



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:29 pm BST

PDB ID : 3NRZ
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Hypoxanthine
Authors : Cao, H.; Paufl, J.M.; Hille, R.
Deposited on : 2010-07-01
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

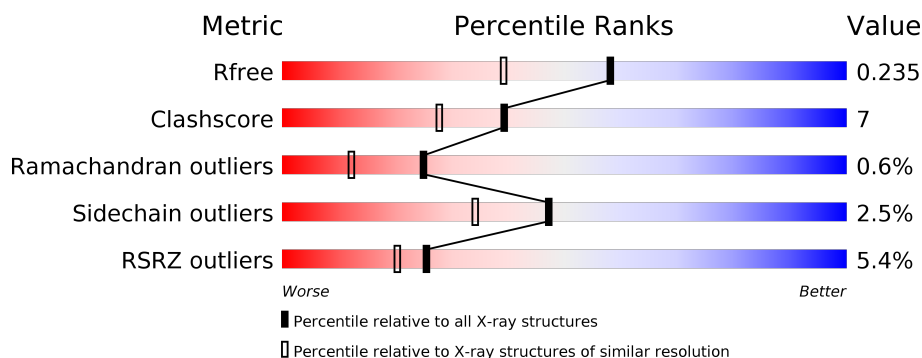
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> <div>•</div> </div>
1	J	164	<div> <div>9%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> <div></div> </div>
2	B	305	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> <div>•</div> </div>
2	K	305	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div>•</div> </div>
3	C	756	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>16%</div> </div> <div>•</div> </div>
3	L	756	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>11%</div> </div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MOS	C	1328	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20353 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			

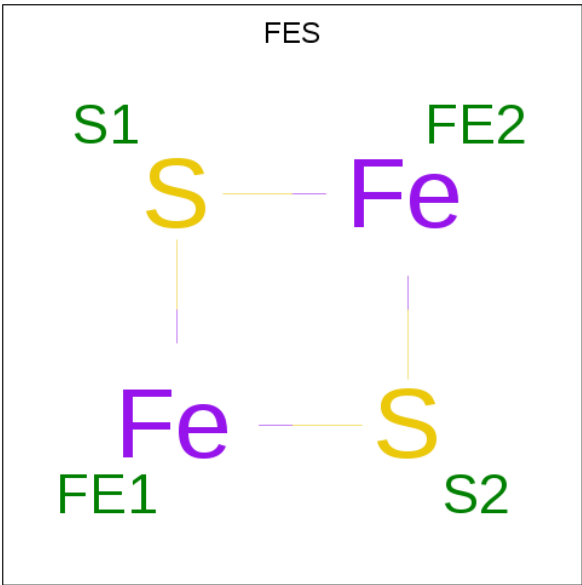
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

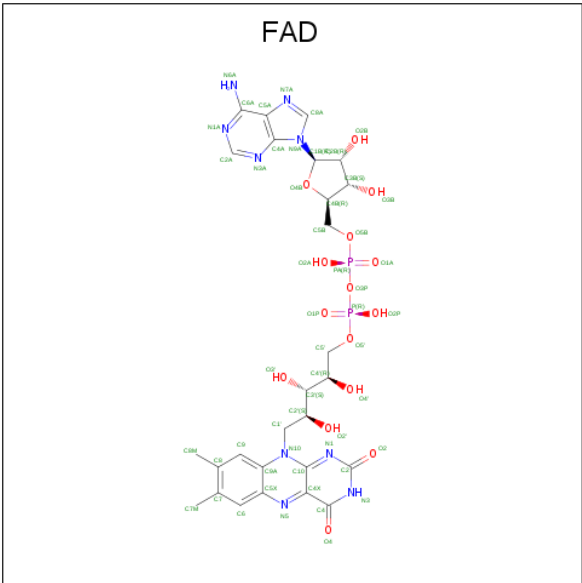
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



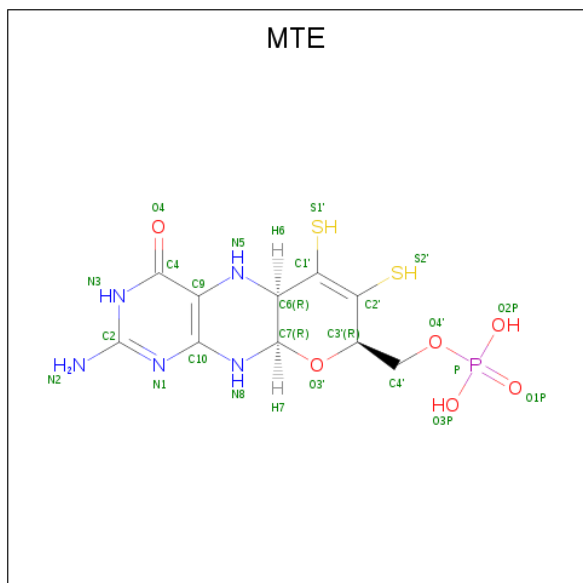
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

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



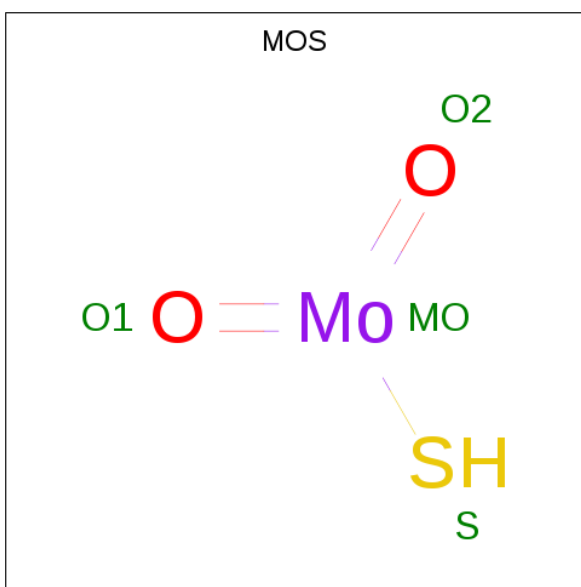
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P S₂).



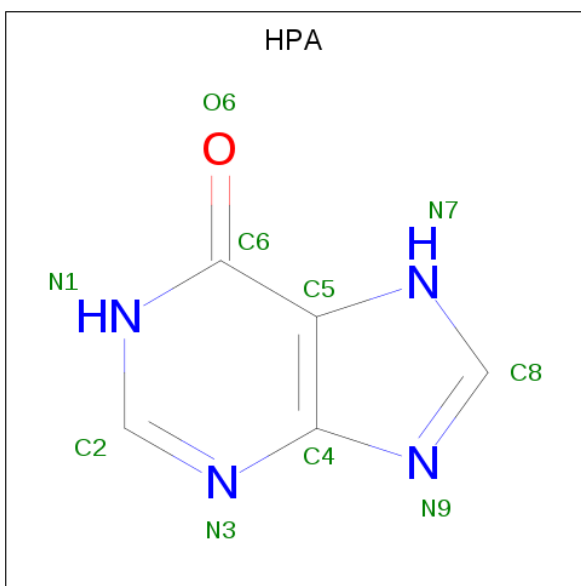
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	L	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO₂S).



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 HYPOXANTHINE (three-letter code: HPA) (formula: $C_5H_4N_4O$).



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

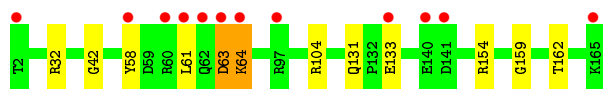
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total 114	O 114	0	0
9	B	114	Total 114	O 114	0	0
9	C	436	Total 436	O 436	0	0
9	J	98	Total 98	O 98	0	0
9	K	75	Total 75	O 75	0	0
9	L	437	Total 437	O 437	0	0

3 Residue-property plots [i](#)

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

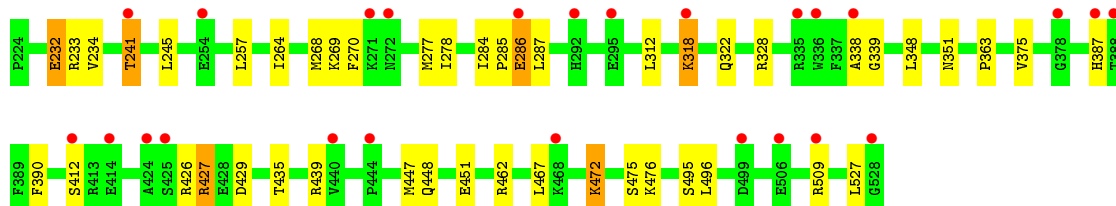
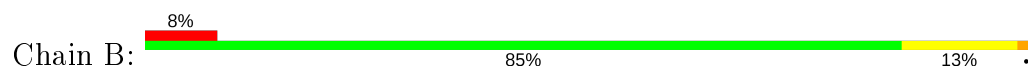
- Molecule 1: Xanthine dehydrogenase/oxidase



