Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:37 PM EDT

PDB ID	:	3SR6 / pdb_00003sr6
Title	:	Crystal Structure of Reduced Bovine Xanthine Oxidase in Complex with Arsenite
Authors	:	Cao, H.; Hille, R.
Deposited on	:	2011-07-07
Resolution	:	2.10 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:

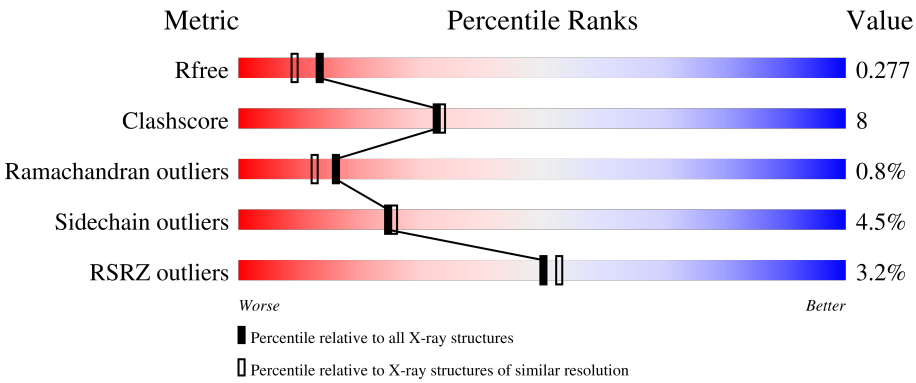
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	5% 79% 20% •
1	J	164	5% 83% 15% •
2	B	305	6% 84% 12% •
2	K	305	5% 84% 13% •
3	C	745	2% 81% 17% •

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Mol	Chain	Length	Quality of chain
3	L	745	2% 79% 19%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19834 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

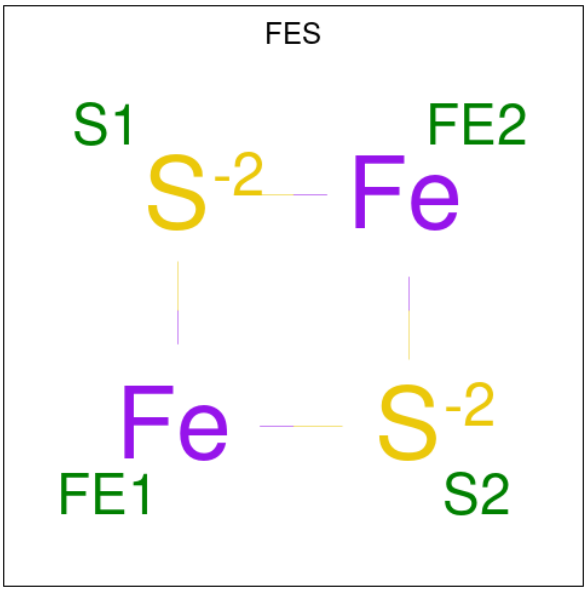
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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

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

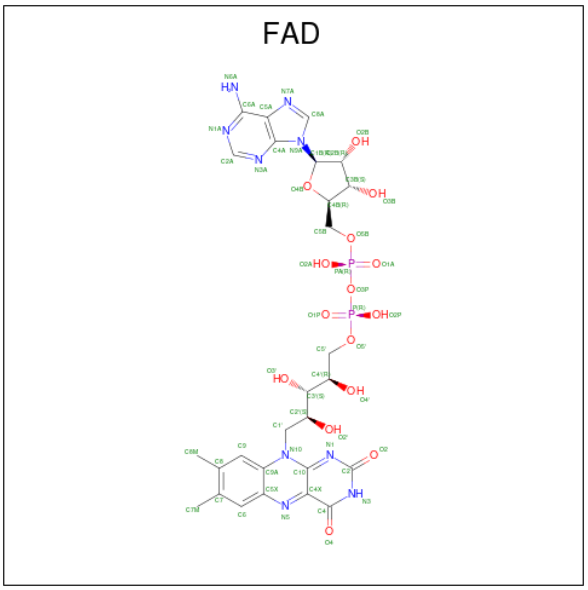
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	745	5761	3643	992	1093	33	0	0	0
3	L	745	5761	3643	992	1093	33	0	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



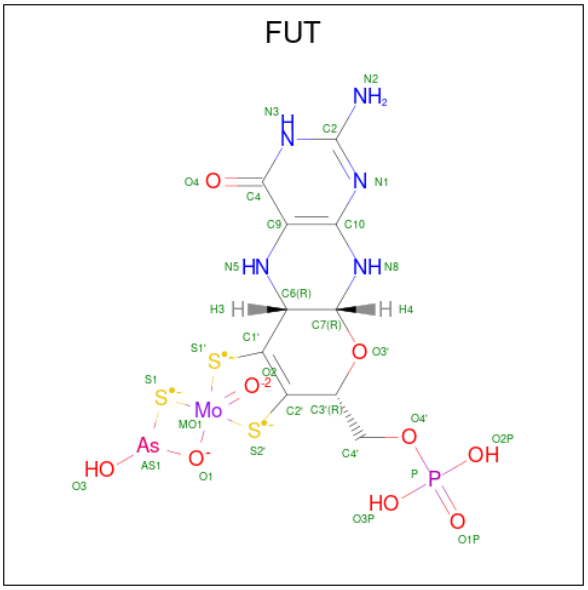
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	A	1	4	2	2	0	0
			Total	Fe	S		
4	J	1	4	2	2	0	0
			Total	Fe	S		
4	J	1	4	2	2	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 Mo-oxo-thioxo-arsenite-molybdopterin (CCD ID: FUT) (formula: $C_{10}H_{13}AsMoN_5O_9PS_3$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	As	C	Mo	N	O	P	S		
6	C	1	30	1	10	1	5	9	1	3	0	0
			Total	As	C	Mo	N	O	P	S		
6	L	1	30	1	10	1	5	9	1	3	0	0

- Molecule 7 is water.

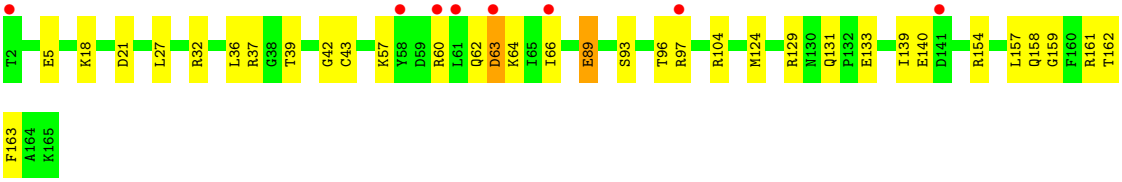
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	63	63	63	0	0
			Total	O		
7	B	88	88	88	0	0
			Total	O		
7	C	299	299	299	0	0
			Total	O		
7	J	51	51	51	0	0
			Total	O		
7	K	82	82	82	0	0
			Total	O		
7	L	259	259	259	0	0

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.

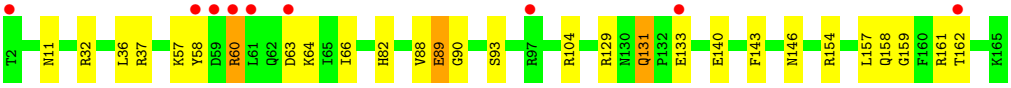
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



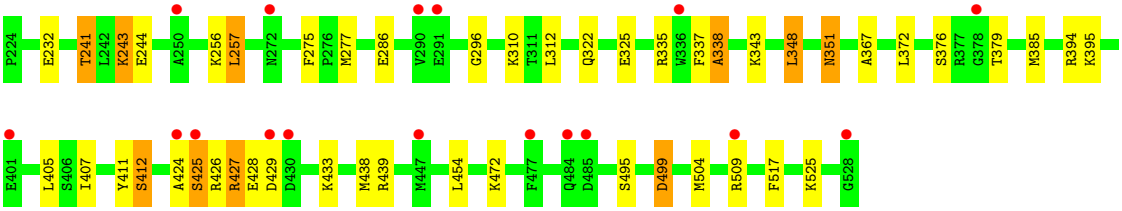
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain J:



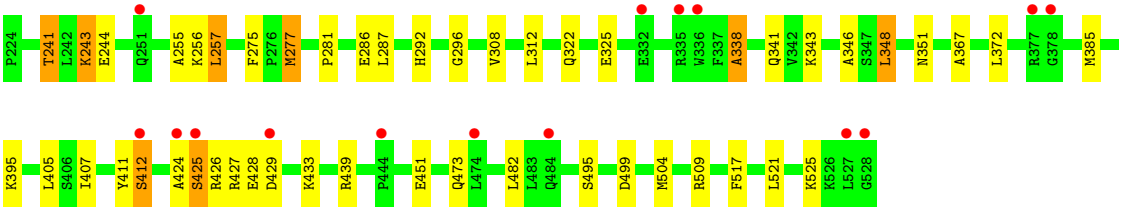
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain B:



