



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:46 PM UTC

PDB ID : 3AMZ / pdb_00003amz
Title : Bovine Xanthine Oxidoreductase urate bound form
Authors : Okamoto, K.; Eger, B.T.; Pai, E.F.; Nishino, T.
Deposited on : 2010-08-27
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

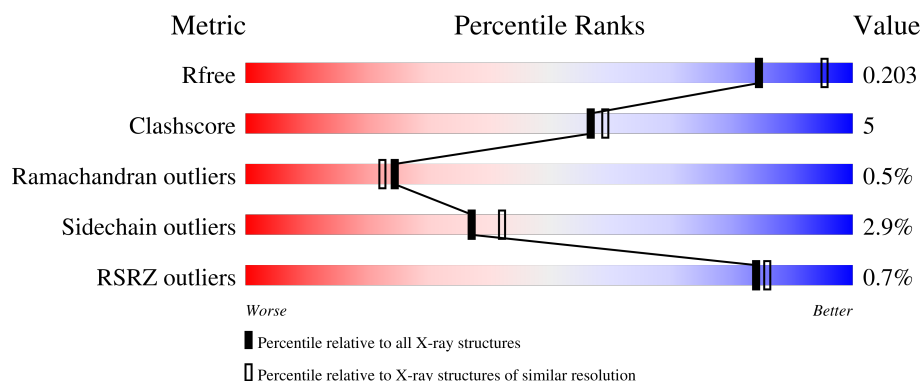
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	1332	% 86% 9% ..
1	B	1332	% 86% 10% ..

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
10	URC	B	1338	-	X	-	-
9	MOS	A	1338	-	-	X	-

2 Entry composition [i](#)

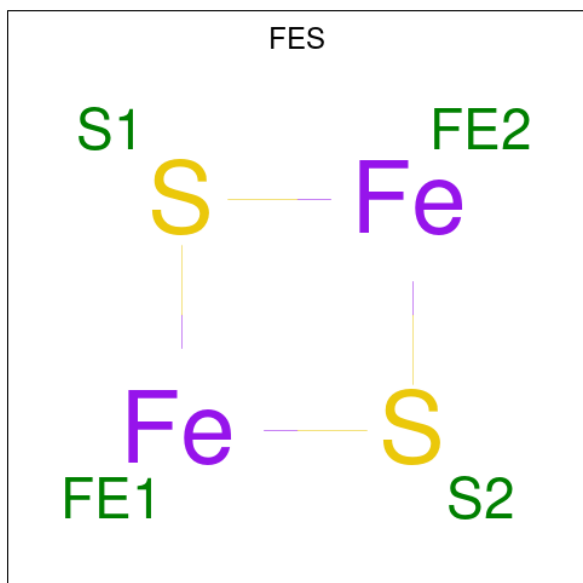
There are 11 unique types of molecules in this entry. The entry contains 22382 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1291	Total	C	N	O	S	0	0	0
			10024	6374	1718	1872	60			
1	B	1289	Total	C	N	O	S	0	0	0
			10013	6368	1716	1869	60			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

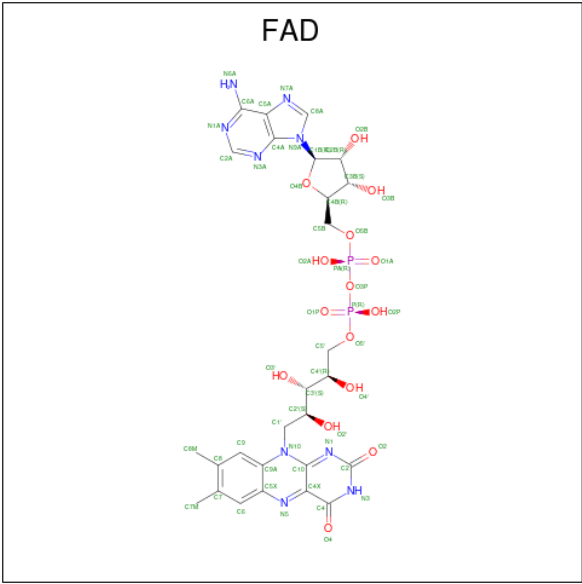


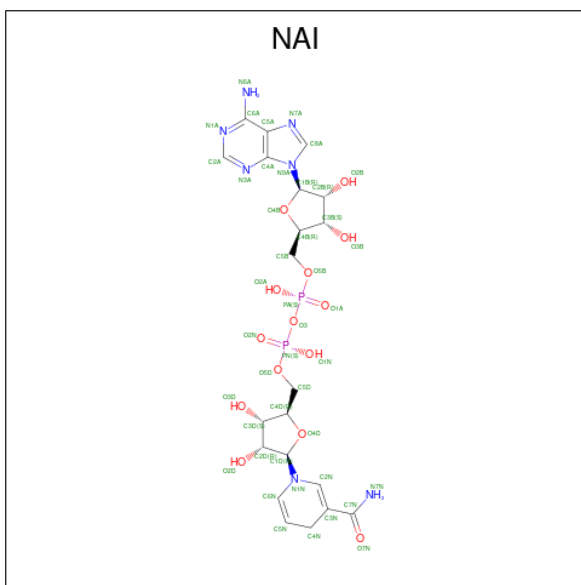
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

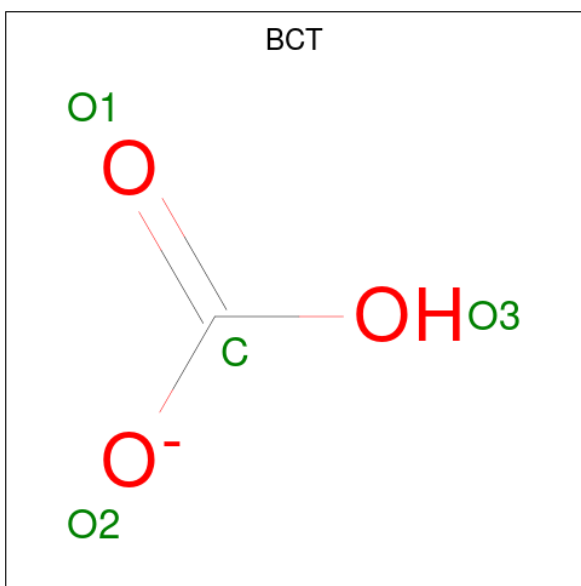
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).





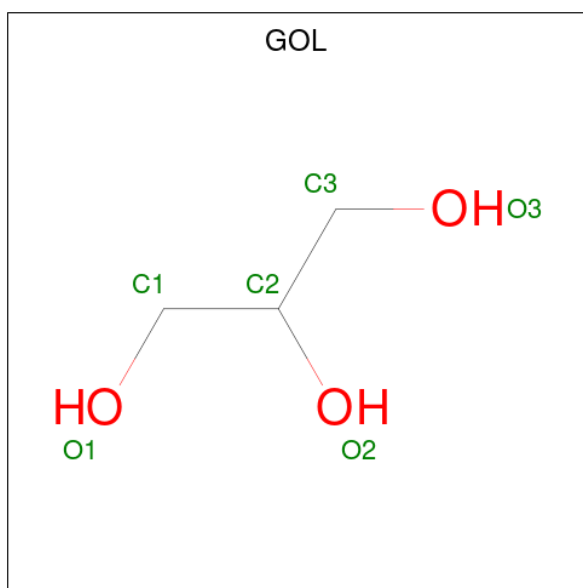
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



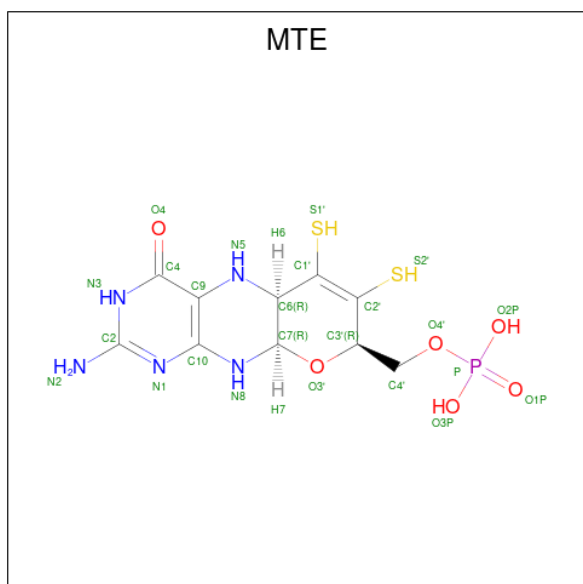
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



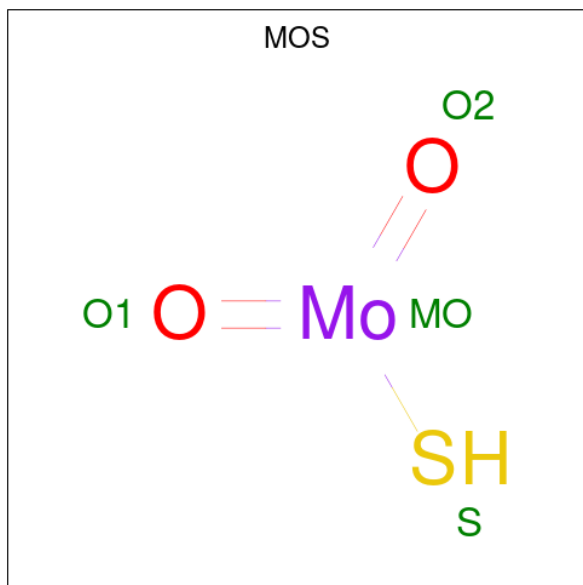
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

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



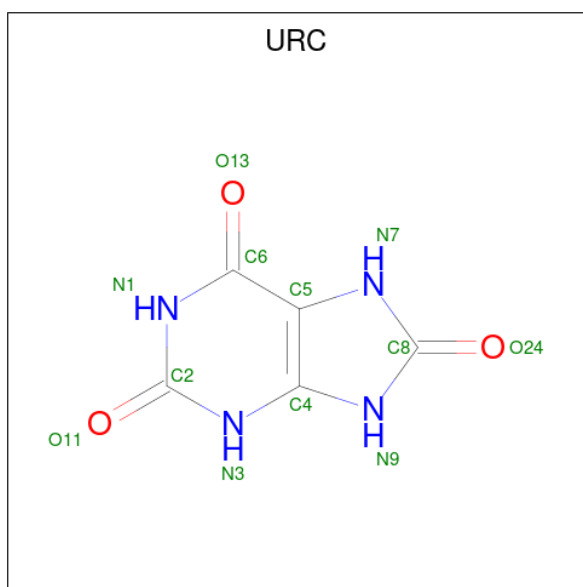
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
8	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

- Molecule 9 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	Mo	O	S		
			3	1	1	1	0	0
9	B	1	Total	Mo	O	S		
			3	1	1	1	0	0