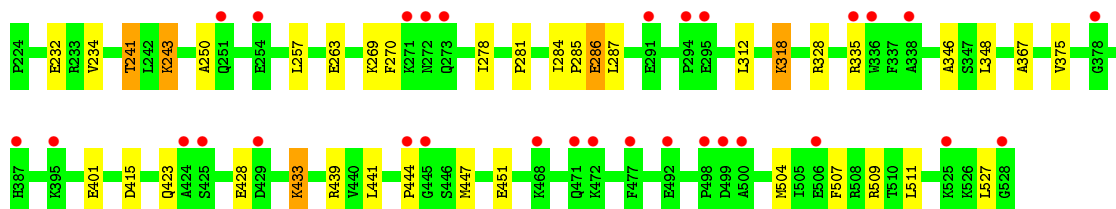
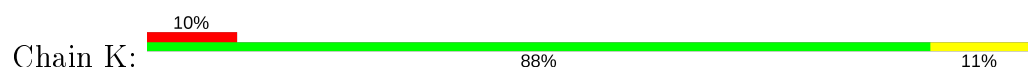
- Molecule 1: Xanthine dehydrogenase/oxidase



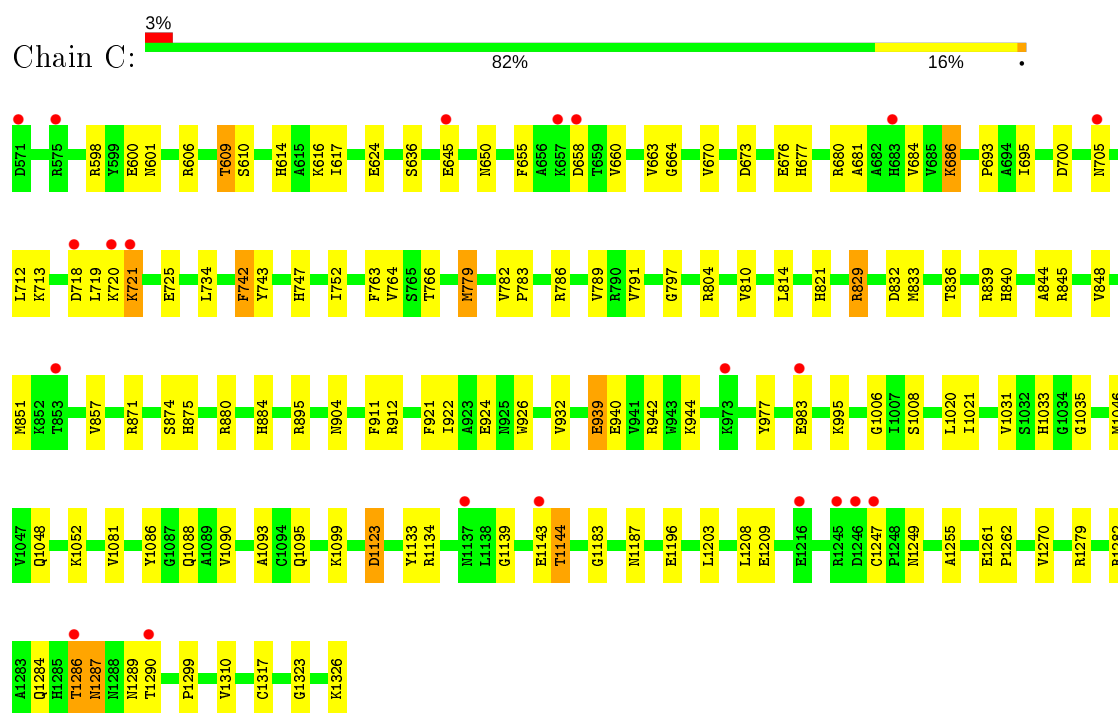
- Molecule 2: Xanthine dehydrogenase/oxidase



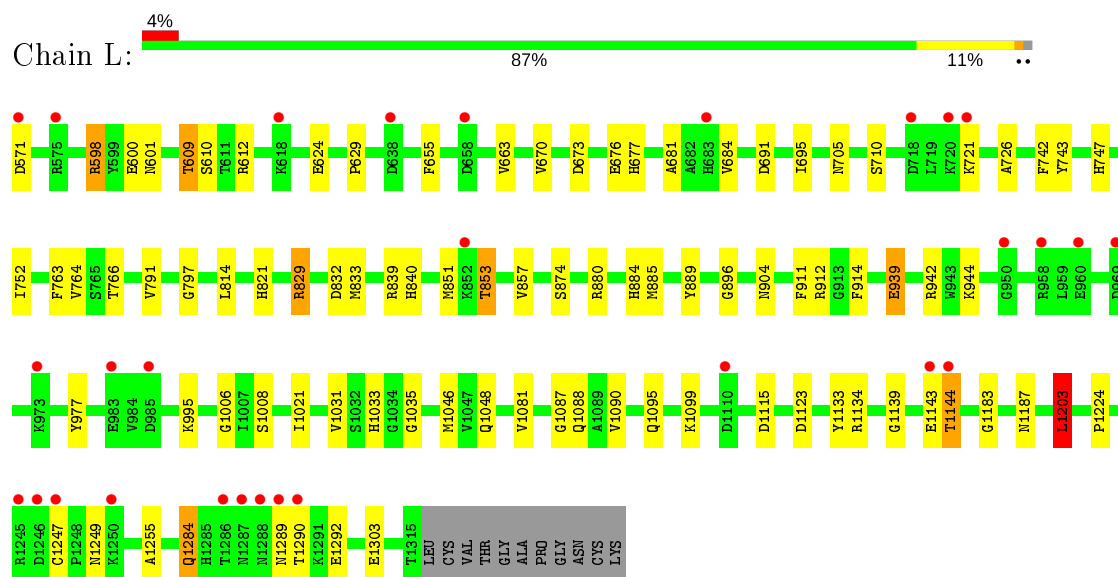
- Molecule 2: Xanthine dehydrogenase/oxidase



- Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.02Å 73.64Å 138.70Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	23.50 – 1.80 23.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (23.50-1.80) 95.1 (23.46-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.234 0.196 , 0.235	Depositor DCC
R_{free} test set	11843 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20353	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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

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, HPA, FES, FAD, MTE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/1277	0.70	0/1723
1	J	0.57	0/1277	0.64	0/1723
2	B	0.50	0/2438	0.62	0/3290
2	K	0.48	0/2438	0.60	0/3290
3	C	0.60	0/5960	0.73	6/8072 (0.1%)
3	L	0.59	0/5888	0.72	6/7974 (0.1%)
All	All	0.57	0/19278	0.69	12/26072 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	839	ARG	NE-CZ-NH2	-14.73	112.94	120.30
3	L	839	ARG	NE-CZ-NH2	-14.27	113.17	120.30
3	L	829	ARG	NE-CZ-NH2	-12.69	113.96	120.30
3	L	839	ARG	NE-CZ-NH1	10.21	125.41	120.30
3	C	829	ARG	NE-CZ-NH2	-10.18	115.21	120.30
3	C	839	ARG	NE-CZ-NH1	9.89	125.25	120.30
3	L	829	ARG	NE-CZ-NH1	9.82	125.21	120.30
3	C	829	ARG	NE-CZ-NH1	8.63	124.62	120.30
3	L	1203	LEU	CA-CB-CG	5.77	128.57	115.30
3	C	839	ARG	CG-CD-NE	-5.60	100.04	111.80
3	C	606	ARG	NE-CZ-NH2	-5.15	117.73	120.30
3	L	839	ARG	CG-CD-NE	-5.12	101.04	111.80

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	11	0
1	J	1255	0	1265	9	0
2	B	2389	0	2459	35	0
2	K	2389	0	2459	38	0
3	C	5832	0	5759	119	1
3	L	5761	0	5685	83	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	3	0
6	C	24	0	10	0	0
6	L	24	0	10	0	0
7	C	4	0	0	2	0
7	L	4	0	0	1	0
8	C	10	0	4	1	0
8	L	10	0	4	0	0
9	A	114	0	0	3	1
9	B	114	0	0	11	0
9	C	436	0	0	13	0
9	J	98	0	0	1	0
9	K	75	0	0	5	0
9	L	437	0	0	9	0
All	All	20353	0	18982	283	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 7.