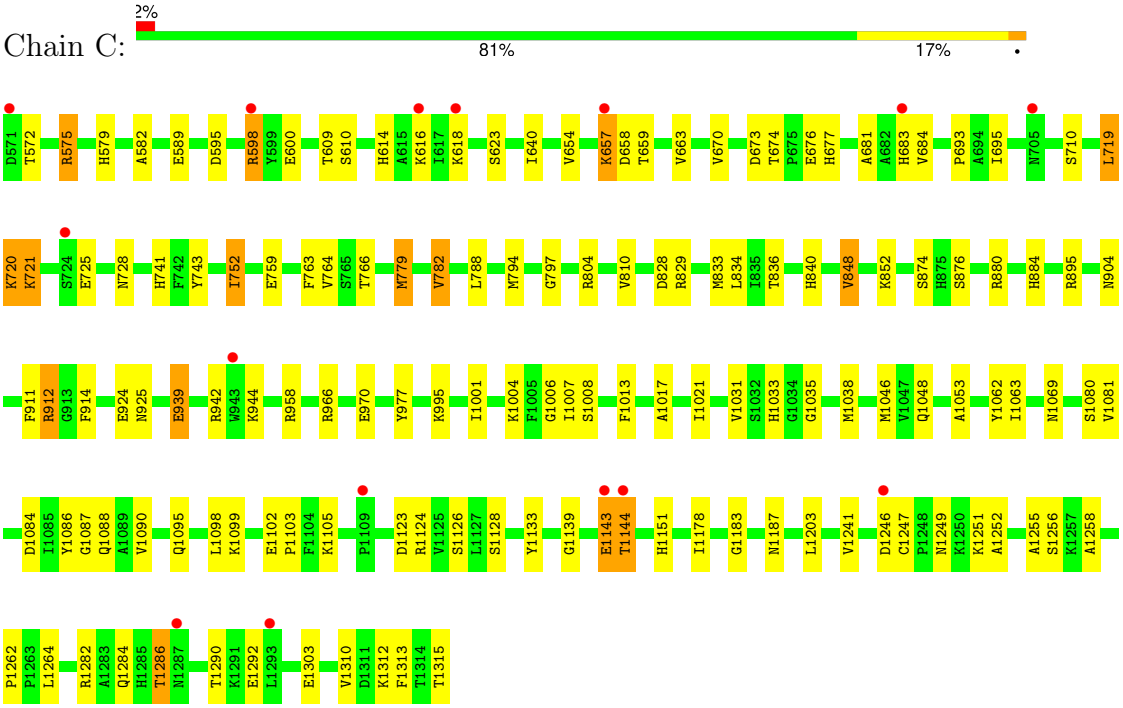
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain K:



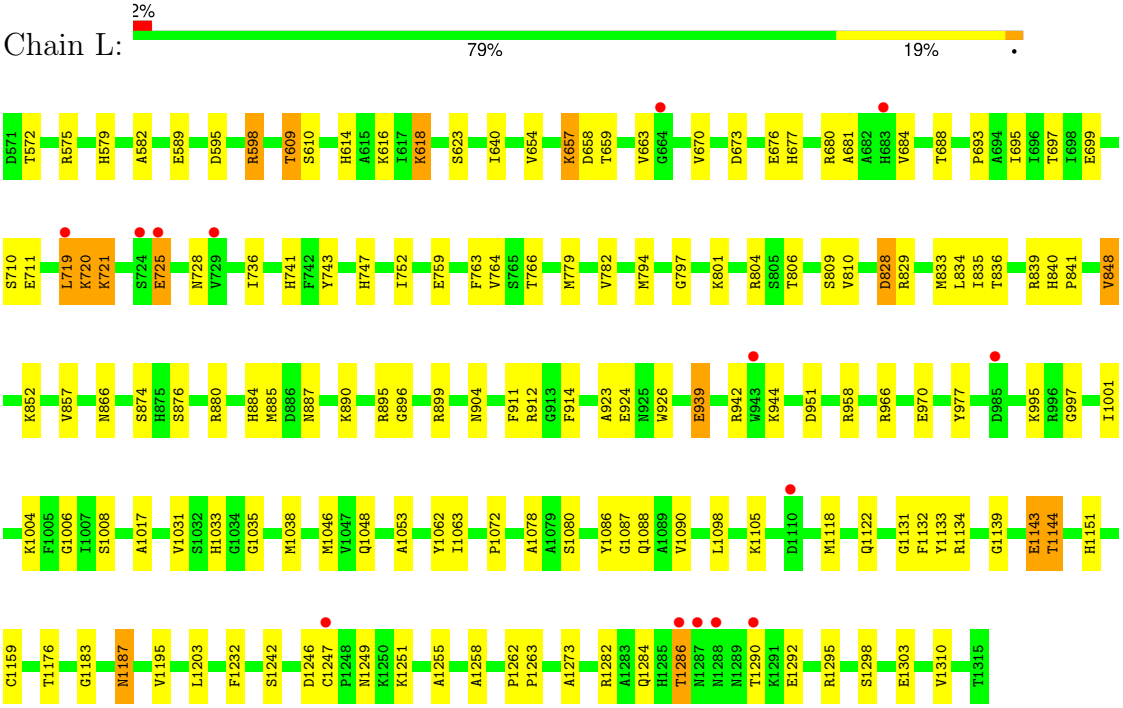
• Molecule 3: Xanthine dehydrogenase/oxidase

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	133.05Å 73.24Å 138.02Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	22.10 – 2.10 22.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (22.10-2.10) 95.8 (22.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.272 0.229 , 0.277	Depositor DCC
R_{free} test set	7451 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19834	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: FAD, FES, FUT

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	0.85	0/1277	0.97	3/1723 (0.2%)
1	J	0.82	1/1277 (0.1%)	1.00	2/1723 (0.1%)
2	B	0.72	0/2438	0.95	2/3290 (0.1%)
2	K	0.74	0/2438	0.93	0/3290
3	C	0.83	0/5888	1.01	13/7974 (0.2%)
3	L	0.85	0/5888	1.01	10/7974 (0.1%)
All	All	0.81	1/19206 (0.0%)	0.99	30/25974 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	88	VAL	CA-CB	5.37	1.61	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	848	VAL	CB-CA-C	-6.73	100.59	110.62
3	C	720	LYS	N-CA-C	-6.18	100.89	110.10
3	L	848	VAL	CB-CA-C	-6.09	101.56	110.81
2	B	337	PHE	N-CA-C	-5.96	102.12	110.35
3	C	1007	ILE	N-CA-C	5.91	116.12	107.37
3	L	1131	GLY	N-CA-C	-5.87	101.92	110.90
3	C	782	VAL	CB-CA-C	5.85	115.06	109.33
3	L	1262	PRO	N-CA-C	5.79	117.76	110.70
3	L	1187	ASN	CA-C-N	5.77	125.24	119.24
3	L	1187	ASN	C-N-CA	5.77	125.24	119.24
3	C	1262	PRO	N-CA-C	5.73	117.69	110.70
1	A	139	ILE	N-CA-C	5.68	115.87	110.42
3	L	835	ILE	N-CA-C	5.57	117.48	111.58
3	L	654	VAL	N-CA-C	-5.50	105.48	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	782	VAL	N-CA-C	-5.42	104.75	109.19
3	L	839	ARG	NE-CZ-NH2	-5.41	114.33	119.20
3	C	575	ARG	CA-C-N	5.34	126.51	119.84
3	C	575	ARG	C-N-CA	5.34	126.51	119.84
1	A	21	ASP	CA-C-N	5.31	125.63	119.47
1	A	21	ASP	C-N-CA	5.31	125.63	119.47
3	C	674	THR	CA-C-N	-5.29	114.22	119.56
3	C	674	THR	C-N-CA	-5.29	114.22	119.56
2	B	335	ARG	N-CA-C	5.26	116.70	110.97
3	C	925	ASN	N-CA-C	5.21	117.38	111.02
3	L	720	LYS	N-CA-C	-5.21	102.33	110.10
3	L	828	ASP	N-CA-C	-5.20	103.67	110.53
3	C	752	ILE	N-CA-C	5.08	113.03	107.60
3	C	654	VAL	N-CA-C	-5.05	105.79	110.53
1	J	131	GLN	CA-C-N	5.01	124.67	119.56
1	J	131	GLN	C-N-CA	5.01	124.67	119.56

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	22	0
1	J	1255	0	1265	19	0
2	B	2389	0	2459	38	0
2	K	2389	0	2459	35	0
3	C	5761	0	5685	102	0
3	L	5761	0	5685	100	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	2	0
5	K	53	0	31	2	0
6	C	30	0	0	2	0
6	L	30	0	0	3	0
7	A	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	88	0	0	6	0
7	C	299	0	0	9	0
7	J	51	0	0	3	0
7	K	82	0	0	3	0
7	L	259	0	0	6	0
All	All	19834	0	18880	298	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 8.

