



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:21 PM UTC

PDB ID : 3NVZ / pdb_00003nvz
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Indole-3-Aldehyde
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

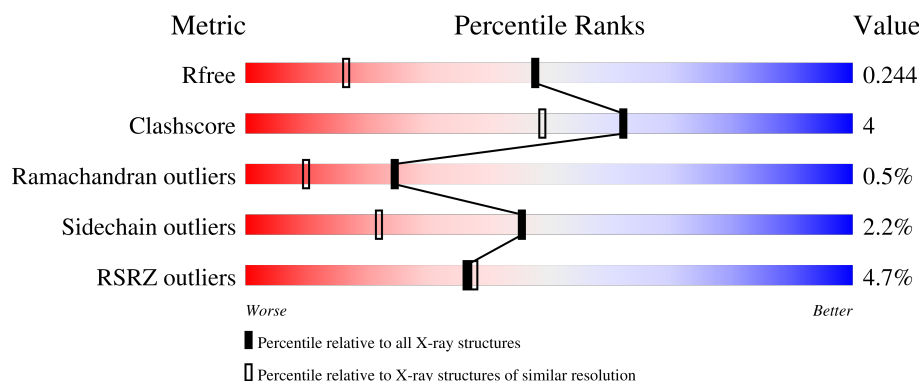
1 Overall quality at a glance

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	6% 93% 7%
1	J	164	10% 90% 9%
2	B	305	9% 90% 9%
2	K	305	10% 93% 6%
3	C	755	2% 89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	755	3% 90% 8% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20672 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			

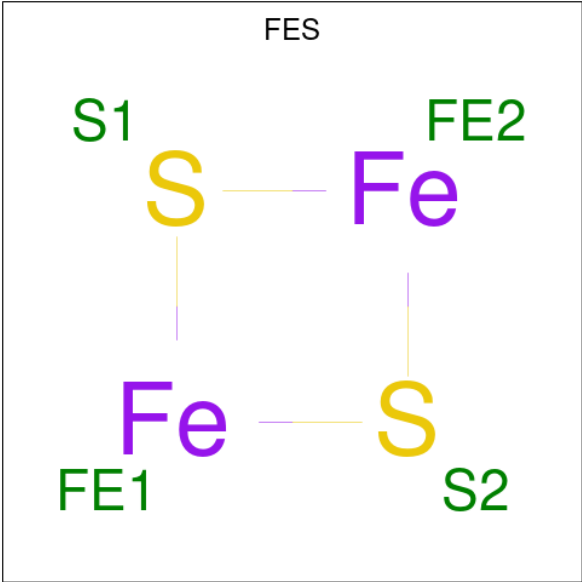
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

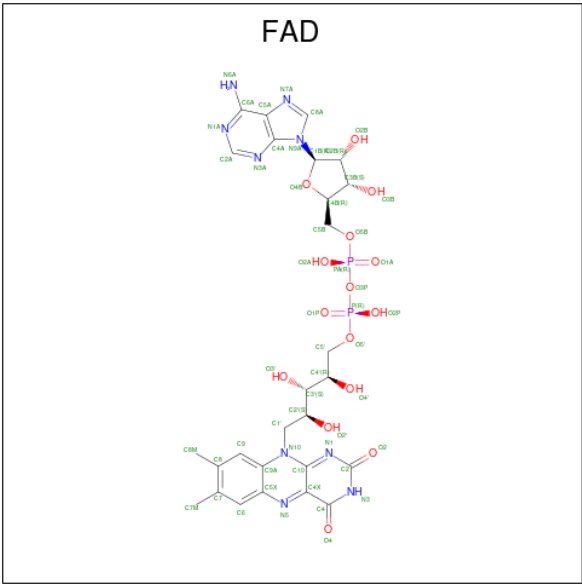
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

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



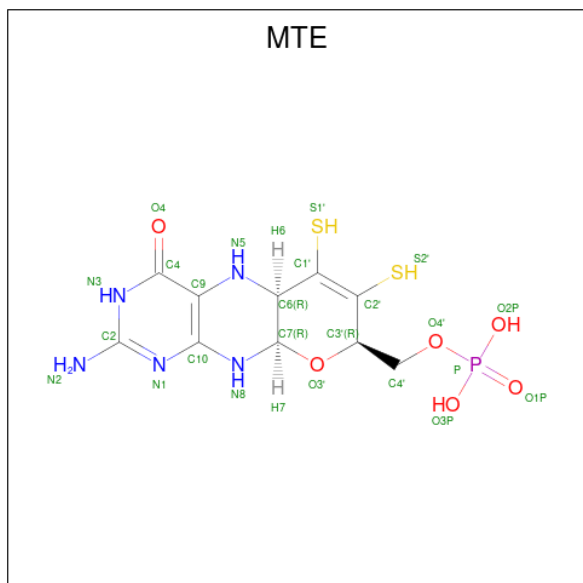
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



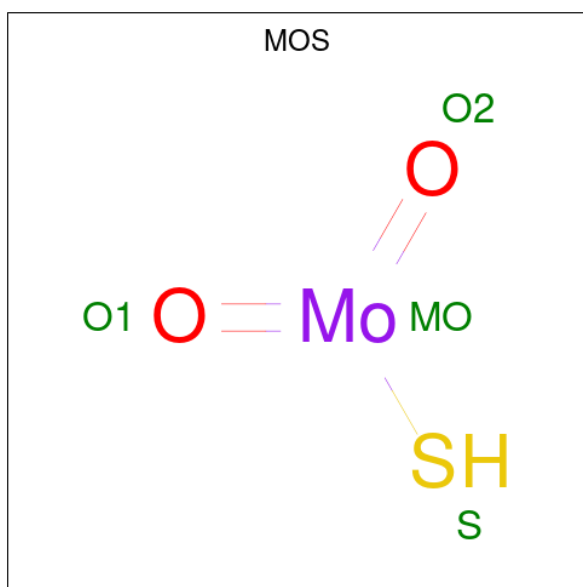
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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: $C_{10}H_{14}N_5O_6PS_2$).



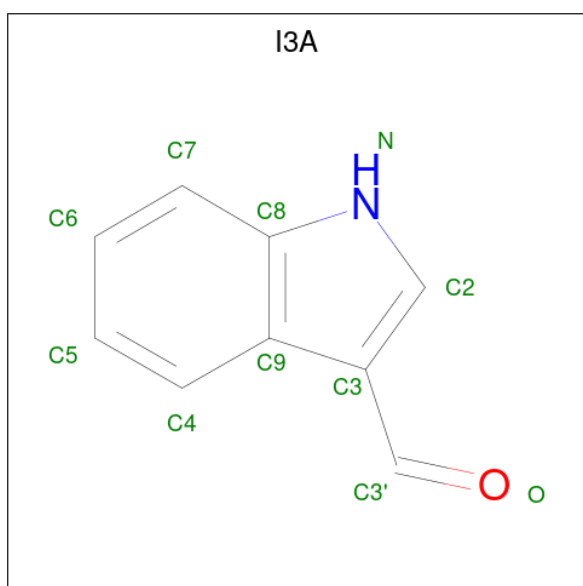
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	L	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- 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 1H-INDOLE-3-CARBALDEHYDE (CCD ID: I3A) (formula: C_9H_7NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	9	1	1		
8	L	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total 114	O 114	0	0
9	B	192	Total 192	O 192	0	0
9	C	538	Total 538	O 538	0	0
9	J	111	Total 111	O 111	0	0
9	K	151	Total 151	O 151	0	0
9	L	494	Total 494	O 494	0	0

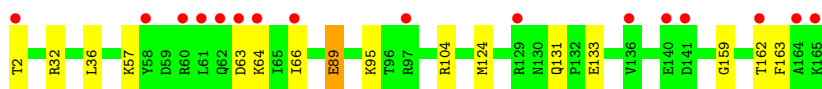
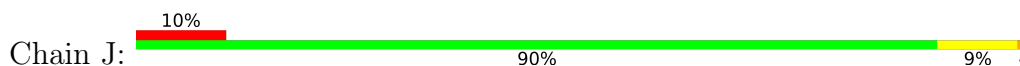
3 Residue-property plots [i](#)