All (283) 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:1081:VAL:HG21	9:C:1338:HOH:O	1.25	1.29
3:C:1052:LYS:HE3	9:C:1342:HOH:O	1.23	1.27
3:L:1081:VAL:HG21	9:L:1366:HOH:O	1.11	1.26
3:C:764:VAL:HB	9:C:1472:HOH:O	1.09	1.23
2:B:241:THR:HB	9:B:558:HOH:O	1.44	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:610:SER:O	3:C:663:VAL:O	1.63	1.15
3:C:779:MET:SD	9:C:445:HOH:O	2.07	1.10
3:L:764:VAL:HB	9:L:1469:HOH:O	0.93	1.09
3:L:598:ARG:NH2	9:L:1437:HOH:O	1.85	1.07
3:C:1046:MET:SD	9:C:1498:HOH:O	2.11	1.06
2:K:243:LYS:HD3	2:K:243:LYS:H	0.95	1.06
3:L:833:MET:SD	9:L:1426:HOH:O	2.11	1.06
1:A:162:THR:HB	9:A:630:HOH:O	1.51	1.05
2:K:243:LYS:HD3	2:K:243:LYS:N	1.70	1.05
3:C:598:ARG:NH2	9:C:1350:HOH:O	1.91	1.04
3:L:726:ALA:HA	3:L:851:MET:HE1	1.38	1.00
2:K:243:LYS:CD	2:K:243:LYS:H	1.71	0.99
2:B:286:GLU:N	9:B:641:HOH:O	1.96	0.98
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.96	0.98
3:L:610:SER:O	3:L:663:VAL:O	1.86	0.93
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.70	0.92
3:L:624:GLU:HB2	3:L:684:VAL:CG1	2.00	0.90
3:C:1046:MET:CE	3:C:1090:VAL:HG21	2.00	0.90
2:K:241:THR:HB	9:K:88:HOH:O	1.69	0.90
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.19	0.90
3:C:1046:MET:HE2	3:C:1090:VAL:HG21	1.52	0.89
3:C:1143:GLU:O	3:C:1144:THR:HG23	1.73	0.89
3:C:779:MET:CG	9:C:445:HOH:O	2.20	0.88
3:L:726:ALA:HA	3:L:851:MET:CE	2.03	0.88
2:K:286:GLU:O	2:K:287:LEU:HB2	1.74	0.87
2:K:241:THR:CG2	2:K:243:LYS:HE2	2.04	0.87
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.57	0.84
3:L:1021:ILE:HD12	3:L:1031:VAL:HG22	1.58	0.83
3:L:1143:GLU:O	3:L:1144:THR:HG23	1.79	0.82
3:C:705:ASN:HB2	9:C:108:HOH:O	1.78	0.82
1:A:159:GLY:O	1:A:162:THR:HG22	1.81	0.80
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.29	0.79
3:L:1289:ASN:HB2	3:L:1292:GLU:HB2	1.65	0.79
1:A:131:GLN:HE21	1:A:133:GLU:H	1.29	0.78
3:L:695:ILE:H	3:L:904:ASN:HD22	1.32	0.77
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.76
3:L:1115:ASP:OD1	9:L:1717:HOH:O	2.04	0.76
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.85	0.75
3:C:1046:MET:CE	3:C:1090:VAL:CG2	2.63	0.75
2:B:285:PRO:HA	9:B:641:HOH:O	1.86	0.75
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:243:LYS:CD	2:K:243:LYS:N	2.41	0.74
2:B:338:ALA:C	9:B:1966:HOH:O	2.26	0.74
3:C:829:ARG:HG3	3:C:833:MET:HE3	1.69	0.74
3:C:624:GLU:HB2	3:C:684:VAL:HG12	1.70	0.73
2:K:439:ARG:NH2	2:K:451:GLU:OE1	2.21	0.73
3:C:742:PHE:CE1	3:C:833:MET:HE1	2.24	0.73
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.69	0.73
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.24	0.72
2:K:241:THR:HG22	9:K:169:HOH:O	1.89	0.72
1:A:32:ARG:NE	9:A:1088:HOH:O	2.05	0.71
2:K:241:THR:HG21	2:K:243:LYS:HE2	1.72	0.70
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.06	0.70
2:K:509:ARG:HG2	9:K:1267:HOH:O	1.93	0.69
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	1.74	0.69
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.07	0.68
3:C:742:PHE:HE1	3:C:833:MET:HE1	1.57	0.68
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.09	0.67
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.77	0.67
2:B:509:ARG:HG2	9:B:35:HOH:O	1.94	0.67
2:B:241:THR:CB	9:B:558:HOH:O	2.17	0.67
2:K:504:MET:HE2	3:L:1303:GLU:HB2	1.77	0.66
2:K:241:THR:HG22	2:K:243:LYS:HE2	1.78	0.66
3:C:845:ARG:NH1	9:C:1508:HOH:O	2.26	0.66
3:L:571:ASP:N	9:L:434:HOH:O	2.28	0.65
2:B:284:ILE:HG22	2:B:285:PRO:O	1.97	0.65
3:C:1046:MET:HE2	3:C:1090:VAL:CG2	2.24	0.64
3:C:1287:ASN:HD22	3:C:1289:ASN:H	1.44	0.64
3:L:840:HIS:HE1	3:L:874:SER:OG	1.80	0.63
3:C:779:MET:HG2	9:C:445:HOH:O	1.89	0.63
3:C:840:HIS:HE1	3:C:874:SER:OG	1.81	0.63
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.34	0.63
2:B:339:GLY:N	9:B:1966:HOH:O	2.32	0.62
3:C:720:LYS:O	3:C:721:LYS:CB	2.47	0.62
3:C:829:ARG:CG	3:C:833:MET:HE3	2.29	0.62
2:B:286:GLU:O	2:B:287:LEU:HB2	1.99	0.62
2:B:318:LYS:N	2:B:318:LYS:HD3	2.15	0.61
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.48	0.61
7:C:1328:MOS:MO	7:C:1328:MOS:O2	1.72	0.60
7:L:1328:MOS:MO	7:L:1328:MOS:O2	1.72	0.60
1:A:32:ARG:NH1	3:C:676:GLU:OE2	2.33	0.60
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.32	0.60
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.33	0.60
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.00	0.60
1:J:42:GLY:O	3:L:829:ARG:HD2	2.02	0.59
3:C:880:ARG:O	3:C:884:HIS:HD2	1.86	0.59
2:B:339:GLY:CA	9:B:1966:HOH:O	2.50	0.59
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.03	0.58
7:C:1328:MOS:O1	8:C:1:HPA:H8	2.02	0.58
3:L:1095:GLN:O	3:L:1099:LYS:HG2	2.03	0.58
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.38	0.58
3:C:1286:THR:O	3:C:1326:LYS:HD3	2.04	0.58
2:K:232:GLU:OE2	3:L:629:PRO:HG2	2.04	0.58
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.52	0.57
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.39	0.57
3:L:829:ARG:HG3	3:L:833:MET:HE3	1.85	0.57
3:C:932:VAL:HG13	3:C:1279:ARG:HH21	1.68	0.57
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.52	0.57
2:K:285:PRO:O	2:K:286:GLU:HB2	2.04	0.56
1:A:42:GLY:O	3:C:829:ARG:HD2	2.06	0.55
2:B:285:PRO:C	2:B:286:GLU:O	2.42	0.55
3:C:725:GLU:HG3	3:C:851:MET:HE1	1.88	0.55
2:K:285:PRO:O	2:K:286:GLU:CB	2.54	0.55
3:C:742:PHE:CE1	3:C:833:MET:CE	2.89	0.55
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.87	0.55
3:C:713:LYS:HD2	3:C:895:ARG:NH1	2.22	0.55
3:L:764:VAL:CG2	3:L:766:THR:HG22	2.36	0.55
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.90	0.55
2:B:285:PRO:CA	9:B:641:HOH:O	2.50	0.55
2:K:509:ARG:HD2	9:K:1767:HOH:O	2.06	0.55
2:K:286:GLU:O	2:K:287:LEU:CB	2.47	0.55
3:C:782:VAL:HG12	3:C:783:PRO:HD2	1.87	0.54
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.88	0.54
3:L:624:GLU:HB2	3:L:684:VAL:HG12	1.88	0.54
3:C:851:MET:CE	3:C:857:VAL:HG21	2.38	0.54
3:C:624:GLU:HG3	3:C:686:LYS:NZ	2.23	0.54
3:C:782:VAL:HG12	3:C:786:ARG:HG3	1.89	0.53
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.90	0.53
2:K:285:PRO:O	2:K:286:GLU:OE1	2.26	0.53
3:L:1134:ARG:NE	9:L:1420:HOH:O	2.41	0.53
2:B:495:SER:HB2	2:B:509:ARG:HH22	1.72	0.53
2:B:234:VAL:HG11	2:B:278:ILE:HD12	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1046:MET:HE1	3:L:1090:VAL:HB	1.90	0.53
2:K:250:ALA:HA	2:K:401:GLU:HG2	1.90	0.53
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.90	0.53
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.50	0.52
3:L:624:GLU:CB	3:L:684:VAL:CG1	2.84	0.52
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.37	0.52
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.08	0.52
3:C:624:GLU:HB2	3:C:684:VAL:CG1	2.38	0.52
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.92	0.52
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.08	0.52
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.45	0.52
3:C:851:MET:HE1	3:C:857:VAL:HG21	1.91	0.52
1:J:159:GLY:O	1:J:162:THR:HG22	2.10	0.52
1:J:131:GLN:HE21	1:J:133:GLU:H	1.56	0.52
3:C:983:GLU:HG2	9:C:1917:HOH:O	2.09	0.52
3:L:829:ARG:HG3	3:L:833:MET:CE	2.40	0.51
3:C:609:THR:HG22	9:C:1982:HOH:O	2.10	0.51
3:C:725:GLU:HG3	3:C:851:MET:CE	2.40	0.51
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.91	0.51
2:B:363:PRO:HG2	2:B:435:THR:HG23	1.93	0.51
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.57	0.51
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.75	0.51
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.92	0.51
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.24	0.51
3:L:612:ARG:NH1	3:L:691:ASP:OD1	2.40	0.51
3:L:601:ASN:O	3:L:821:HIS:HD2	1.93	0.50
3:C:617:ILE:HD11	3:C:660:VAL:HG13	1.92	0.50
3:C:601:ASN:O	3:C:821:HIS:HD2	1.95	0.50