- Molecule 10 is URIC ACID (CCD ID: URC) (formula: $\text{C}_5\text{H}_4\text{N}_4\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			12	5	4	3		
10	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1019	Total	O	0	0
			1019	1019		
11	B	1010	Total	O	0	0
			1010	1010		

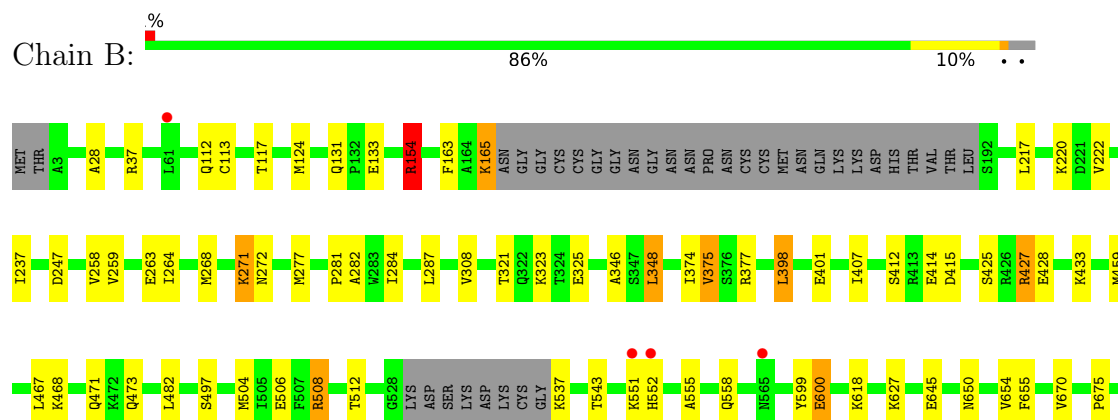
3 Residue-property plots

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

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.21Å 124.53Å 148.03Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	34.83 – 2.10 34.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.83-2.10) 99.8 (34.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.151 , 0.202 0.152 , 0.203	Depositor DCC
R_{free} test set	8881 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22382	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 3.05% 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: URC, FAD, MOS, CA, FES, BCT, MTE, GOL, NAI

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	1.28	9/10243 (0.1%)	1.13	27/13863 (0.2%)
1	B	1.26	14/10232 (0.1%)	1.11	16/13848 (0.1%)
All	All	1.27	23/20475 (0.1%)	1.12	43/27711 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
All	All	1	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ASP	CA-C	8.91	1.64	1.52
1	B	258	VAL	CA-CB	6.84	1.63	1.54
1	B	1011	VAL	CA-CB	6.38	1.60	1.53
1	A	4	ASP	N-CA	-6.25	1.38	1.46
1	B	117	THR	C-O	-6.12	1.18	1.24
1	B	508	ARG	CD-NE	-6.01	1.37	1.46
1	B	259	VAL	CA-CB	5.92	1.62	1.54
1	B	543	THR	CA-CB	5.78	1.62	1.53
1	A	931	ALA	CA-CB	5.71	1.62	1.53
1	B	1290	THR	CA-CB	5.60	1.62	1.53
1	B	282	ALA	CA-CB	5.47	1.62	1.53
1	B	734	LEU	N-CA	5.39	1.52	1.46
1	B	28	ALA	CA-CB	5.28	1.61	1.53
1	B	796	GLY	C-O	5.27	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ILE	CA-CB	5.25	1.60	1.54
1	A	922	ILE	CA-CB	-5.21	1.48	1.54
1	A	622	VAL	CA-CB	5.14	1.60	1.54
1	A	777	ALA	N-CA	5.14	1.52	1.46
1	B	1195	VAL	CA-CB	5.13	1.60	1.54
1	B	154	ARG	CD-NE	-5.13	1.39	1.46
1	A	1200	VAL	CA-CB	5.09	1.60	1.54
1	A	197	ASN	N-CA	-5.05	1.41	1.46
1	A	96	THR	CA-C	5.03	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH2	-8.21	111.81	119.20
1	B	154	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	A	1332	VAL	CB-CA-C	7.77	126.16	111.40
1	B	1262	PRO	CA-C-N	-7.71	111.71	120.04
1	B	1262	PRO	C-N-CA	-7.71	111.71	120.04
1	A	62	GLN	N-CA-C	-7.40	105.42	114.75
1	A	684	VAL	CB-CA-C	7.15	120.07	111.20
1	A	97	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	B	508	ARG	NE-CZ-NH2	-6.88	113.00	119.20
1	A	684	VAL	N-CA-CB	-6.79	103.50	112.26
1	A	60	ARG	N-CA-C	-6.55	99.23	109.25
1	A	222	VAL	CA-C-N	-6.50	113.69	120.38
1	A	222	VAL	C-N-CA	-6.50	113.69	120.38
1	B	154	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	B	1011	VAL	CB-CA-C	6.34	117.50	110.71
1	A	4	ASP	CB-CA-C	6.26	122.88	110.42
1	A	89	GLU	CA-CB-CG	6.05	126.20	114.10
1	B	427	ARG	NE-CZ-NH2	-5.96	113.84	119.20
1	B	508	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	A	131	GLN	CA-C-N	5.79	125.46	119.56
1	A	131	GLN	C-N-CA	5.79	125.46	119.56
1	A	97	ARG	CG-CD-NE	-5.77	99.30	112.00
1	A	1235	ILE	CA-C-N	-5.66	113.72	119.83
1	A	1235	ILE	C-N-CA	-5.66	113.72	119.83
1	A	412	SER	N-CA-CB	-5.57	101.65	110.06
1	A	980	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	B	835	ILE	N-CA-C	5.48	116.53	111.81
1	A	1131	GLY	N-CA-C	-5.45	102.57	110.90
1	B	375	VAL	N-CA-CB	-5.32	101.98	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1262	PRO	N-CA-C	5.32	117.19	110.70
1	A	223	PRO	CA-C-N	5.26	125.19	119.78
1	A	223	PRO	C-N-CA	5.26	125.19	119.78
1	B	743	TYR	N-CA-C	-5.24	102.64	110.23
1	B	154	ARG	CB-CG-CD	-5.22	99.29	111.30
1	A	1262	PRO	N-CA-C	5.18	117.02	110.70
1	A	1331	ARG	CB-CG-CD	-5.13	99.49	111.30
1	A	262	THR	N-CA-C	-5.12	107.03	113.28
1	B	654	VAL	N-CA-C	-5.11	105.72	110.53
1	A	89	GLU	N-CA-C	5.08	118.74	112.54
1	B	1137	ASN	N-CA-C	5.08	118.77	112.58
1	B	982	SER	N-CA-C	5.04	116.46	111.07
1	A	592	TYR	N-CA-C	-5.02	102.77	110.14
1	A	1332	VAL	N-CA-CB	5.00	120.00	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1332	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1286	THR	Peptide

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	10024	0	10027	98	0
1	B	10013	0	10017	84	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	4	0
4	B	53	0	31	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	44	0	25	4	0
5	B	44	0	27	3	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	12	0	16	0	0
7	B	6	0	8	1	0
8	A	24	0	10	1	0
8	B	24	0	10	0	0
9	A	3	0	0	2	0
9	B	3	0	0	1	0
10	A	12	0	4	0	0
10	B	12	0	4	0	0
11	A	1019	0	0	19	0
11	B	1010	0	0	22	0
All	All	22382	0	20210	187	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 5.