All (298) 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:H	2:K:243:LYS:HD3	1.20	1.04
3:C:1315:THR:CA	7:C:1464:HOH:O	2.06	1.00
3:L:924:GLU:OE1	3:L:942:ARG:NH1	1.95	0.99
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.96	0.98
3:C:1315:THR:C	7:C:1464:HOH:O	2.06	0.98
2:B:243:LYS:H	2:B:243:LYS:HD3	1.26	0.97
2:K:241:THR:HG23	2:K:243:LYS:HG2	1.46	0.95
2:B:241:THR:HG22	2:B:244:GLU:HG3	1.48	0.92
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.52	0.92
2:K:241:THR:CG2	2:K:243:LYS:HG2	2.00	0.90
2:B:241:THR:HG23	2:B:243:LYS:HG2	1.54	0.89
1:J:60:ARG:HA	7:J:293:HOH:O	1.71	0.88
3:C:1046:MET:HE2	3:C:1090:VAL:HG21	1.56	0.88
3:C:640:ILE:HG12	3:C:779:MET:HE1	1.56	0.88
3:L:890:LYS:HD3	7:L:116:HOH:O	1.74	0.88
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.05	0.86
2:K:495:SER:HB2	2:K:509:ARG:HH22	1.40	0.86
2:B:495:SER:HB2	2:B:509:ARG:HH22	1.41	0.86
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.39	0.85
2:B:427:ARG:HD2	7:B:529:HOH:O	1.76	0.83
2:K:241:THR:HG22	2:K:244:GLU:HG3	1.60	0.83
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.78	0.83
1:A:104:ARG:HH11	1:A:162:THR:HG23	1.44	0.82
3:C:695:ILE:H	3:C:904:ASN:HD22	1.26	0.82
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.63	0.81
3:L:572:THR:HA	3:L:575:ARG:HD3	1.63	0.80
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.29	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:243:LYS:HD3	2:K:243:LYS:N	1.98	0.79
3:L:695:ILE:H	3:L:904:ASN:HD22	1.29	0.79
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.65	0.79
2:K:243:LYS:H	2:K:243:LYS:CD	1.91	0.77
3:L:640:ILE:HG12	3:L:779:MET:HE1	1.66	0.77
2:B:243:LYS:HD3	2:B:243:LYS:N	1.99	0.77
3:L:720:LYS:O	3:L:721:LYS:CB	2.33	0.76
1:A:93:SER:HB2	3:C:589:GLU:OE1	1.86	0.76
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.75
3:C:1315:THR:O	7:C:1464:HOH:O	2.04	0.75
3:C:572:THR:HA	3:C:575:ARG:HD3	1.69	0.74
1:J:93:SER:HB2	3:L:589:GLU:OE1	1.86	0.74
3:C:1315:THR:HA	7:C:1464:HOH:O	1.76	0.74
3:L:779:MET:HG2	3:L:810:VAL:HG13	1.70	0.74
3:L:880:ARG:O	3:L:884:HIS:HD2	1.68	0.74
2:B:241:THR:CG2	2:B:244:GLU:HG3	2.18	0.74
3:C:1046:MET:HE2	3:C:1090:VAL:CG2	2.17	0.74
2:B:310:LYS:HE3	7:B:97:HOH:O	1.88	0.73
2:K:495:SER:HB2	2:K:509:ARG:NH2	2.04	0.72
1:J:131:GLN:HE21	1:J:133:GLU:H	1.36	0.72
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.73	0.71
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.73	0.71
3:L:1282:ARG:HA	3:L:1286:THR:HG23	1.71	0.70
3:C:720:LYS:O	3:C:721:LYS:CB	2.38	0.69
2:B:499:ASP:OD1	7:B:550:HOH:O	2.11	0.69
3:L:663:VAL:HG12	3:L:834:LEU:HD11	1.75	0.69
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.06	0.68
3:L:680:ARG:NH2	7:L:1323:HOH:O	2.27	0.67
2:B:322:GLN:O	2:B:412:SER:HB3	1.94	0.67
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	1.77	0.67
1:A:32:ARG:NH1	3:C:676:GLU:OE2	2.21	0.67
2:K:241:THR:HG22	2:K:244:GLU:H	1.60	0.67
2:B:495:SER:HB2	2:B:509:ARG:NH2	2.09	0.67
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.29	0.66
3:C:880:ARG:O	3:C:884:HIS:HD2	1.78	0.66
6:L:1316:FUT:MO1	6:L:1316:FUT:O2	1.66	0.66
2:B:243:LYS:H	2:B:243:LYS:CD	1.96	0.66
3:L:764:VAL:CG2	3:L:766:THR:HG22	2.25	0.65
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.77	0.65
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.12	0.65
2:B:241:THR:HG22	2:B:244:GLU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.32	0.64
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.79	0.64
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.33	0.64
6:C:1316:FUT:O2	6:C:1316:FUT:MO1	1.66	0.64
3:L:1286:THR:HG22	3:L:1310:VAL:O	1.98	0.64
3:L:958:ARG:NH1	7:L:1334:HOH:O	2.19	0.64
2:K:241:THR:CG2	2:K:244:GLU:HG3	2.27	0.64
1:J:159:GLY:O	1:J:162:THR:HG22	1.98	0.63
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.81	0.63
3:L:880:ARG:O	3:L:884:HIS:CD2	2.52	0.63
3:C:663:VAL:HG12	3:C:834:LEU:HD11	1.80	0.62
3:L:840:HIS:HE1	3:L:874:SER:OG	1.81	0.62
1:A:159:GLY:O	1:A:162:THR:HG22	1.99	0.62
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.82	0.62
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.99	0.62
2:K:322:GLN:O	2:K:412:SER:HB3	2.00	0.61
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.15	0.61
3:L:1046:MET:HE2	3:L:1090:VAL:CG2	2.31	0.61
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.36	0.61
2:B:504:MET:HE2	3:C:1303:GLU:HB2	1.82	0.61
1:A:104:ARG:NH1	1:A:162:THR:HG23	2.14	0.60
2:B:424:ALA:O	2:B:425:SER:HB3	2.02	0.60
3:L:610:SER:O	3:L:663:VAL:O	2.20	0.59
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.03	0.59
3:L:951:ASP:HB3	7:L:116:HOH:O	2.03	0.59
3:L:794:MET:HE3	3:L:1038:MET:HB3	1.84	0.59
3:L:609:THR:HG22	7:L:59:HOH:O	2.01	0.58
3:C:720:LYS:O	3:C:721:LYS:HB3	2.03	0.58
2:K:424:ALA:O	2:K:425:SER:HB3	2.04	0.58
3:L:720:LYS:O	3:L:721:LYS:HB3	2.04	0.58
2:B:325:GLU:HB2	2:B:412:SER:OG	2.03	0.58
2:K:325:GLU:HB2	2:K:412:SER:OG	2.03	0.58
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.16	0.58
1:J:82:HIS:HE1	7:J:172:HOH:O	1.87	0.58
3:L:880:ARG:HD2	3:L:914:PHE:HB3	1.86	0.57
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	2.02	0.57
2:K:241:THR:HG23	2:K:243:LYS:CG	2.27	0.57
1:A:104:ARG:HD3	1:A:162:THR:HG21	1.86	0.57
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.87	0.57
3:C:600:GLU:HG2	3:L:598:ARG:O	2.05	0.56
3:C:840:HIS:HE1	3:C:874:SER:OG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.71	0.55
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.42	0.55
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.53	0.55
3:C:640:ILE:HG12	3:C:779:MET:CE	2.34	0.55
3:L:806:THR:HA	3:L:809:SER:HB2	1.88	0.54
3:C:1123:ASP:O	3:L:1134:ARG:NH1	2.40	0.54
1:A:157:LEU:O	1:A:161:ARG:HB2	2.07	0.54
3:C:598:ARG:CD	7:C:1422:HOH:O	2.55	0.54
3:C:610:SER:O	3:C:663:VAL:O	2.26	0.54
3:C:1282:ARG:NH2	3:C:1292:GLU:OE2	2.30	0.54
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.90	0.54
3:L:720:LYS:O	3:L:721:LYS:HB2	2.08	0.54
1:A:57:LYS:HE2	1:A:66:ILE:HD11	1.91	0.53
3:C:794:MET:HE3	3:C:1038:MET:HB3	1.90	0.53
2:K:424:ALA:O	2:K:425:SER:CB	2.56	0.53
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.07	0.53
2:K:338:ALA:N	7:K:214:HOH:O	2.43	0.52
2:B:394:ARG:HD2	7:B:530:HOH:O	2.09	0.52
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.91	0.52
1:A:154:ARG:NH1	1:A:158:GLN:OE1	2.43	0.52
1:J:37:ARG:HD3	3:L:595:ASP:O	2.10	0.51
3:L:887:ASN:ND2	3:L:924:GLU:OE2	2.43	0.51
3:C:759:GLU:OE2	3:L:1062:TYR:OH	2.25	0.51
3:C:1264:LEU:HD23	3:C:1264:LEU:C	2.35	0.51
2:K:257:LEU:O	5:K:606:FAD:H2B	2.10	0.51
3:L:711:GLU:HA	3:L:899:ARG:HD2	1.93	0.51
3:C:598:ARG:HD2	7:C:1422:HOH:O	2.09	0.51
2:B:257:LEU:O	5:B:606:FAD:H2B	2.11	0.51
7:B:544:HOH:O	3:C:683:HIS:HB2	2.10	0.51
2:B:241:THR:HG23	2:B:243:LYS:CG	2.34	0.50
3:C:1062:TYR:OH	3:L:759:GLU:OE2	2.25	0.50
3:C:1046:MET:HE3	3:C:1046:MET:HA	1.94	0.50
3:C:1128:SER:HB2	3:L:1072:PRO:HG3	1.93	0.50
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.94	0.50
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.41	0.49
2:B:424:ALA:O	2:B:425:SER:CB	2.60	0.49
3:L:1046:MET:HE3	3:L:1046:MET:HA	1.93	0.49
3:C:695:ILE:H	3:C:904:ASN:ND2	2.04	0.49
2:K:241:THR:HG21	2:K:243:LYS:HG2	1.90	0.49
3:L:579:HIS:HB3	3:L:582:ALA:HB2	1.94	0.49
3:L:840:HIS:CE1	3:L:874:SER:OG	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:741:HIS:HA	3:C:911:PHE:CE1	2.46	0.49
3:C:598:ARG:NE	7:C:1422:HOH:O	2.45	0.49
3:C:876:SER:HB3	3:C:914:PHE:HE2	1.77	0.49
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.94	0.48
2:B:296:GLY:HA2	2:B:411:TYR:CD1	2.47	0.48
3:C:728:ASN:HD21	3:C:852:LYS:HD3	1.77	0.48