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.94	0.50
3:L:853:THR:HG22	3:L:944:LYS:NZ	2.27	0.49
3:L:880:ARG:O	3:L:884:HIS:HD2	1.94	0.49
1:A:131:GLN:NE2	1:A:133:GLU:H	2.06	0.49
3:C:616:LYS:HD2	3:C:658:ASP:O	2.13	0.49
3:C:924:GLU:OE1	3:C:942:ARG:CZ	2.57	0.49
3:C:614:HIS:HD2	3:C:693:PRO:O	1.95	0.49
3:C:718:ASP:OD1	3:C:720:LYS:O	2.31	0.49
2:K:504:MET:CE	3:L:1303:GLU:HB2	2.41	0.49
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.33	0.49
3:C:645:GLU:OE2	3:C:650:ASN:HB3	2.13	0.49
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.78	0.49
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:LEU:HD11	2:B:257:LEU:HD21	1.94	0.49
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.46	0.48
2:K:284:ILE:HG22	2:K:285:PRO:O	2.13	0.48
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.58	0.48
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.49	0.48
2:B:232:GLU:OE2	3:C:680:ARG:NH1	2.47	0.48
3:L:1046:MET:CE	3:L:1087:GLY:HA2	2.43	0.48
1:J:97:ARG:HG2	1:J:97:ARG:HH11	1.78	0.48
3:L:764:VAL:HG23	3:L:791:VAL:HG22	1.96	0.48
3:L:609:THR:HG22	9:L:60:HOH:O	2.13	0.47
3:L:684:VAL:O	3:L:684:VAL:CG1	2.62	0.47
3:C:734:LEU:HD21	3:C:921:PHE:CE2	2.48	0.47
3:L:829:ARG:CG	3:L:833:MET:HE3	2.45	0.47
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.15	0.47
3:C:764:VAL:HG23	3:C:791:VAL:HG22	1.95	0.47
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.97	0.47
2:B:427:ARG:HD2	9:B:531:HOH:O	2.13	0.47
3:C:1209:GLU:O	3:C:1299:PRO:HG3	2.15	0.47
3:C:747:HIS:HD2	3:C:832:ASP:OD1	1.98	0.47
3:C:1046:MET:HE1	3:C:1090:VAL:CG2	2.45	0.47
2:K:423:GLN:HB3	2:K:433:LYS:HG2	1.97	0.47
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.97	0.46
2:K:241:THR:CB	9:K:88:HOH:O	2.42	0.46
3:C:598:ARG:HD3	3:L:600:GLU:OE2	2.16	0.46
1:A:154:ARG:NE	3:C:1196:GLU:OE2	2.46	0.46
3:C:1134:ARG:NH1	3:L:1123:ASP:O	2.48	0.46
3:L:624:GLU:HB2	3:L:684:VAL:HG11	1.94	0.46
1:A:104:ARG:HE	1:A:162:THR:HG21	1.81	0.46
3:C:995:LYS:NZ	3:C:1284:GLN:NE2	2.59	0.46
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.17	0.45
3:C:1021:ILE:HG12	3:C:1093:ALA:CB	2.47	0.45
3:L:752:ILE:CD1	3:L:763:PHE:CE1	2.95	0.45
1:J:32:ARG:NH1	9:J:315:HOH:O	2.39	0.45
3:L:1046:MET:CE	3:L:1090:VAL:HG21	2.43	0.45
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.52	0.45
3:L:624:GLU:HB2	3:L:684:VAL:HG13	1.92	0.45
3:C:844:ALA:HB2	3:C:922:ILE:HD13	1.98	0.45
3:L:889:TYR:OH	3:L:942:ARG:HD3	2.17	0.45
2:B:285:PRO:O	2:B:286:GLU:HB2	2.17	0.44
2:K:415:ASP:OD2	2:K:444:PRO:HA	2.18	0.44
2:B:264:ILE:O	2:B:268:MET:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.82	0.44
3:L:609:THR:CG2	9:L:60:HOH:O	2.64	0.44
3:L:673:ASP:OD2	3:L:677:HIS:HD2	2.00	0.44
3:L:684:VAL:O	3:L:684:VAL:HG12	2.16	0.44
3:L:747:HIS:HD2	3:L:832:ASP:OD1	2.01	0.44
2:K:269:LYS:HG2	2:K:270:PHE:CE1	2.52	0.44
3:C:695:ILE:H	3:C:904:ASN:ND2	2.10	0.44
3:C:624:GLU:HB3	3:C:684:VAL:HG11	2.00	0.44
2:B:285:PRO:O	2:B:286:GLU:CB	2.65	0.43
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.81	0.43
3:C:680:ARG:O	3:C:684:VAL:HG23	2.18	0.43
2:K:346:ALA:HB1	5:K:606:FAD:H4'	2.00	0.43
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.64	0.43
2:B:390:PHE:O	2:B:462:ARG:HD2	2.17	0.43
3:C:1020:LEU:C	3:C:1021:ILE:HD13	2.38	0.43
2:K:257:LEU:O	5:K:606:FAD:H2B	2.19	0.43
3:L:752:ILE:HD12	3:L:763:PHE:CE1	2.53	0.43
2:B:232:GLU:HG2	2:B:233:ARG:HG3	2.00	0.43
2:B:448:GLN:HE21	2:B:475:SER:HB2	1.84	0.43
3:C:1033:HIS:HD2	3:C:1035:GLY:N	2.10	0.43
3:C:764:VAL:HG21	3:C:789:VAL:CG1	2.49	0.43
3:C:782:VAL:CG1	3:C:783:PRO:HD2	2.48	0.43
2:K:263:GLU:HB3	5:K:606:FAD:H52A	2.01	0.43
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.34	0.43
2:B:269:LYS:HG2	2:B:270:PHE:CE1	2.54	0.43
2:B:472:LYS:O	2:B:472:LYS:HG3	2.12	0.43
2:K:367:ALA:O	2:K:439:ARG:HD3	2.19	0.43
3:L:880:ARG:HD2	3:L:914:PHE:HB3	2.01	0.43
2:B:322:GLN:O	2:B:412:SER:HB3	2.19	0.42
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.32	0.42
2:K:318:LYS:N	2:K:318:LYS:HD3	2.34	0.42
2:K:441:LEU:HB3	2:K:451:GLU:HB2	2.01	0.42
3:C:1021:ILE:HG12	3:C:1093:ALA:HB1	2.01	0.42
3:C:624:GLU:HG3	3:C:686:LYS:HZ1	1.83	0.42
3:C:1021:ILE:HD12	3:C:1031:VAL:HG13	2.01	0.42
3:C:624:GLU:CB	3:C:684:VAL:CG1	2.96	0.42
2:B:496:LEU:H	2:B:509:ARG:NH2	2.17	0.42
3:C:1203:LEU:HD13	3:C:1270:VAL:HG21	2.01	0.42
3:L:670:VAL:HG11	3:L:681:ALA:CB	2.50	0.42
3:L:655:PHE:CE1	3:L:814:LEU:HD23	2.54	0.42
1:A:58:TYR:CE1	1:A:63:ASP:O	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:507:PHE:CZ	2:K:511:LEU:HD11	2.55	0.42
3:C:1123:ASP:O	3:L:1134:ARG:CZ	2.68	0.42
3:L:840:HIS:CE1	3:L:874:SER:OG	2.67	0.42
3:C:720:LYS:O	3:C:721:LYS:HB3	2.19	0.41
3:C:940:GLU:O	3:C:944:LYS:HG3	2.20	0.41
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.85	0.41
2:K:241:THR:HG22	2:K:243:LYS:CE	2.49	0.41
2:K:281:PRO:HB2	2:K:287:LEU:CD1	2.50	0.41
2:B:426:ARG:NH2	2:B:429:ASP:O	2.53	0.41
2:B:387:HIS:CE1	2:B:467:LEU:HD11	2.56	0.41
2:K:232:GLU:OE1	3:L:677:HIS:HE1	2.02	0.41
1:J:45:GLU:CD	3:L:1224:PRO:HD2	2.40	0.41
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.85	0.41
3:C:1046:MET:HE1	3:C:1086:TYR:O	2.20	0.41
3:L:885:MET:SD	3:L:896:GLY:HA3	2.60	0.41
2:B:284:ILE:O	2:B:286:GLU:O	2.37	0.41
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.56	0.41
3:C:995:LYS:HZ1	3:C:1284:GLN:NE2	2.16	0.41
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	2.02	0.41
1:J:74:LEU:O	1:J:76:PRO:HD3	2.21	0.41
3:L:851:MET:CE	3:L:857:VAL:HG21	2.50	0.41
3:L:995:LYS:NZ	3:L:1284:GLN:NE2	2.67	0.41
1:A:32:ARG:NH2	9:A:1088:HOH:O	2.54	0.40
2:B:375:VAL:HG13	9:B:560:HOH:O	2.21	0.40
2:K:234:VAL:HG11	2:K:278:ILE:HD12	2.03	0.40
3:C:600:GLU:HG2	3:L:598:ARG:O	2.22	0.40
3:C:720:LYS:O	3:C:721:LYS:HB2	2.20	0.40
3:C:939:GLU:H	3:C:939:GLU:CD	2.23	0.40
3:L:1048:GLN:NE2	3:L:1187:ASN:HD22	2.18	0.40
3:L:851:MET:HE2	3:L:857:VAL:CG2	2.51	0.40
3:C:1134:ARG:NH1	9:C:1926:HOH:O	2.53	0.40
3:C:804:ARG:HG3	3:C:836:THR:O	2.21	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:871:ARG:NH1	9:A:173:HOH:O[1_565]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	12
1	J	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
2	B	303/305 (99%)	291 (96%)	12 (4%)	0	100	100
2	K	303/305 (99%)	292 (96%)	10 (3%)	1 (0%)	41	27
3	C	754/756 (100%)	733 (97%)	15 (2%)	6 (1%)	19	7
3	L	743/756 (98%)	724 (97%)	13 (2%)	6 (1%)	19	7
All	All	2427/2450 (99%)	2349 (97%)	64 (3%)	14 (1%)	25	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	721	LYS
3	C	1008	SER
3	C	1144	THR
3	L	721	LYS
3	L	1008	SER
3	L	1144	THR
3	L	912	ARG
1	A	64	LYS
3	C	912	ARG
2	K	286	GLU
3	L	1139	GLY
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%)	134 (98%)	3 (2%)	52	39
1	J	137/137 (100%)	136 (99%)	1 (1%)	84	81
2	B	261/261 (100%)	249 (95%)	12 (5%)	27	13
2	K	261/261 (100%)	251 (96%)	10 (4%)	33	18
3	C	632/632 (100%)	619 (98%)	13 (2%)	53	42
3	L	624/632 (99%)	612 (98%)	12 (2%)	57	46
All	All	2052/2060 (100%)	2001 (98%)	51 (2%)	47	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	63	ASP
1	A	64	LYS
2	B	232	GLU
2	B	241	THR
2	B	277	MET
2	B	286	GLU
2	B	312	LEU
2	B	318	LYS
2	B	328	ARG
2	B	348	LEU
2	B	351	ASN
2	B	427	ARG
2	B	472	LYS
2	B	476	LYS
3	C	609	THR
3	C	636	SER
3	C	686	LYS
3	C	742	PHE
3	C	743	TYR
3	C	779	MET
3	C	911	PHE
3	C	939	GLU
3	C	1123	ASP
3	C	1208	LEU
3	C	1286	THR
3	C	1287	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1290	THR
1	J	93	SER
2	K	241	THR
2	K	243	LYS
2	K	312	LEU
2	K	318	LYS
2	K	328	ARG
2	K	335	ARG
2	K	348	LEU
2	K	375	VAL
2	K	428	GLU
2	K	433	LYS
3	L	598	ARG
3	L	609	THR
3	L	705	ASN
3	L	710	SER
3	L	742	PHE
3	L	743	TYR
3	L	853	THR
3	L	911	PHE
3	L	939	GLU
3	L	1203	LEU
3	L	1284	GLN
3	L	1290	THR