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

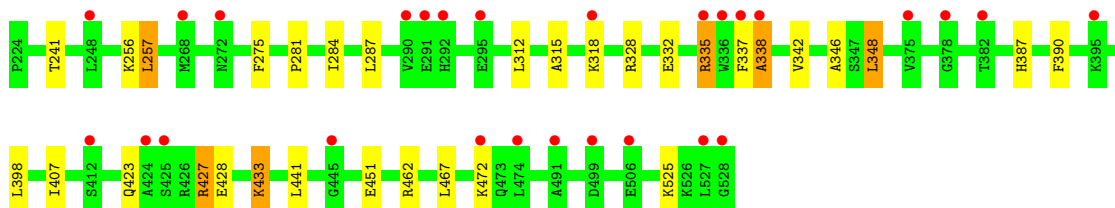
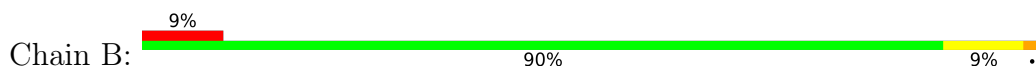
- Molecule 1: Xanthine dehydrogenase/oxidase



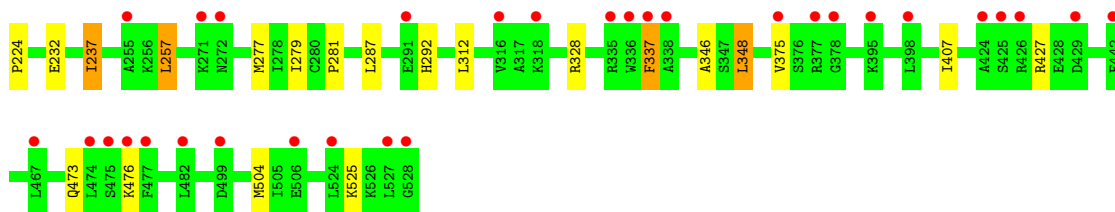
- Molecule 1: Xanthine dehydrogenase/oxidase



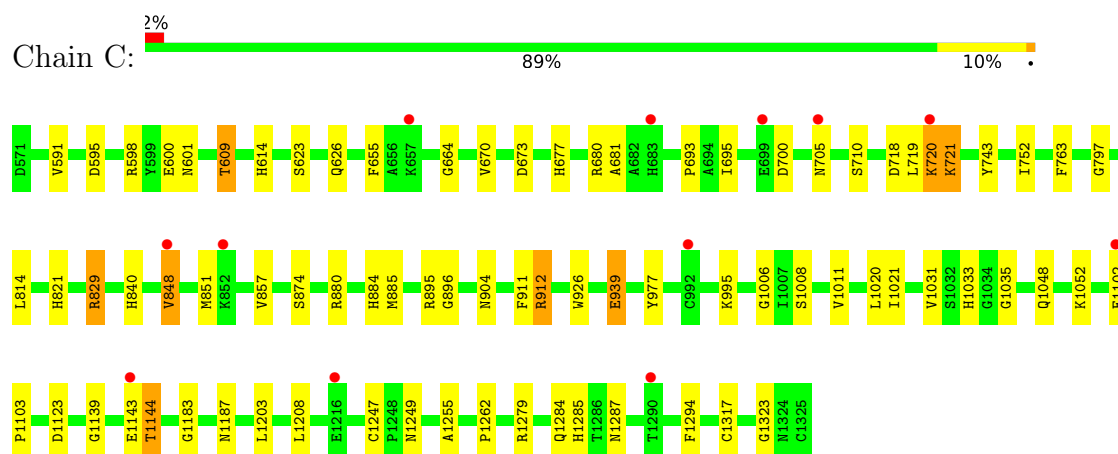
- Molecule 2: Xanthine dehydrogenase/oxidase



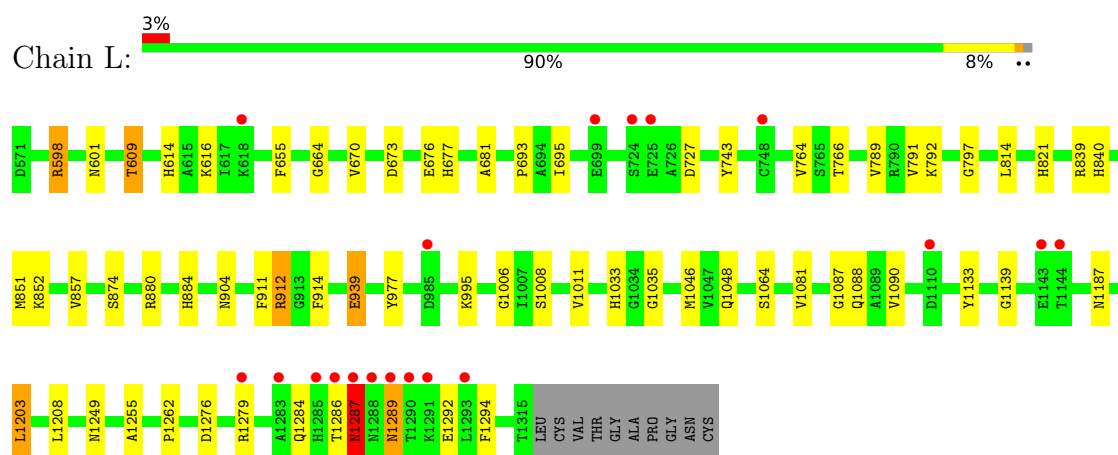
- Molecule 2: Xanthine dehydrogenase/oxidase



- 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	133.41Å 73.70Å 138.92Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	45.20 – 1.60 45.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.20-1.60) 95.6 (45.20-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.246 0.212 , 0.244	Depositor DCC
R_{free} test set	17094 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20672	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, MTE, FES, FAD, I3A

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	0.71	0/1277	0.82	0/1723
1	J	0.71	0/1277	0.79	0/1723
2	B	0.61	0/2438	0.81	1/3290 (0.0%)
2	K	0.57	0/2438	0.79	0/3290
3	C	0.71	0/5951	0.82	3/8061 (0.0%)
3	L	0.68	0/5888	0.81	1/7974 (0.0%)
All	All	0.67	0/19269	0.81	5/26061 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1262	PRO	N-CA-C	7.56	119.92	110.70
3	C	1262	PRO	N-CA-C	6.82	119.02	110.70
3	C	829	ARG	NE-CZ-NH2	-6.12	113.69	119.20
3	C	720	LYS	N-CA-C	-5.10	102.31	109.96
2	B	335	ARG	N-CA-C	5.07	116.49	111.07