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.62	0.48
3:C:880:ARG:HD2	3:C:914:PHE:HB3	1.95	0.48
3:L:1078:ALA:HB1	6:L:1316:FUT:O1	2.13	0.48
2:K:292:HIS:HE1	7:K:544:HOH:O	1.96	0.48
3:C:1178:ILE:HD12	3:C:1241:VAL:HG22	1.94	0.48
3:L:736:ILE:HG13	3:L:1298:SER:HB3	1.96	0.48
1:A:27:LEU:CD1	1:A:39:THR:HG22	2.43	0.48
3:L:1017:ALA:HB1	3:L:1086:TYR:CD2	2.49	0.48
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.60	0.48
3:L:1195:VAL:HA	3:L:1263:PRO:HG2	1.96	0.48
2:B:232:GLU:OE1	3:C:677:HIS:HE1	1.96	0.48
3:L:885:MET:SD	3:L:896:GLY:HA3	2.54	0.48
2:B:241:THR:HG21	2:B:243:LYS:HG2	1.91	0.47
2:K:372:LEU:HD11	2:K:385:MET:HE2	1.96	0.47
3:L:1031:VAL:HB	3:L:1063:ILE:HG12	1.96	0.47
3:L:728:ASN:HD21	3:L:852:LYS:HD3	1.79	0.47
3:L:1159:CYS:O	3:L:1176:THR:HA	2.15	0.47
3:C:958:ARG:HG2	3:C:958:ARG:HH11	1.80	0.47
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.50	0.47
2:K:296:GLY:HA2	2:K:411:TYR:CD1	2.49	0.47
3:L:1290:THR:C	3:L:1292:GLU:H	2.23	0.47
3:C:880:ARG:O	3:C:884:HIS:CD2	2.63	0.47
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.50	0.47
3:L:719:LEU:HD13	3:L:895:ARG:HB2	1.96	0.47
3:L:1053:ALA:O	3:L:1098:LEU:HD11	2.15	0.47
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.31	0.47
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.95	0.47
2:B:286:GLU:HB3	2:B:405:LEU:HD11	1.96	0.47
3:C:752:ILE:CD1	3:C:763:PHE:CE1	2.94	0.46
3:L:958:ARG:HG2	3:L:958:ARG:HH11	1.80	0.46
3:L:1143:GLU:O	3:L:1144:THR:HG23	2.15	0.46
3:C:614:HIS:HD2	3:C:693:PRO:O	1.98	0.46
3:L:876:SER:HB3	3:L:914:PHE:HE2	1.80	0.46
3:C:616:LYS:HD2	3:C:658:ASP:O	2.16	0.46
3:L:997:GLY:HA3	3:L:1273:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.80	0.46
2:B:509:ARG:HG2	7:B:108:HOH:O	2.16	0.46
3:L:1295:ARG:HA	7:L:264:HOH:O	2.14	0.46
1:A:32:ARG:NH2	7:A:932:HOH:O	2.48	0.46
2:B:372:LEU:HD11	2:B:385:MET:HE2	1.96	0.46
3:L:829:ARG:O	3:L:833:MET:HG3	2.16	0.46
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.23	0.46
3:L:1080:SER:HB3	3:L:1258:ALA:HB1	1.97	0.45
3:C:911:PHE:O	3:C:912:ARG:C	2.58	0.45
3:C:719:LEU:CD1	3:C:895:ARG:HB2	2.46	0.45
3:C:1126:SER:HB2	3:L:1132:PHE:CD1	2.51	0.45
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.31	0.45
2:B:472:LYS:HE2	2:B:472:LYS:HB3	1.72	0.45
3:L:614:HIS:HD2	3:L:693:PRO:O	1.99	0.45
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.81	0.45
1:A:62:GLN:O	1:A:63:ASP:CB	2.64	0.45
1:J:154:ARG:NH1	1:J:158:GLN:OE1	2.50	0.45
1:A:62:GLN:O	1:A:63:ASP:HB3	2.17	0.45
3:C:1315:THR:HB	7:C:1464:HOH:O	2.16	0.45
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.17	0.45
2:K:348:LEU:HD13	2:K:407:ILE:HD13	1.98	0.45
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.35	0.45
1:A:42:GLY:O	3:C:829:ARG:HD2	2.17	0.44
2:B:351:ASN:HD22	2:B:351:ASN:C	2.25	0.44
1:J:157:LEU:O	1:J:161:ARG:HB2	2.16	0.44
2:K:255:ALA:HB2	2:K:277:MET:HG2	1.99	0.44
2:K:256:LYS:HG3	2:K:275:PHE:CG	2.51	0.44
3:C:829:ARG:CG	3:C:833:MET:HE3	2.48	0.44
2:K:451:GLU:HG2	7:K:153:HOH:O	2.18	0.44
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.98	0.44
3:C:1013:PHE:CD1	3:C:1013:PHE:C	2.96	0.44
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.42	0.44
2:B:438:MET:HG2	2:B:454:LEU:HD22	2.00	0.44
1:J:104:ARG:HD3	1:J:162:THR:CG2	2.48	0.44
1:J:146:ASN:ND2	2:K:341:GLN:HE22	2.15	0.44
3:C:1151:HIS:CD2	3:C:1251:LYS:HB3	2.53	0.44
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.66	0.44
3:C:1252:ALA:HB3	3:C:1256:SER:O	2.18	0.44
3:L:618:LYS:NZ	3:L:688:THR:HG21	2.33	0.44
3:C:720:LYS:O	3:C:721:LYS:HB2	2.16	0.43
3:L:670:VAL:HG11	3:L:681:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1118:MET:O	3:L:1122:GLN:HG3	2.17	0.43
3:C:579:HIS:HB3	3:C:582:ALA:HB2	1.99	0.43
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.53	0.43
3:C:719:LEU:HD13	3:C:895:ARG:HB2	1.99	0.43
3:C:840:HIS:CE1	3:C:874:SER:OG	2.70	0.43
3:C:1031:VAL:HB	3:C:1063:ILE:HG12	2.00	0.43
3:C:1282:ARG:HG2	3:C:1286:THR:HG21	2.01	0.43
2:K:308:VAL:HG21	2:K:348:LEU:HG	2.01	0.43
2:K:367:ALA:O	2:K:439:ARG:NH1	2.46	0.43
3:L:779:MET:SD	3:L:779:MET:C	3.02	0.43
3:C:1081:VAL:O	3:C:1084:ASP:HB2	2.19	0.43
3:L:779:MET:HB2	3:L:779:MET:HE2	1.72	0.43
1:A:124:MET:HE2	1:A:163:PHE:CD1	2.54	0.42
3:L:697:THR:HB	3:L:699:GLU:OE1	2.19	0.42
3:L:657:LYS:HB3	3:L:657:LYS:HE3	1.69	0.42
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	2.01	0.42
3:C:1143:GLU:O	3:C:1144:THR:HG23	2.19	0.42
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.19	0.42
3:C:1312:LYS:HD3	7:C:415:HOH:O	2.18	0.42
3:C:1080:SER:HB3	3:C:1258:ALA:HB1	2.00	0.42
1:J:58:TYR:HE2	7:J:293:HOH:O	2.02	0.42
2:K:517:PHE:CZ	2:K:521:LEU:HD11	2.55	0.42
6:L:1316:FUT:O2	6:L:1316:FUT:S1	2.78	0.42
2:B:338:ALA:HB2	5:B:606:FAD:C6	2.50	0.42
2:B:517:PHE:CG	3:C:1313:PHE:CZ	3.08	0.42
3:L:804:ARG:HG3	3:L:836:THR:O	2.19	0.42
3:C:1053:ALA:O	3:C:1098:LEU:HD11	2.19	0.41
2:K:256:LYS:HG3	2:K:275:PHE:CD2	2.55	0.41
2:K:281:PRO:HB2	2:K:287:LEU:HD12	2.01	0.41
3:C:1290:THR:C	3:C:1292:GLU:H	2.28	0.41
3:C:804:ARG:HG3	3:C:836:THR:O	2.21	0.41
2:K:504:MET:HG2	3:L:1303:GLU:CD	2.45	0.41
1:A:96:THR:O	1:A:97:ARG:HG3	2.21	0.41
2:B:351:ASN:C	2:B:351:ASN:ND2	2.79	0.41
2:K:473:GLN:HE21	2:K:482:LEU:HD12	1.85	0.41
1:A:5:GLU:HG2	1:A:18:LYS:HG2	2.02	0.41
3:C:1102:GLU:N	3:C:1103:PRO:CD	2.84	0.41
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.21	0.41
2:B:376:SER:OG	2:B:379:THR:OG1	2.30	0.41
2:K:286:GLU:HB3	2:K:405:LEU:HD11	2.03	0.41
3:L:841:PRO:HD2	3:L:866:ASN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:958:ARG:HH11	3:L:958:ARG:CG	2.34	0.41
3:C:657:LYS:HB3	3:C:657:LYS:HE3	1.72	0.41
3:C:914:PHE:CD1	6:C:1316:FUT:AS1	3.34	0.41
3:C:1124:ARG:HB3	3:L:1134:ARG:HG3	2.02	0.41
1:J:11:ASN:OD1	1:J:90:GLY:HA3	2.20	0.41
3:L:1046:MET:CE	3:L:1087:GLY:HA2	2.38	0.41
2:B:367:ALA:O	2:B:439:ARG:NH1	2.50	0.41
3:L:719:LEU:CD1	3:L:895:ARG:HB2	2.51	0.41
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.68	0.41
3:C:752:ILE:HD11	3:C:763:PHE:CE1	2.54	0.40
1:A:37:ARG:HD3	3:C:595:ASP:O	2.21	0.40
1:A:104:ARG:HD3	1:A:162:THR:CG2	2.51	0.40
2:B:256:LYS:HG3	2:B:275:PHE:CD2	2.56	0.40
3:L:1046:MET:CE	3:L:1090:VAL:HB	2.51	0.40
3:L:1151:HIS:CD2	3:L:1251:LYS:HB3	2.56	0.40
3:L:1286:THR:CG2	3:L:1310:VAL:HB	2.51	0.40
3:C:939:GLU:CD	3:C:939:GLU:H	2.29	0.40
3:L:741:HIS:HA	3:L:911:PHE:CE1	2.57	0.40
3:L:747:HIS:CE1	3:L:801:LYS:HG2	2.56	0.40
3:L:966:ARG:O	3:L:970:GLU:HB2	2.20	0.40
3:C:876:SER:HB3	3:C:914:PHE:CE2	2.55	0.40
3:L:725:GLU:HG2	3:L:857:VAL:HG11	2.03	0.40
3:C:966:ARG:O	3:C:970:GLU:HB2	2.22	0.40
3:L:616:LYS:HD2	3:L:658:ASP:O	2.21	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%)	154 (95%)	6 (4%)	2 (1%)	10 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	10	7
2	B	303/305 (99%)	291 (96%)	10 (3%)	2 (1%)	18	15
2	K	303/305 (99%)	290 (96%)	11 (4%)	2 (1%)	18	15
3	C	743/745 (100%)	717 (96%)	20 (3%)	6 (1%)	16	12
3	L	743/745 (100%)	724 (97%)	13 (2%)	6 (1%)	16	12
All	All	2416/2428 (100%)	2329 (96%)	67 (3%)	20 (1%)	16	12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	338	ALA
2	B	425	SER
3	C	721	LYS
2	K	338	ALA
2	K	425	SER
3	L	721	LYS
1	A	64	LYS
3	C	912	ARG
3	C	1008	SER
3	L	1008	SER
1	A	63	ASP
3	C	797	GLY
3	C	1144	THR
1	J	64	LYS
3	L	797	GLY
3	L	912	ARG
3	L	1144	THR
3	C	1139	GLY
1	J	63	ASP
3	L	1139	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%)	133 (97%)	4 (3%)	37	42
1	J	137/137 (100%)	133 (97%)	4 (3%)	37	42
2	B	261/261 (100%)	244 (94%)	17 (6%)	15	13
2	K	261/261 (100%)	244 (94%)	17 (6%)	15	13
3	C	624/624 (100%)	599 (96%)	25 (4%)	28	29
3	L	624/624 (100%)	600 (96%)	24 (4%)	29	32
All	All	2044/2044 (100%)	1953 (96%)	91 (4%)	24	25