All (187) 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)
1:A:3:ALA:HB1	1:A:228:ARG:H	1.08	1.09
1:A:60:ARG:O	1:A:61:LEU:HB2	1.47	1.08
1:B:272:ASN:HB3	11:B:1988:HOH:O	1.65	0.95
1:B:217:LEU:O	1:B:220:LYS:HG2	1.70	0.92
1:A:3:ALA:HB1	1:A:228:ARG:N	1.86	0.90
4:A:3005:FAD:C4X	5:A:1333:NAI:C6N	2.50	0.90
4:B:4005:FAD:C4X	5:B:1333:NAI:C6N	2.52	0.88
1:B:37:ARG:HD3	11:B:1467:HOH:O	1.74	0.88
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.77	0.85
1:A:377:ARG:NE	11:A:2032:HOH:O	2.09	0.84
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.41	0.83
1:A:60:ARG:O	1:A:61:LEU:CB	2.27	0.83
1:A:237:ILE:CD1	1:A:277:MET:HE3	2.08	0.82
1:A:237:ILE:HD12	1:A:277:MET:HE3	1.61	0.82
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	1.98	0.81
1:B:131:GLN:HE21	1:B:133:GLU:H	1.27	0.80
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.44	0.80
1:A:3:ALA:O	1:A:4:ASP:C	2.23	0.80
1:A:154:ARG:CD	1:A:1196:GLU:OE2	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HD2	11:A:1470:HOH:O	1.81	0.79
1:A:1330:LEU:HG	11:A:2358:HOH:O	1.83	0.78
1:B:165:LYS:O	1:B:165:LYS:HE3	1.84	0.77
1:B:506:GLU:HG3	11:B:1384:HOH:O	1.86	0.76
1:A:552:HIS:HB2	11:A:2208:HOH:O	1.85	0.75
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.51	0.74
1:A:995:LYS:NZ	1:A:1284:GLN:HE21	1.85	0.73
1:A:154:ARG:HD2	11:A:1444:HOH:O	1.89	0.72
1:A:1279:ARG:HG2	1:A:1294:PHE:HE2	1.56	0.70
1:A:3:ALA:O	1:A:5:GLU:N	2.25	0.69
1:A:439:ARG:HH11	1:A:439:ARG:HB3	1.58	0.68
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.57	0.68
1:B:627:LYS:NZ	11:B:2302:HOH:O	2.28	0.67
1:B:467:LEU:O	1:B:471:GLN:HG2	1.94	0.67
1:A:415:ASP:OD2	1:A:444:PRO:HA	1.95	0.66
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.95	0.66
1:A:131:GLN:HE21	1:A:133:GLU:H	1.44	0.66
1:A:237:ILE:HD12	1:A:277:MET:CE	2.25	0.66
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.92	0.65
1:B:1212:HIS:HD2	11:B:2345:HOH:O	1.80	0.64
1:B:154:ARG:HD2	11:B:1705:HOH:O	1.98	0.63
1:A:1249:ASN:O	1:A:1255:ALA:HA	1.98	0.63
1:B:433:LYS:HE2	1:B:504:MET:SD	2.38	0.63
1:B:323:LYS:NZ	11:B:1485:HOH:O	2.18	0.62
1:B:1312:LYS:HE2	11:B:2314:HOH:O	1.99	0.62
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.64	0.62
1:A:1319:THR:HG22	11:A:2095:HOH:O	2.00	0.62
1:A:995:LYS:HZ3	1:A:1284:GLN:HE21	1.48	0.61
1:A:154:ARG:HD2	1:A:1196:GLU:OE2	2.00	0.61
1:A:624:GLU:HB3	11:A:2199:HOH:O	2.00	0.60
9:A:1338:MOS:MO	9:A:1338:MOS:O1	1.72	0.59
1:B:348:LEU:HD13	1:B:407:ILE:HD13	1.84	0.58
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.85	0.58
1:A:562:GLU:HB2	11:A:2245:HOH:O	2.04	0.58
4:A:3005:FAD:C4	5:A:1333:NAI:C6N	2.81	0.58
1:B:425:SER:OG	1:B:433:LYS:NZ	2.38	0.57
1:B:427:ARG:NH2	1:B:1171:HIS:O	2.37	0.57
1:A:1180:MET:HE1	1:A:1266:LEU:HD12	1.85	0.57
1:B:645:GLU:HG2	1:B:650:ASN:ND2	2.16	0.57
1:A:645:GLU:HG2	1:A:650:ASN:ND2	2.19	0.57
4:B:4005:FAD:C4	5:B:1333:NAI:C6N	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLN:HE21	1:A:429:ASP:H	1.53	0.56
1:B:695:ILE:HG23	1:B:700:ASP:HB3	1.87	0.56
1:A:541:THR:HG23	1:A:992:CYS:HB2	1.88	0.56
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.36	0.56
1:A:1326:LYS:N	1:A:1327:PRO:CD	2.70	0.55
1:A:237:ILE:CD1	1:A:277:MET:CE	2.82	0.55
1:B:980:ARG:HD2	11:B:2278:HOH:O	2.07	0.55
1:A:197:ASN:O	1:A:200:GLU:HG3	2.06	0.54
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.55	0.54
1:B:1106:LYS:O	1:B:1109:PRO:HD3	2.08	0.54
1:A:322:GLN:O	1:A:412:SER:HB3	2.08	0.54
1:B:264:ILE:HD11	4:B:4005:FAD:H3B	1.89	0.54
1:B:552:HIS:CE1	1:B:1172:LYS:NZ	2.73	0.53
1:B:346:ALA:HB1	4:B:4005:FAD:H4'	1.90	0.53
1:A:1140:TYR:OH	1:A:1145:ASN:ND2	2.41	0.53
1:B:1203:LEU:C	1:B:1203:LEU:HD23	2.34	0.52
1:A:508:ARG:O	1:A:512:THR:HG23	2.08	0.52
1:A:256:LYS:HG3	1:A:275:PHE:CD2	2.45	0.52
1:A:655:PHE:HE1	1:A:814:LEU:CD2	2.23	0.52
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.56	0.52
1:A:220:LYS:HG2	1:A:221:ASP:N	2.25	0.51
1:A:719:LEU:HD22	1:A:860:GLU:HG3	1.93	0.51
1:B:1105:LYS:NZ	11:B:2048:HOH:O	2.23	0.51
1:A:37:ARG:HD3	1:A:595:ASP:O	2.11	0.51
1:A:154:ARG:HD3	1:A:1196:GLU:CD	2.35	0.50
1:A:980:ARG:HD2	11:A:2318:HOH:O	2.12	0.50
1:B:508:ARG:O	1:B:512:THR:HG23	2.11	0.50
1:A:263:GLU:HB2	11:A:2103:HOH:O	2.11	0.50
1:A:59:ASP:OD2	1:A:62:GLN:HB2	2.12	0.50
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.44	0.50
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.47	0.49
1:A:220:LYS:HE3	11:A:2267:HOH:O	2.11	0.49
1:A:1057:PRO:HD2	1:A:1060:LYS:HD2	1.95	0.49
1:A:1212:HIS:HD2	11:A:1528:HOH:O	1.95	0.48
1:A:35:GLY:N	11:A:2071:HOH:O	2.47	0.48
1:B:401:GLU:HB2	11:B:1713:HOH:O	2.13	0.48
1:B:428:GLU:HG2	11:B:1891:HOH:O	2.12	0.48
1:B:473:GLN:HE21	1:B:482:LEU:HD12	1.79	0.48
1:A:529:LYS:HG2	11:A:2066:HOH:O	2.13	0.48
1:B:271:LYS:HE2	11:B:2010:HOH:O	2.13	0.48
1:B:414:GLU:O	1:B:415:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ASP:OD1	1:A:541:THR:HB	2.14	0.48
4:A:3005:FAD:C4	5:A:1333:NAI:H6N	2.44	0.48
1:A:1178:ILE:CG2	1:A:1180:MET:CE	2.92	0.47
1:A:1132:PHE:CD1	1:B:1126:SER:HB2	2.49	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.57	0.47
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.96	0.47
1:A:376:SER:HB3	1:A:379:THR:OG1	2.15	0.47
1:B:459:MET:HE2	1:B:512:THR:HG21	1.97	0.47
1:A:1180:MET:HE2	1:A:1180:MET:HB2	1.63	0.46
1:B:247:ASP:OD1	1:B:377:ARG:HD3	2.14	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.15	0.46
1:B:1289:ASN:O	1:B:1290:THR:HB	2.16	0.46
1:B:912:ARG:N	9:B:1337:MOS:S	2.89	0.46
1:B:847:LYS:NZ	11:B:1471:HOH:O	2.37	0.46
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.80	0.46
1:B:468:LYS:HG3	11:B:1428:HOH:O	2.15	0.46
1:B:555:ALA:O	1:B:1238:GLU:HA	2.16	0.46
1:B:263:GLU:HB3	4:B:4005:FAD:H52A	1.98	0.45
1:A:723:PHE:CE2	1:A:847:LYS:HG2	2.51	0.45
1:A:902:LYS:NZ	11:A:2313:HOH:O	2.27	0.45
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.47	0.45
1:A:474:LEU:O	1:A:475:SER:HB2	2.16	0.45
1:A:217:LEU:O	1:A:220:LYS:HD3	2.16	0.45
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.97	0.45
1:A:618:LYS:HA	1:A:618:LYS:HD2	1.67	0.45
1:A:237:ILE:HD11	1:A:277:MET:HE3	1.96	0.45
1:B:1153:PHE:HB2	1:B:1155:TYR:CZ	2.52	0.45
1:B:1213:TYR:HD1	11:B:2360:HOH:O	2.00	0.45
1:B:1122:GLN:NE2	11:B:1906:HOH:O	2.50	0.44
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.77	0.44
1:A:1082:SER:HB2	8:A:1337:MTE:O3P	2.17	0.44
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.44
1:B:112:GLN:HB3	1:B:1039:GLY:O	2.17	0.44
1:A:723:PHE:CZ	1:A:847:LYS:HG2	2.53	0.44
1:A:35:GLY:HA2	11:A:2071:HOH:O	2.17	0.44
4:A:3005:FAD:C4X	5:A:1333:NAI:C5N	2.96	0.44
1:A:195:LEU:HD22	1:A:1189:ALA:HA	2.00	0.44
1:A:970:GLU:HG2	1:A:1179:VAL:HG21	2.00	0.44
1:A:1212:HIS:HE1	11:A:1816:HOH:O	2.00	0.44
1:A:256:LYS:HE2	1:A:275:PHE:CE2	2.52	0.43
1:A:613:ALA:O	1:A:904:ASN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:HB2	1:B:412:SER:HB3	2.00	0.43
1:A:598:ARG:HG3	1:B:600:GLU:HG2	2.00	0.43
1:B:268:MET:CE	11:B:2245:HOH:O	2.67	0.43
1:B:1212:HIS:HE1	11:B:2011:HOH:O	2.00	0.43
1:B:113:CYS:HA	1:B:1039:GLY:HA2	2.00	0.43
1:A:55:LEU:CD2	1:A:85:VAL:HG22	2.49	0.43
1:B:374:ILE:HD13	1:B:398:LEU:HD22	2.01	0.43
1:B:1140:TYR:OH	1:B:1145:ASN:ND2	2.51	0.43
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.43
1:A:348:LEU:HD13	1:A:407:ILE:HD13	2.01	0.43
1:A:362:ASN:N	1:A:363:PRO:CD	2.82	0.43
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.18	0.43
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.84	0.43
1:B:794:MET:HE3	1:B:1038:MET:HB3	2.00	0.43
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.22	0.43
1:B:308:VAL:HG21	1:B:348:LEU:HG	2.01	0.43
1:A:712:LEU:HG	11:A:1380:HOH:O	2.19	0.42
1:B:237:ILE:HD13	1:B:277:MET:HE3	2.01	0.42
4:B:4005:FAD:C4	5:B:1333:NAI:H6N	2.49	0.42
1:A:325:GLU:HB2	1:A:412:SER:OG	2.19	0.42
1:B:124:MET:HE2	1:B:163:PHE:CD1	2.54	0.42
1:A:995:LYS:NZ	1:A:1284:GLN:NE2	2.63	0.42
1:B:1031:VAL:HB	1:B:1063:ILE:HG12	2.01	0.42
1:A:599:TYR:HA	1:B:599:TYR:HA	2.02	0.42
1:A:926:TRP:CZ3	1:A:927:MET:HE2	2.54	0.42
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.20	0.41
1:A:447:MET:O	1:A:477:PHE:HA	2.20	0.41
1:A:1178:ILE:HG21	1:A:1180:MET:CE	2.50	0.41
1:B:268:MET:HE3	11:B:2245:HOH:O	2.20	0.41
1:A:995:LYS:HZ1	1:A:1284:GLN:HE21	1.64	0.41
1:A:1203:LEU:HD12	1:A:1203:LEU:C	2.45	0.41
1:B:1134:ARG:HG2	11:B:1419:HOH:O	2.20	0.41
1:B:237:ILE:CD1	1:B:277:MET:HE3	2.50	0.41
1:A:35:GLY:CA	11:A:2071:HOH:O	2.69	0.41
1:A:541:THR:HG22	1:A:542:TYR:HD1	1.84	0.41
1:A:912:ARG:N	9:A:1338:MOS:S	2.94	0.41
1:B:272:ASN:CB	11:B:1988:HOH:O	2.42	0.41
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.86	0.41
1:A:946:MET:HE3	1:A:946:MET:HB2	1.87	0.40
1:B:645:GLU:CG	1:B:650:ASN:HD22	2.26	0.40
1:B:675:PRO:HB3	7:B:1335:GOL:H12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:GLU:OE1	1:B:1106:LYS:HD2	2.22	0.40
1:A:555:ALA:O	1:A:1238:GLU:HA	2.20	0.40
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	2.02	0.40
1:B:618:LYS:HA	1:B:618:LYS:HD2	1.91	0.40

There are no symmetry-related clashes.

