Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 04:17 AM EDT

PDB ID	:	3NVV
Title	:	Crystal Structure of Bovine Xanthine Oxidase in Complex with Arsenite
Authors	:	Cao, H.; Hille, R.
Deposited on	:	2010-07-08
Resolution	:	1.82 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 (i) 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 (i)) were used in the production of this report:

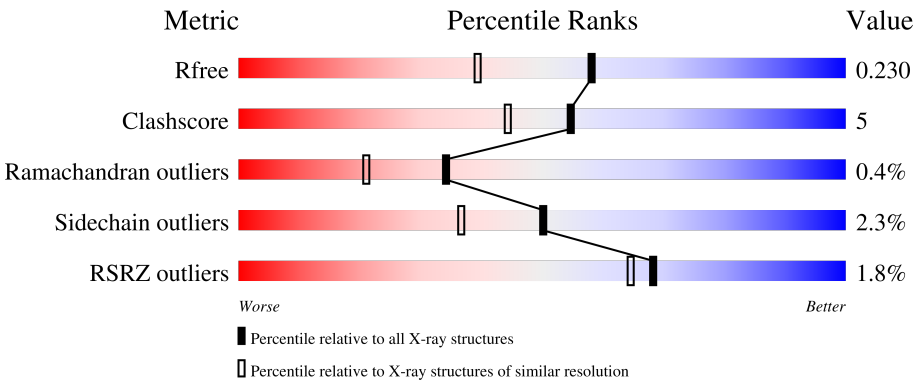
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 <=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	2%, 89%, 10%
1	J	164	3%, 85%, 13%
2	B	334	3%, 90%, 9%
2	K	334	6%, 81%, 9%, 9%
3	C	755	89%, 10%

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Mol	Chain	Length	Quality of chain
3	L	755	% 86% 12% ••

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20671 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
			Total	C	N	O	S			
1	A	164	1255	788	225	230	12	0	0	0
1	J	164	1255	788	225	230	12	0	0	0

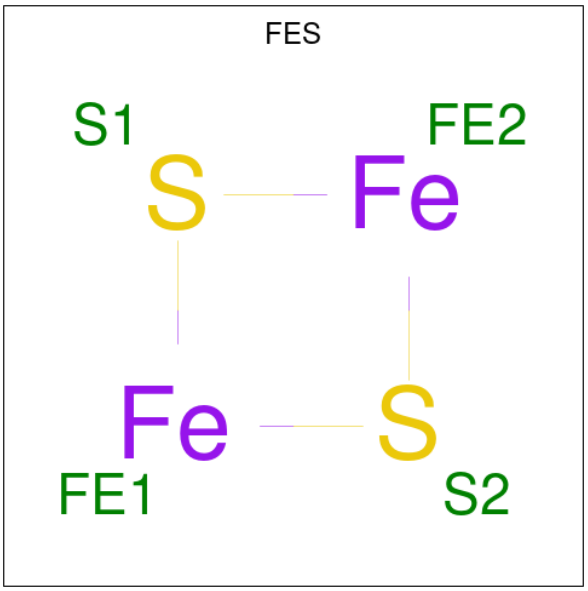
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	334	2630	1700	437	479	14	0	0	0
2	K	305	2389	1539	402	435	13	0	0	0

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

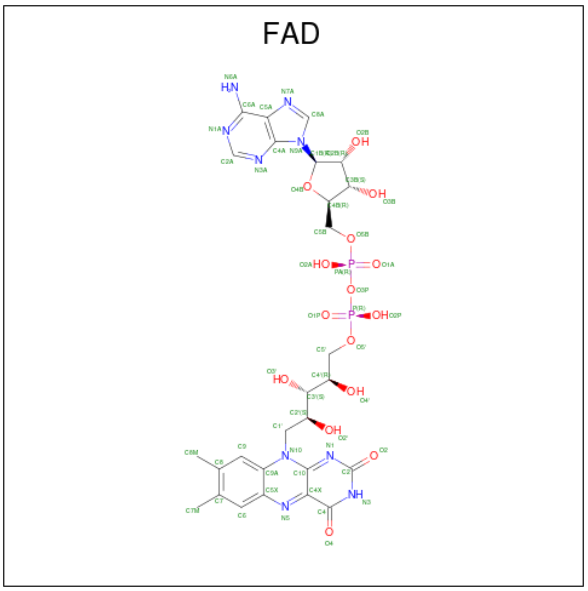
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	755	5823	3680	1003	1105	35	0	0	0
3	L	745	5761	3643	992	1093	33	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



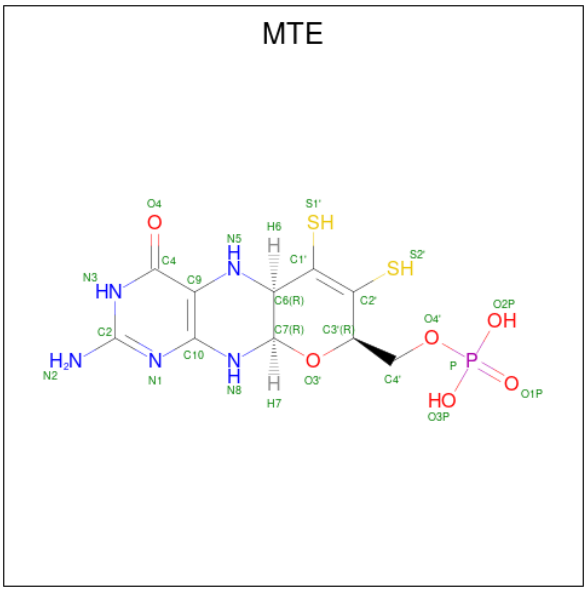
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	J	1	4	2	2	0	0
			Total	Fe	S		
4	J	1	4	2	2	0	0

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



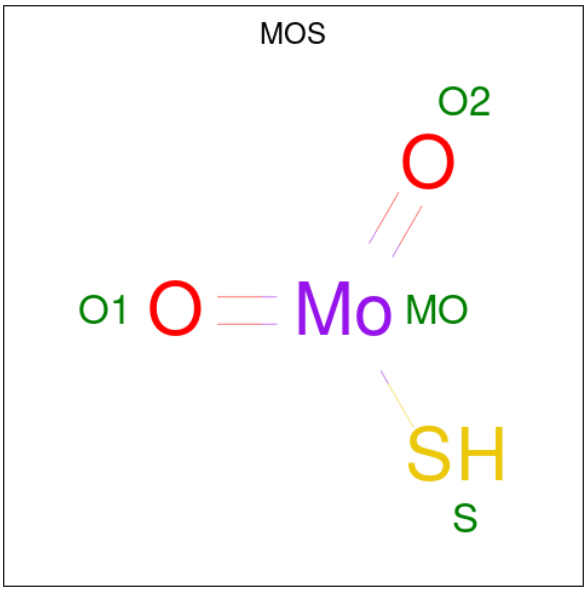
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
5	K	1	53	27	9	15	2	0	0

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



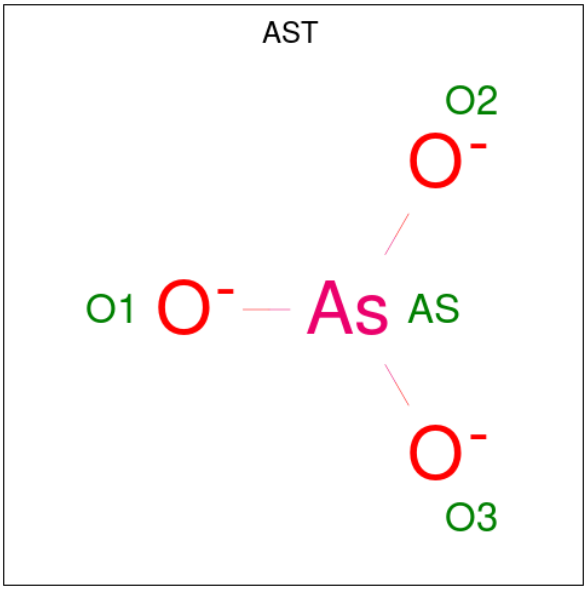
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	C	1	24	10	5	6	1	2	0	0
			Total	C	N	O	P	S		
6	L	1	24	10	5	6	1	2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



