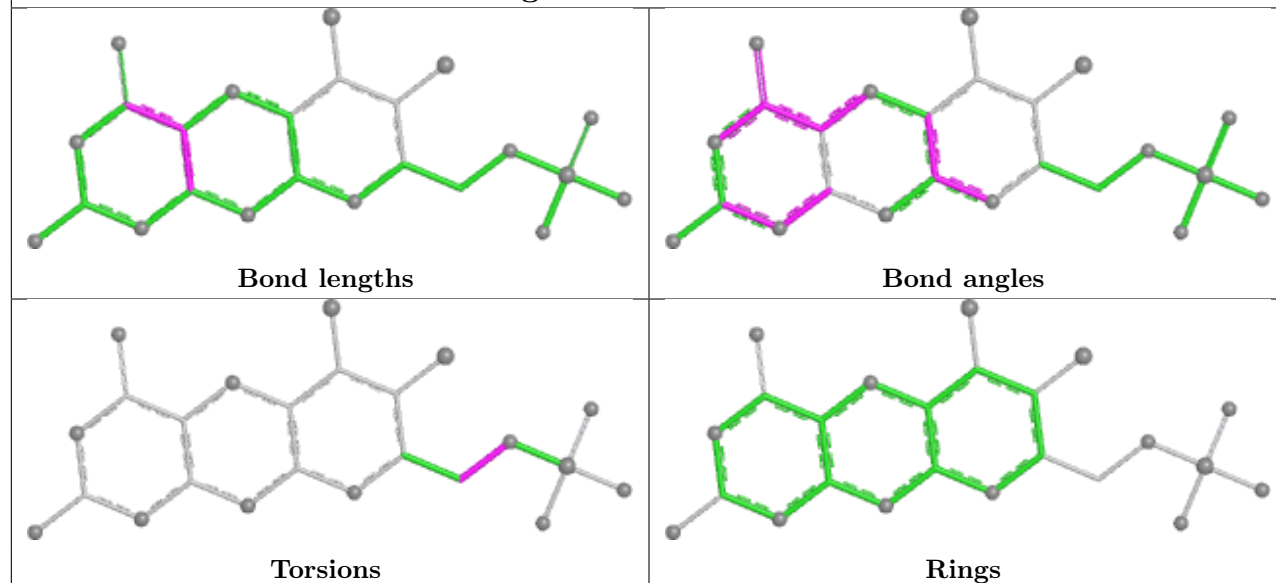
There are no ring outliers.

3 monomers are involved in 3 short contacts:

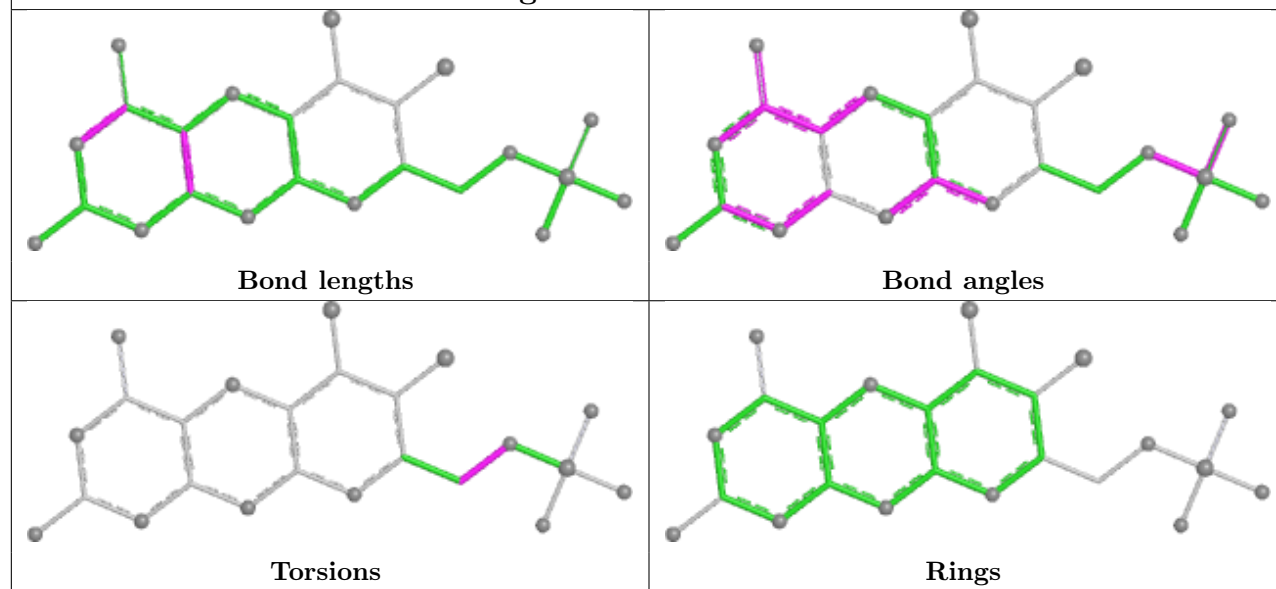
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1328	MOS	1	0
7	C	1328	MOS	1	0
5	K	606	FAD	1	0