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	1283/1332 (96%)	1234 (96%)	42 (3%)	7 (0%)	24	22
1	B	1281/1332 (96%)	1239 (97%)	37 (3%)	5 (0%)	30	28
All	All	2564/2664 (96%)	2473 (96%)	79 (3%)	12 (0%)	24	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	539	ASP
1	A	61	LEU
1	A	912	ARG
1	A	1008	SER
1	B	1008	SER
1	B	912	ARG
1	A	1139	GLY
1	A	797	GLY
1	B	797	GLY
1	B	1139	GLY
1	B	1290	THR

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	1095/1128 (97%)	1059 (97%)	36 (3%)	33	37
1	B	1094/1128 (97%)	1067 (98%)	27 (2%)	42	48
All	All	2189/2256 (97%)	2126 (97%)	63 (3%)	37	42

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	61	LEU
1	A	62	GLN
1	A	64	LYS
1	A	89	GLU
1	A	154	ARG
1	A	165	LYS
1	A	200	GLU
1	A	211	ILE
1	A	225	LYS
1	A	256	LYS
1	A	312	LEU
1	A	323	LYS
1	A	348	LEU
1	A	398	LEU
1	A	439	ARG
1	A	468	LYS
1	A	513	LEU
1	A	541	THR
1	A	548	LEU
1	A	551	LYS
1	A	645	GLU
1	A	684	VAL
1	A	719	LEU
1	A	743	TYR
1	A	792	LYS
1	A	857	VAL

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Mol	Chain	Res	Type
1	A	970	GLU
1	A	983	GLU
1	A	989	LYS
1	A	1203	LEU
1	A	1208	LEU
1	A	1287	ASN
1	A	1316	LEU
1	A	1326	LYS
1	A	1330	LEU
1	B	154	ARG
1	B	165	LYS
1	B	222	VAL
1	B	271	LYS
1	B	321	THR
1	B	348	LEU
1	B	375	VAL
1	B	398	LEU
1	B	497	SER
1	B	537	LYS
1	B	551	LYS
1	B	600	GLU
1	B	743	TYR
1	B	818	LYS
1	B	845	ARG
1	B	852	LYS
1	B	857	VAL
1	B	899	ARG
1	B	973	LYS
1	B	982	SER
1	B	983	GLU
1	B	989	LYS
1	B	1011	VAL
1	B	1208	LEU
1	B	1318	VAL
1	B	1326	LYS
1	B	1330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN

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Mol	Chain	Res	Type
1	A	251	GLN
1	A	322	GLN
1	A	556	ASN
1	A	567	GLN
1	A	650	ASN
1	A	705	ASN
1	A	728	ASN
1	A	869	ASN
1	A	1088	GLN
1	A	1145	ASN
1	A	1212	HIS
1	A	1284	GLN
1	B	62	GLN
1	B	131	GLN
1	B	146	ASN
1	B	226	GLN
1	B	251	GLN
1	B	333	GLN
1	B	387	HIS
1	B	473	GLN
1	B	565	ASN
1	B	626	GLN
1	B	650	ASN
1	B	1088	GLN
1	B	1122	GLN
1	B	1145	ASN
1	B	1212	HIS
1	B	1220	HIS
1	B	1284	GLN
1	B	1288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	FAD	B	4005	-	58,58,58	1.28	5 (8%)	85,89,89	1.88	21 (24%)
2	FES	B	4001	1	0,4,4	-	-	-	-	-
5	NAI	A	1333	-	47,48,48	1.58	6 (12%)	64,73,73	2.19	16 (25%)
10	URC	B	1338	9	13,13,13	3.40	5 (38%)	17,19,19	4.53	12 (70%)
5	NAI	B	1333	-	47,48,48	1.50	8 (17%)	64,73,73	1.93	15 (23%)
4	FAD	A	3005	-	58,58,58	1.35	6 (10%)	85,89,89	1.93	21 (24%)
9	MOS	B	1337	8,10	0,2,3	-	-	-	-	-
8	MTE	A	1337	9	21,26,26	1.79	2 (9%)	19,40,40	2.42	10 (52%)
7	GOL	A	1336	-	5,5,5	0.36	0	5,5,5	0.48	0
7	GOL	A	1335	-	5,5,5	1.04	0	5,5,5	1.91	1 (20%)
6	BCT	B	1334	-	3,3,3	0.65	0	2,3,3	0.63	0
7	GOL	B	1335	-	5,5,5	0.55	0	5,5,5	0.76	0
10	URC	A	1339	9	13,13,13	3.65	5 (38%)	17,19,19	4.44	8 (47%)
6	BCT	A	1334	-	3,3,3	0.59	0	2,3,3	0.22	0
9	MOS	A	1338	8,10	0,2,3	-	-	-	-	-
2	FES	A	3002	1	0,4,4	-	-	-	-	-
2	FES	B	4002	1	0,4,4	-	-	-	-	-
8	MTE	B	1336	9	21,26,26	2.12	4 (19%)	19,40,40	2.05	7 (36%)
2	FES	A	3001	1	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAI	A	1333	-	-	2/29/72/72	0/5/5/5
10	URC	A	1339	9	-	-	0/2/2/2
10	URC	B	1338	9	-	-	0/2/2/2
5	NAI	B	1333	-	-	3/29/72/72	0/5/5/5
4	FAD	B	4005	-	-	1/34/50/50	0/6/6/6
4	FAD	A	3005	-	-	0/34/50/50	0/6/6/6
8	MTE	A	1337	9	-	1/6/34/34	0/3/3/3
2	FES	B	4001	1	-	-	0/1/1/1
2	FES	A	3002	1	-	-	0/1/1/1
8	MTE	B	1336	9	-	1/6/34/34	0/3/3/3
2	FES	B	4002	1	-	-	0/1/1/1
7	GOL	A	1336	-	-	2/4/4/4	-
7	GOL	A	1335	-	-	1/4/4/4	-
7	GOL	B	1335	-	-	4/4/4/4	-
2	FES	A	3001	1	-	-	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1338	URC	O24-C8	8.26	1.40	1.23
10	A	1339	URC	O24-C8	8.20	1.40	1.23
8	B	1336	MTE	O4-C4	7.20	1.37	1.23
10	A	1339	URC	C8-N7	6.72	1.54	1.38
10	B	1338	URC	C8-N7	6.49	1.54	1.38
8	A	1337	MTE	O4-C4	5.50	1.34	1.23
5	B	1333	NAI	C4N-C3N	-5.48	1.39	1.50
5	A	1333	NAI	PN-O3	5.42	1.65	1.59
5	A	1333	NAI	C4N-C3N	-4.85	1.40	1.50
10	A	1339	URC	C8-N9	4.79	1.50	1.38
4	B	4005	FAD	C2A-N1A	4.38	1.41	1.33
10	B	1338	URC	C8-N9	4.33	1.48	1.38
4	A	3005	FAD	C4X-N5	4.24	1.39	1.30
4	A	3005	FAD	P-O3P	4.10	1.63	1.59
4	A	3005	FAD	C1'-C2'	3.88	1.58	1.52
8	A	1337	MTE	C10-N8	3.87	1.39	1.35
8	B	1336	MTE	C10-N8	3.64	1.39	1.35
5	B	1333	NAI	PN-O3	3.62	1.63	1.59
5	A	1333	NAI	C4N-C5N	-3.27	1.40	1.49
5	A	1333	NAI	C7N-N7N	-3.23	1.24	1.33
4	B	4005	FAD	C2A-N3A	3.20	1.39	1.33
10	A	1339	URC	O11-C2	3.16	1.30	1.23
10	A	1339	URC	C5-C4	3.15	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1333	NAI	C6N-N1N	3.05	1.44	1.37
5	B	1333	NAI	C4N-C5N	-3.02	1.41	1.49
8	B	1336	MTE	C6-N5	3.00	1.49	1.46
4	A	3005	FAD	C2A-N1A	2.95	1.39	1.33
4	B	4005	FAD	C1'-C2'	2.78	1.56	1.52
4	A	3005	FAD	C8A-N7A	2.68	1.36	1.31
8	B	1336	MTE	C7-C6	2.68	1.55	1.53
5	B	1333	NAI	C7N-N7N	-2.59	1.25	1.33
4	B	4005	FAD	C8A-N7A	2.50	1.36	1.31
4	B	4005	FAD	C4X-N5	2.49	1.36	1.30
10	B	1338	URC	C5-C4	2.46	1.42	1.37
5	B	1333	NAI	C4A-N9A	-2.38	1.32	1.37
5	B	1333	NAI	C6N-C5N	2.29	1.40	1.33
5	B	1333	NAI	C5A-N7A	-2.27	1.34	1.39
5	A	1333	NAI	C6N-N1N	2.27	1.42	1.37
4	A	3005	FAD	PA-O3P	2.15	1.61	1.59
5	A	1333	NAI	C6N-C5N	2.14	1.39	1.33
10	B	1338	URC	O11-C2	2.06	1.27	1.23