Some 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
1	A	146	ASN
2	B	351	ASN
2	B	448	GLN
2	B	473	GLN
3	C	585	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1033	HIS
3	C	1048	GLN
3	C	1220	HIS
3	C	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
1	J	131	GLN
1	J	146	ASN
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	728	ASN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MOS	L	1328	6	0,3,3	0.00	-	-		
8	HPA	C	1	-	8,11,11	2.20	4 (50%)	5,15,15	2.09	2 (40%)
5	FAD	B	606	-	51,58,58	1.46	7 (13%)	60,89,89	1.69	7 (11%)
8	HPA	L	1	-	8,11,11	1.68	2 (25%)	5,15,15	2.55	2 (40%)
4	FES	A	602	1	0,4,4	0.00	-	-		
4	FES	J	601	1	0,4,4	0.00	-	-		
6	MTE	C	1327	7	21,26,26	1.60	2 (9%)	21,40,40	2.10	8 (38%)
4	FES	J	602	1	0,4,4	0.00	-	-		
6	MTE	L	1327	7	21,26,26	1.66	3 (14%)	21,40,40	2.34	6 (28%)
4	FES	A	601	1	0,4,4	0.00	-	-		
5	FAD	K	606	-	51,58,58	1.45	6 (11%)	60,89,89	1.76	11 (18%)
7	MOS	C	1328	6	0,3,3	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HPA	C	1	-	-	-	0/2/2/2
5	FAD	B	606	-	-	1/30/50/50	0/6/6/6
8	HPA	L	1	-	-	-	0/2/2/2
4	FES	J	601	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
6	MTE	C	1327	7	-	2/6/34/34	0/3/3/3
4	FES	J	602	1	-	-	0/1/1/1
6	MTE	L	1327	7	-	3/6/34/34	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
5	FAD	K	606	-	-	0/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1327	MTE	C4-C9	5.79	1.49	1.41
6	L	1327	MTE	C4-C9	5.29	1.48	1.41
5	B	606	FAD	C10-N1	4.87	1.39	1.33
5	K	606	FAD	C2A-N3A	4.46	1.39	1.32
5	K	606	FAD	C10-N1	4.44	1.39	1.33
5	B	606	FAD	C2A-N3A	4.38	1.39	1.32
5	K	606	FAD	C4X-N5	4.16	1.39	1.33
5	B	606	FAD	C4X-N5	3.90	1.38	1.33
6	L	1327	MTE	C9-C10	3.76	1.48	1.41
8	C	1	HPA	C2-N3	3.62	1.37	1.32
6	C	1327	MTE	C9-C10	3.42	1.47	1.41
5	K	606	FAD	C4-N3	3.40	1.39	1.33
8	C	1	HPA	C6-C5	-3.17	1.35	1.41
5	B	606	FAD	C4-N3	3.09	1.38	1.33
5	K	606	FAD	C2A-N1A	2.81	1.39	1.33
8	C	1	HPA	C6-N1	2.75	1.37	1.33
5	B	606	FAD	C2A-N1A	2.62	1.38	1.33
8	L	1	HPA	C2-N3	2.53	1.36	1.32
5	K	606	FAD	C5X-N5	2.25	1.39	1.35
5	B	606	FAD	C1'-N10	2.20	1.50	1.48
5	B	606	FAD	C4X-C10	2.20	1.41	1.38
6	L	1327	MTE	C4-N3	2.06	1.36	1.33
8	C	1	HPA	C2-N1	2.04	1.37	1.33
8	L	1	HPA	C6-C5	-2.04	1.37	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1327	MTE	C4-C9-N5	6.87	124.89	119.12
5	K	606	FAD	C4-N3-C2	6.60	120.71	115.14
5	B	606	FAD	N3A-C2A-N1A	-5.96	119.36	128.68
5	K	606	FAD	N3A-C2A-N1A	-5.96	119.37	128.68
5	B	606	FAD	C4-N3-C2	5.88	120.10	115.14
5	K	606	FAD	C1'-N10-C9A	4.65	121.95	118.29
5	B	606	FAD	C1'-N10-C9A	4.51	121.84	118.29
8	L	1	HPA	N3-C2-N1	-4.31	121.94	128.68
5	B	606	FAD	C4X-N5-C5X	4.19	120.96	116.77
6	L	1327	MTE	C4-N3-C2	4.15	122.52	115.93
6	C	1327	MTE	C4-N3-C2	4.04	122.36	115.93
6	C	1327	MTE	C4-C9-N5	3.81	122.32	119.12
5	K	606	FAD	C4X-N5-C5X	3.79	120.56	116.77
8	C	1	HPA	N3-C2-N1	-3.66	122.96	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1327	MTE	O2P-P-O4'	-3.33	97.88	106.73
6	L	1327	MTE	O2P-P-O4'	-3.26	98.07	106.73
8	L	1	HPA	C2-N1-C6	3.03	120.95	115.88
6	L	1327	MTE	C2-N1-C10	3.01	121.28	114.54
6	C	1327	MTE	O3P-P-O2P	2.84	118.50	107.64
5	K	606	FAD	C4-C4X-N5	2.73	121.72	118.60
6	C	1327	MTE	C2-N1-C10	2.71	120.61	114.54
8	C	1	HPA	C2-N1-C6	2.60	120.23	115.88
5	B	606	FAD	C5X-C9A-N10	2.51	119.53	117.72
5	B	606	FAD	C4X-C4-N3	-2.50	120.01	123.43
5	K	606	FAD	C5'-C4'-C3'	-2.44	107.49	112.20
6	C	1327	MTE	O3P-P-O4'	-2.43	100.27	106.73
5	K	606	FAD	C4X-C4-N3	-2.35	120.22	123.43
6	L	1327	MTE	N3-C2-N1	-2.29	121.82	125.42
5	K	606	FAD	C10-C4X-N5	-2.25	119.70	121.26
6	C	1327	MTE	C10-N8-C7	-2.21	119.34	123.67
6	L	1327	MTE	O3P-P-O2P	2.19	116.01	107.64
5	B	606	FAD	C10-C4X-N5	-2.17	119.76	121.26
5	K	606	FAD	C1'-C2'-C3'	-2.12	103.86	109.79
5	K	606	FAD	C4-C4X-C10	-2.08	118.58	119.95
5	K	606	FAD	O3'-C3'-C2'	-2.04	103.88	108.81
6	C	1327	MTE	C9-C4-N3	-2.02	118.27	124.01