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

- Molecule 8 is ARSENITE (three-letter code: AST) (formula: AsO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	O		
8	C	1	3	1	2	0	0
8	L	1	3	1	2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	94	Total O 94 94	0	0
9	B	137	Total O 137 137	0	0
9	C	465	Total O 465 465	0	0
9	J	99	Total O 99 99	0	0
9	K	105	Total O 105 105	0	0
9	L	474	Total O 474 474	0	0

3 Residue-property plots (i)

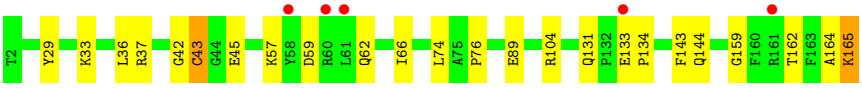
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:

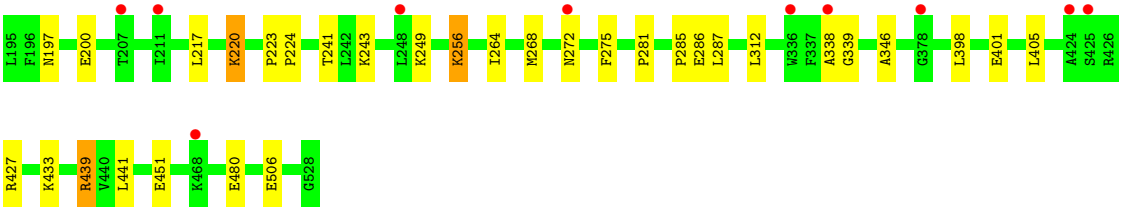
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain J:



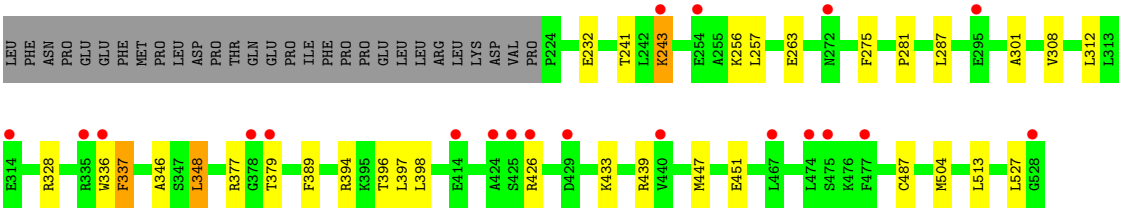
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain B:



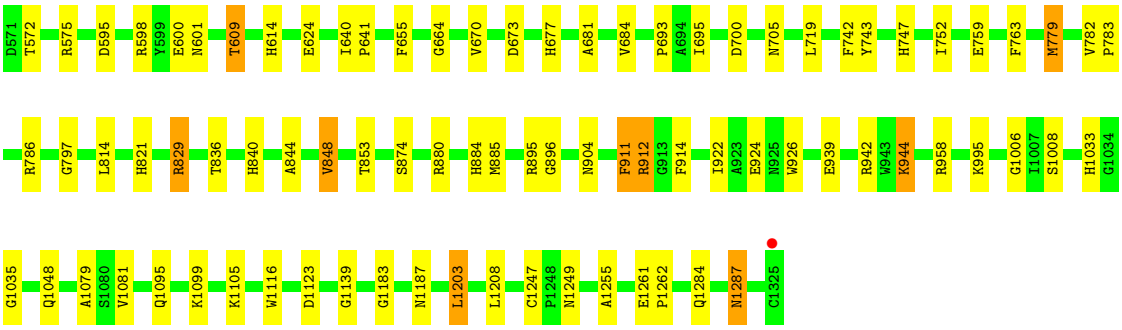
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain K:



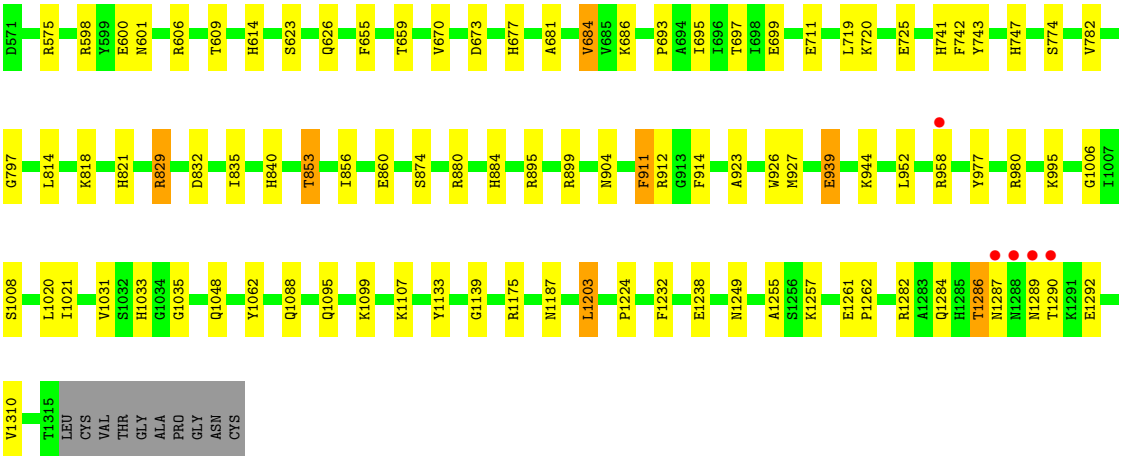
• Molecule 3: Xanthine dehydrogenase/oxidase

Chain C:



- Molecule 3: Xanthine dehydrogenase/oxidase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.77Å 73.42Å 138.16Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	131.80 – 1.82 131.80 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.2 (131.80-1.82) 97.2 (131.80-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.229 0.193 , 0.230	Depositor DCC
R_{free} test set	11464 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20671	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, FAD, MOS, AST, FES

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	0.62	0/1277	0.67	0/1723
1	J	0.57	0/1277	0.64	0/1723
2	B	0.49	0/2689	0.60	2/3637 (0.1%)
2	K	0.47	0/2438	0.59	1/3290 (0.0%)
3	C	0.63	0/5951	0.69	5/8061 (0.1%)
3	L	0.58	0/5888	0.67	5/7974 (0.1%)
All	All	0.57	0/19520	0.66	13/26408 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	829	ARG	NE-CZ-NH2	-10.72	114.94	120.30
3	C	829	ARG	NE-CZ-NH1	8.37	124.48	120.30
3	L	829	ARG	NE-CZ-NH2	-7.93	116.33	120.30
3	C	1203	LEU	CA-CB-CG	7.90	133.47	115.30
3	L	829	ARG	NE-CZ-NH1	7.46	124.03	120.30
3	L	1203	LEU	CA-CB-CG	6.56	130.38	115.30
2	K	398	LEU	CA-CB-CG	5.81	128.66	115.30
3	C	848	VAL	CB-CA-C	-5.70	100.56	111.40
2	B	398	LEU	CA-CB-CG	5.49	127.93	115.30
3	L	980	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	B	439	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	C	1203	LEU	CB-CG-CD1	5.13	119.72	111.00
3	L	606	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	11	0
1	J	1255	0	1265	20	0
2	B	2630	0	2697	18	0
2	K	2389	0	2459	23	0
3	C	5823	0	5744	74	1
3	L	5761	0	5685	66	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	3	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	3	0	0	1	0
8	L	3	0	0	1	0
9	A	94	0	0	0	0
9	B	137	0	0	3	0
9	C	465	0	0	4	0
9	J	99	0	0	1	0
9	K	105	0	0	1	0
9	L	474	0	0	3	1
All	All	20671	0	19197	200	1

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 5.