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1339	URC	O24-C8-N9	-16.03	96.44	125.56
10	B	1338	URC	O24-C8-N9	-14.94	98.41	125.56
5	A	1333	NAI	N3A-C2A-N1A	-7.23	117.64	128.58
5	B	1333	NAI	N3A-C2A-N1A	-6.94	118.08	128.58
4	B	4005	FAD	N3A-C2A-N1A	-6.46	118.81	128.58
4	A	3005	FAD	N3A-C2A-N1A	-6.29	119.06	128.58
5	A	1333	NAI	N9A-C8A-N7A	-5.90	105.57	113.94
4	A	3005	FAD	O3'-C3'-C2'	-5.61	96.18	108.93
4	A	3005	FAD	C5A-C4A-N3A	-5.15	119.63	126.72
10	B	1338	URC	N7-C8-N9	-4.90	100.28	107.22
10	B	1338	URC	C6-C5-N7	4.89	141.03	131.54
10	A	1339	URC	N7-C8-N9	-4.83	100.37	107.22
4	A	3005	FAD	C9A-C5X-N5	-4.80	117.36	122.45
5	A	1333	NAI	C4A-N9A-C8A	4.60	110.57	105.74
5	A	1333	NAI	C1D-N1N-C2N	-4.57	113.61	121.14
5	B	1333	NAI	C1D-N1N-C2N	-4.52	113.70	121.14
5	B	1333	NAI	C5A-C4A-N3A	-4.35	120.73	126.72
5	A	1333	NAI	C5A-C4A-N3A	-4.35	120.73	126.72
8	A	1337	MTE	C7-C6-N5	4.25	112.04	107.87
5	B	1333	NAI	O3-PN-O2N	-4.22	98.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1336	MTE	C7-C6-N5	4.20	111.99	107.87
8	A	1337	MTE	C2-N1-C10	4.16	120.69	113.36
4	B	4005	FAD	O3'-C3'-C2'	-4.13	99.55	108.93
4	A	3005	FAD	C2A-N3A-C4A	4.11	121.87	111.83
5	A	1333	NAI	C2A-N3A-C4A	4.02	121.64	111.83
5	A	1333	NAI	O1N-PN-O2N	3.93	130.75	112.44
4	B	4005	FAD	C4-N3-C2	-3.86	118.78	125.64
7	A	1335	GOL	O2-C2-C3	-3.84	93.27	109.18
5	A	1333	NAI	C5A-N7A-C8A	3.84	109.48	103.45
4	B	4005	FAD	C5A-C4A-N3A	-3.81	121.47	126.72
8	B	1336	MTE	C2-N1-C10	3.73	119.93	113.36
5	B	1333	NAI	C2A-N3A-C4A	3.67	120.79	111.83
4	B	4005	FAD	N9A-C8A-N7A	-3.67	108.74	113.94
10	A	1339	URC	C6-C5-N7	3.64	138.59	131.54
4	B	4005	FAD	C9A-C5X-N5	-3.63	118.60	122.45
10	B	1338	URC	C5-C4-N9	3.61	113.40	108.31
5	B	1333	NAI	O1N-PN-O2N	3.54	128.91	112.44
8	A	1337	MTE	C9-C4-N3	3.47	121.67	112.13
4	B	4005	FAD	C5A-N7A-C8A	3.45	108.88	103.45
4	B	4005	FAD	C2A-N3A-C4A	3.45	120.26	111.83
5	A	1333	NAI	N3A-C4A-N9A	3.43	133.00	127.17
5	B	1333	NAI	C2A-N1A-C6A	3.42	124.36	118.73
4	A	3005	FAD	C10-C4X-N5	-3.41	117.85	124.81
4	B	4005	FAD	C5'-C4'-C3'	-3.41	105.79	112.22
4	A	3005	FAD	C5X-N5-C4X	3.38	123.55	118.09
5	A	1333	NAI	O3-PN-O2N	-3.32	100.72	110.70
8	A	1337	MTE	O4-C4-C9	-3.27	119.38	127.26
8	A	1337	MTE	C2-N3-C4	-3.26	119.20	125.11
5	A	1333	NAI	O2B-C2B-C1B	-3.20	99.10	110.10
4	B	4005	FAD	C10-C4X-N5	-3.18	118.32	124.81
4	B	4005	FAD	C5X-N5-C4X	3.17	123.22	118.09
4	A	3005	FAD	C5'-C4'-C3'	-3.11	106.35	112.22
10	B	1338	URC	C6-N1-C2	-3.09	122.11	126.37
4	A	3005	FAD	C4-N3-C2	-3.08	120.18	125.64
8	A	1337	MTE	O2P-P-O4'	-3.07	98.66	106.67
8	B	1336	MTE	C9-C4-N3	3.03	120.45	112.13
5	B	1333	NAI	N9A-C8A-N7A	-2.97	109.72	113.94
4	A	3005	FAD	O4'-C4'-C3'	2.96	116.18	109.25
5	B	1333	NAI	C6N-N1N-C2N	-2.93	116.19	119.32
4	B	4005	FAD	O2'-C2'-C3'	-2.93	102.40	109.25
5	A	1333	NAI	C6N-N1N-C2N	-2.90	116.21	119.32
5	B	1333	NAI	N3A-C4A-N9A	2.89	132.08	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3005	FAD	C5A-C4A-N9A	2.87	108.94	105.81
8	B	1336	MTE	C2-N3-C4	-2.86	119.92	125.11
10	B	1338	URC	O11-C2-N3	-2.85	116.80	121.86
10	B	1338	URC	C5-C6-N1	2.81	119.86	112.13
8	A	1337	MTE	O2P-P-O1P	2.81	121.77	110.83
4	B	4005	FAD	O2-C2-N1	-2.79	117.16	121.80
4	B	4005	FAD	N3A-C4A-N9A	2.78	131.89	127.17
5	A	1333	NAI	C2A-N1A-C6A	2.75	123.25	118.73
4	A	3005	FAD	C4A-C5A-N7A	-2.73	107.46	110.58
5	A	1333	NAI	C2B-C1B-N9A	2.72	120.07	113.30
10	B	1338	URC	C5-N7-C8	2.72	112.32	108.82
5	B	1333	NAI	O4D-C1D-N1N	2.72	113.26	108.08
10	A	1339	URC	C5-C6-N1	2.68	119.49	112.13
8	B	1336	MTE	O4-C4-C9	-2.67	120.82	127.26
10	B	1338	URC	O24-C8-N7	2.67	130.41	125.56
4	A	3005	FAD	O2'-C2'-C3'	-2.66	103.01	109.25
4	A	3005	FAD	C6-C5X-C9A	2.65	122.69	119.05
5	A	1333	NAI	O4D-C4D-C3D	-2.62	99.94	105.15
8	B	1336	MTE	O3'-C7-N8	2.62	110.99	108.61
4	B	4005	FAD	C4X-C10-N10	2.62	120.23	116.48
4	A	3005	FAD	O5'-C5'-C4'	-2.60	102.43	109.36
10	B	1338	URC	C4-C5-N7	-2.58	104.60	107.36
10	A	1339	URC	O24-C8-N7	2.57	130.23	125.56
4	A	3005	FAD	C4X-C10-N10	2.55	120.14	116.48
4	B	4005	FAD	O4B-C1B-N9A	-2.53	103.23	108.09
10	A	1339	URC	C6-N1-C2	-2.52	122.90	126.37
4	A	3005	FAD	N3A-C4A-N9A	2.50	131.42	127.17
10	B	1338	URC	O13-C6-N1	-2.48	115.46	120.11
8	A	1337	MTE	O3'-C7-N8	2.47	110.85	108.61
4	B	4005	FAD	C6-C5X-C9A	2.40	122.34	119.05
4	A	3005	FAD	C5A-N7A-C8A	2.38	107.19	103.45
5	B	1333	NAI	C1D-N1N-C6N	-2.38	115.74	120.77
10	B	1338	URC	N9-C4-N3	-2.34	122.55	128.19
4	A	3005	FAD	C4-C4X-N5	2.34	121.44	118.21
5	B	1333	NAI	C4A-N9A-C8A	2.34	108.19	105.74
8	A	1337	MTE	O3'-C7-C6	-2.28	107.44	108.96
4	B	4005	FAD	C4X-C4-N3	2.20	118.85	113.25
8	A	1337	MTE	C4-C9-N5	2.20	122.26	116.27
4	A	3005	FAD	O2P-P-O3P	2.19	113.18	107.27
4	B	4005	FAD	C4A-C5A-N7A	-2.18	108.09	110.58
4	B	4005	FAD	O3B-C3B-C4B	-2.17	104.86	111.08
8	B	1336	MTE	C4-C9-N5	2.17	122.17	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1333	NAI	C4A-C5A-N7A	-2.16	108.11	110.58
10	A	1339	URC	O13-C6-C5	-2.08	122.24	127.26
10	A	1339	URC	C5-C4-N9	2.08	111.24	108.31
5	B	1333	NAI	C3D-C2D-C1D	2.07	105.39	101.46
4	A	3005	FAD	O2'-C2'-C1'	2.07	118.69	110.20
5	B	1333	NAI	C4A-C5A-N7A	-2.04	108.24	110.58
4	B	4005	FAD	C4-C4X-C10	2.03	120.41	116.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

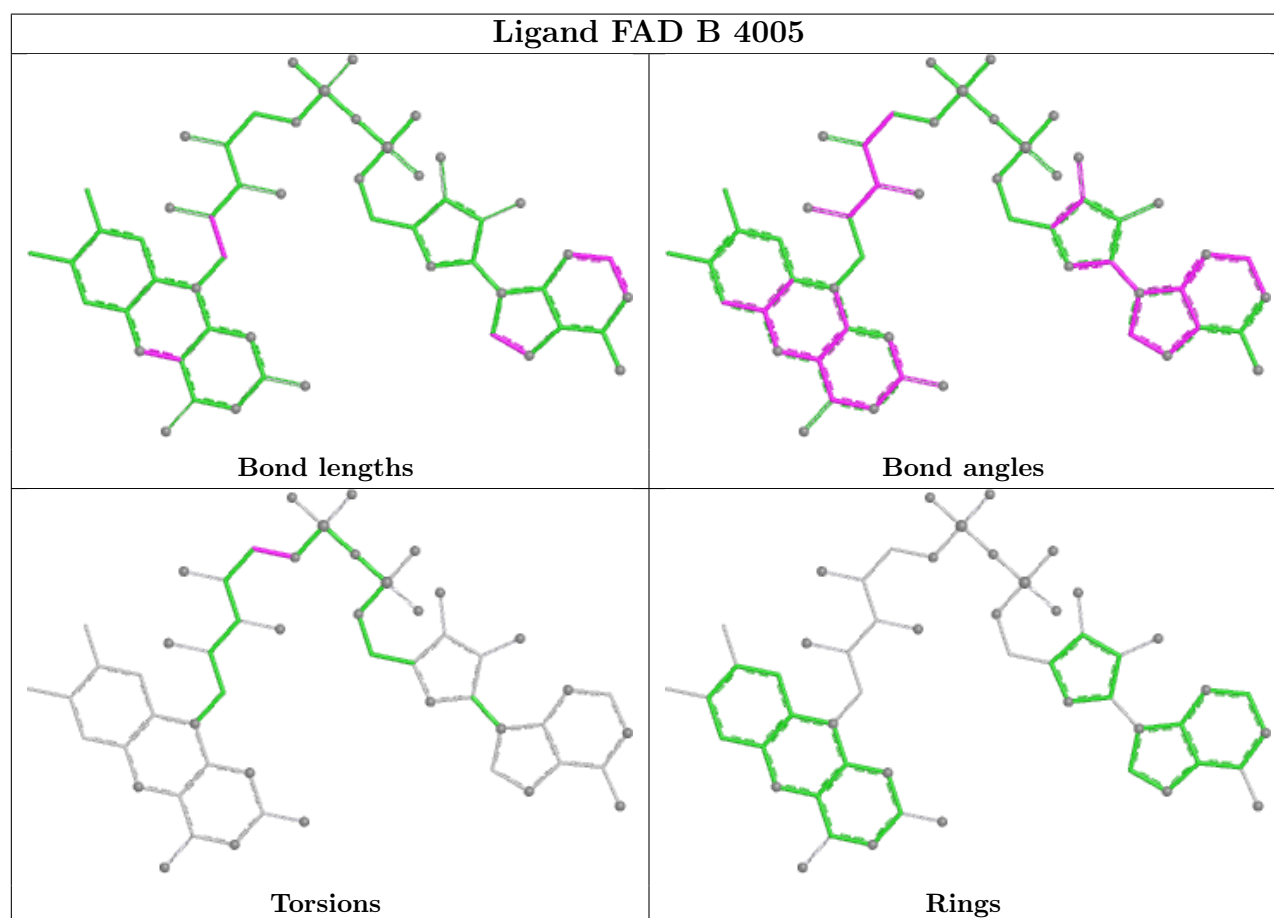
Mol	Chain	Res	Type	Atoms
7	A	1336	GOL	O1-C1-C2-C3
5	A	1333	NAI	C2D-C1D-N1N-C6N
5	B	1333	NAI	C2D-C1D-N1N-C6N
8	B	1336	MTE	C3'-C4'-O4'-P
7	A	1335	GOL	C1-C2-C3-O3
7	B	1335	GOL	O1-C1-C2-C3
7	B	1335	GOL	C1-C2-C3-O3
7	A	1336	GOL	O1-C1-C2-O2
8	A	1337	MTE	C3'-C4'-O4'-P
7	B	1335	GOL	O2-C2-C3-O3
7	B	1335	GOL	O1-C1-C2-O2
5	A	1333	NAI	O4D-C1D-N1N-C6N
4	B	4005	FAD	C4'-C5'-O5'-P
5	B	1333	NAI	O4D-C1D-N1N-C6N
5	B	1333	NAI	O4D-C4D-C5D-O5D