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	1255	0	1265	5	0
1	J	1255	0	1265	16	0
2	B	2389	0	2459	21	0
2	K	2389	0	2459	11	0
3	C	5823	0	5746	58	0
3	L	5761	0	5685	47	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	1	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	7	2	0
8	L	11	0	7	1	0
9	A	114	0	0	0	0
9	B	192	0	0	4	0
9	C	538	0	0	4	0
9	J	111	0	0	5	0
9	K	151	0	0	2	0
9	L	494	0	0	3	0
All	All	20672	0	18975	154	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 (154) 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:1502:HOH:O	1.11	1.22
3:L:1081:VAL:HG21	9:L:1363:HOH:O	1.03	1.19
2:B:241:THR:HB	9:B:752:HOH:O	1.03	1.18
3:L:764:VAL:HB	9:L:1454:HOH:O	0.94	1.11
3:C:1143:GLU:O	3:C:1144:THR:HG23	1.62	0.98
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	1.46	0.95
3:C:1102:GLU:HG2	3:C:1103:PRO:HD3	1.54	0.87
1:J:32:ARG:NE	9:J:1229:HOH:O	1.92	0.86
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.22	0.85
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.42	0.84
1:A:131:GLN:HE21	1:A:133:GLU:H	1.27	0.82
3:L:695:ILE:H	3:L:904:ASN:HD22	1.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.17	0.79
3:C:680:ARG:NH2	9:C:2132:HOH:O	2.13	0.79
3:L:1046:MET:HE2	3:L:1090:VAL:CG2	2.14	0.78
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.77
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.33	0.75
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.73
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.71	0.73
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.32	0.70
1:A:42:GLY:O	3:C:829:ARG:HD2	1.90	0.70
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.08	0.69
3:C:705:ASN:OD1	9:C:1525:HOH:O	2.10	0.69
1:J:131:GLN:HE21	1:J:133:GLU:H	1.41	0.68
1:J:159:GLY:O	1:J:162:THR:HG22	1.93	0.68
3:L:851:MET:HE2	3:L:857:VAL:HG11	1.77	0.67
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.13	0.67
3:L:840:HIS:HE1	3:L:874:SER:OG	1.77	0.67
3:L:1046:MET:HE3	3:L:1046:MET:HA	1.76	0.66
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.15	0.65
3:C:601:ASN:O	3:C:821:HIS:HD2	1.80	0.64
3:L:1011:VAL:HG23	8:L:1:I3A:H5	1.80	0.64
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.80	0.63
3:C:720:LYS:O	3:C:721:LYS:CB	2.47	0.63
3:C:1011:VAL:HG23	8:C:1:I3A:H5	1.81	0.62
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.35	0.62
2:K:237:ILE:HG13	2:K:277:MET:HE1	1.82	0.61
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.81	0.61
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.82	0.61
3:C:623:SER:HA	3:C:626:GLN:HE21	1.66	0.61
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.98	0.61
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.12	0.61
7:L:1327:MOS:O2	7:L:1327:MOS:MO	1.72	0.60
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.84	0.60
3:C:840:HIS:HE1	3:C:874:SER:OG	1.85	0.60
3:L:609:THR:HG22	9:L:500:HOH:O	2.01	0.60
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.00	0.59
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.67	0.59
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.14	0.59
3:L:609:THR:HG23	3:L:664:GLY:HA2	1.86	0.58
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.51	0.58
9:B:1039:HOH:O	3:C:680:ARG:HG2	2.04	0.57
2:K:281:PRO:HB2	2:K:287:LEU:CD1	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.88	0.56
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.53	0.56
3:C:718:ASP:OD2	3:C:720:LYS:O	2.24	0.56
1:J:32:ARG:CZ	9:J:1229:HOH:O	2.44	0.56
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.89	0.55
3:C:719:LEU:HD12	3:C:895:ARG:NH1	2.21	0.55
2:B:315:ALA:HA	2:B:318:LYS:HE2	1.89	0.55
3:L:764:VAL:HG23	3:L:791:VAL:HG22	1.87	0.55
3:C:880:ARG:O	3:C:884:HIS:HD2	1.89	0.55
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.42	0.55
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.88	0.55
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.88	0.55
3:C:720:LYS:O	3:C:721:LYS:HB2	2.07	0.54
3:L:727:ASP:HB3	3:L:852:LYS:HE2	1.90	0.54
2:B:241:THR:HG23	9:B:138:HOH:O	2.08	0.54
3:L:792:LYS:NZ	3:L:1064:SER:O	2.41	0.54
1:J:32:ARG:NH2	9:J:1229:HOH:O	2.42	0.53
3:L:764:VAL:HG21	3:L:789:VAL:CG1	2.39	0.53
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.90	0.52
2:K:348:LEU:HD13	2:K:407:ILE:HD13	1.91	0.52
3:L:880:ARG:O	3:L:884:HIS:HD2	1.93	0.51
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.11	0.51
3:C:614:HIS:HD2	3:C:693:PRO:O	1.93	0.51
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.75	0.51
3:L:609:THR:CG2	3:L:664:GLY:HA2	2.40	0.51
2:K:427:ARG:NE	2:K:504:MET:HE3	2.25	0.51
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.57	0.50
2:B:332:GLU:HA	2:B:335:ARG:HG3	1.93	0.50
3:C:600:GLU:HG2	3:L:598:ARG:O	2.12	0.50
2:B:256:LYS:HG3	2:B:275:PHE:CD2	2.47	0.50
3:C:851:MET:HE2	3:C:857:VAL:HG11	1.92	0.50
3:C:1285:HIS:HD2	9:C:334:HOH:O	1.95	0.49
2:K:292:HIS:HE1	9:K:543:HOH:O	1.95	0.49
2:B:427:ARG:HG2	2:B:428:GLU:HG2	1.94	0.49
3:C:1021:ILE:HD12	3:C:1031:VAL:HG22	1.94	0.48
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.60	0.48
1:A:10:VAL:O	1:A:13:LYS:HG2	2.13	0.48
3:L:1286:THR:OG1	3:L:1287:ASN:N	2.47	0.48
3:C:1020:LEU:C	3:C:1021:ILE:HD13	2.39	0.48
1:J:63:ASP:O	1:J:64:LYS:HG3	2.14	0.47
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:601:ASN:O	3:L:821:HIS:HD2	1.98	0.47
3:L:614:HIS:HD2	3:L:693:PRO:O	1.97	0.47
2:K:224:PRO:N	9:K:812:HOH:O	2.47	0.47
3:L:839:ARG:NH2	3:L:912:ARG:O	2.39	0.46
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.40	0.46
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.51	0.46
3:C:1102:GLU:HG2	3:C:1103:PRO:CD	2.36	0.46
3:C:1011:VAL:CG2	8:C:1:I3A:H5	2.45	0.46
3:C:912:ARG:N	7:C:1327:MOS:S	2.89	0.46
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.51	0.46
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.14	0.45
2:B:427:ARG:HG2	2:B:427:ARG:O	2.16	0.45
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.17	0.45
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.65	0.45
3:C:1143:GLU:O	3:C:1144:THR:CG2	2.50	0.45
1:J:104:ARG:HD3	1:J:162:THR:CG2	2.47	0.45
3:L:1279:ARG:HG2	3:L:1294:PHE:HE2	1.82	0.44
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.50	0.44
2:B:281:PRO:HB2	2:B:287:LEU:CD1	2.48	0.44
2:B:284:ILE:HB	2:B:287:LEU:HD12	1.99	0.44
2:B:390:PHE:O	2:B:462:ARG:HD2	2.18	0.44
2:B:423:GLN:HB3	2:B:433:LYS:HG2	1.99	0.44
3:L:609:THR:HG23	3:L:664:GLY:CA	2.47	0.43
2:K:337:PHE:CD2	2:K:337:PHE:C	2.96	0.43
2:K:473:GLN:O	2:K:476:LYS:HB2	2.19	0.43
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.83	0.43
3:C:911:PHE:O	3:C:912:ARG:C	2.62	0.43
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.18	0.43
3:L:911:PHE:O	3:L:912:ARG:C	2.61	0.43
3:C:601:ASN:O	3:C:821:HIS:CD2	2.68	0.42
1:J:95:LYS:CE	9:J:708:HOH:O	2.66	0.42
3:C:752:ILE:HD11	3:C:763:PHE:CE1	2.51	0.42
2:B:441:LEU:HB3	2:B:451:GLU:HB2	2.01	0.42
1:J:32:ARG:NH1	9:J:684:HOH:O	2.47	0.42
2:B:342:VAL:HG23	9:B:942:HOH:O	2.20	0.42
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.49	0.42
3:L:1046:MET:HE3	3:L:1046:MET:CA	2.48	0.42
3:L:670:VAL:HG11	3:L:681:ALA:HB3	2.02	0.42
2:B:337:PHE:O	2:B:338:ALA:O	2.37	0.42
2:B:348:LEU:HD13	2:B:407:ILE:HD13	2.02	0.41
2:B:281:PRO:HB2	2:B:287:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1021:ILE:CD1	3:C:1031:VAL:HG13	2.50	0.41
3:L:1289:ASN:HB3	3:L:1292:GLU:HB2	2.02	0.41
3:C:939:GLU:H	3:C:939:GLU:CD	2.27	0.41
1:J:36:LEU:HD22	1:J:89:GLU:HG3	2.02	0.41
2:B:387:HIS:CE1	2:B:467:LEU:HD11	2.55	0.41
2:B:346:ALA:HB1	5:B:606:FAD:H4'	2.03	0.41
3:C:885:MET:SD	3:C:896:GLY:HA3	2.60	0.41
1:A:43:CYS:HA	3:C:829:ARG:HB2	2.02	0.41
1:A:129:ARG:HD3	1:A:129:ARG:HA	1.78	0.41
2:K:257:LEU:HA	2:K:279:ILE:O	2.21	0.41
3:L:840:HIS:CE1	3:L:874:SER:OG	2.67	0.41
2:B:257:LEU:HD13	2:B:281:PRO:HG3	2.01	0.41
3:C:1279:ARG:HG2	3:C:1294:PHE:HE2	1.85	0.40
2:K:346:ALA:HB1	5:K:606:FAD:H4'	2.03	0.40
3:L:880:ARG:HD2	3:L:914:PHE:HB3	2.03	0.40
1:J:124:MET:HE2	1:J:163:PHE:CD1	2.56	0.40
2:K:232:GLU:OE1	3:L:677:HIS:HE1	2.03	0.40
2:B:338:ALA:HB1	2:B:342:VAL:HB	2.03	0.40
3:C:591:VAL:HG13	3:C:595:ASP:HB2	2.02	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%)	156 (96%)	6 (4%)	0	100	100
1	J	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
2	B	303/305 (99%)	295 (97%)	7 (2%)	1 (0%)	36	20
2	K	303/305 (99%)	296 (98%)	7 (2%)	0	100	100
3	C	753/755 (100%)	733 (97%)	14 (2%)	6 (1%)	16	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	743/755 (98%)	728 (98%)	10 (1%)	5 (1%)	18	6
All	All	2426/2448 (99%)	2365 (98%)	49 (2%)	12 (0%)	24	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	338	ALA
3	C	721	LYS
3	C	1008	SER
3	C	1144	THR
3	L	1008	SER
3	L	912	ARG
3	C	912	ARG
3	L	1139	GLY
3	L	1287	ASN
3	L	797	GLY
3	C	797	GLY
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%)	25	7
1	J	137/137 (100%)	135 (98%)	2 (2%)	57	35
2	B	261/261 (100%)	252 (97%)	9 (3%)	32	11
2	K	261/261 (100%)	253 (97%)	8 (3%)	35	13
3	C	631/631 (100%)	621 (98%)	10 (2%)	55	33
3	L	624/631 (99%)	614 (98%)	10 (2%)	55	33
All	All	2051/2058 (100%)	2006 (98%)	45 (2%)	45	22