All (200) 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:243:LYS:HD3	2:K:243:LYS:H	1.05	1.12
3:C:641:PRO:HD2	3:C:779:MET:CE	1.84	1.06
2:K:243:LYS:HD3	2:K:243:LYS:N	1.75	0.99
3:C:641:PRO:HD2	3:C:779:MET:HE1	1.44	0.99
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:952:LEU:CD2	3:L:958:ARG:HG2	1.97	0.95
2:K:241:THR:HB	2:K:243:LYS:HE2	1.49	0.94
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.04	0.91
3:L:697:THR:HB	3:L:699:GLU:OE1	1.72	0.88
2:K:243:LYS:H	2:K:243:LYS:CD	1.81	0.83
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.59	0.82
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.23	0.81
3:L:695:ILE:H	3:L:904:ASN:HD22	1.27	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.28	0.80
3:C:641:PRO:HD2	3:C:779:MET:HE2	1.63	0.80
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.45	0.80
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.31	0.76
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.75
1:A:57:LYS:HE2	1:A:66:ILE:HD11	1.66	0.75
1:J:159:GLY:O	1:J:162:THR:HG22	1.86	0.75
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.05	0.75
3:L:1289:ASN:HB2	3:L:1292:GLU:HB2	1.70	0.74
1:J:131:GLN:HE21	1:J:133:GLU:H	1.36	0.74
3:L:952:LEU:HD23	3:L:958:ARG:HG2	1.69	0.74
2:K:439:ARG:NH2	2:K:451:GLU:OE1	2.19	0.73
3:C:640:ILE:HG23	3:C:779:MET:HE2	1.69	0.72
3:C:575:ARG:HD2	9:C:365:HOH:O	1.93	0.69
1:J:134:PRO:O	1:J:165:LYS:HA	1.93	0.69
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.91	0.68
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.24	0.68
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.76	0.67
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	1.92	0.67
3:L:623:SER:HA	3:L:626:GLN:HE21	1.60	0.67
3:C:640:ILE:HG23	3:C:779:MET:CE	2.25	0.65
3:C:572:THR:HA	3:C:575:ARG:HD3	1.77	0.65
3:L:952:LEU:HD21	3:L:958:ARG:HG2	1.75	0.65
3:C:840:HIS:HE1	3:C:874:SER:OG	1.79	0.65
3:C:779:MET:CE	3:C:814:LEU:HD13	2.27	0.64
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.13	0.63
3:C:1287:ASN:C	3:C:1287:ASN:HD22	2.01	0.63
3:L:1020:LEU:C	3:L:1021:ILE:HD13	2.20	0.62
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.82	0.61
3:L:699:GLU:H	3:L:699:GLU:CD	2.03	0.61
2:K:243:LYS:N	2:K:243:LYS:CD	2.54	0.61
7:C:1327:MOS:O2	7:C:1327:MOS:MO	1.72	0.61
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:601:ASN:O	3:C:821:HIS:HD2	1.83	0.60
3:C:705:ASN:HB2	9:C:114:HOH:O	2.01	0.60
7:L:1327:MOS:O2	7:L:1327:MOS:MO	1.73	0.58
2:B:217:LEU:O	2:B:220:LYS:HD2	2.04	0.58
3:L:914:PHE:CD1	8:L:1:AST:AS	3.17	0.58
3:L:1021:ILE:HD12	3:L:1031:VAL:HA	1.86	0.58
3:L:853:THR:HG22	3:L:944:LYS:NZ	2.19	0.57
2:K:281:PRO:HB2	2:K:287:LEU:HD12	1.85	0.57
3:L:840:HIS:HE1	3:L:874:SER:OG	1.87	0.57
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.18	0.57
2:B:241:THR:HG22	2:B:243:LYS:H	1.70	0.56
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.52	0.56
3:L:601:ASN:O	3:L:821:HIS:HD2	1.87	0.56
3:L:614:HIS:HD2	3:L:693:PRO:O	1.88	0.56
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.54	0.55
1:J:164:ALA:HB1	1:J:165:LYS:HG3	1.89	0.55
3:L:880:ARG:O	3:L:884:HIS:HD2	1.88	0.55
3:C:609:THR:HG22	9:C:338:HOH:O	2.07	0.55
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.89	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	0.54
3:C:942:ARG:HH11	3:C:942:ARG:HG2	1.73	0.54
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.56	0.54
2:K:232:GLU:OE1	3:L:677:HIS:HE1	1.91	0.53
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.73	0.53
2:K:394:ARG:NH2	9:K:1351:HOH:O	2.41	0.53
2:B:264:ILE:O	2:B:268:MET:HG3	2.08	0.53
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.56	0.53
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.90	0.52
2:K:287:LEU:HD22	2:K:301:ALA:HB3	1.91	0.52
3:C:779:MET:HE1	3:C:814:LEU:HD13	1.91	0.52
3:C:614:HIS:HD2	3:C:693:PRO:O	1.92	0.52
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.40	0.52
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.43	0.52
1:A:42:GLY:O	3:C:829:ARG:HD2	2.11	0.51
3:C:624:GLU:CB	3:C:684:VAL:CG1	2.87	0.51
3:C:914:PHE:CD1	8:C:1:AST:AS	3.24	0.51
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.92	0.51
1:A:125:TYR:CZ	1:A:129:ARG:HD2	2.46	0.51
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.93	0.51
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.59	0.51
3:L:856:ILE:HD11	3:L:927:MET:CE	2.41	0.50
1:J:43:CYS:HA	3:L:829:ARG:HB2	1.92	0.50
1:J:104:ARG:HH11	1:J:162:THR:CG2	2.20	0.50
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.92	0.50
3:C:624:GLU:HB2	3:C:684:VAL:CG1	2.42	0.50
3:L:1286:THR:OG1	3:L:1287:ASN:N	2.44	0.50
2:B:480:GLU:HG2	9:B:602:HOH:O	2.13	0.49
3:C:782:VAL:CG1	3:C:783:PRO:HD2	2.42	0.49
3:C:779:MET:HE3	3:C:814:LEU:HD13	1.92	0.49
3:L:1020:LEU:O	3:L:1021:ILE:HD13	2.13	0.49
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.95	0.49
3:L:719:LEU:HD11	3:L:895:ARG:CB	2.43	0.49
3:C:600:GLU:HG2	3:L:598:ARG:O	2.13	0.48
3:C:719:LEU:HD11	3:C:895:ARG:CB	2.42	0.48
1:J:42:GLY:O	3:L:829:ARG:HD2	2.13	0.48
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.61	0.48
3:L:623:SER:HA	3:L:626:GLN:NE2	2.28	0.48
3:C:640:ILE:HG12	3:C:779:MET:HE3	1.95	0.48
3:L:719:LEU:HD13	3:L:860:GLU:OE2	2.14	0.48
3:C:885:MET:SD	3:C:896:GLY:HA3	2.54	0.48
1:J:29:TYR:CD1	1:J:33:LYS:HD3	2.49	0.48
2:K:257:LEU:O	5:K:606:FAD:H2B	2.14	0.47
2:B:249:LYS:HG2	2:B:401:GLU:O	2.14	0.47
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.97	0.47
1:A:61:LEU:HD21	2:B:285:PRO:HA	1.95	0.47
2:K:308:VAL:HG21	2:K:348:LEU:HG	1.96	0.47
3:C:884:HIS:HE1	3:C:1006:GLY:N	2.02	0.47
2:B:441:LEU:HB3	2:B:451:GLU:HB2	1.95	0.47
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.23	0.46
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.16	0.46
2:B:506:GLU:HG2	9:C:493:HOH:O	2.15	0.46
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.34	0.46
2:B:339:GLY:CA	9:B:2064:HOH:O	2.63	0.46
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.45	0.46
3:C:624:GLU:HB3	3:C:684:VAL:CG1	2.46	0.46
3:C:641:PRO:CD	3:C:779:MET:HE1	2.29	0.45
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.31	0.45
3:L:853:THR:HG22	3:L:944:LYS:HZ2	1.79	0.45
2:B:338:ALA:C	9:B:2064:HOH:O	2.55	0.45
2:K:337:PHE:O	2:K:337:PHE:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:256:LYS:HE3	2:K:275:PHE:CE2	2.52	0.45
1:A:165:LYS:HD3	1:A:165:LYS:HA	1.67	0.45
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.99	0.45
3:C:624:GLU:HB3	3:C:684:VAL:HG11	1.98	0.45
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.80	0.45
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.82	0.45
3:L:880:ARG:HD2	3:L:914:PHE:HB3	1.99	0.45
3:L:1257:LYS:HE3	9:L:2028:HOH:O	2.17	0.45
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.34	0.45
1:J:29:TYR:HA	1:J:33:LYS:HD2	2.00	0.44
3:L:1095:GLN:O	3:L:1099:LYS:HG2	2.17	0.44
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.17	0.44
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.99	0.44
2:K:377:ARG:HE	2:K:377:ARG:HB3	1.56	0.44
3:L:609:THR:HG21	3:L:835:ILE:HD11	1.99	0.44
1:A:37:ARG:HD3	3:C:595:ASP:O	2.17	0.44
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.15	0.44
3:C:1079:ALA:O	3:C:1081:VAL:HG13	2.17	0.44
3:C:1105:LYS:HG2	3:C:1116:TRP:CD2	2.52	0.44
3:C:853:THR:HG22	3:C:944:LYS:HD3	2.00	0.44
3:C:705:ASN:O	3:C:705:ASN:CG	2.56	0.43
1:J:144:GLN:HE22	2:K:336:TRP:HA	1.84	0.43
3:C:624:GLU:HB2	3:C:684:VAL:HG13	2.01	0.43
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.18	0.43
2:K:257:LEU:HD13	2:K:281:PRO:HG3	2.00	0.43
3:L:711:GLU:HA	3:L:899:ARG:HD2	2.00	0.43
3:L:995:LYS:HZ3	3:L:1284:GLN:HE21	1.65	0.43
3:C:782:VAL:HG12	3:C:786:ARG:HG3	2.01	0.43
2:K:389:PHE:O	2:K:396:THR:HA	2.18	0.43
3:C:782:VAL:HG12	3:C:783:PRO:HD2	2.01	0.43
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.66	0.43
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.19	0.43
3:L:1175:ARG:HA	3:L:1238:GLU:O	2.19	0.43
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.82	0.43
1:A:58:TYR:CD2	2:B:220:LYS:HG3	2.54	0.42
3:L:1107:LYS:NZ	9:L:1489:HOH:O	2.49	0.42
3:C:911:PHE:O	3:C:912:ARG:C	2.57	0.42
3:L:1282:ARG:HA	3:L:1286:THR:HG23	2.01	0.42
2:B:223:PRO:HA	2:B:224:PRO:HD3	1.97	0.42
1:J:37:ARG:NH1	9:J:2129:HOH:O	2.26	0.42
1:J:74:LEU:O	1:J:76:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:844:ALA:HB2	3:C:922:ILE:HD13	2.02	0.42
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.55	0.42
3:L:719:LEU:HD11	3:L:895:ARG:HB2	2.00	0.42
3:L:747:HIS:HD2	3:L:832:ASP:OD1	2.03	0.42
3:C:601:ASN:O	3:C:821:HIS:CD2	2.70	0.42
1:A:36:LEU:HD22	1:A:89:GLU:CG	2.50	0.42
2:K:487:CYS:HA	2:K:513:LEU:HD22	2.01	0.42
3:L:741:HIS:HA	3:L:911:PHE:CE1	2.55	0.42
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.35	0.42
1:J:45:GLU:CD	3:L:1224:PRO:HD2	2.40	0.41
1:J:59:ASP:HB3	1:J:62:GLN:HB2	2.02	0.41
2:K:504:MET:HE1	9:L:524:HOH:O	2.20	0.41
2:B:197:ASN:O	2:B:200:GLU:HG2	2.21	0.41
3:C:1287:ASN:C	3:C:1287:ASN:ND2	2.72	0.41
3:L:719:LEU:HD11	3:L:895:ARG:HB3	2.02	0.41
2:B:281:PRO:HB2	2:B:287:LEU:HD13	2.03	0.41
2:B:286:GLU:HB3	2:B:405:LEU:HD11	2.03	0.41
2:B:346:ALA:HB1	5:B:606:FAD:H4'	2.03	0.41
3:C:719:LEU:HD11	3:C:895:ARG:HB3	2.03	0.41
3:C:759:GLU:OE2	3:L:1062:TYR:OH	2.32	0.41
3:L:684:VAL:O	3:L:686:LYS:HD2	2.21	0.41
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.56	0.41
3:C:598:ARG:HD3	3:L:600:GLU:OE2	2.21	0.40
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.56	0.40
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.56	0.40
3:C:848:VAL:HG21	3:C:926:TRP:HB2	2.04	0.40
2:K:263:GLU:HB3	5:K:606:FAD:H52A	2.03	0.40
3:L:695:ILE:H	3:L:904:ASN:ND2	2.07	0.40
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.87	0.40
3:L:1286:THR:HG22	3:L:1310:VAL:O	2.20	0.40
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:958:ARG:NH2	9:L:1506:HOH:O[2_655]	1.88	0.32