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	89	GLU
1	A	129	ARG
1	A	140	GLU
2	B	241	THR
2	B	243	LYS
2	B	257	LEU
2	B	277	MET
2	B	312	LEU
2	B	343	LYS
2	B	348	LEU
2	B	351	ASN
2	B	395	LYS
2	B	412	SER
2	B	426	ARG
2	B	427	ARG
2	B	428	GLU
2	B	429	ASP
2	B	433	LYS
2	B	499	ASP
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	618	LYS
3	C	623	SER
3	C	657	LYS
3	C	659	THR
3	C	684	VAL
3	C	710	SER
3	C	719	LEU

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Mol	Chain	Res	Type
3	C	725	GLU
3	C	743	TYR
3	C	779	MET
3	C	782	VAL
3	C	828	ASP
3	C	848	VAL
3	C	939	GLU
3	C	944	LYS
3	C	1001	ILE
3	C	1004	LYS
3	C	1021	ILE
3	C	1105	LYS
3	C	1143	GLU
3	C	1203	LEU
3	C	1246	ASP
3	C	1286	THR
1	J	60	ARG
1	J	89	GLU
1	J	129	ARG
1	J	140	GLU
2	K	241	THR
2	K	243	LYS
2	K	257	LEU
2	K	277	MET
2	K	312	LEU
2	K	343	LYS
2	K	348	LEU
2	K	351	ASN
2	K	395	LYS
2	K	412	SER
2	K	426	ARG
2	K	427	ARG
2	K	428	GLU
2	K	429	ASP
2	K	433	LYS
2	K	499	ASP
2	K	525	LYS
3	L	598	ARG
3	L	609	THR
3	L	618	LYS
3	L	623	SER
3	L	657	LYS

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Mol	Chain	Res	Type
3	L	659	THR
3	L	684	VAL
3	L	710	SER
3	L	719	LEU
3	L	725	GLU
3	L	743	TYR
3	L	782	VAL
3	L	828	ASP
3	L	848	VAL
3	L	939	GLU
3	L	944	LYS
3	L	1001	ILE
3	L	1004	LYS
3	L	1105	LYS
3	L	1143	GLU
3	L	1203	LEU
3	L	1242	SER
3	L	1246	ASP
3	L	1286	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	112	GLN
1	A	131	GLN
1	A	144	GLN
1	A	146	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	728	ASN
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS

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Mol	Chain	Res	Type
3	C	1048	GLN
3	C	1212	HIS
3	C	1284	GLN
1	J	62	GLN
1	J	82	HIS
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	261	ASN
2	K	273	GLN
2	K	292	HIS
2	K	333	GLN
2	K	351	ASN
2	K	471	GLN
2	K	473	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	728	ASN
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1033	HIS
3	L	1043	HIS
3	L	1048	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FAD	K	606	-	58,58,58	1.09	5 (8%)	85,89,89	1.63	17 (20%)
6	FUT	C	1316	-	24,34,34	2.02	5 (20%)	22,57,57	2.70	8 (36%)
4	FES	J	601	1	0,4,4	-	-	-		
4	FES	A	602	1	0,4,4	-	-	-		
4	FES	A	601	1	0,4,4	-	-	-		
4	FES	J	602	1	0,4,4	-	-	-		
6	FUT	L	1316	-	24,34,34	1.43	2 (8%)	22,57,57	2.72	11 (50%)
5	FAD	B	606	-	58,58,58	1.13	7 (12%)	85,89,89	1.79	21 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	K	606	-	-	3/34/50/50	0/6/6/6
6	FUT	C	1316	-	-	2/6/58/58	0/5/5/5
4	FES	J	601	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1
4	FES	J	602	1	-	-	0/1/1/1
6	FUT	L	1316	-	-	2/6/58/58	0/5/5/5
5	FAD	B	606	-	-	1/34/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1316	FUT	C9-C10	6.65	1.50	1.38
6	L	1316	FUT	C9-C10	5.16	1.47	1.38
5	K	606	FAD	C4X-N5	3.76	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1316	FUT	MO1-S2'	-3.41	2.33	2.39
6	C	1316	FUT	C7-C6	-3.03	1.51	1.53
5	B	606	FAD	C4X-N5	2.98	1.37	1.30
5	B	606	FAD	C2A-N3A	2.75	1.38	1.33
5	K	606	FAD	C2A-N3A	2.67	1.38	1.33
5	K	606	FAD	C10-N1	2.52	1.38	1.33
5	K	606	FAD	C8A-N7A	2.49	1.36	1.31
5	K	606	FAD	C2A-N1A	2.47	1.38	1.33
5	B	606	FAD	C2A-N1A	2.43	1.38	1.33
6	C	1316	FUT	C9-C4	2.39	1.49	1.41
5	B	606	FAD	C10-N1	2.27	1.37	1.33
5	B	606	FAD	C5A-N7A	-2.22	1.35	1.39
6	C	1316	FUT	C4-N3	-2.21	1.34	1.38
5	B	606	FAD	P-O3P	2.21	1.61	1.59
6	L	1316	FUT	C4-N3	-2.14	1.34	1.38
5	B	606	FAD	C8A-N7A	2.00	1.35	1.31

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1316	FUT	O3'-C7-N8	8.37	116.20	108.61
5	B	606	FAD	N3A-C2A-N1A	-6.05	119.42	128.58
5	K	606	FAD	N3A-C2A-N1A	-5.25	120.64	128.58
6	L	1316	FUT	C2'-C1'-S1'	5.08	123.03	120.15
6	L	1316	FUT	C2-N1-C10	4.85	121.92	113.36
6	L	1316	FUT	C1'-C2'-S2'	4.70	122.82	120.15
5	B	606	FAD	C5A-C4A-N3A	-4.62	120.35	126.72
5	K	606	FAD	N9A-C8A-N7A	-4.54	107.49	113.94
5	K	606	FAD	C5A-C4A-N3A	-4.23	120.89	126.72
6	L	1316	FUT	O4-C4-C9	-4.04	117.51	127.26
5	K	606	FAD	C5A-N7A-C8A	4.00	109.74	103.45
6	C	1316	FUT	C2-N1-C10	3.79	120.06	113.36
5	B	606	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
6	L	1316	FUT	C7-C6-N5	3.60	111.40	107.87
6	C	1316	FUT	O4'-C4'-C3'	3.54	117.31	108.58
6	C	1316	FUT	O2P-P-O4'	-3.52	97.49	106.67
5	B	606	FAD	C2A-N3A-C4A	3.43	120.20	111.83
5	B	606	FAD	O4'-C4'-C3'	3.27	116.89	109.25
5	B	606	FAD	C5X-C9A-N10	3.26	120.92	117.97
5	B	606	FAD	N3A-C4A-N9A	3.26	132.71	127.17
5	B	606	FAD	C4-N3-C2	-3.23	119.90	125.64
6	L	1316	FUT	O2P-P-O4'	-3.19	98.36	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1316	FUT	O3'-C7-C6	-3.15	106.86	108.96
5	K	606	FAD	C2A-N3A-C4A	3.14	119.49	111.83
5	B	606	FAD	C5A-N7A-C8A	3.13	108.37	103.45
5	K	606	FAD	O2P-P-O3P	3.06	115.54	107.27
6	C	1316	FUT	C4-C9-N5	3.04	124.56	116.27
6	C	1316	FUT	O3P-P-O2P	2.93	118.78	107.80
5	K	606	FAD	N3A-C4A-N9A	2.93	132.14	127.17
6	L	1316	FUT	C9-C4-N3	2.78	119.77	112.13
5	K	606	FAD	C4A-C5A-N7A	-2.74	107.45	110.58
5	B	606	FAD	C4X-C10-N10	2.74	120.40	116.48
5	B	606	FAD	O4-C4-C4X	-2.62	119.61	126.53
5	K	606	FAD	C4X-C10-N10	2.62	120.23	116.48
5	K	606	FAD	C4-N3-C2	-2.61	121.01	125.64
5	B	606	FAD	C4-C4X-C10	2.59	121.38	116.93
5	B	606	FAD	C5'-C4'-C3'	-2.57	107.37	112.22
5	B	606	FAD	C2B-C1B-N9A	2.53	119.58	113.30
6	L	1316	FUT	O3P-P-O2P	2.51	117.20	107.80
5	K	606	FAD	C4A-N9A-C8A	2.46	108.32	105.74
6	C	1316	FUT	C2'-C1'-S1'	2.41	121.52	120.15
6	L	1316	FUT	O4'-C4'-C3'	2.39	114.47	108.58
6	L	1316	FUT	C4-C9-N5	2.38	122.76	116.27
5	K	606	FAD	O2A-PA-O3P	2.37	113.67	107.27
5	B	606	FAD	C5A-C6A-N6A	-2.36	117.45	123.29
5	B	606	FAD	C6-C5X-C9A	2.29	122.20	119.05
5	B	606	FAD	C9A-C5X-N5	-2.27	120.04	122.45
5	K	606	FAD	C4X-C4-N3	2.24	118.95	113.25
5	B	606	FAD	C4X-C10-N1	-2.23	119.12	124.59
5	K	606	FAD	C10-C4X-N5	-2.23	120.25	124.81
5	B	606	FAD	C10-C4X-N5	-2.17	120.38	124.81
5	B	606	FAD	C4X-C4-N3	2.12	118.65	113.25
6	C	1316	FUT	C9-C4-N3	2.11	117.93	112.13
5	K	606	FAD	O3B-C3B-C4B	-2.09	105.07	111.08
5	K	606	FAD	O4-C4-C4X	-2.09	121.02	126.53
5	K	606	FAD	C7M-C7-C6	-2.03	116.00	119.57
5	B	606	FAD	C4A-C5A-N7A	-2.01	108.28	110.58