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	61	LEU
1	A	89	GLU
1	A	129	ARG
1	A	140	GLU
1	A	165	LYS
2	B	257	LEU
2	B	312	LEU
2	B	328	ARG
2	B	348	LEU
2	B	398	LEU
2	B	427	ARG
2	B	433	LYS
2	B	472	LYS
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	710	SER
3	C	743	TYR
3	C	848	VAL
3	C	939	GLU
3	C	1123	ASP
3	C	1203	LEU
3	C	1208	LEU
3	C	1287	ASN
1	J	2	THR
1	J	89	GLU
2	K	237	ILE
2	K	257	LEU
2	K	312	LEU
2	K	328	ARG
2	K	337	PHE
2	K	348	LEU
2	K	375	VAL
2	K	525	LYS
3	L	598	ARG
3	L	609	THR
3	L	616	LYS
3	L	743	TYR
3	L	939	GLU
3	L	1203	LEU
3	L	1208	LEU
3	L	1276	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	1287	ASN
3	L	1289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	146	ASN
2	B	226	GLN
2	B	251	GLN
2	B	261	ASN
2	B	272	ASN
2	B	351	ASN
2	B	471	GLN
2	B	473	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	683	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	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
1	J	131	GLN
1	J	146	ASN
2	K	226	GLN
2	K	252	HIS
2	K	261	ASN
2	K	292	HIS
2	K	322	GLN
2	K	351	ASN
2	K	387	HIS
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	677	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	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 oligosaccharides 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	B	606	-	58,58,58	1.15	6 (10%)	85,89,89	1.56	13 (15%)
7	MOS	C	1327	6	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MTE	L	1326	7	21,26,26	1.55	2 (9%)	19,40,40	1.94	6 (31%)
5	FAD	K	606	-	58,58,58	1.15	5 (8%)	85,89,89	1.56	12 (14%)
8	I3A	L	1	-	12,12,12	2.55	4 (33%)	16,16,16	2.34	7 (43%)
4	FES	J	602	1	0,4,4	-	-	-	-	-
8	I3A	C	1	-	12,12,12	2.57	4 (33%)	16,16,16	2.48	6 (37%)
4	FES	J	601	1	0,4,4	-	-	-	-	-
4	FES	A	601	1	0,4,4	-	-	-	-	-
4	FES	A	602	1	0,4,4	-	-	-	-	-
6	MTE	C	1326	7	21,26,26	1.58	1 (4%)	19,40,40	2.08	9 (47%)
7	MOS	L	1327	6	0,3,3	-	-	-	-	-