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%)	158 (98%)	4 (2%)	0	100	100
1	J	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	25	12
2	B	332/334 (99%)	317 (96%)	15 (4%)	0	100	100
2	K	303/334 (91%)	290 (96%)	13 (4%)	0	100	100
3	C	753/755 (100%)	736 (98%)	13 (2%)	4 (0%)	29	15
3	L	743/755 (98%)	722 (97%)	17 (2%)	4 (0%)	29	15
All	All	2455/2506 (98%)	2380 (97%)	66 (3%)	9 (0%)	34	21

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/137 (100%)	132 (96%)	5 (4%)	35	19
1	J	137/137 (100%)	136 (99%)	1 (1%)	84	80
2	B	290/290 (100%)	284 (98%)	6 (2%)	53	41
2	K	261/290 (90%)	252 (97%)	9 (3%)	37	22
3	C	631/631 (100%)	620 (98%)	11 (2%)	60	50
3	L	624/631 (99%)	608 (97%)	16 (3%)	46	32
All	All	2080/2116 (98%)	2032 (98%)	48 (2%)	50	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	82	HIS
1	A	93	SER
1	A	140	GLU
1	A	165	LYS
2	B	220	LYS
2	B	256	LYS
2	B	272	ASN
2	B	312	LEU
2	B	427	ARG
2	B	433	LYS
3	C	609	THR
3	C	742	PHE
3	C	743	TYR
3	C	779	MET
3	C	911	PHE
3	C	939	GLU
3	C	944	LYS
3	C	1123	ASP
3	C	1203	LEU
3	C	1208	LEU
3	C	1287	ASN
1	J	165	LYS
2	K	243	LYS
2	K	312	LEU
2	K	328	ARG
2	K	337	PHE
2	K	348	LEU
2	K	379	THR
2	K	397	LEU