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1316	FUT	C3'-C4'-O4'-P
5	K	606	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	L	1316	FUT	C3'-C4'-O4'-P
5	K	606	FAD	O4B-C4B-C5B-O5B
5	K	606	FAD	C3B-C4B-C5B-O5B
6	C	1316	FUT	O3'-C3'-C4'-O4'
6	L	1316	FUT	O3'-C3'-C4'-O4'
5	B	606	FAD	C4'-C5'-O5'-P

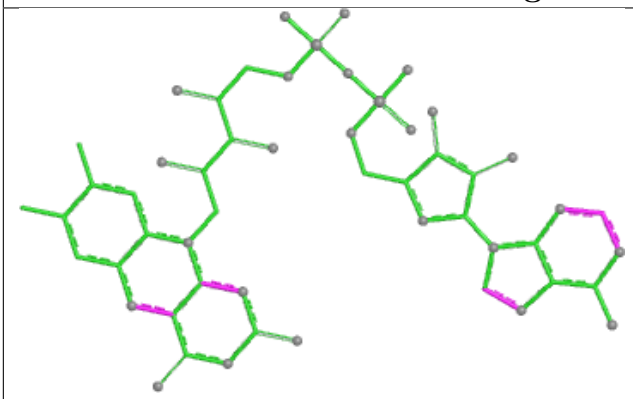
There are no ring outliers.

4 monomers are involved in 9 short contacts:

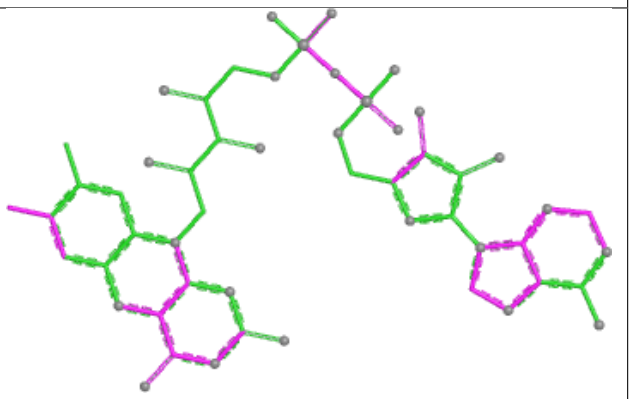
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	606	FAD	2	0
6	C	1316	FUT	2	0
6	L	1316	FUT	3	0
5	B	606	FAD	2	0

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 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.