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	B	606	-	-	0/34/50/50	0/6/6/6
6	MTE	L	1326	7	-	1/6/34/34	0/3/3/3
5	FAD	K	606	-	-	0/34/50/50	0/6/6/6
8	I3A	L	1	-	-	0/2/2/2	0/2/2/2
4	FES	J	602	1	-	-	0/1/1/1
8	I3A	C	1	-	-	0/2/2/2	0/2/2/2
4	FES	J	601	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
6	MTE	C	1326	7	-	1/6/34/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1326	MTE	C9-C10	5.93	1.48	1.38
6	L	1326	MTE	C9-C10	5.61	1.48	1.38
8	C	1	I3A	C9-C3	-4.79	1.39	1.45
8	L	1	I3A	C3'-C3	4.69	1.54	1.45
8	C	1	I3A	C3'-C3	4.63	1.54	1.45
8	L	1	I3A	C9-C3	-4.51	1.39	1.45
5	K	606	FAD	C4X-N5	4.32	1.40	1.30
5	B	606	FAD	C4X-N5	4.19	1.39	1.30
8	C	1	I3A	C8-N	-3.04	1.32	1.37
5	B	606	FAD	C2A-N3A	2.97	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	606	FAD	C2A-N3A	2.91	1.39	1.33
8	L	1	I3A	C2-C3	-2.90	1.33	1.38
5	K	606	FAD	C2A-N1A	2.83	1.39	1.33
8	C	1	I3A	C2-C3	-2.80	1.33	1.38
8	L	1	I3A	C8-N	-2.74	1.33	1.37
5	K	606	FAD	C8A-N7A	2.72	1.36	1.31
5	B	606	FAD	P-O3P	2.68	1.62	1.59
5	B	606	FAD	C10-N1	2.62	1.38	1.33
5	K	606	FAD	C10-N1	2.59	1.38	1.33
5	B	606	FAD	C2A-N1A	2.27	1.38	1.33
5	B	606	FAD	C8A-N7A	2.24	1.36	1.31
6	L	1326	MTE	C9-C4	2.19	1.48	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-6.19	119.21	128.58
8	L	1	I3A	C9-C3-C2	6.08	109.46	106.12
8	C	1	I3A	C9-C3-C2	5.85	109.33	106.12
5	K	606	FAD	N3A-C2A-N1A	-5.64	120.04	128.58
5	K	606	FAD	C5A-C4A-N3A	-4.25	120.86	126.72
6	L	1326	MTE	C2-N1-C10	4.22	120.80	113.36
8	C	1	I3A	C9-C3-C3'	-4.15	124.48	129.24
6	C	1326	MTE	O4-C4-C9	-3.99	117.64	127.26
5	K	606	FAD	N9A-C8A-N7A	-3.93	108.36	113.94
5	B	606	FAD	C5A-C4A-N3A	-3.92	121.32	126.72
6	C	1326	MTE	C2-N1-C10	3.80	120.07	113.36
6	L	1326	MTE	O4-C4-C9	-3.47	118.89	127.26
5	K	606	FAD	C5A-N7A-C8A	3.46	108.88	103.45
8	L	1	I3A	C8-C9-C3	-3.45	104.19	106.53
5	B	606	FAD	N9A-C8A-N7A	-3.44	109.05	113.94
5	K	606	FAD	C4-N3-C2	-3.38	119.64	125.64
5	B	606	FAD	C2A-N3A-C4A	3.36	120.04	111.83
8	C	1	I3A	O-C3'-C3	-3.36	120.92	125.41
5	K	606	FAD	C2A-N3A-C4A	3.28	119.84	111.83
5	B	606	FAD	C4X-C10-N10	3.19	121.05	116.48
8	L	1	I3A	O-C3'-C3	-3.08	121.28	125.41
6	C	1326	MTE	O3P-P-O4'	-3.05	98.71	106.67
8	C	1	I3A	C8-C9-C3	-3.05	104.47	106.53
5	K	606	FAD	C4X-C10-N10	3.00	120.77	116.48
8	L	1	I3A	C9-C3-C3'	-2.99	125.81	129.24
5	B	606	FAD	C5A-N7A-C8A	2.95	108.08	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	C4-N3-C2	-2.94	120.43	125.64
8	C	1	I3A	C3-C2-N	-2.91	108.71	110.20
5	B	606	FAD	C10-C4X-N5	-2.87	118.95	124.81
8	C	1	I3A	C4-C9-C8	2.84	121.79	118.84
8	L	1	I3A	C3-C2-N	-2.82	108.76	110.20
6	L	1326	MTE	C4-C9-N5	2.80	123.90	116.27
5	K	606	FAD	C10-C4X-N5	-2.72	119.26	124.81
5	K	606	FAD	C4A-C5A-N7A	-2.67	107.52	110.58
5	K	606	FAD	N3A-C4A-N9A	2.65	131.67	127.17
5	K	606	FAD	C4X-C4-N3	2.57	119.78	113.25
6	L	1326	MTE	C9-C4-N3	2.50	119.00	112.13
6	C	1326	MTE	C4-C9-N5	2.50	123.08	116.27
5	B	606	FAD	C4X-C4-N3	2.48	119.58	113.25
5	B	606	FAD	N3A-C4A-N9A	2.45	131.33	127.17
6	L	1326	MTE	O3'-C7-N8	2.37	110.76	108.61
6	L	1326	MTE	O2P-P-O4'	-2.35	100.55	106.67
6	C	1326	MTE	O3P-P-O2P	2.27	116.31	107.80
6	C	1326	MTE	C7-C6-N5	2.24	110.07	107.87
5	B	606	FAD	C4-C4X-N5	2.22	121.27	118.21
6	C	1326	MTE	O4-C4-N3	2.21	124.27	120.11
8	L	1	I3A	C4-C9-C8	2.17	121.09	118.84
6	C	1326	MTE	C9-C4-N3	2.16	118.06	112.13
5	K	606	FAD	C4-C4X-N5	2.15	121.17	118.21
5	B	606	FAD	O4-C4-C4X	-2.14	120.87	126.53
6	C	1326	MTE	O2P-P-O4'	-2.14	101.09	106.67
8	L	1	I3A	C7-C8-C9	-2.12	120.13	122.19
5	B	606	FAD	C4A-C5A-N7A	-2.10	108.18	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1326	MTE	C3'-C4'-O4'-P
6	L	1326	MTE	C3'-C4'-O4'-P

There are no ring outliers.

6 monomers are involved in 7 short contacts:

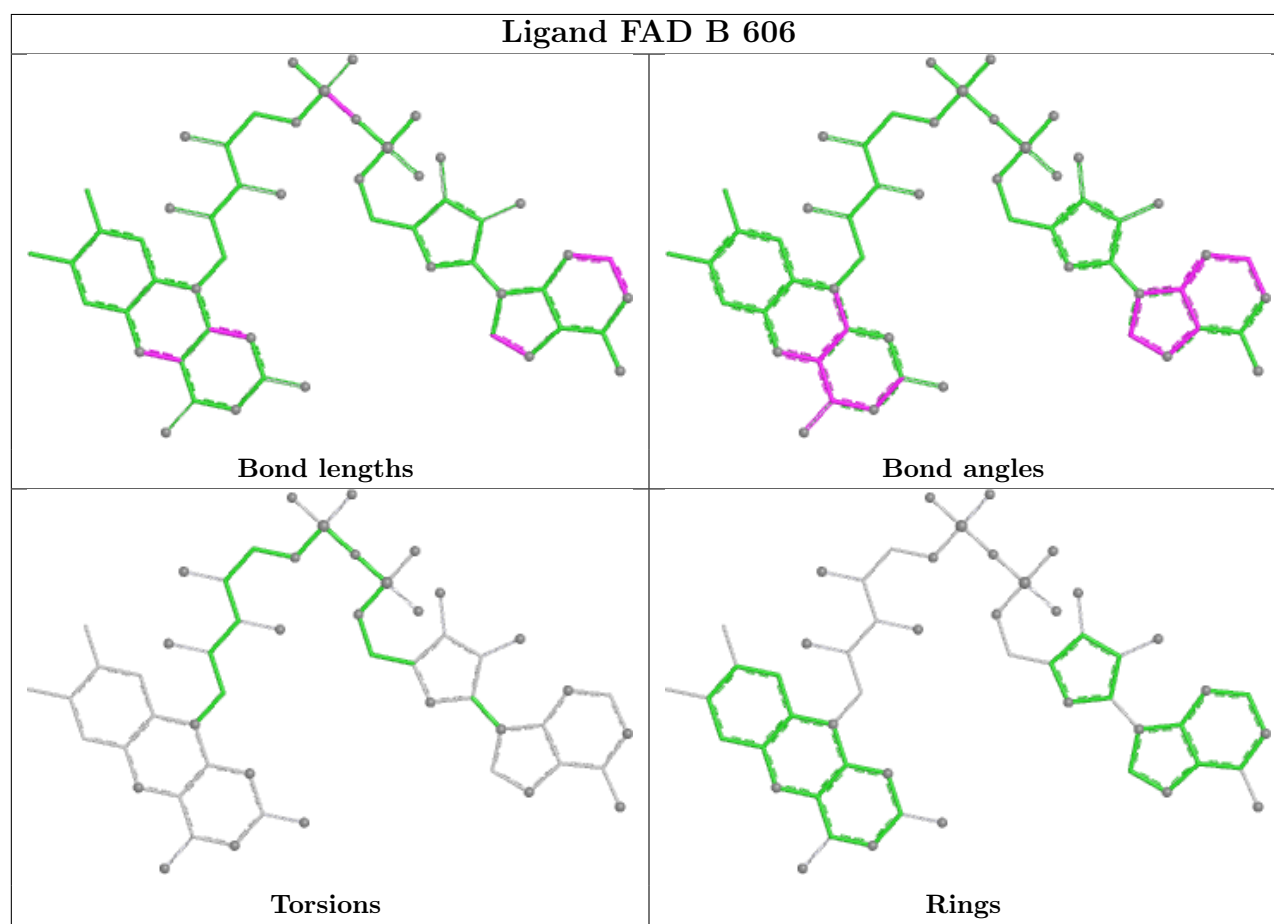
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	FAD	1	0
7	C	1327	MOS	1	0

Continued on next page...