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Mol	Chain	Res	Type
2	K	426	ARG
2	K	433	LYS
3	L	575	ARG
3	L	659	THR
3	L	684	VAL
3	L	720	LYS
3	L	725	GLU
3	L	742	PHE
3	L	743	TYR
3	L	774	SER
3	L	782	VAL
3	L	818	LYS
3	L	853	THR
3	L	911	PHE
3	L	939	GLU
3	L	1203	LEU
3	L	1286	THR
3	L	1290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	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	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1088	GLN
3	C	1284	GLN
3	C	1287	ASN
3	C	1324	ASN

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Mol	Chain	Res	Type
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	292	HIS
2	K	351	ASN
2	K	473	GLN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1016	GLN
3	L	1033	HIS
3	L	1048	GLN
3	L	1212	HIS
3	L	1220	HIS
3	L	1284	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
8	AST	L	1	-	0,2,3	-	-	0,1,3	-	-
4	FES	J	602	1	0,4,4	-	-	-		
5	FAD	K	606	-	54,58,58	1.19	4 (7%)	71,89,89	1.45	13 (18%)
4	FES	A	601	1	0,4,4	-	-	-		
4	FES	A	602	1	0,4,4	-	-	-		
7	MOS	L	1327	6	0,3,3	-	-	-		
5	FAD	B	606	-	54,58,58	1.18	5 (9%)	71,89,89	1.47	11 (15%)
7	MOS	C	1327	6	0,3,3	-	-	-		
4	FES	J	601	1	0,4,4	-	-	-		
8	AST	C	1	-	0,2,3	-	-	0,1,3	-	-
6	MTE	C	1326	7	19,26,26	1.26	2 (10%)	20,40,40	2.37	10 (50%)
6	MTE	L	1326	7	19,26,26	1.24	1 (5%)	20,40,40	2.17	8 (40%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	606	FAD	C2A-N3A	4.22	1.38	1.32
6	L	1326	MTE	C9-C10	4.17	1.49	1.41
5	B	606	FAD	C2A-N3A	4.04	1.38	1.32
5	B	606	FAD	C4X-N5	3.74	1.38	1.30
5	K	606	FAD	C4X-N5	3.58	1.38	1.30
6	C	1326	MTE	C9-C10	3.36	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C10-N1	3.28	1.39	1.33
5	K	606	FAD	C10-N1	2.96	1.39	1.33
5	K	606	FAD	C2A-N1A	2.82	1.38	1.33
5	B	606	FAD	C2A-N1A	2.38	1.38	1.33
5	B	606	FAD	P-O3P	2.32	1.62	1.59
6	C	1326	MTE	C4-N3	2.23	1.36	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	606	FAD	N3A-C2A-N1A	-7.29	118.78	128.67
5	K	606	FAD	N3A-C2A-N1A	-6.08	120.42	128.67
6	L	1326	MTE	C2-N3-C4	5.46	123.56	115.96
6	L	1326	MTE	C4-C9-N5	4.23	124.60	118.57
6	C	1326	MTE	C2-N3-C4	4.12	121.69	115.96
6	C	1326	MTE	O3'-C7-C6	-3.90	106.36	108.96
6	C	1326	MTE	C4-C9-N5	3.30	123.28	118.57
5	B	606	FAD	O4B-C1B-N9A	-3.21	104.49	108.75
6	C	1326	MTE	O2P-P-O4'	-3.07	98.67	106.67
5	K	606	FAD	O3'-C3'-C2'	-3.05	102.00	108.93
6	C	1326	MTE	C2-N1-C10	2.90	121.49	114.59
6	C	1326	MTE	O3'-C7-N8	2.83	111.18	108.61
5	K	606	FAD	C4-N3-C2	-2.81	120.66	125.64
6	L	1326	MTE	C7-C6-N5	2.77	110.58	107.87
6	C	1326	MTE	O3P-P-O2P	2.70	117.91	107.80
6	L	1326	MTE	O3P-P-O4'	-2.67	99.71	106.67
5	B	606	FAD	C4X-C4-N3	2.62	119.92	113.25
5	K	606	FAD	C4X-C4-N3	2.58	119.82	113.25
5	K	606	FAD	O4B-C1B-N9A	-2.56	105.35	108.75
6	C	1326	MTE	O3P-P-O4'	-2.52	100.11	106.67
5	B	606	FAD	C10-C4X-N5	-2.51	119.68	124.81
5	K	606	FAD	O2P-P-O3P	2.48	113.97	107.27
5	K	606	FAD	C10-C4X-N5	-2.45	119.81	124.81
5	K	606	FAD	C4X-C10-N10	2.45	119.98	116.48
6	C	1326	MTE	O4'-C4'-C3'	2.42	114.54	108.58
5	B	606	FAD	C4-C4X-N5	2.39	121.50	118.21
5	B	606	FAD	O2A-PA-O3P	2.35	113.63	107.27
5	B	606	FAD	C4X-C10-N10	2.35	119.85	116.48
5	K	606	FAD	C5'-C4'-C3'	-2.31	107.87	112.22
6	C	1326	MTE	N1-C2-N3	-2.29	121.97	125.48
5	B	606	FAD	C1'-C2'-C3'	-2.28	103.48	109.66
5	B	606	FAD	C9A-C5X-N5	-2.26	120.06	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1326	MTE	O4'-C4'-C3'	2.24	114.10	108.58
5	K	606	FAD	C1'-C2'-C3'	-2.23	103.60	109.66
5	B	606	FAD	C4-N3-C2	-2.23	121.68	125.64
5	B	606	FAD	O2P-P-O3P	2.17	113.13	107.27
6	L	1326	MTE	C9-C4-N3	-2.16	118.45	123.91
5	K	606	FAD	O2A-PA-O3P	2.09	112.91	107.27
5	K	606	FAD	C9A-C5X-N5	-2.08	120.25	122.45
6	L	1326	MTE	C2-N1-C10	2.07	119.50	114.59
5	K	606	FAD	C4-C4X-N5	2.06	121.05	118.21
6	L	1326	MTE	N1-C2-N3	-2.05	122.34	125.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1326	MTE	C3'-C4'-O4'-P
6	C	1326	MTE	C3'-C4'-O4'-P
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

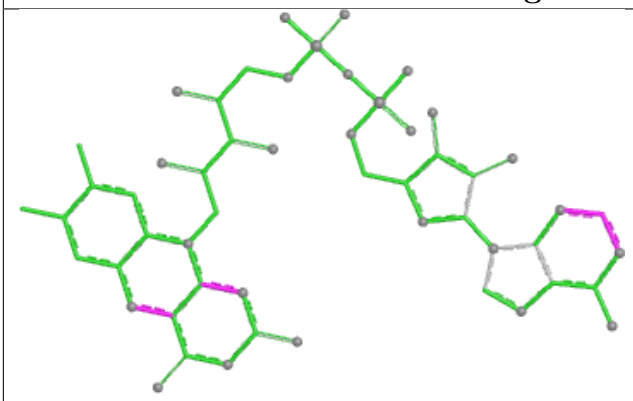
6 monomers are involved in 8 short contacts:

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

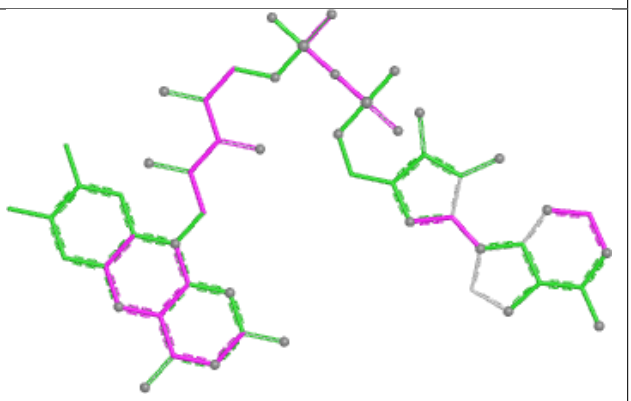
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