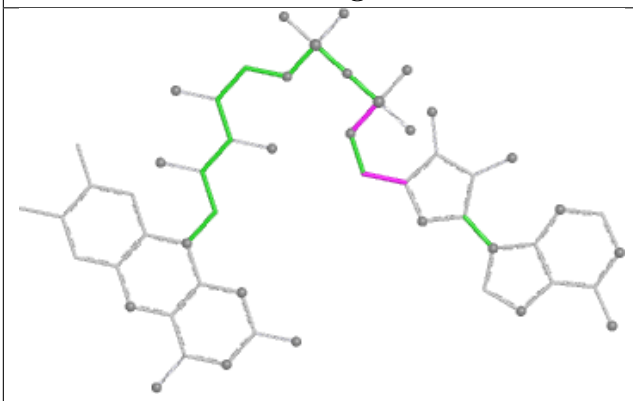
Ligand FAD K 606



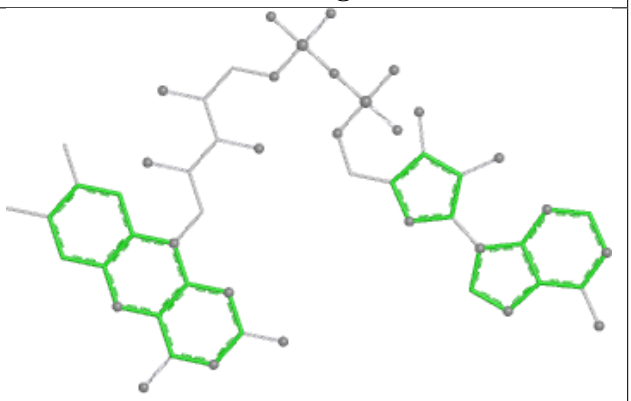
Bond lengths



Bond angles

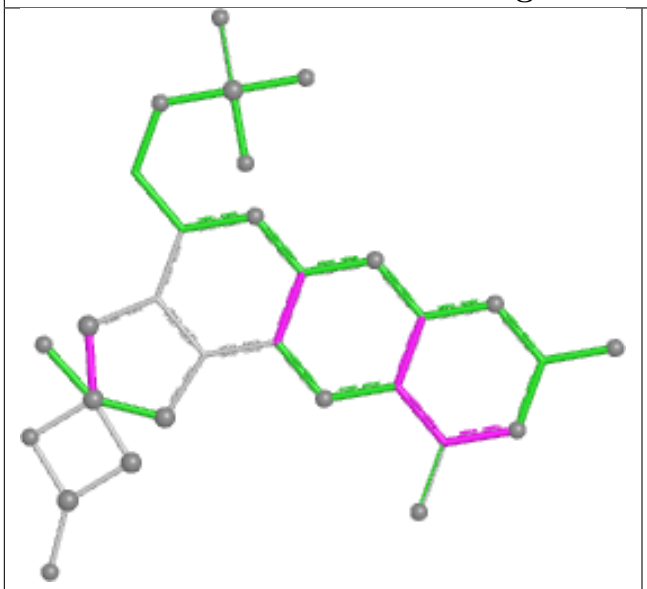


Torsions

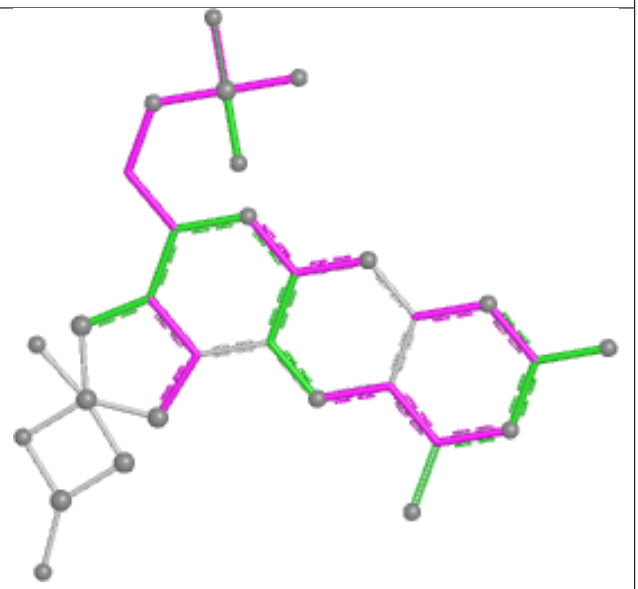


Rings

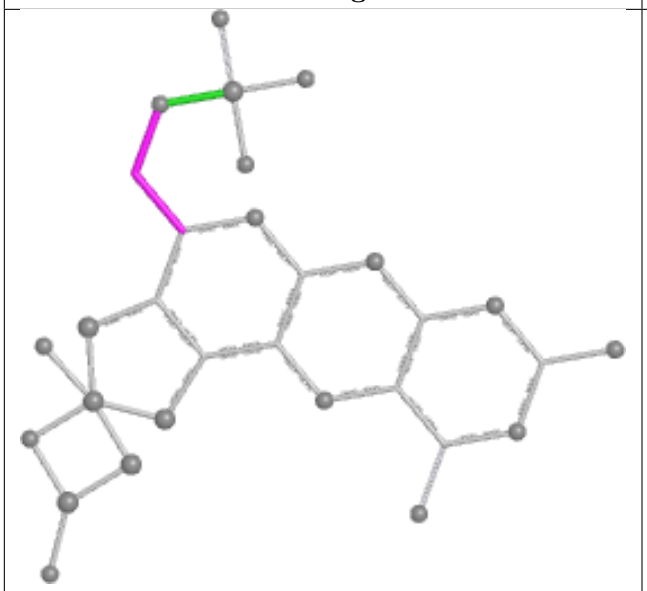
Ligand FUT C 1316



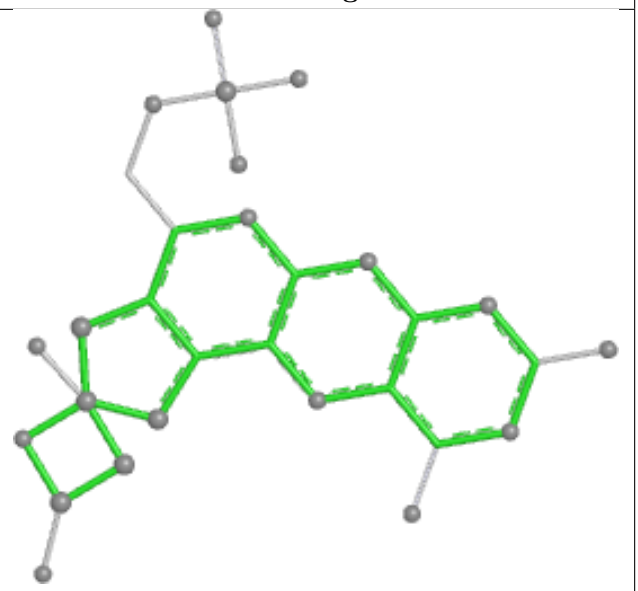
Bond lengths



Bond angles

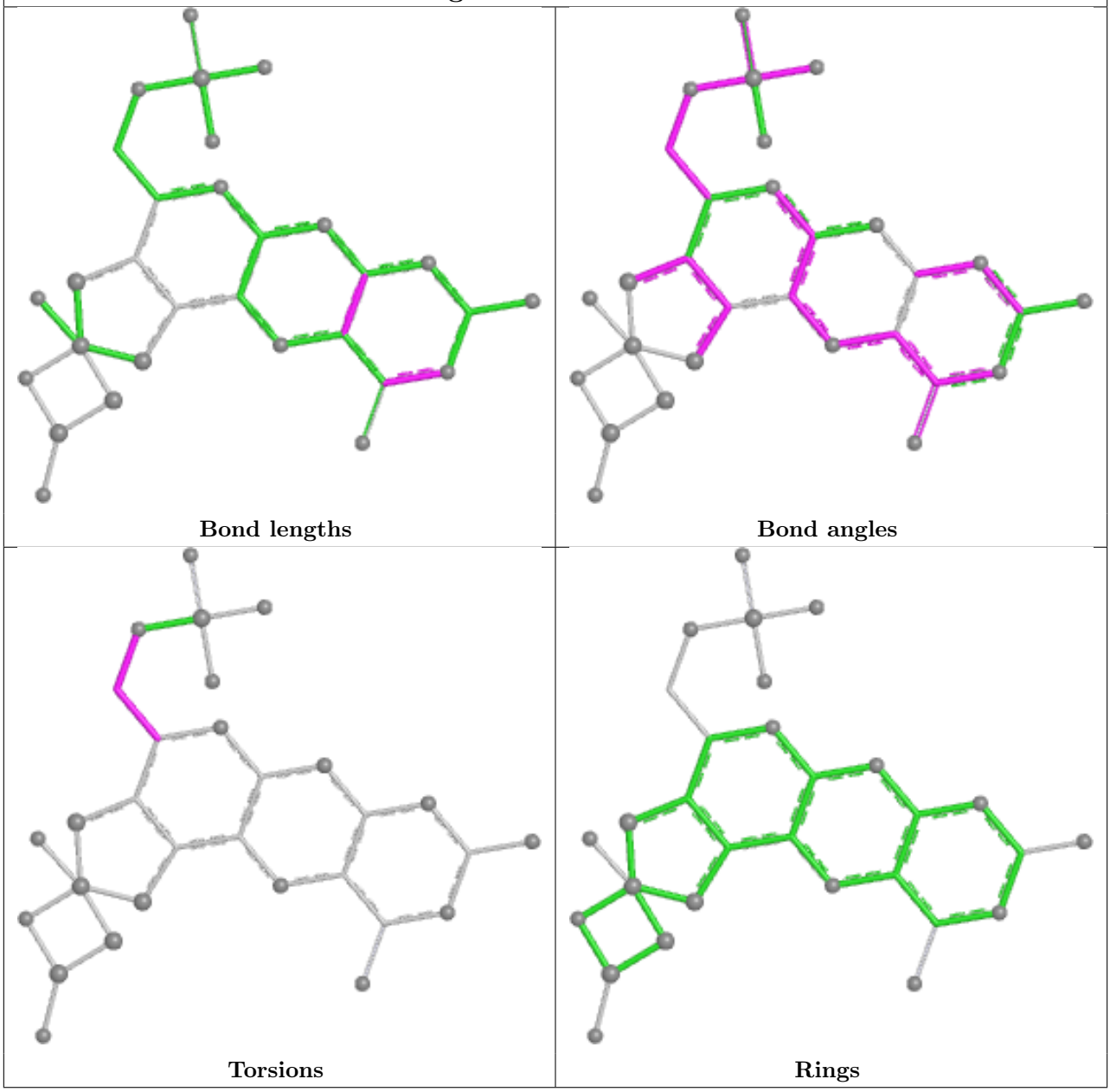


Torsions

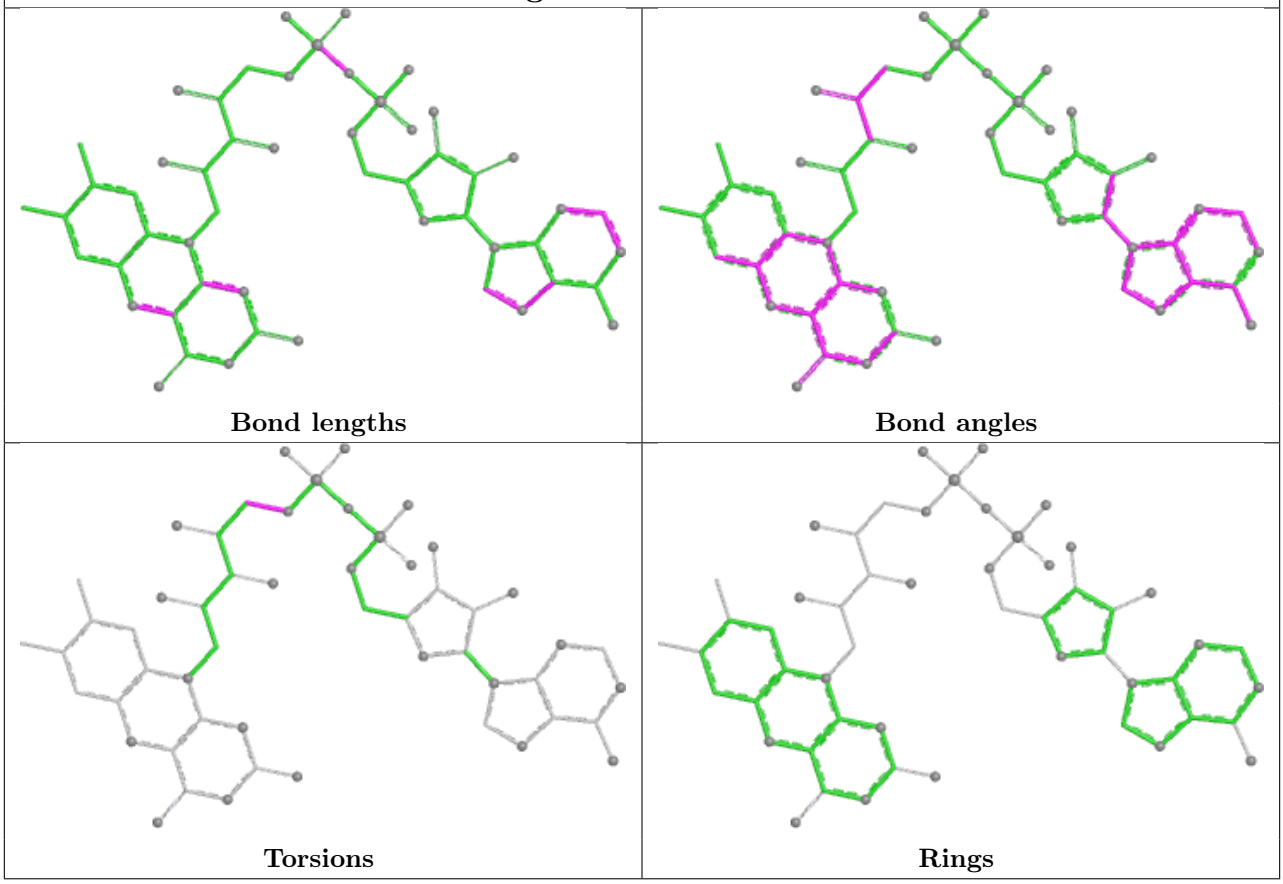


Rings

Ligand FUT L 1316



Ligand FAD B 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 (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%)	0.28	8 (4%)	35	37	11, 22, 41, 56	0
1	J	164/164 (100%)	0.24	9 (5%)	30	32	11, 23, 41, 56	0
2	B	305/305 (100%)	0.60	17 (5%)	30	32	19, 30, 41, 46	0
2	K	305/305 (100%)	0.54	15 (4%)	35	37	19, 30, 41, 46	0
3	C	745/745 (100%)	0.14	15 (2%)	65	67	11, 22, 35, 48	0
3	L	745/745 (100%)	0.16	14 (1%)	66	69	11, 22, 35, 48	0
All	All	2428/2428 (100%)	0.27	78 (3%)	50	53	11, 24, 39, 56	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	4.7
3	L	1288	ASN	4.6
1	J	2	THR	4.4
1	J	61	LEU	4.0
2	B	528	GLY	4.0
3	C	1287	ASN	3.8
2	B	401	GLU	3.6
2	B	378	GLY	3.5
1	A	63	ASP	3.4
1	A	2	THR	3.3
1	J	59	ASP	3.3
2	K	378	GLY	3.2
2	K	424	ALA	3.1
3	L	1290	THR	3.0
1	A	58	TYR	3.0
2	B	424	ALA	2.9
3	C	616	LYS	2.9
3	L	664	GLY	2.9
1	J	58	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	336	TRP	2.9
1	A	97	ARG	2.9
3	C	943	TRP	2.8
1	A	141	ASP	2.8
2	K	429	ASP	2.8
3	L	725	GLU	2.7
2	K	335	ARG	2.7
1	J	63	ASP	2.7
3	C	683	HIS	2.7
3	L	1286	THR	2.7
3	C	724	SER	2.6
2	B	484	GLN	2.6
3	L	683	HIS	2.5
1	J	60	ARG	2.5
3	L	1287	ASN	2.5
2	K	251	GLN	2.5
2	B	250	ALA	2.5
2	B	509	ARG	2.5
2	K	528	GLY	2.5
3	L	724	SER	2.4
3	C	571	ASP	2.4
3	L	1247	CYS	2.4
2	K	425	SER	2.4
1	J	162	THR	2.4