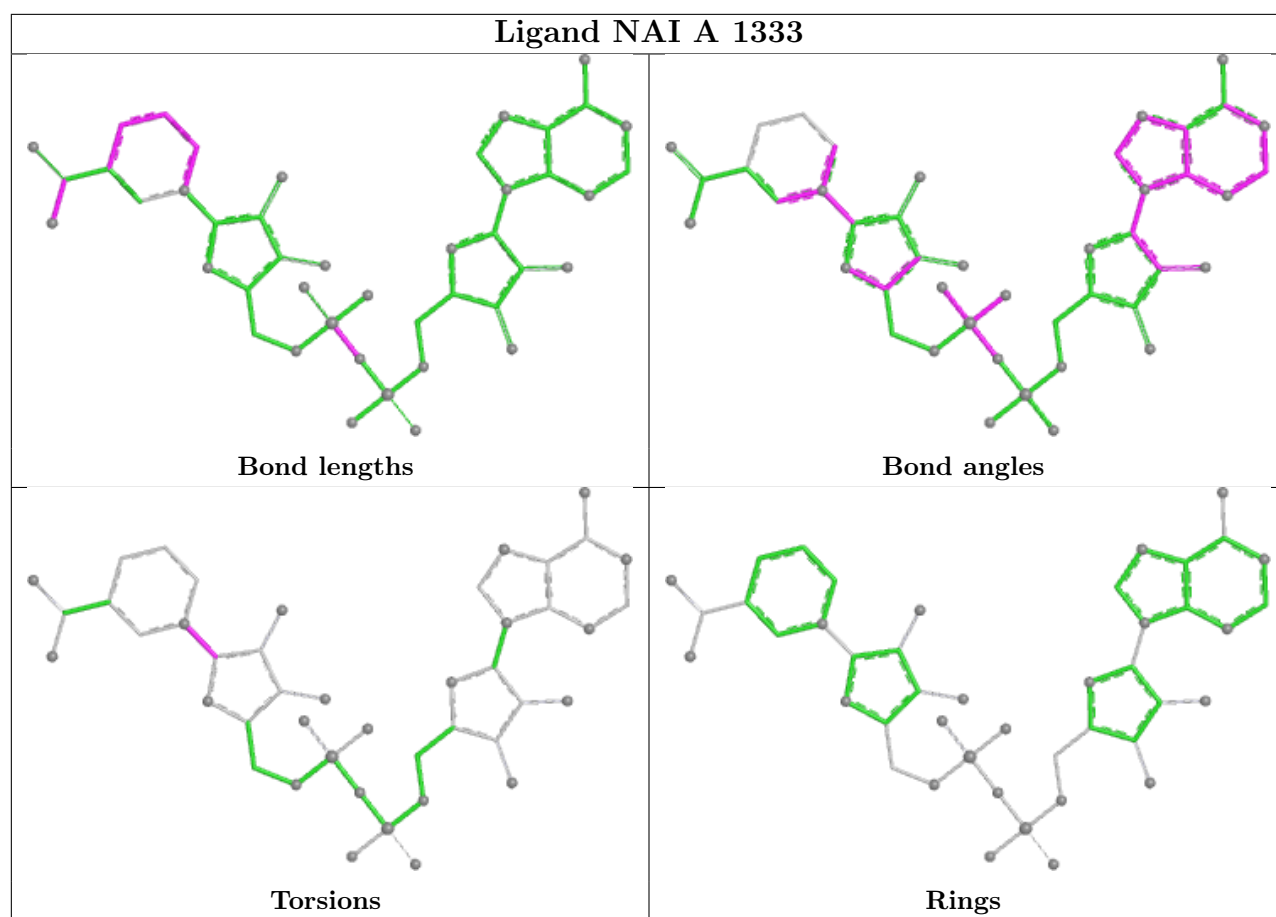
There are no ring outliers.

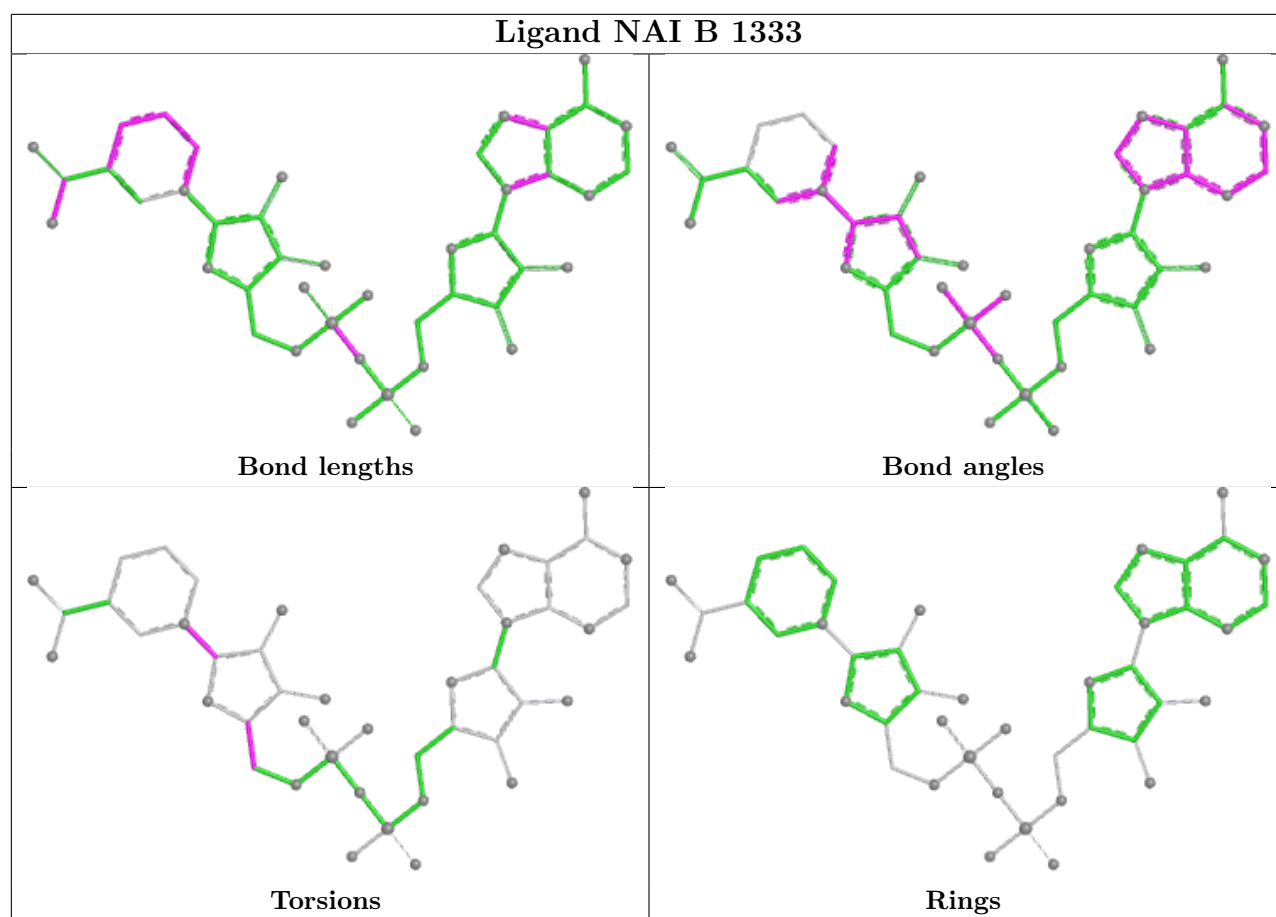
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4005	FAD	6	0
5	A	1333	NAI	4	0
5	B	1333	NAI	3	0
4	A	3005	FAD	4	0
9	B	1337	MOS	1	0
8	A	1337	MTE	1	0
7	B	1335	GOL	1	0
9	A	1338	MOS	2	0

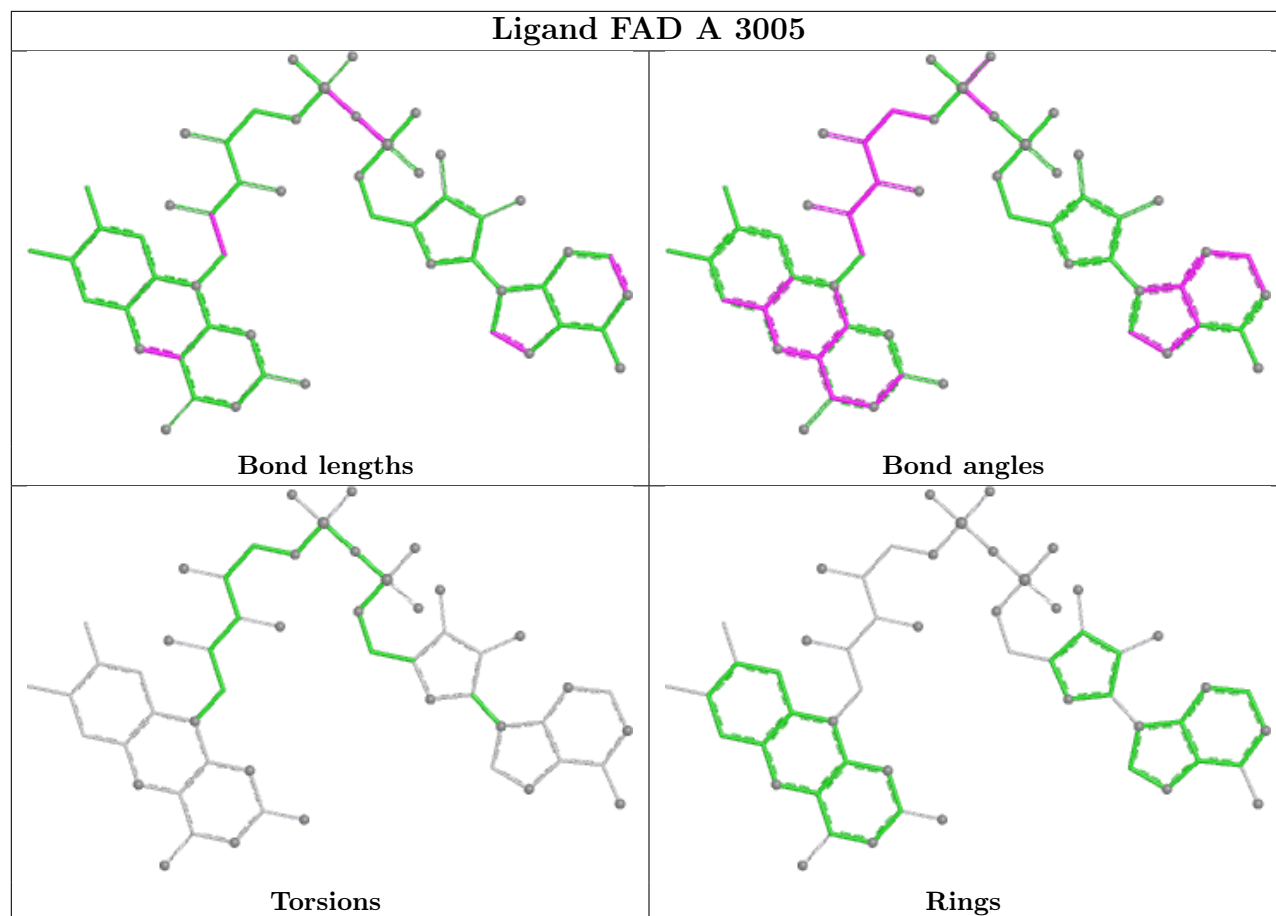
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