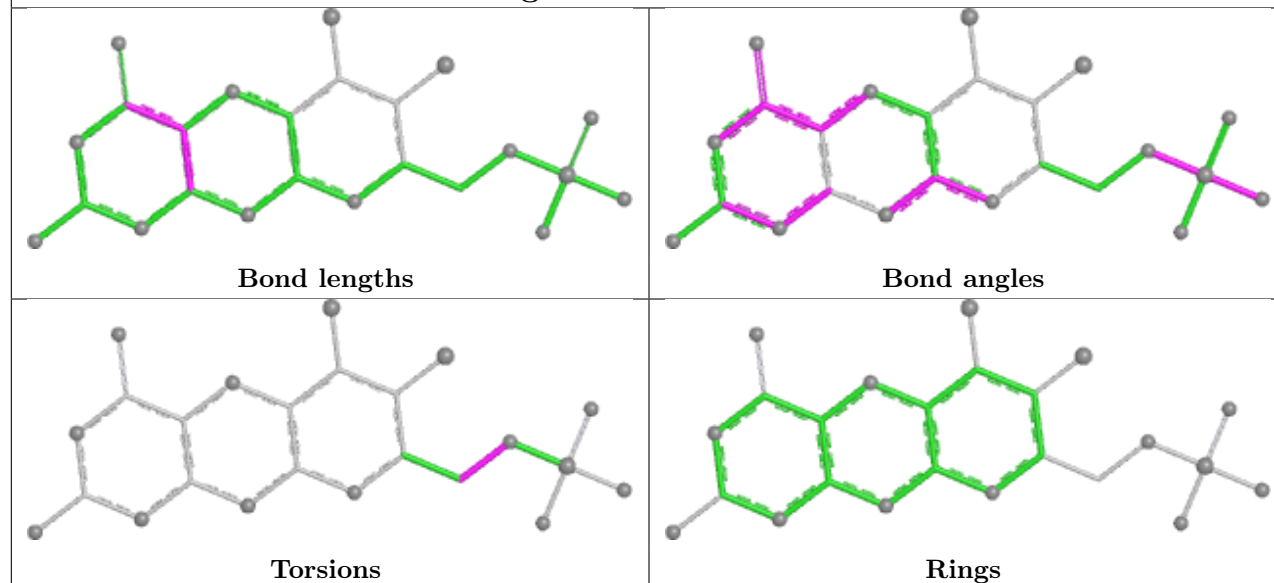
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	606	FAD	1	0
8	L	1	I3A	1	0
8	C	1	I3A	2	0
7	L	1327	MOS	1	0

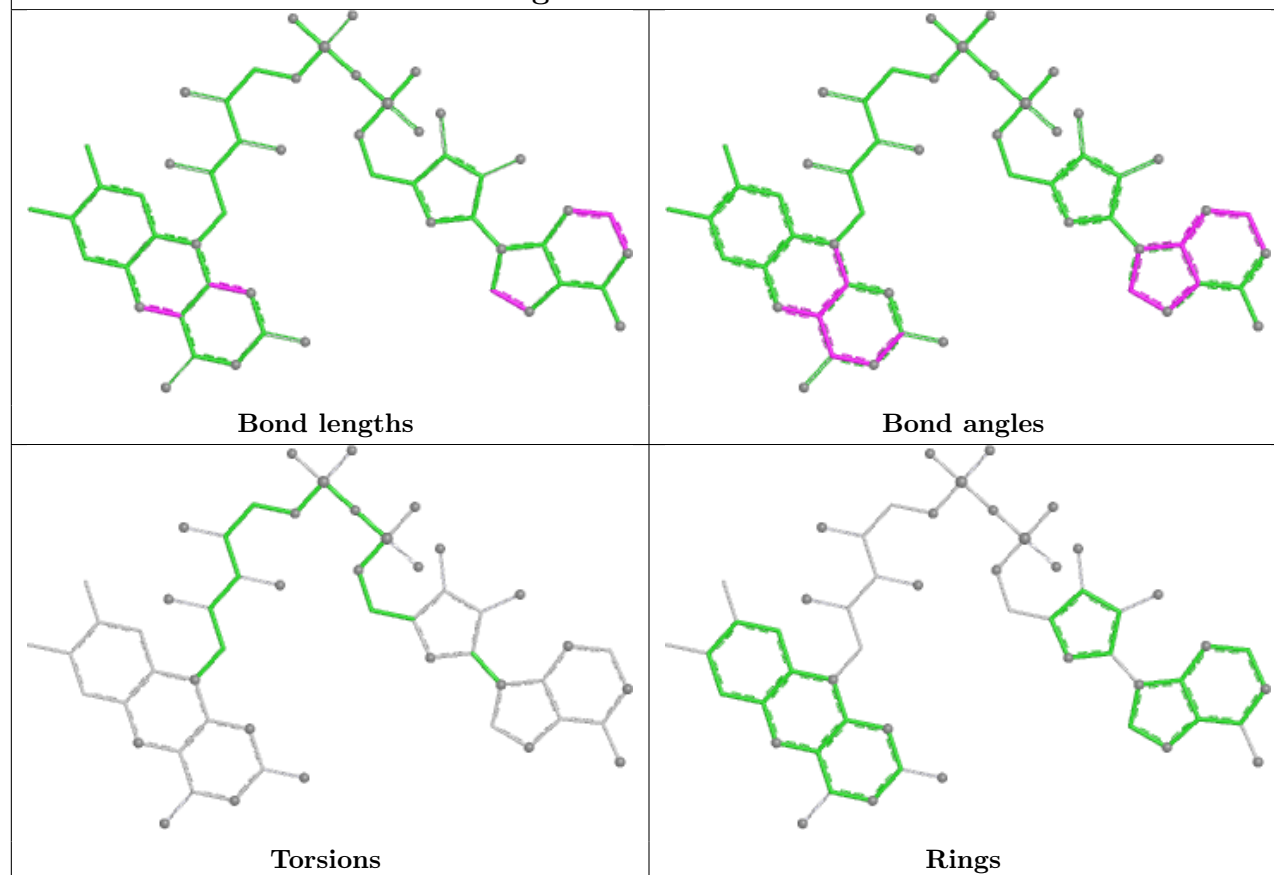
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