2	B	477	PHE	2.4
3	C	1293	LEU	2.4
3	C	1143	GLU	2.4
3	C	1246	ASP	2.3
3	C	598	ARG	2.3
3	L	1110	ASP	2.3
2	B	291	GLU	2.3
2	K	332	GLU	2.3
2	B	272	ASN	2.3
1	J	97	ARG	2.3
2	K	336	TRP	2.3
2	K	412	SER	2.2
3	L	943	TRP	2.2
3	C	618	LYS	2.2
2	K	444	PRO	2.2
3	C	1144	THR	2.2
2	B	485	ASP	2.2
2	K	377	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	527	LEU	2.1
3	L	719	LEU	2.1
3	C	657	LYS	2.1
3	C	705	ASN	2.1
1	J	133	GLU	2.1
2	B	429	ASP	2.1
1	A	66	ILE	2.1
2	K	474	LEU	2.1
2	B	447	MET	2.1
2	B	430	ASP	2.1
3	L	985	ASP	2.1
3	C	1109	PRO	2.1
3	L	729	VAL	2.1
2	K	484	GLN	2.1
2	B	290	VAL	2.0
2	B	425	SER	2.0
1	A	60	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 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(Å^2)	Q<0.9
5	FAD	B	606	53/53	0.96	0.06	14,20,24,28	0
5	FAD	K	606	53/53	0.97	0.06	17,22,24,24	0
6	FUT	L	1316	30/30	0.98	0.06	13,20,32,40	0
4	FES	J	602	4/4	0.99	0.02	12,13,14,15	0
4	FES	A	601	4/4	0.99	0.03	10,12,14,15	0
4	FES	A	602	4/4	0.99	0.03	14,15,17,19	0

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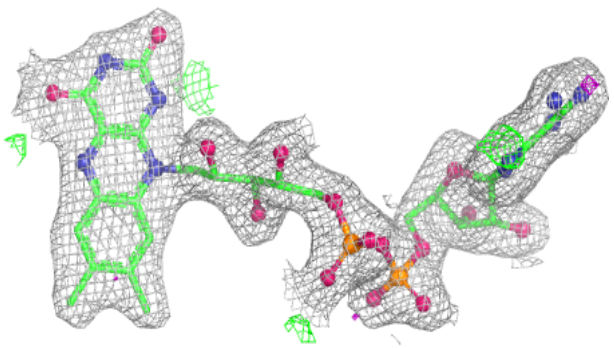
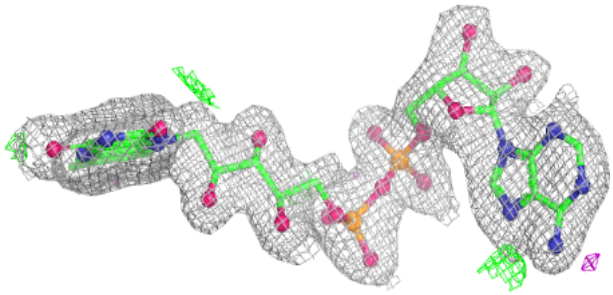
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	FUT	C	1316	30/30	0.99	0.05	15,17,33,40	0
4	FES	J	601	4/4	0.99	0.03	14,14,14,17	0

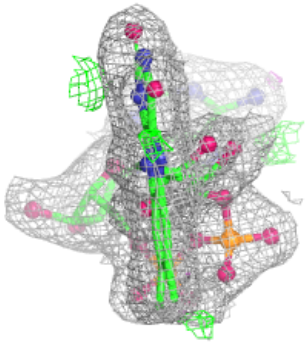
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

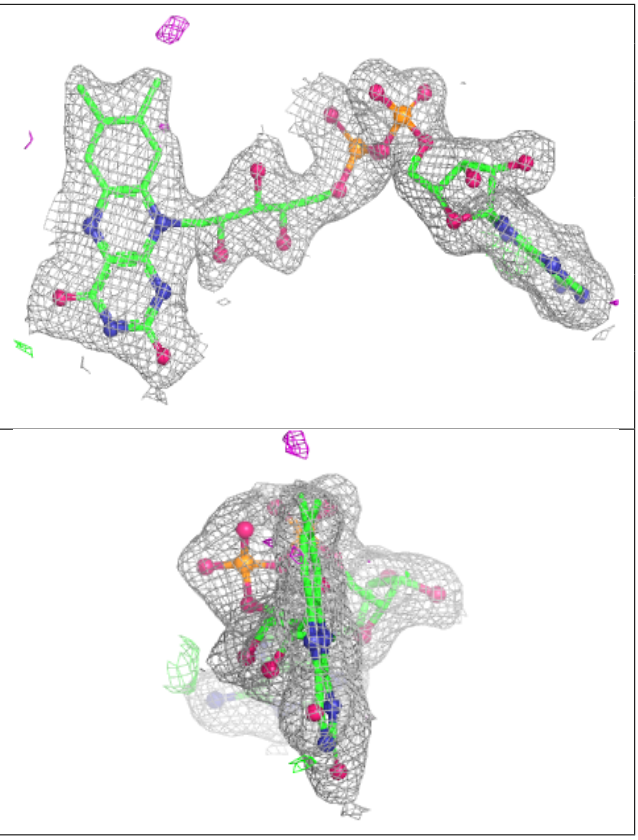






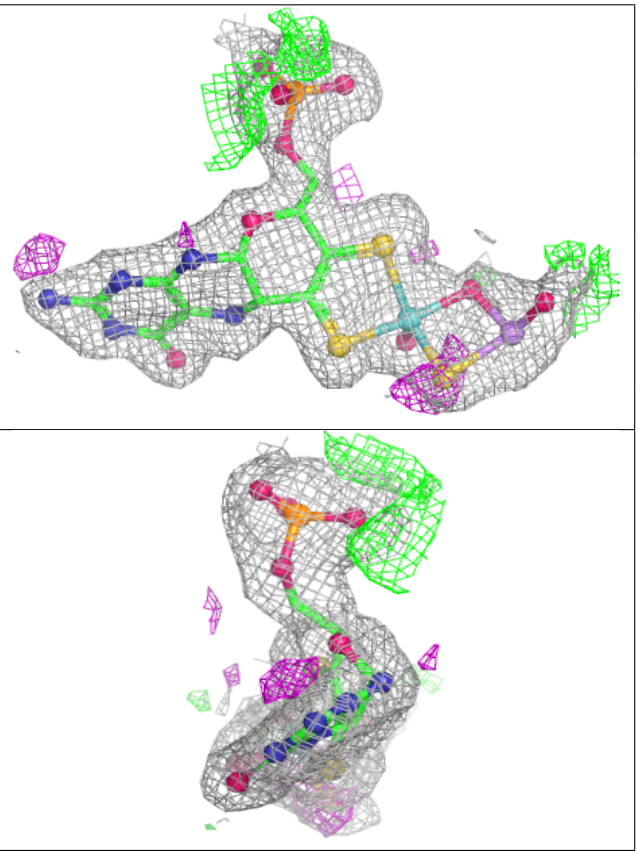
Electron density around FAD K 606:

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



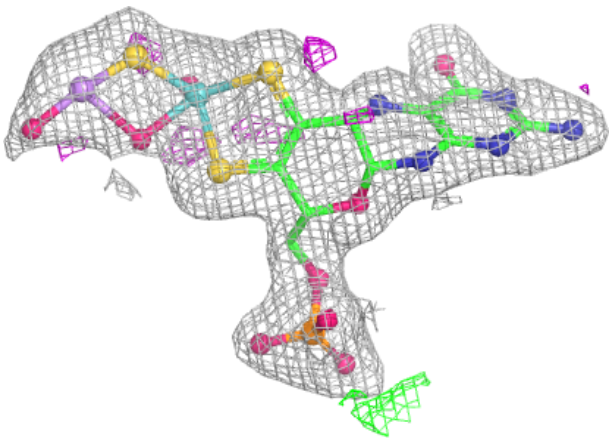
Electron density around FUT L 1316:

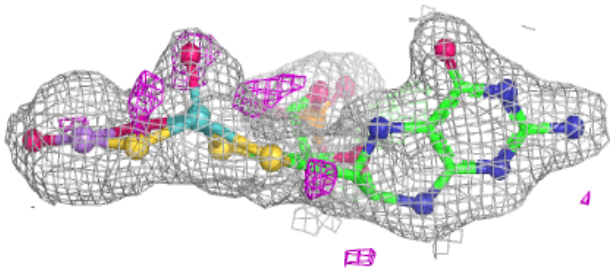
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FUT C 1316:

$2mF_o$-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.