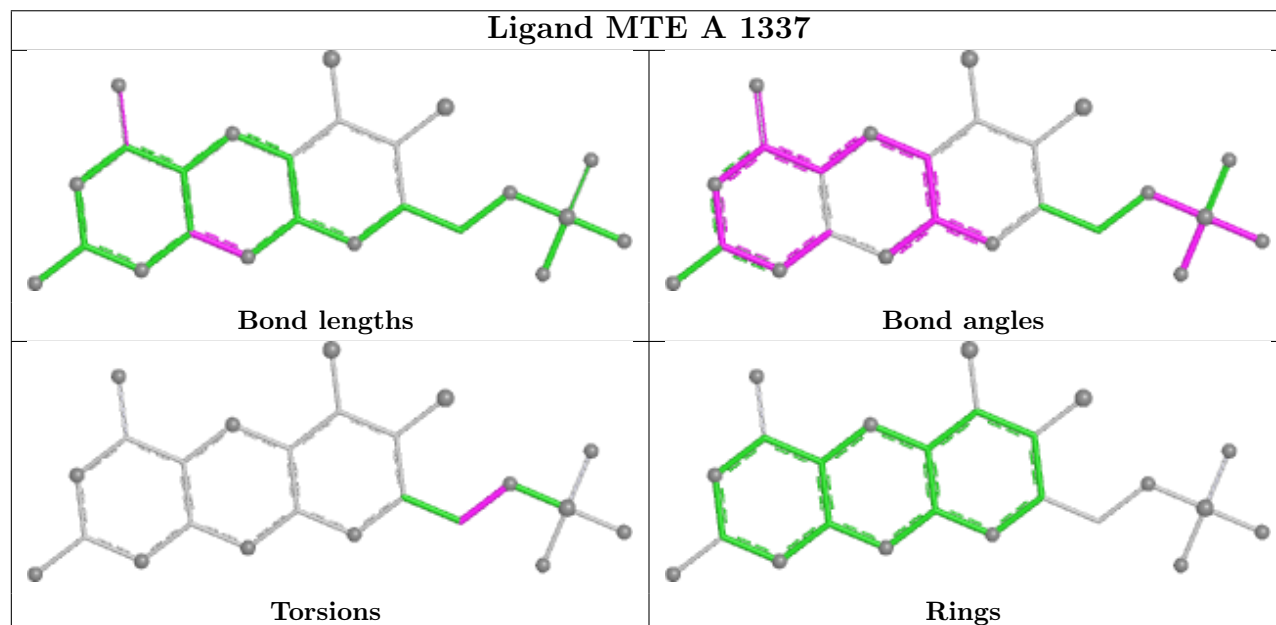


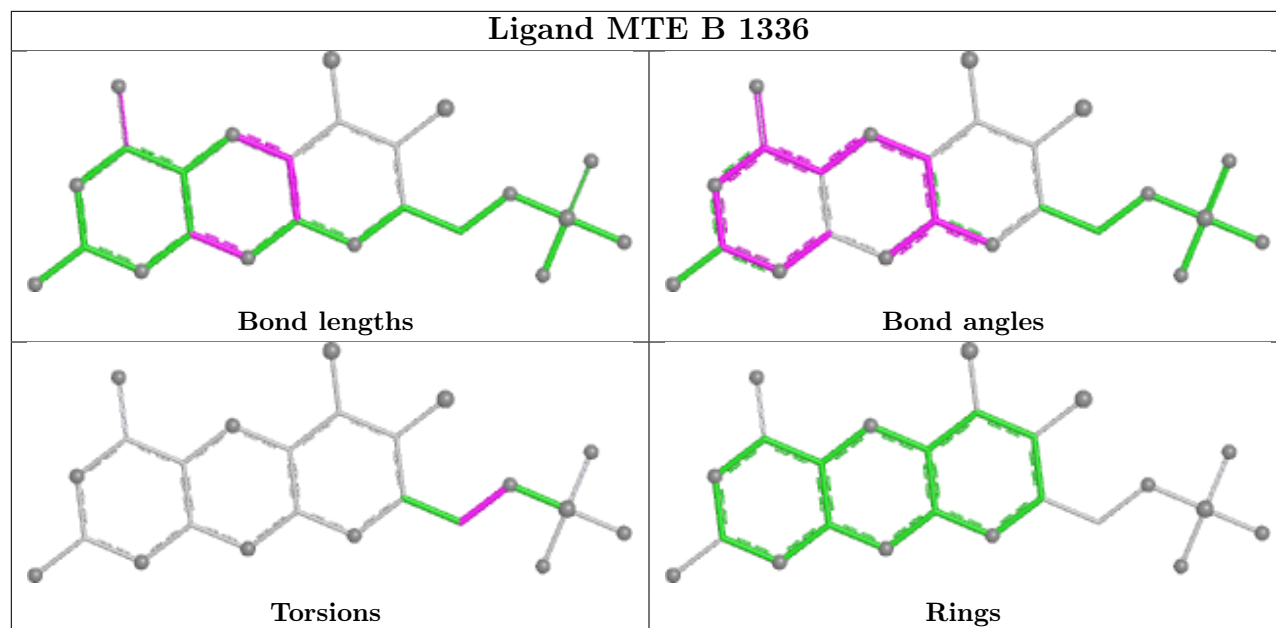


Ligand FAD A 3005



Ligand MTE A 1337





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	1291/1332 (96%)	-0.60	11 (0%) 81 83	12, 22, 39, 66	0
1	B	1289/1332 (96%)	-0.65	8 (0%) 85 87	12, 22, 39, 65	0
All	All	2580/2664 (96%)	-0.63	19 (0%) 84 86	12, 22, 39, 66	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	LEU	4.7
1	B	1318	VAL	4.3
1	A	378	GLY	2.9
1	A	528	GLY	2.8
1	A	1318	VAL	2.7
1	A	61	LEU	2.7
1	A	1287	ASN	2.6
1	B	1287	ASN	2.6
1	A	60	ARG	2.6
1	B	1288	ASN	2.5
1	B	565	ASN	2.4
1	A	552	HIS	2.4
1	B	551	LYS	2.4
1	B	61	LEU	2.3
1	A	1286	THR	2.2
1	A	1288	ASN	2.2
1	B	552	HIS	2.1
1	B	1290	THR	2.1
1	A	3	ALA	2.1

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

There are no oligosaccharides in this entry.

6.4 Ligands

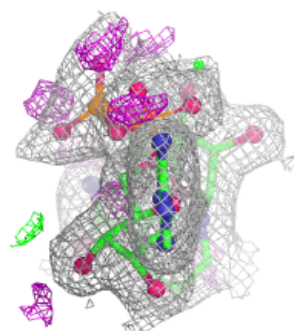
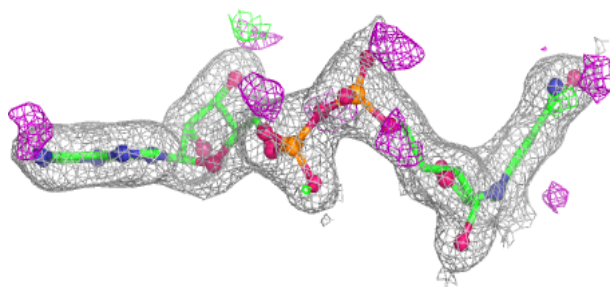
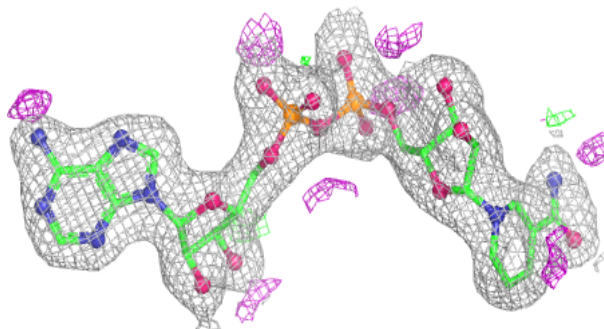
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1335	6/6	0.88	0.11	28,39,39,41	0
10	URC	A	1339	12/12	0.90	0.11	30,34,37,39	0
10	URC	B	1338	12/12	0.92	0.10	31,38,41,43	0
7	GOL	B	1335	6/6	0.94	0.08	29,35,39,40	0
6	BCT	A	1334	4/4	0.96	0.06	17,20,20,22	0
5	NAI	A	1333	44/44	0.96	0.06	18,25,29,33	0
7	GOL	A	1336	6/6	0.96	0.06	23,27,31,32	0
5	NAI	B	1333	44/44	0.97	0.05	18,25,28,31	0
4	FAD	A	3005	53/53	0.98	0.05	14,19,24,28	0
4	FAD	B	4005	53/53	0.98	0.04	15,18,21,28	0
8	MTE	A	1337	24/24	0.99	0.04	14,19,24,25	0
8	MTE	B	1336	24/24	0.99	0.03	15,20,23,25	0
9	MOS	A	1338	3/4	0.99	0.10	25,25,27,40	0
9	MOS	B	1337	3/4	0.99	0.10	27,27,27,39	0
6	BCT	B	1334	4/4	0.99	0.03	16,17,18,19	0
3	CA	A	3008	1/1	0.99	0.03	20,20,20,20	0
2	FES	A	3002	4/4	1.00	0.01	15,15,17,18	0
2	FES	B	4001	4/4	1.00	0.02	14,15,16,16	0
2	FES	B	4002	4/4	1.00	0.02	14,15,16,16	0
2	FES	A	3001	4/4	1.00	0.01	15,15,16,17	0
3	CA	B	4008	1/1	1.00	0.02	19,19,19,19	0