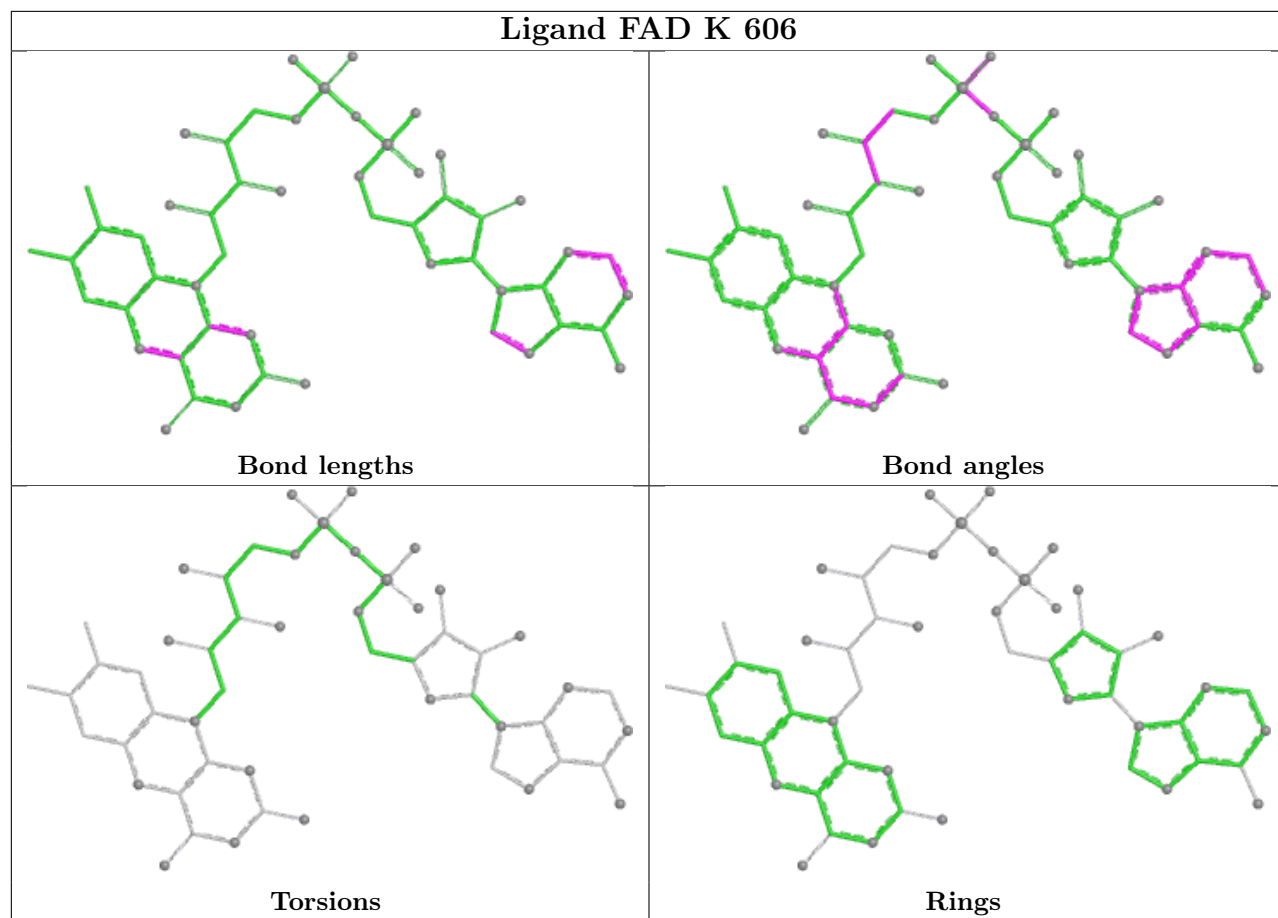
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