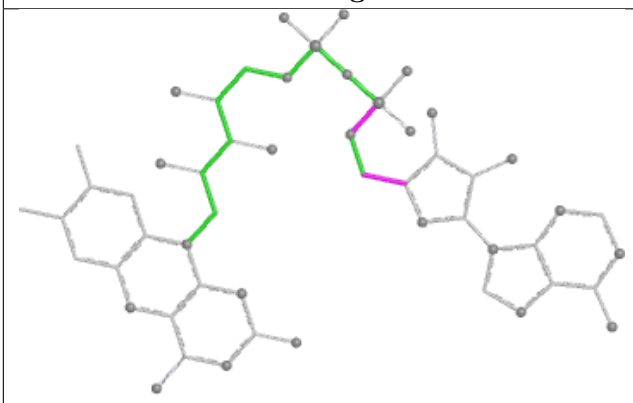
Ligand FAD K 606



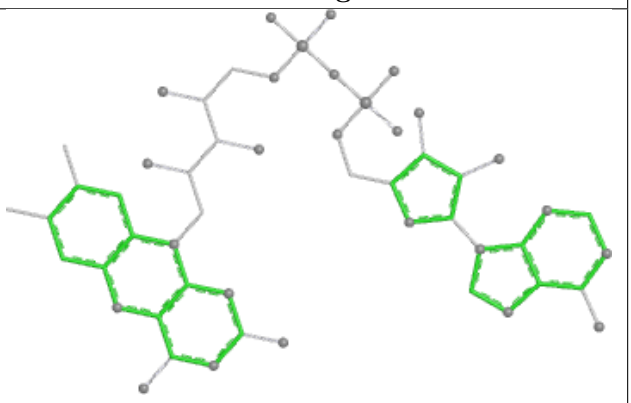
Bond lengths



Bond angles

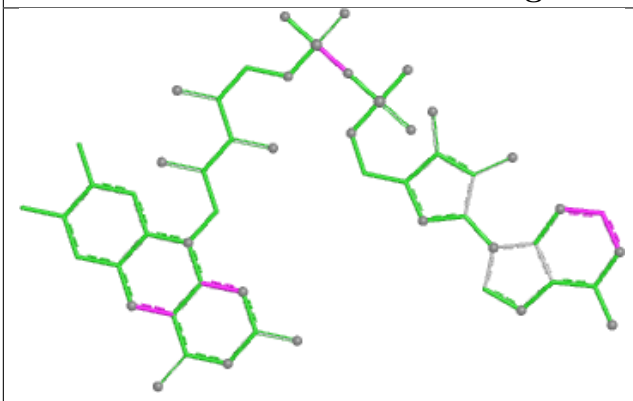


Torsions

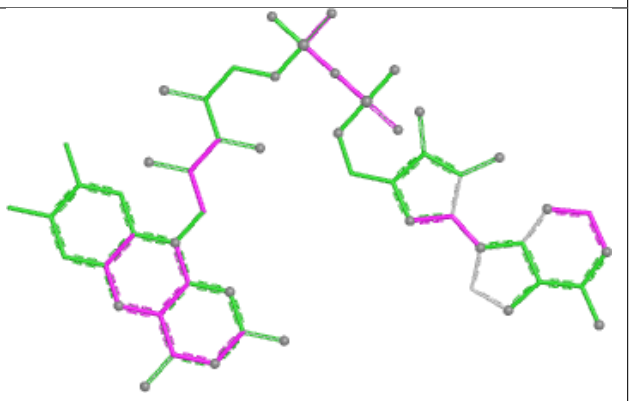


Rings

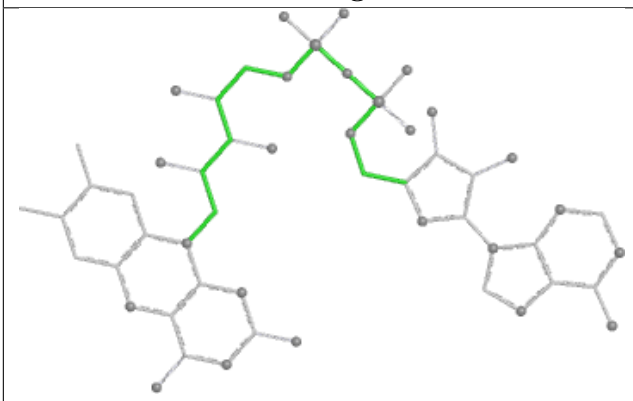
Ligand FAD B 606



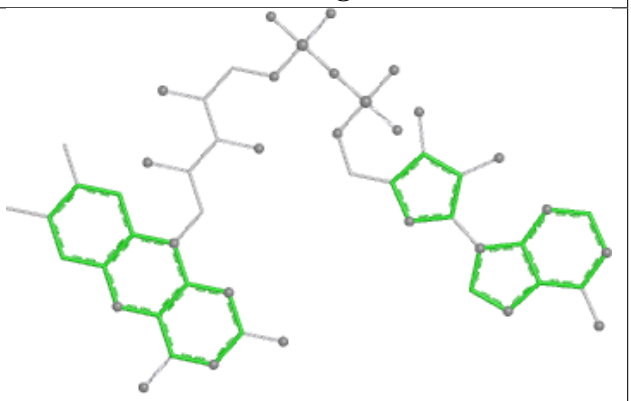
Bond lengths



Bond angles

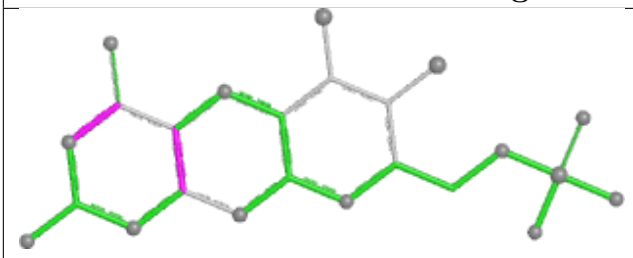


Torsions

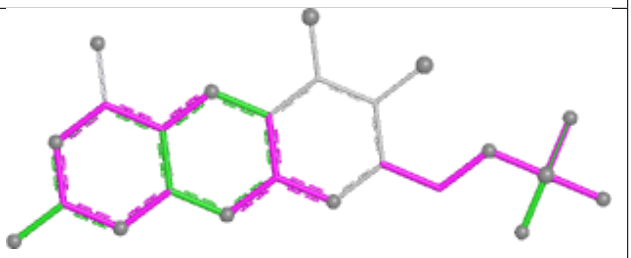


Rings

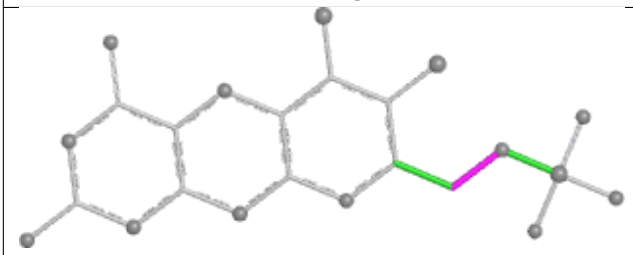
Ligand MTE C 1326



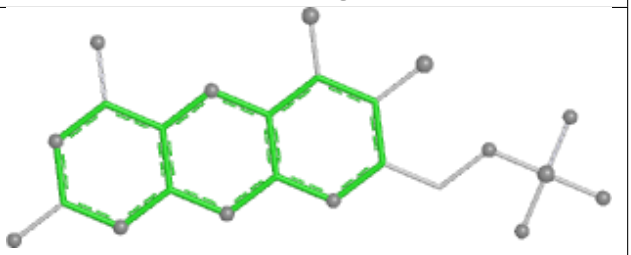
Bond lengths



Bond angles

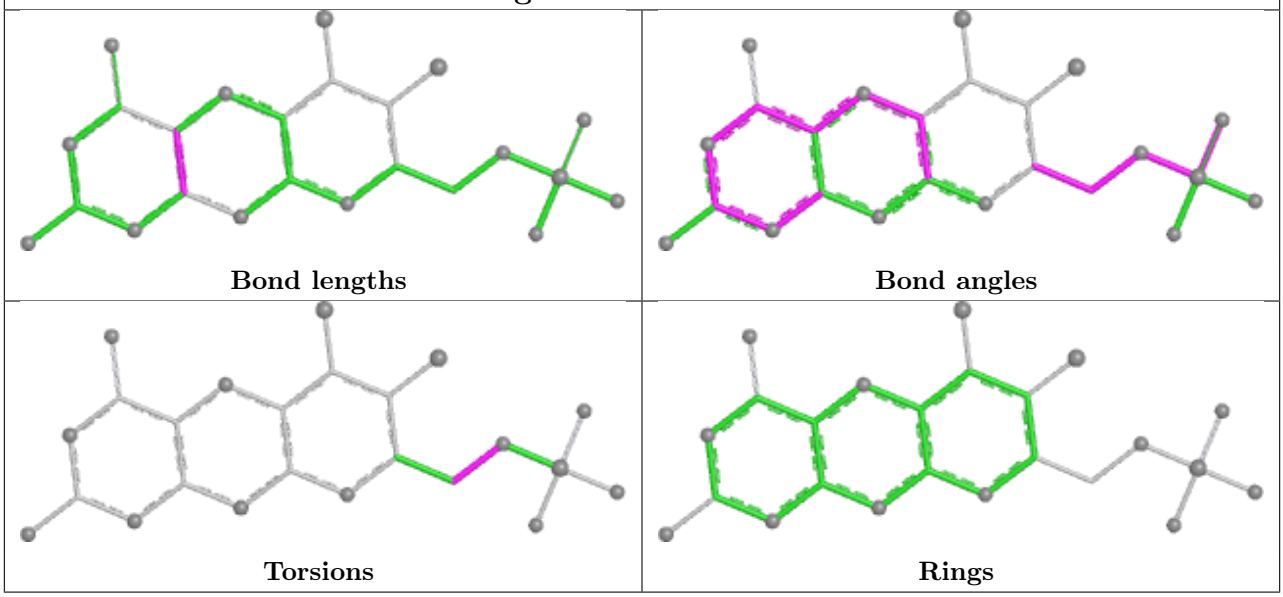


Torsions



Rings

Ligand MTE L 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.06	3 (1%)	68	64	10, 20, 34, 43	0
1	J	164/164 (100%)	-0.03	5 (3%)	50	44	13, 22, 42, 52	0
2	B	334/334 (100%)	0.26	10 (2%)	50	44	17, 29, 42, 50	0
2	K	305/334 (91%)	0.38	20 (6%)	18	14	21, 33, 45, 49	0
3	C	755/755 (100%)	-0.22	1 (0%)	95	93	11, 18, 28, 35	0
3	L	745/755 (98%)	-0.16	5 (0%)	87	86	12, 20, 34, 60	0
All	All	2467/2506 (98%)	-0.04	44 (1%)	68	64	10, 22, 40, 60	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1290	THR	7.3
1	J	61	LEU	6.1
3	L	1288	ASN	6.1
1	J	58	TYR	6.1
1	A	61	LEU	6.0
2	B	424	ALA	4.2
2	K	424	ALA	4.2