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1327	MTE	C4'-O4'-P-O3P
6	L	1327	MTE	C4'-O4'-P-O3P
6	C	1327	MTE	C3'-C4'-O4'-P
6	L	1327	MTE	C3'-C4'-O4'-P
6	L	1327	MTE	C4'-O4'-P-O2P
5	B	606	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

4 monomers are involved in 6 short contacts:

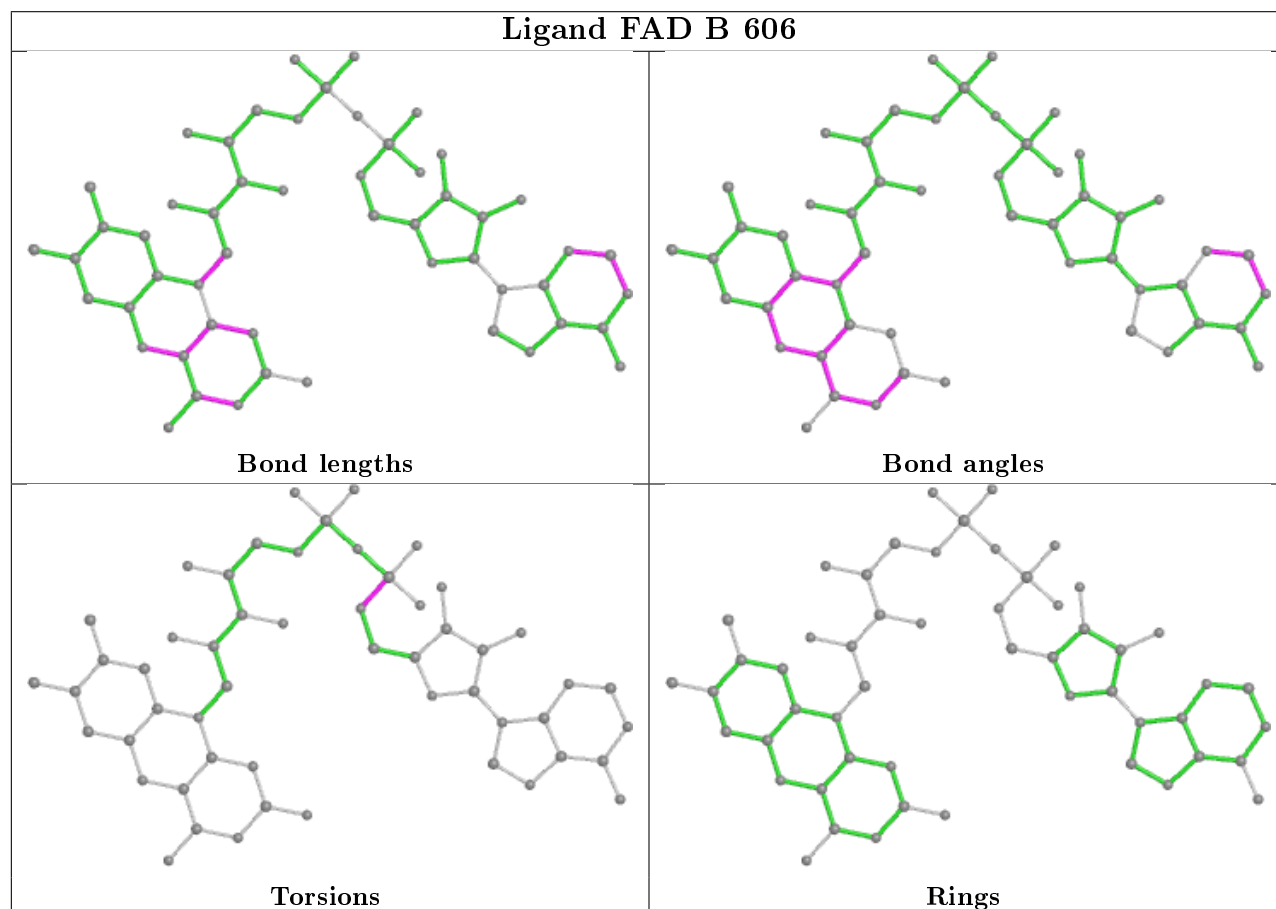
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1328	MOS	1	0
8	C	1	HPA	1	0
5	K	606	FAD	3	0

Continued on next page...

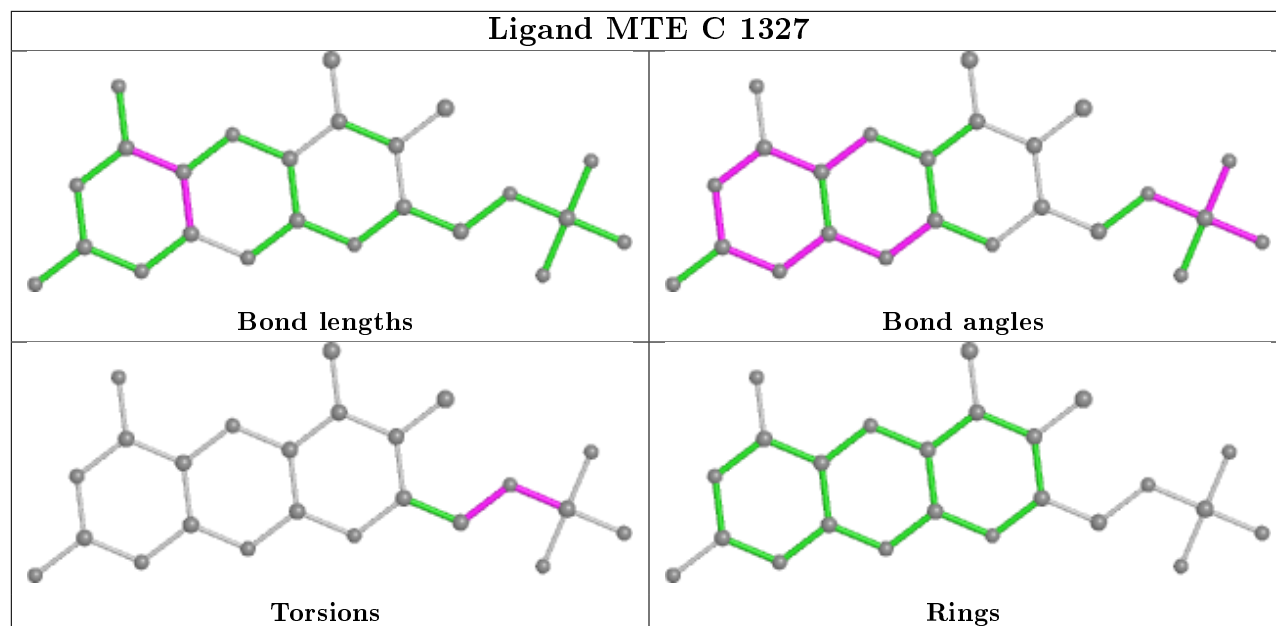
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1328	MOS	2	0

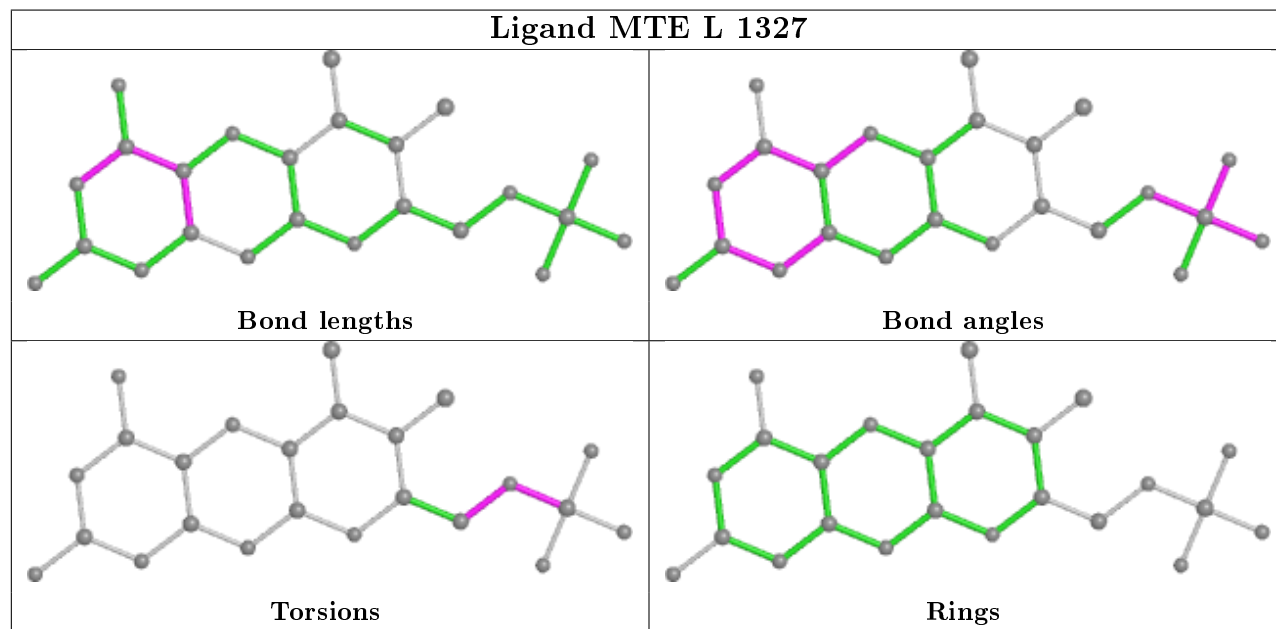
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