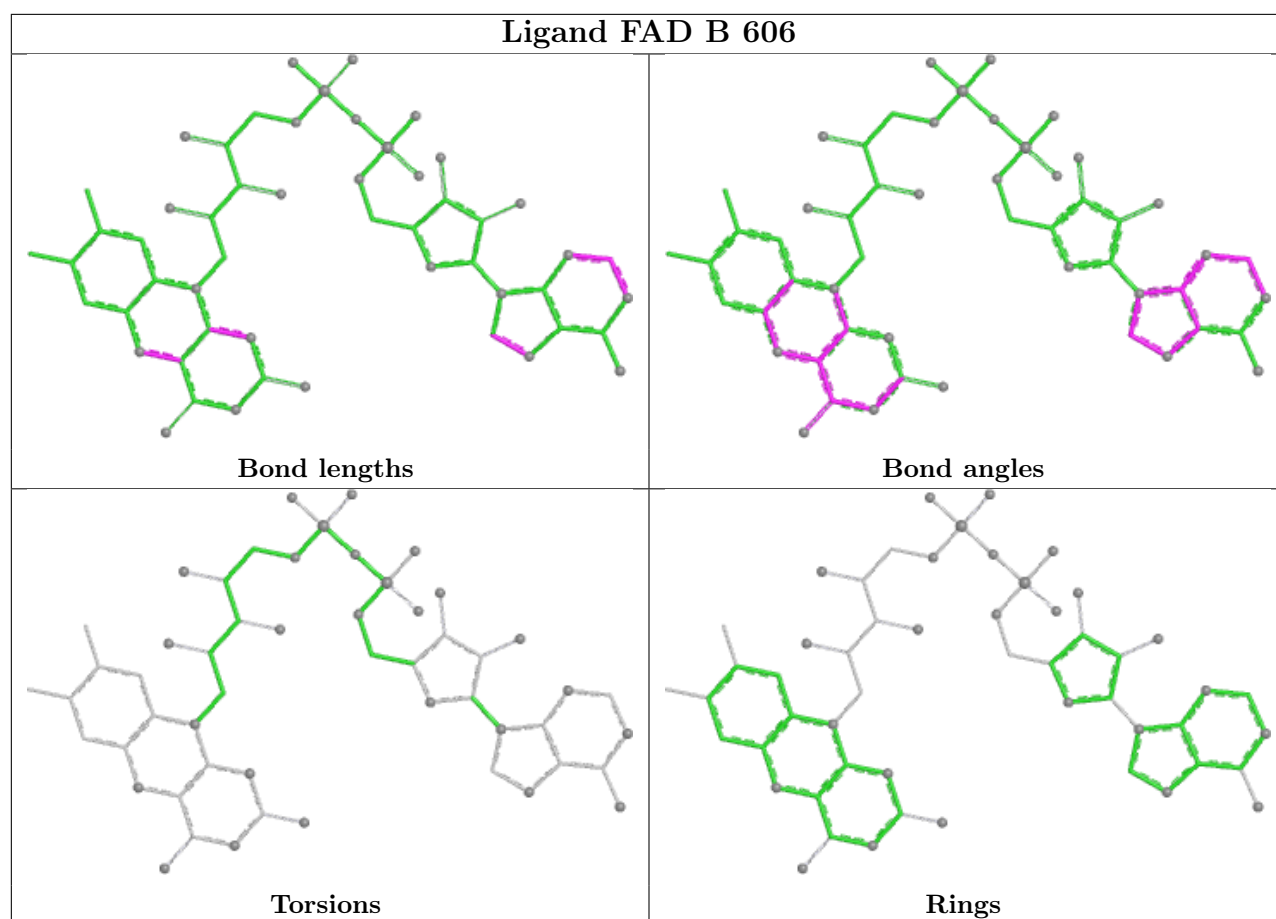
Ligand MTE L 1327



Ligand MTE C 1327







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.03	5 (3%)	52 55	7, 13, 25, 34	0
1	J	164/164 (100%)	0.29	14 (8%)	16 16	9, 16, 33, 43	0
2	B	334/334 (100%)	0.50	19 (5%)	29 30	11, 19, 29, 40	0
2	K	305/334 (91%)	0.77	27 (8%)	15 15	14, 23, 33, 37	0
3	C	756/756 (100%)	-0.29	7 (0%)	81 84	6, 12, 21, 25	0
3	L	745/756 (98%)	-0.10	20 (2%)	56 59	7, 14, 25, 45	0
All	All	2468/2508 (98%)	0.06	92 (3%)	45 47	6, 15, 29, 45	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	58	TYR	7.8
2	B	424	ALA	6.6
2	K	528	GLY	6.3
3	L	1288	ASN	5.8
1	J	61	LEU	5.2
1	A	61	LEU	4.8
3	L	1289	ASN	4.3
3	L	1287	ASN	4.3
3	L	1290	THR	4.2
2	K	378	GLY	4.1
2	K	336	TRP	4.0
2	K	338	ALA	4.0
2	K	424	ALA	4.0
1	J	64	LYS	3.8
2	K	254	GLU	3.8
1	J	2	THR	3.7
2	K	291	GLU	3.6
2	K	499	ASP	3.6
1	A	2	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	K	429	ASP	3.5
2	B	222	VAL	3.5
3	C	657	LYS	3.5
2	B	202	MET	3.5
2	B	272	ASN	3.4
2	K	335	ARG	3.3
1	J	140	GLU	3.2
3	L	1286	THR	3.1
1	A	165	LYS	3.1
2	B	425	SER	3.1
2	K	316	VAL	3.0