2	K	336	TRP	4.1
3	L	1287	ASN	3.8
2	K	378	GLY	3.8
2	K	429	ASP	3.8
2	K	425	SER	3.6
2	B	211	ILE	3.5
2	K	254	GLU	3.2
2	K	414	GLU	3.2
2	K	272	ASN	3.2
2	B	425	SER	3.1
2	B	336	TRP	3.0
2	B	207	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	1289	ASN	3.0
2	K	379	THR	3.0
2	B	248	LEU	2.9
3	L	958	ARG	2.9
2	B	338	ALA	2.9
1	J	133	GLU	2.8
2	K	474	LEU	2.8
2	K	475	SER	2.8
1	A	60	ARG	2.7
2	K	335	ARG	2.7
1	A	2	THR	2.5
2	B	272	ASN	2.4
2	K	467	LEU	2.3
1	J	60	ARG	2.3
2	B	378	GLY	2.2
3	C	1325	CYS	2.2
2	K	295	GLU	2.2
2	K	477	PHE	2.2
2	K	243	LYS	2.1
2	K	440	VAL	2.1
2	K	314	GLU	2.1
2	K	528	GLY	2.1
2	B	468	LYS	2.0
1	J	161	ARG	2.0
2	K	426	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

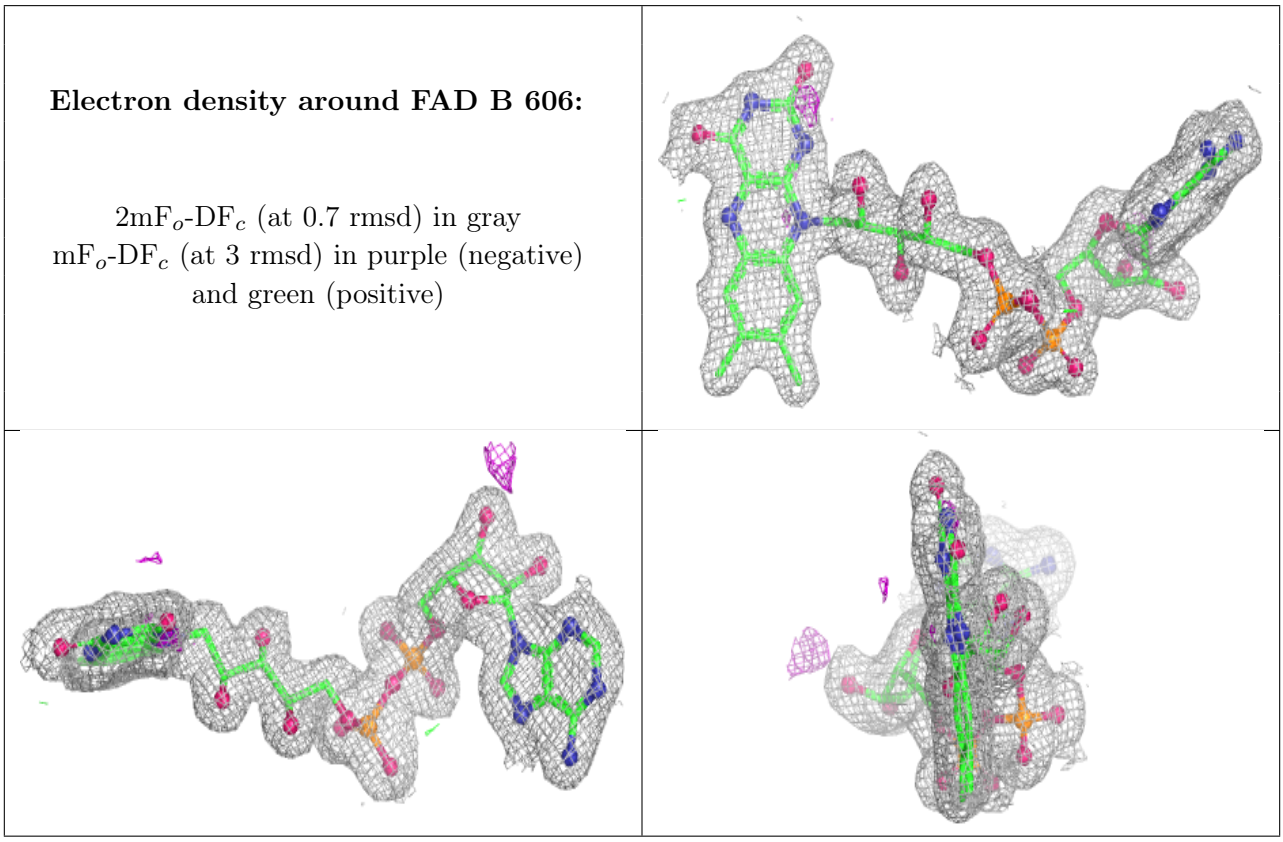
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	B	606	53/53	0.96	0.10	17,21,27,29	0
5	FAD	K	606	53/53	0.97	0.09	20,26,28,30	0
6	MTE	C	1326	24/24	0.98	0.09	9,12,17,19	0
6	MTE	L	1326	24/24	0.98	0.08	12,14,19,21	0
4	FES	J	601	4/4	0.99	0.08	14,14,16,16	0
4	FES	J	602	4/4	0.99	0.09	15,15,16,16	0
4	FES	A	602	4/4	0.99	0.09	14,15,16,16	0
7	MOS	C	1327	4/4	0.99	0.11	18,20,24,32	0
7	MOS	L	1327	4/4	0.99	0.10	12,19,19,29	0
8	AST	C	1	3/4	0.99	0.08	21,21,22,23	0
8	AST	L	1	3/4	0.99	0.09	26,26,26,31	0
4	FES	A	601	4/4	1.00	0.10	13,14,14,15	0