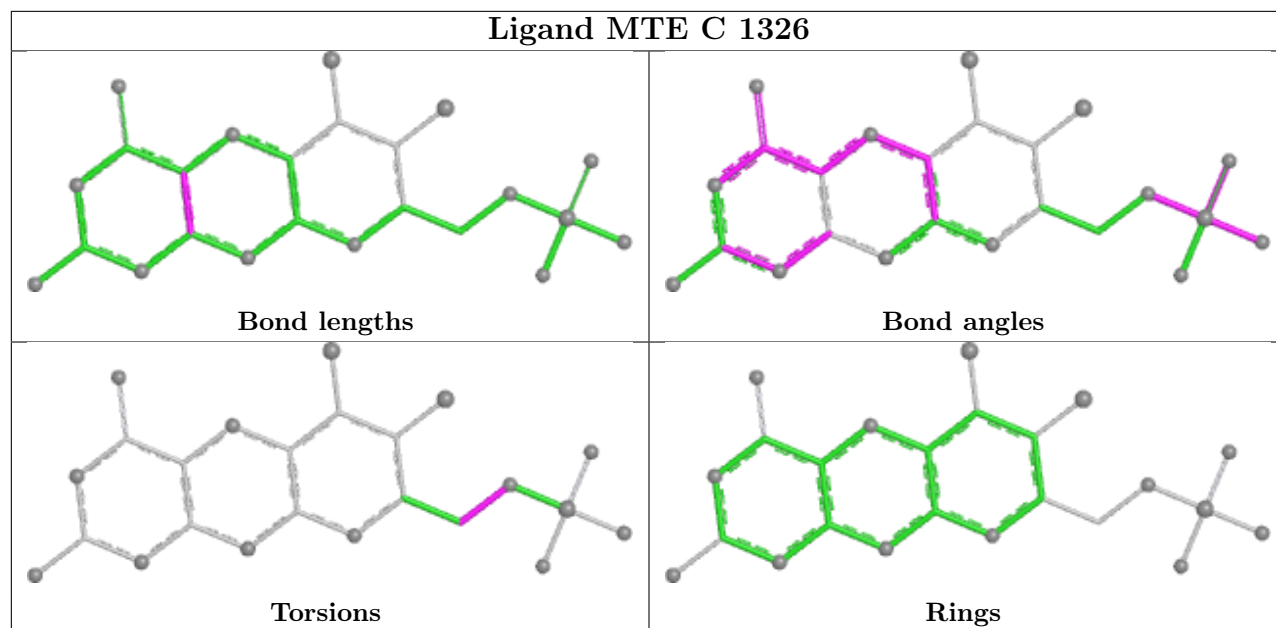


Ligand MTE L 1326



Ligand FAD K 606





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%)	0.25	10 (6%)	27 27	10, 17, 32, 36	0
1	J	164/164 (100%)	0.47	16 (9%)	13 13	12, 19, 38, 49	0
2	B	305/305 (100%)	0.71	27 (8%)	15 15	14, 23, 34, 39	0
2	K	305/305 (100%)	0.88	31 (10%)	12 12	17, 27, 38, 42	0
3	C	755/755 (100%)	-0.02	12 (1%)	70 74	10, 16, 26, 34	0
3	L	745/755 (98%)	0.13	19 (2%)	57 60	11, 18, 30, 52	0
All	All	2438/2448 (99%)	0.28	115 (4%)	36 38	10, 19, 33, 52	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	58	TYR	11.4
2	K	528	GLY	7.2
2	B	528	GLY	6.2
3	L	1288	ASN	6.0
1	J	61	LEU	5.8
3	L	1287	ASN	5.1
2	B	424	ALA	5.1
1	J	2	THR	5.0
1	A	61	LEU	4.9
2	K	424	ALA	4.7
3	L	985	ASP	4.5
3	L	1290	THR	4.4
2	K	378	GLY	4.2
3	C	1143	GLU	3.9
2	K	429	ASP	3.9
3	C	683	HIS	3.7
1	A	141	ASP	3.7
3	L	1110	ASP	3.4
2	K	336	TRP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	992	CYS	3.4
2	B	412	SER	3.4
3	L	1289	ASN	3.3
3	C	720	LYS	3.3
2	K	291	GLU	3.2
2	B	499	ASP	3.2
1	J	165	LYS	3.2
1	J	162	THR	3.2
2	K	335	ARG	3.1
3	L	1286	THR	3.1
2	K	499	ASP	3.0
2	K	527	LEU	3.0
2	B	425	SER	3.0
3	L	618	LYS	3.0
2	B	272	ASN	3.0
2	K	474	LEU	3.0
1	A	2	THR	2.9
2	K	338	ALA	2.9
3	C	1216	GLU	2.9
2	K	272	ASN	2.9
2	B	268	MET	2.9
2	K	395	LYS	2.9
2	B	336	TRP	2.8
2	B	335	ARG	2.8
3	L	724	SER	2.8
2	B	375	VAL	2.8
2	K	375	VAL	2.8
1	J	164	ALA	2.7
2	K	442	PHE	2.7
1	A	140	GLU	2.7
2	B	506	GLU	2.7
3	L	725	GLU	2.7
2	B	290	VAL	2.6
1	A	97	ARG	2.6
2	B	291	GLU	2.6
2	K	426	ARG	2.6
1	J	63	ASP	2.6
1	J	62	GLN	2.6
3	L	748	CYS	2.6
2	B	292	HIS	2.6
2	K	425	SER	2.6
3	C	657	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	475	SER	2.5
1	J	64	LYS	2.5
1	J	97	ARG	2.5
3	L	699	GLU	2.5
2	B	445	GLY	2.5
2	K	477	PHE	2.5
2	B	338	ALA	2.4
3	L	1279	ARG	2.4
3	C	1290	THR	2.4
3	L	1143	GLU	2.4
2	B	378	GLY	2.4
2	K	377	ARG	2.3
2	B	318	LYS	2.3
2	B	395	LYS	2.3
1	A	165	LYS	2.3
3	C	852	LYS	2.3
2	B	491	ALA	2.3
3	C	1102	GLU	2.3
1	J	136	VAL	2.3
2	B	527	LEU	2.3
2	K	318	LYS	2.3
2	K	255	ALA	2.2
2	B	474	LEU	2.2
2	K	271	LYS	2.2
2	B	295	GLU	2.2
3	L	1291	LYS	2.2
2	B	248	LEU	2.2
2	K	524	LEU	2.2
1	J	140	GLU	2.2
2	K	506	GLU	2.2
2	K	337	PHE	2.2
2	K	316	VAL	2.2
3	C	848	VAL	2.2
3	L	1283	ALA	2.2
1	A	137	GLU	2.2
1	A	58	TYR	2.2
1	A	96	THR	2.2
2	B	382	THR	2.2
2	K	398	LEU	2.1
2	B	472	LYS	2.1
3	L	1144	THR	2.1
1	J	66	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	467	LEU	2.1
2	K	482	LEU	2.1
3	C	699	GLU	2.1
1	J	60	ARG	2.1
2	B	337	PHE	2.1
3	L	1285	HIS	2.1
3	C	705	ASN	2.1
1	J	141	ASP	2.1
1	J	129	ARG	2.1
3	L	1293	LEU	2.0
1	A	60	ARG	2.0
2	K	476	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

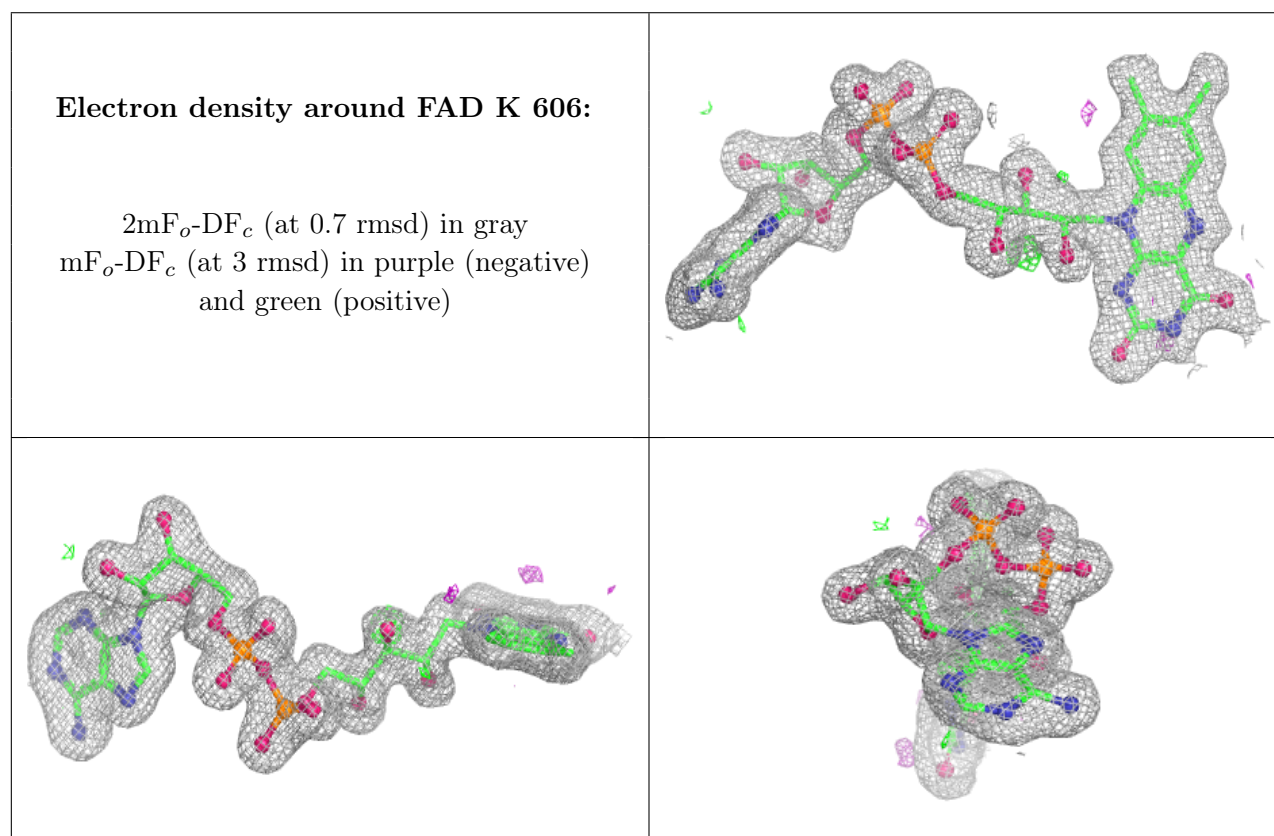
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	I3A	C	1	11/11	0.71	0.19	27,29,30,30	0
8	I3A	L	1	11/11	0.75	0.17	32,34,35,35	0
5	FAD	K	606	53/53	0.96	0.07	16,21,23,25	0
6	MTE	L	1326	24/24	0.97	0.06	15,18,25,25	0
5	FAD	B	606	53/53	0.97	0.06	14,17,21,22	0
6	MTE	C	1326	24/24	0.97	0.06	13,16,19,20	0
7	MOS	C	1327	4/4	0.98	0.16	20,20,23,33	0
7	MOS	L	1327	4/4	0.98	0.15	22,22,25,34	0
4	FES	A	602	4/4	0.99	0.04	12,12,14,14	0
4	FES	J	602	4/4	0.99	0.03	13,14,14,15	0
4	FES	J	601	4/4	1.00	0.03	13,13,15,15	0

Continued on next page...