1	J	165	LYS	3.0
1	J	60	ARG	3.0
3	L	1001	ILE	3.0
2	B	200	GLU	3.0
1	A	60	ARG	3.0
1	J	141	ASP	2.9
2	B	499	ASP	2.9
2	K	475	SER	2.9
2	K	474	LEU	2.8
3	C	779	MET	2.8
3	L	683	HIS	2.8
1	J	136	VAL	2.8
3	L	992	CYS	2.8
3	C	1290	THR	2.7
2	B	211	ILE	2.7
2	B	207	THR	2.7
1	J	164	ALA	2.7
3	C	1250	LYS	2.6
2	K	272	ASN	2.6
1	J	63	ASP	2.6
3	C	992	CYS	2.6
2	B	335	ARG	2.6
2	B	336	TRP	2.5
2	K	468	LYS	2.5
2	B	429	ASP	2.5
3	L	1276	ASP	2.5
3	L	985	ASP	2.4
2	K	527	LEU	2.4
3	L	1143	GLU	2.4
2	K	318	LYS	2.4
2	B	219	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	2.3
3	L	983	GLU	2.3
3	C	683	HIS	2.3
3	L	748	CYS	2.3
2	B	195	LEU	2.2
3	L	1293	LEU	2.2
1	A	58	TYR	2.2
1	J	133	GLU	2.2
2	B	220	LYS	2.2
2	K	243	LYS	2.2
2	K	467	LEU	2.2
3	L	770	MET	2.2
3	L	725	GLU	2.2
3	L	958	ARG	2.2
2	B	528	GLY	2.2
1	J	129	ARG	2.2
2	K	477	PHE	2.2
1	J	62	GLN	2.1
2	B	295	GLU	2.1
2	K	482	LEU	2.1
2	K	425	SER	2.1
2	K	377	ARG	2.1
2	K	337	PHE	2.1
2	K	230	GLU	2.1
2	B	218	ARG	2.1
3	L	657	LYS	2.1
3	L	852	LYS	2.1
3	C	720	LYS	2.0
2	K	445	GLY	2.0
2	K	317	ALA	2.0
3	L	979	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