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

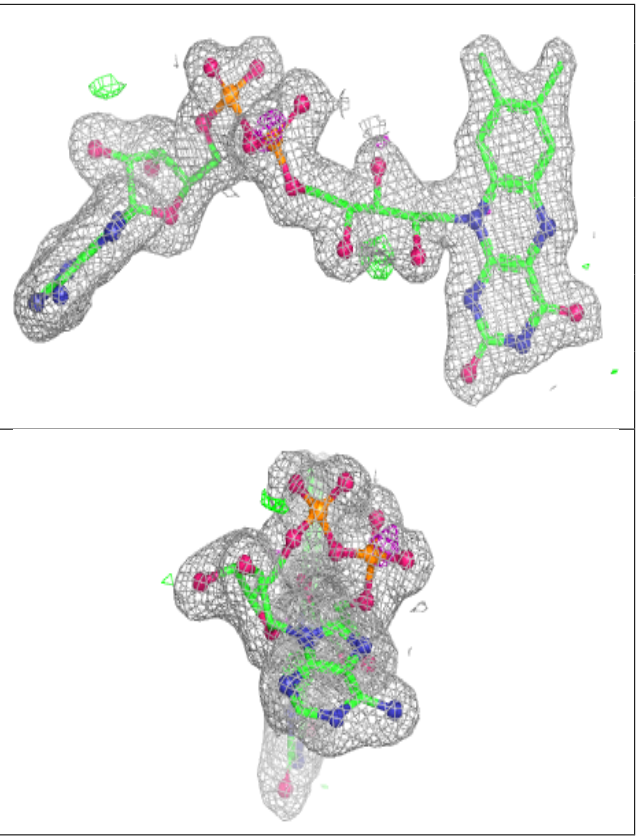
Electron density around FAD B 606:

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



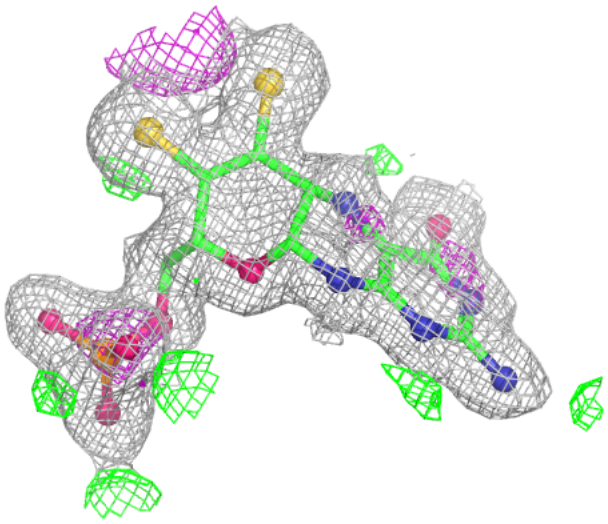
Electron density around FAD K 606:

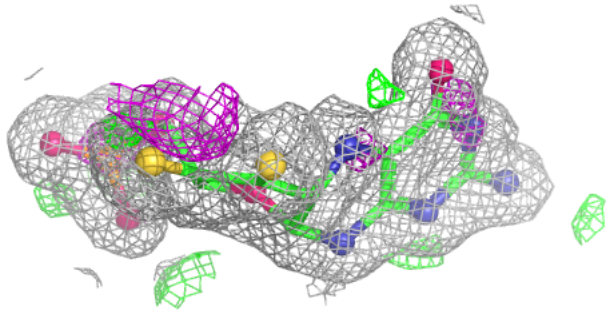
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

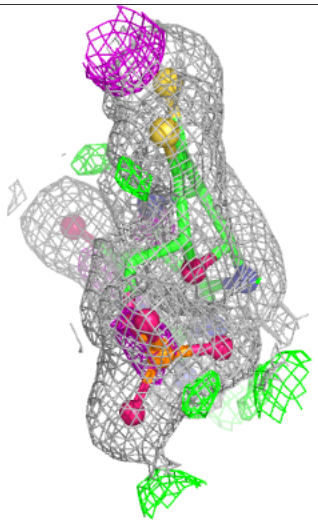


Electron density around MTE C 1326:

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

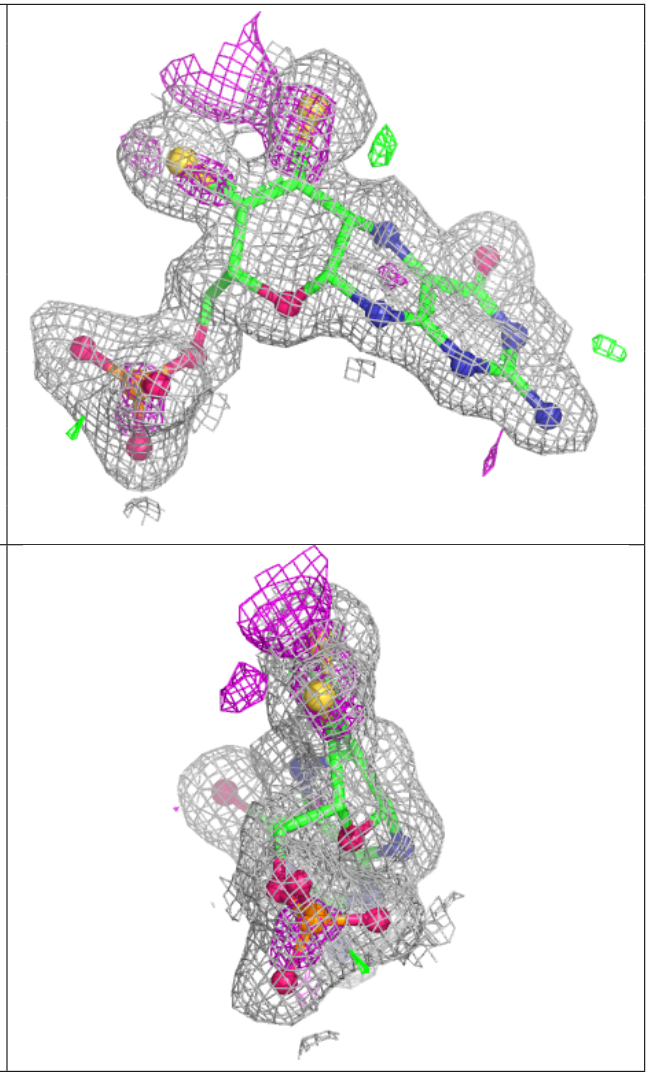






Electron density around MTE L 1326:

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



6.5 Other polymers (i)

There are no such residues in this entry.