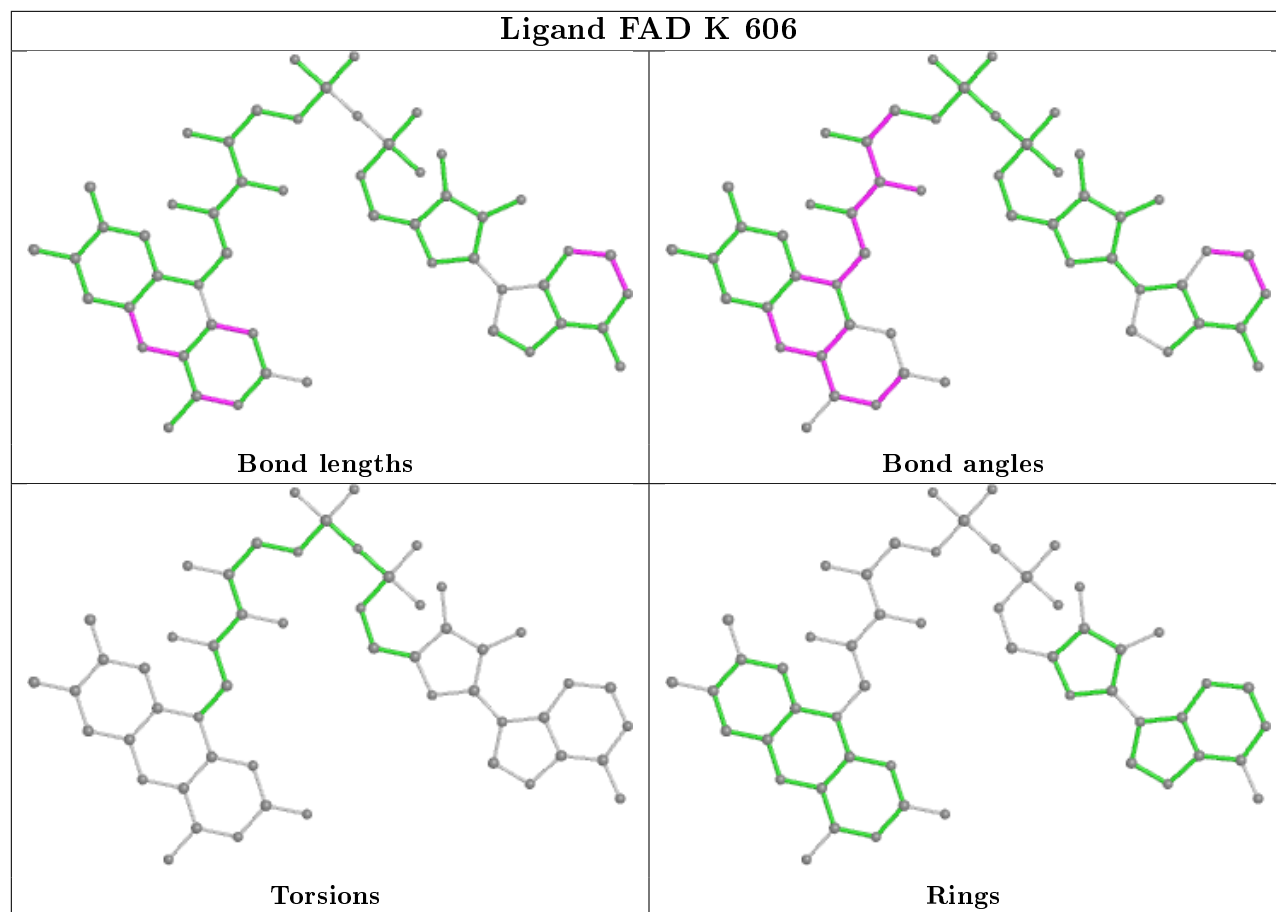


Ligand MTE C 1327



Ligand MTE L 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%)	0.32	12 (7%) 15 11	8, 19, 36, 45	0
1	J	164/164 (100%)	0.39	14 (8%) 10 8	11, 21, 41, 52	0
2	B	305/305 (100%)	0.55	25 (8%) 11 9	16, 27, 41, 45	0
2	K	305/305 (100%)	0.61	30 (9%) 7 5	19, 32, 44, 50	0
3	C	756/756 (100%)	0.01	21 (2%) 53 47	10, 18, 30, 38	0
3	L	745/756 (98%)	0.09	29 (3%) 39 33	10, 20, 33, 56	0
All	All	2439/2450 (99%)	0.22	131 (5%) 25 20	8, 21, 39, 56	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	2	THR	8.4
3	L	1290	THR	8.0
1	A	63	ASP	7.4
3	L	1288	ASN	7.3
1	J	61	LEU	7.2
2	K	528	GLY	6.5
2	K	336	TRP	6.2
2	B	336	TRP	5.9
1	J	58	TYR	5.6
1	A	2	THR	5.5
2	K	272	ASN	5.5
1	J	63	ASP	5.2
1	J	60	ARG	5.2
1	A	61	LEU	5.0
1	J	62	GLN	4.9
2	B	528	GLY	4.9
3	C	1143	GLU	4.8
2	B	424	ALA	4.6
2	K	429	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	272	ASN	4.5
3	L	1287	ASN	4.5
2	B	271	LYS	4.4
2	B	499	ASP	4.2
2	K	499	ASP	4.2
3	L	1143	GLU	4.1
2	K	445	GLY	4.0
3	L	1110	ASP	4.0
1	A	58	TYR	3.9
1	J	165	LYS	3.9
2	K	335	ARG	3.9
1	A	97	ARG	3.9
2	K	295	GLU	3.9
3	C	683	HIS	3.7
3	L	720	LYS	3.5
2	B	338	ALA	3.5
3	C	1286	THR	3.4
3	L	1289	ASN	3.4
2	K	254	GLU	3.3
1	A	60	ARG	3.3
1	J	97	ARG	3.3
3	C	1247	CYS	3.3
2	K	492	GLU	3.3
2	K	477	PHE	3.2
3	L	985	ASP	3.2
2	K	425	SER	3.2
3	L	683	HIS	3.1
2	K	498	PRO	3.1
2	K	424	ALA	3.1
3	C	1137	ASN	3.1
2	K	378	GLY	3.1
3	L	1246	ASP	3.1
1	J	59	ASP	3.0
3	L	1144	THR	3.0
3	C	1245	ARG	3.0
3	L	618	LYS	3.0
3	C	1290	THR	3.0
2	K	525	LYS	3.0
3	C	720	LYS	2.9
2	B	335	ARG	2.9
2	K	251	GLN	2.9
1	A	141	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	638	ASP	2.8
3	C	571	ASP	2.8
2	K	471	GLN	2.8
1	A	133	GLU	2.8
1	A	64	LYS	2.8
3	L	1245	ARG	2.8
3	C	718	ASP	2.7
3	L	950	GLY	2.7
1	J	137	GLU	2.6
2	K	500	ALA	2.6
2	K	271	LYS	2.6
2	B	414	GLU	2.6
2	B	509	ARG	2.6
3	L	1286	THR	2.6
3	C	705	ASN	2.6
2	B	444	PRO	2.5
3	C	1246	ASP	2.5
2	K	387	HIS	2.5
2	B	468	LYS	2.5
2	K	395	LYS	2.5
3	L	658	ASP	2.5
3	L	721	LYS	2.5
2	B	254	GLU	2.5
3	L	575	ARG	2.5
2	K	444	PRO	2.5
3	C	657	LYS	2.4
2	K	506	GLU	2.4
3	C	973	LYS	2.4
3	L	969	ASP	2.4
3	C	658	ASP	2.4
3	C	721	LYS	2.4
3	L	958	ARG	2.3
2	B	387	HIS	2.3
3	L	1250	LYS	2.3
2	K	338	ALA	2.3
2	B	292	HIS	2.3
2	B	286	GLU	2.3
2	B	378	GLY	2.3
2	K	291	GLU	2.3
2	K	468	LYS	2.2
3	L	852	LYS	2.2
2	B	412	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	960	GLU	2.2
2	B	318	LYS	2.2
1	A	140	GLU	2.2
2	K	294	PRO	2.2
2	B	388	THR	2.2
3	C	645	GLU	2.2
1	A	62	GLN	2.2
2	B	440	VAL	2.2
2	B	506	GLU	2.1
1	J	64	LYS	2.1
3	L	1247	CYS	2.1
2	K	273	GLN	2.1
3	C	1216	GLU	2.1
2	B	425	SER	2.1
1	A	165	LYS	2.1
3	L	718	ASP	2.1
3	C	575	ARG	2.1
2	B	295	GLU	2.1
3	L	571	ASP	2.1
2	K	472	LYS	2.1
3	L	973	LYS	2.0
3	C	983	GLU	2.0
3	L	983	GLU	2.0
2	B	241	THR	2.0
1	J	140	GLU	2.0
1	J	141	ASP	2.0
3	C	853	THR	2.0
1	J	133	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