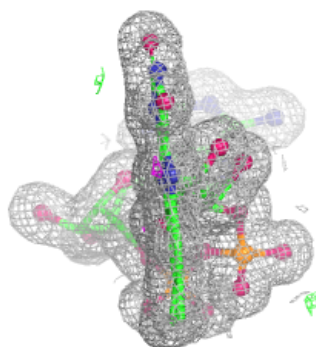
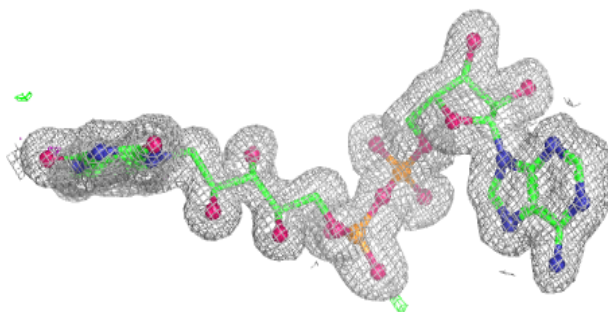
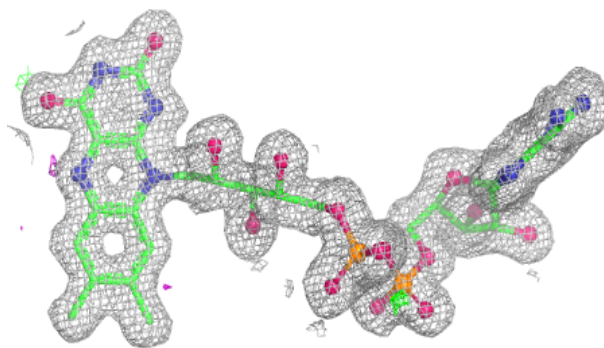
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GUN	C	503	11/11	0.90	0.09	17,18,19,19	0
8	GUN	L	503	11/11	0.91	0.09	18,19,20,20	0
5	FAD	B	606	53/53	0.97	0.05	10,12,15,16	0
5	FAD	K	606	53/53	0.97	0.06	13,17,18,18	0
6	MTE	L	1327	24/24	0.99	0.04	8,10,12,13	0
7	MOS	L	1328	4/4	0.99	0.08	12,12,12,22	0
4	FES	J	601	4/4	0.99	0.02	9,10,10,10	0
6	MTE	C	1327	24/24	0.99	0.04	6,8,10,11	0
7	MOS	C	1328	4/4	1.00	0.07	11,12,15,23	0
4	FES	A	601	4/4	1.00	0.01	7,8,8,9	0
4	FES	J	602	4/4	1.00	0.02	10,10,10,11	0
4	FES	A	602	4/4	1.00	0.02	9,9,10,10	0

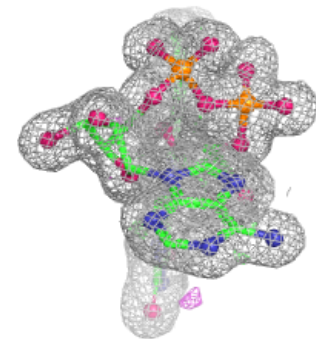
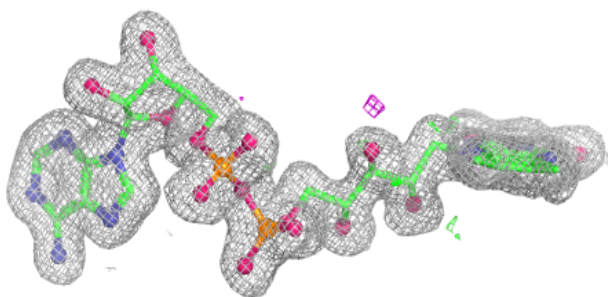
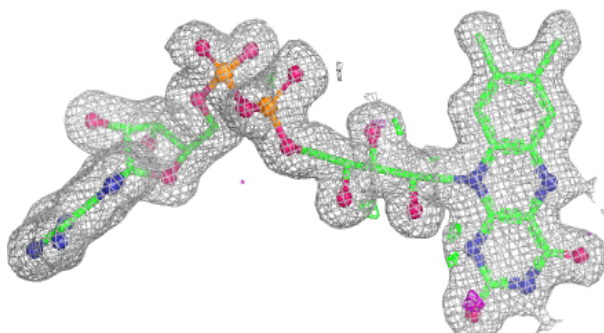
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