Continued from previous page...

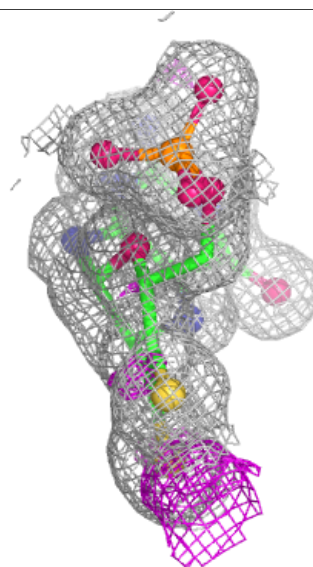
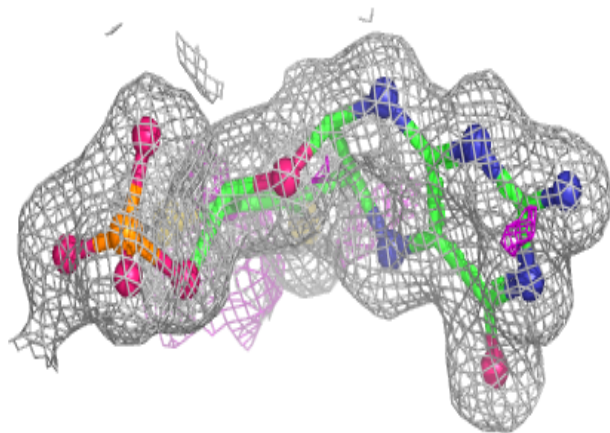
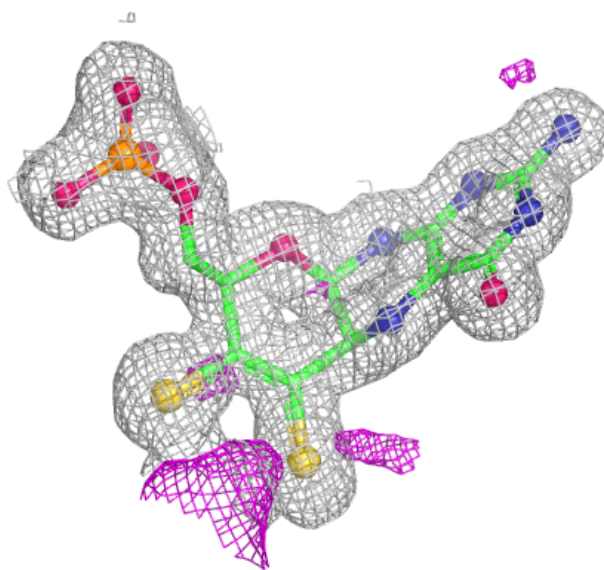
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FES	A	601	4/4	1.00	0.02	11,11,13,13	0

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.



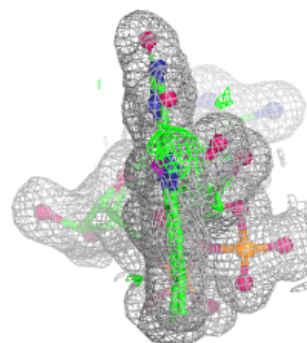
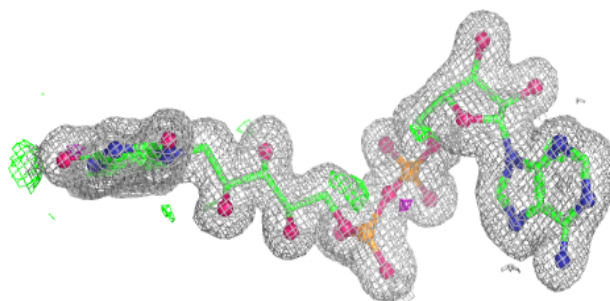
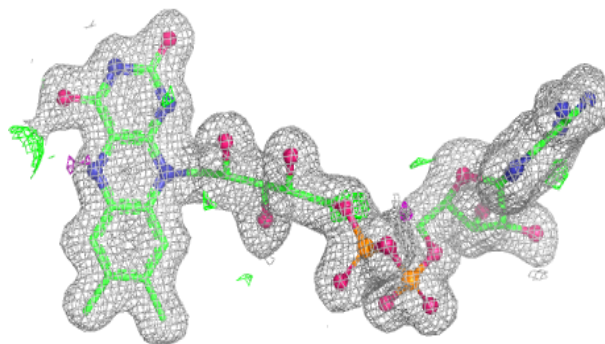
Electron density around MTE L 1326:

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



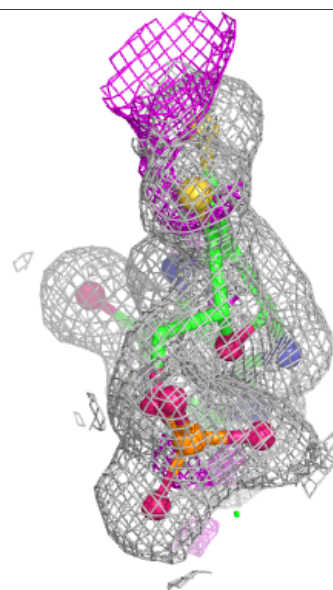
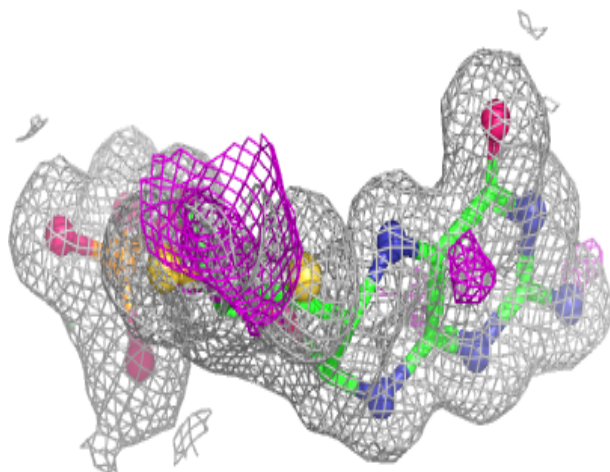
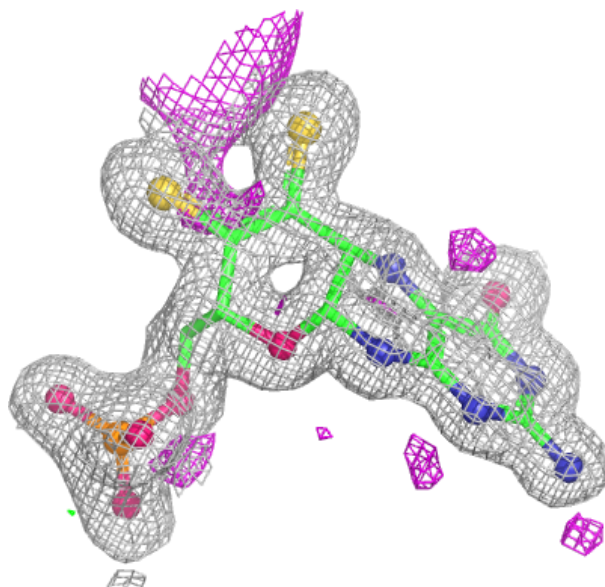
Electron density around FAD B 606:

$2mF_o - DF_c$ (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 ⓘ

There are no such residues in this entry.