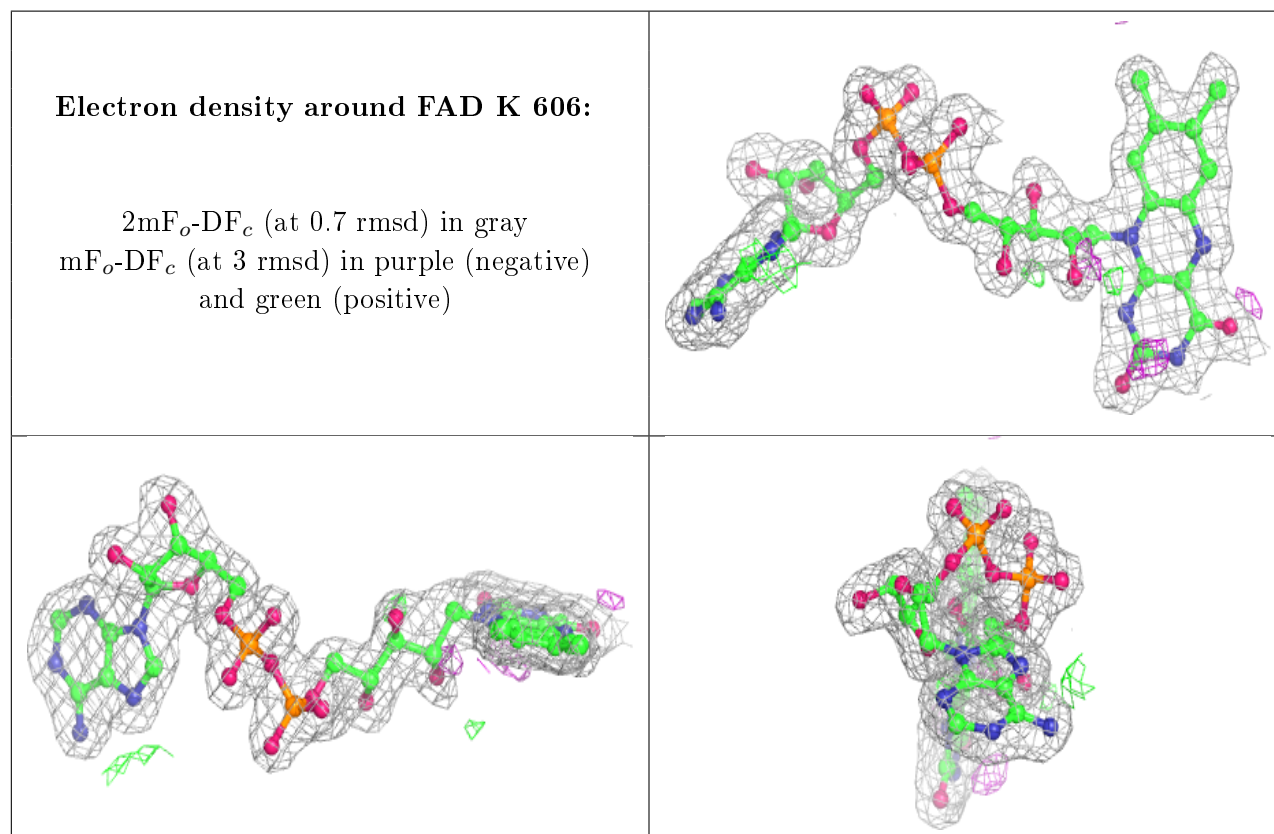
6.4 Ligands [i](#)

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

median, 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.

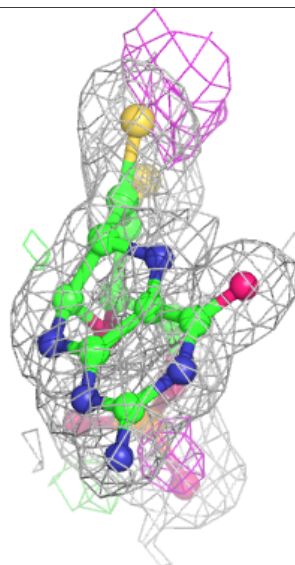
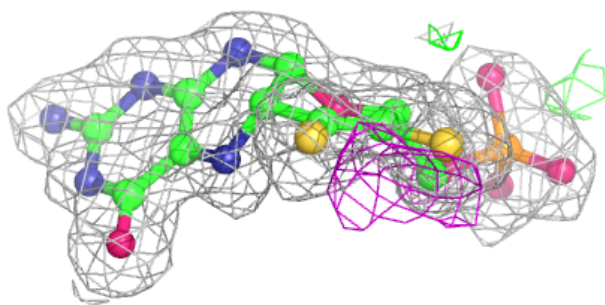
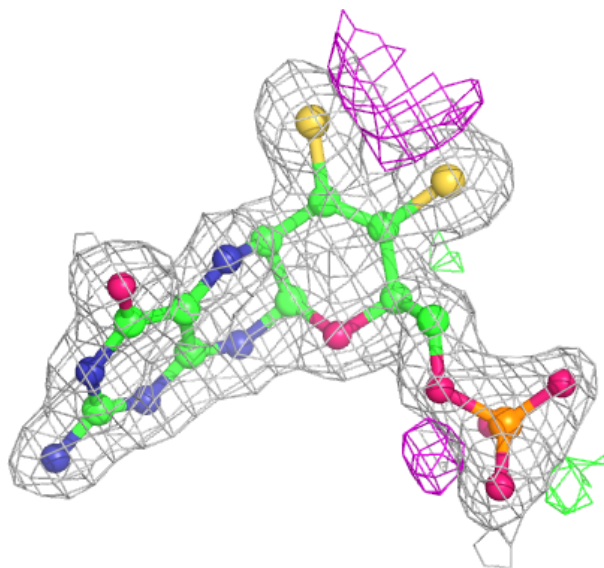
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	HPA	C	1	10/10	0.75	0.19	25,27,29,29	0
8	HPA	L	1	10/10	0.81	0.15	25,26,28,29	0
5	FAD	K	606	53/53	0.96	0.09	17,24,27,29	0
6	MTE	C	1327	24/24	0.97	0.08	11,14,25,28	0
5	FAD	B	606	53/53	0.97	0.09	15,18,24,27	0
6	MTE	L	1327	24/24	0.98	0.07	12,16,26,29	0
4	FES	J	601	4/4	0.99	0.07	11,11,12,13	0
7	MOS	L	1328	4/4	0.99	0.09	23,26,27,35	0
7	MOS	C	1328	4/4	0.99	0.10	22,26,27,35	0
4	FES	A	601	4/4	1.00	0.09	10,10,11,11	0
4	FES	J	602	4/4	1.00	0.06	13,13,14,14	0
4	FES	A	602	4/4	1.00	0.06	11,12,12,13	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.



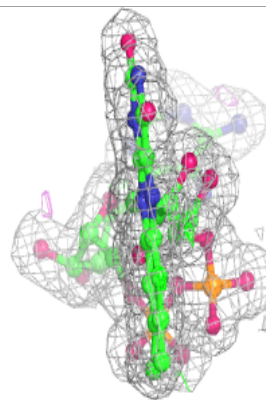
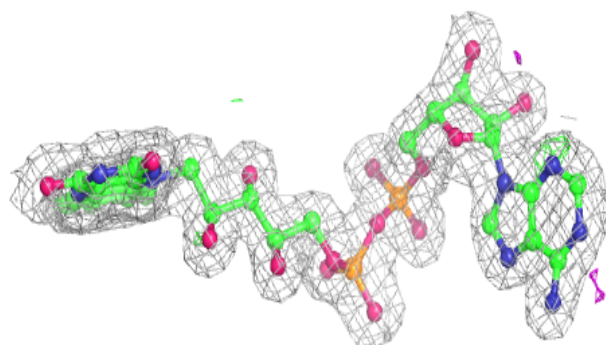
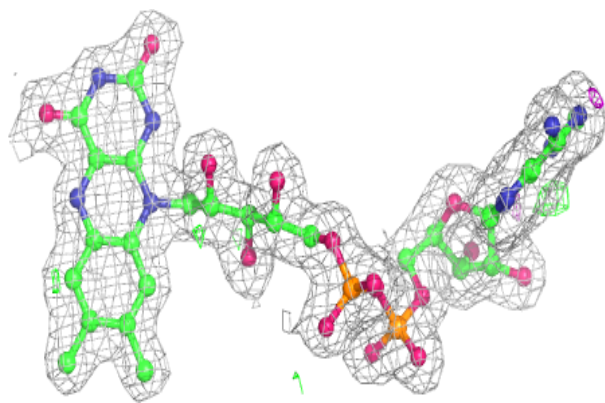
Electron density around MTE C 1327:

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



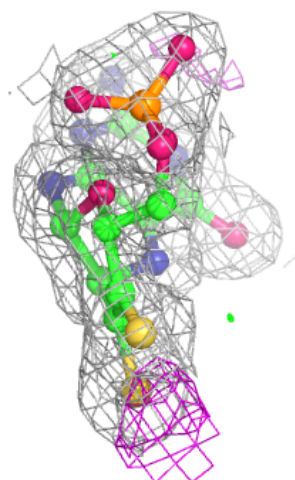
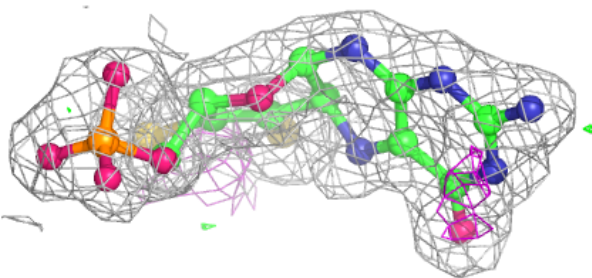
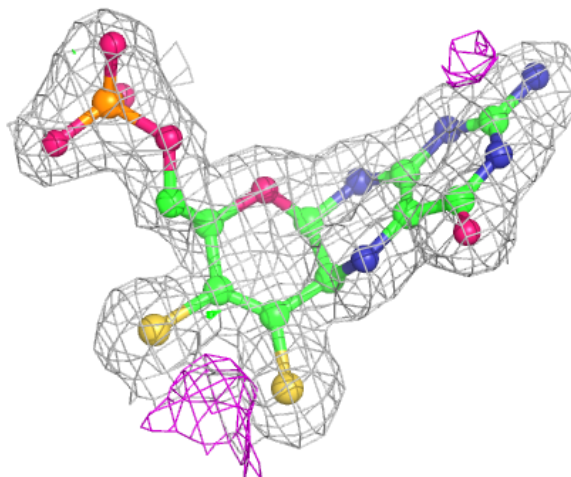
Electron density around FAD B 606:

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



Electron density around MTE 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.