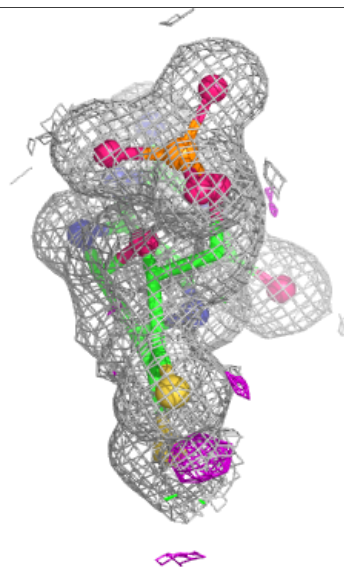
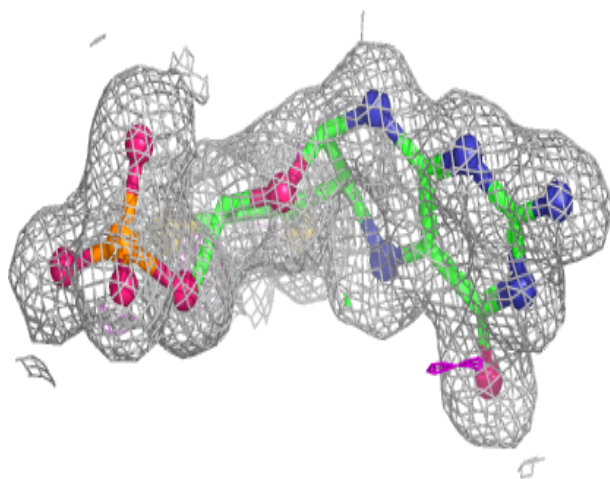
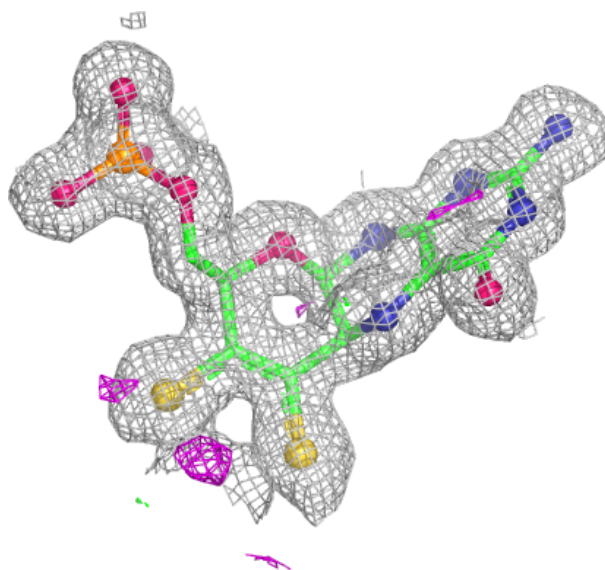
**Electron density around FAD K 606:**

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



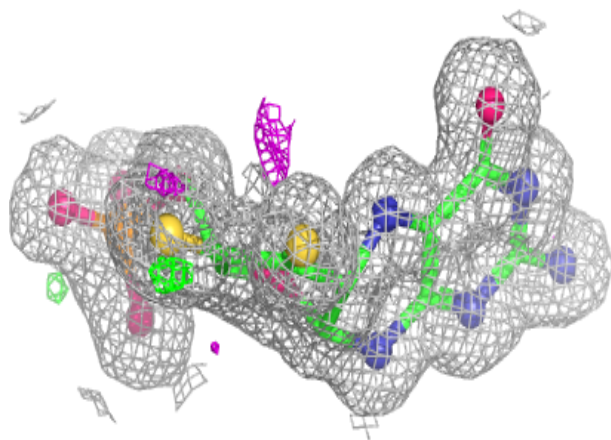
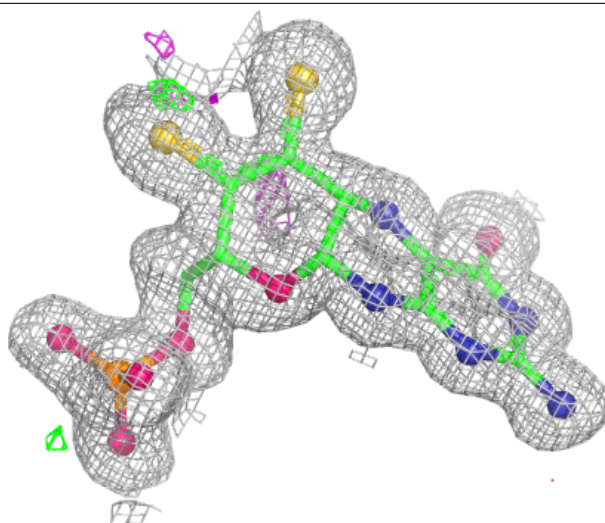
Electron density around MTE L 1327:

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



Electron density around MTE C 1327:

$2mF_o-DF_c$ (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.