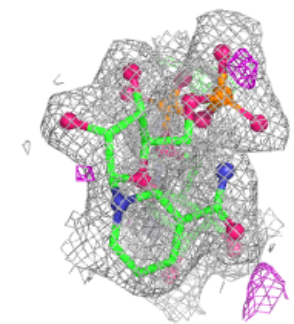
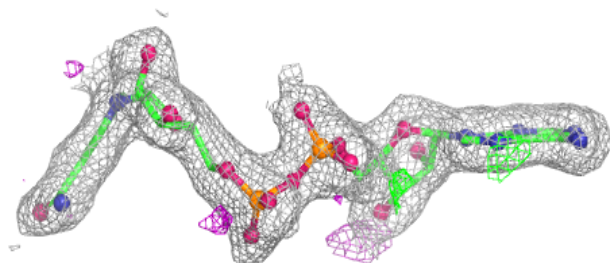
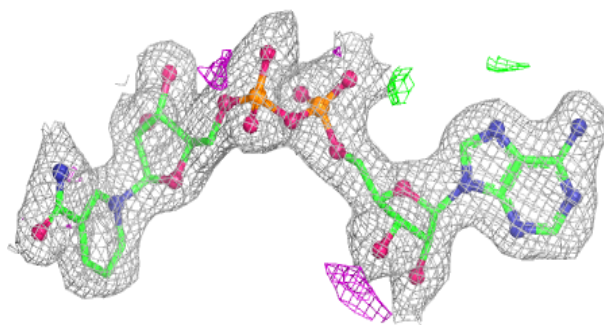
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 1333:

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

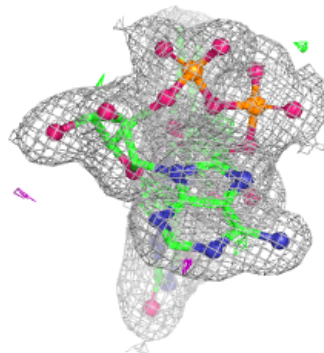
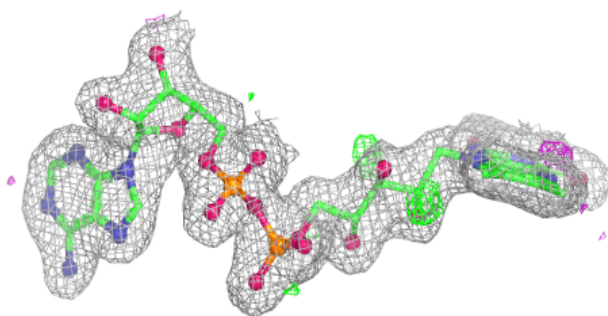
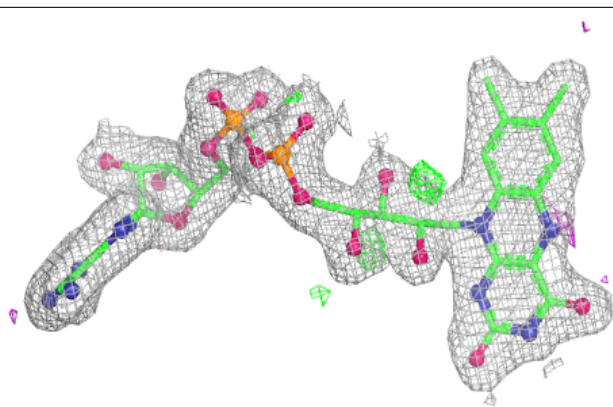
**Electron density around NAI B 1333:**

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

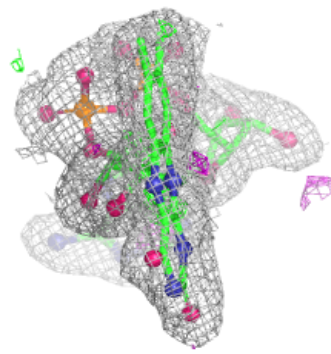
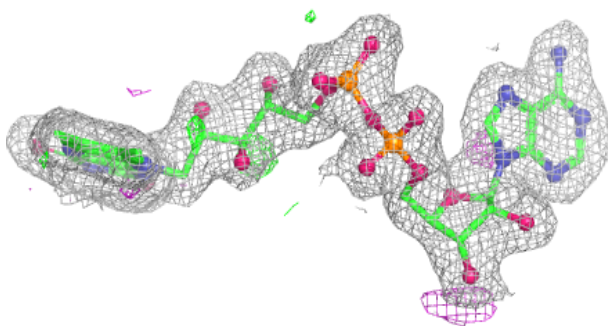
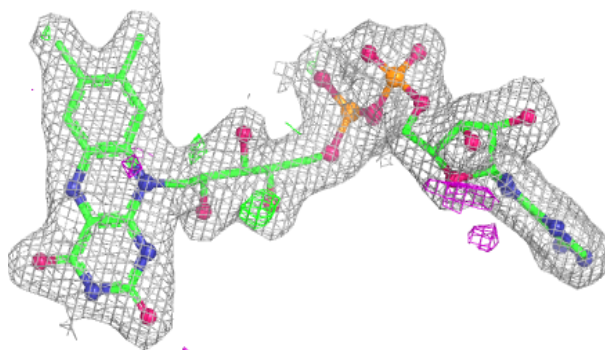


Electron density around FAD A 3005:

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

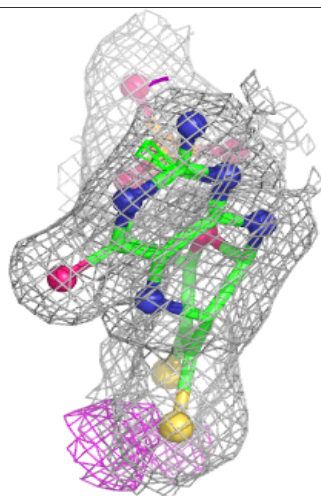
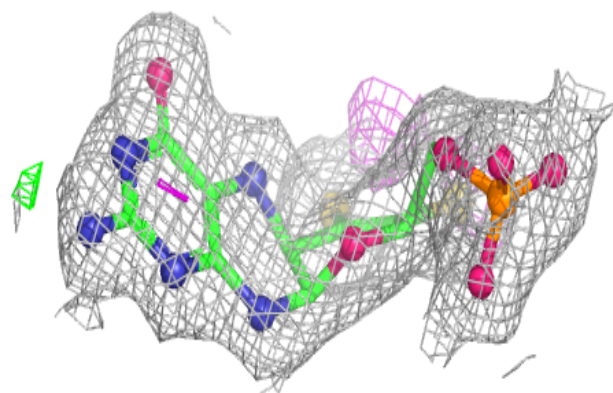
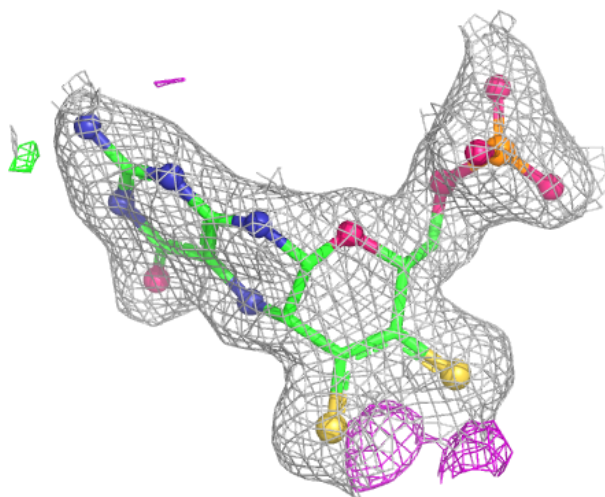
**Electron density around FAD B 4005:**

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



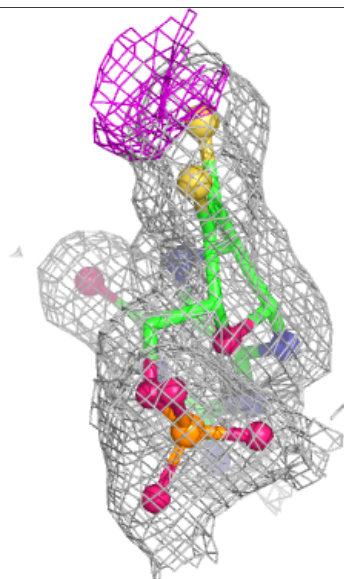
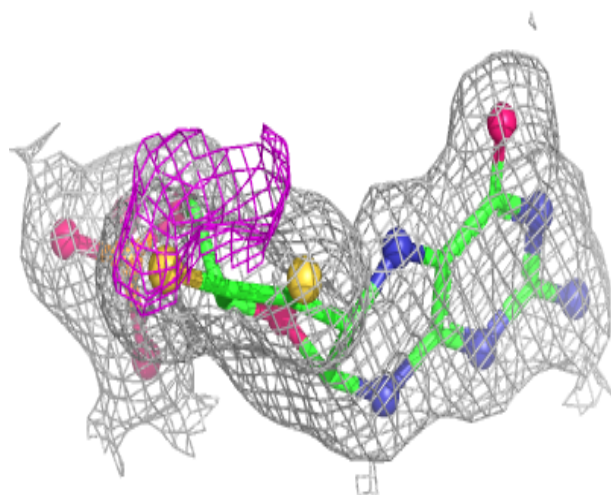
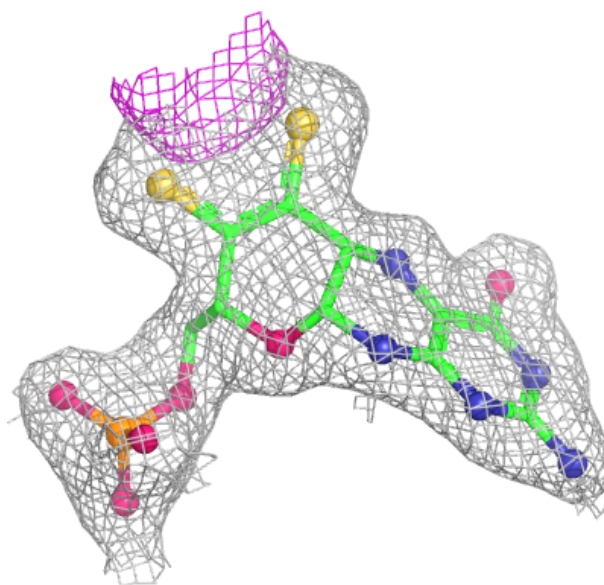
Electron density around MTE A 1337:

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



Electron density around MTE B 1336:

$2mF_o-DF_c$ (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.