



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:41 PM UTC

PDB ID : 4YSW / pdb_00004ysw
Title : Structure of rat xanthine oxidoreductase, C-terminal deletion protein variant, NADH bound form
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Matsumura, T.; Eger, B.T.; Pai, E.F.
Deposited on : 2015-03-17
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

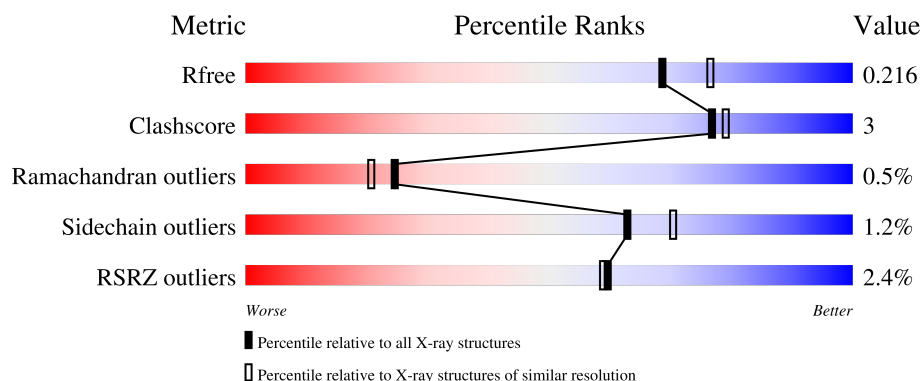
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

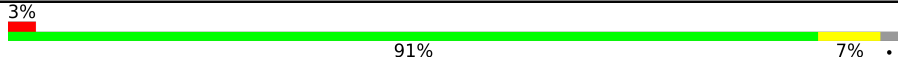
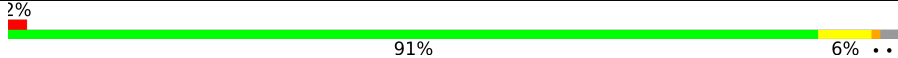
The reported resolution of this entry is 1.99 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1315	
1	B	1315	

2 Entry composition [i](#)

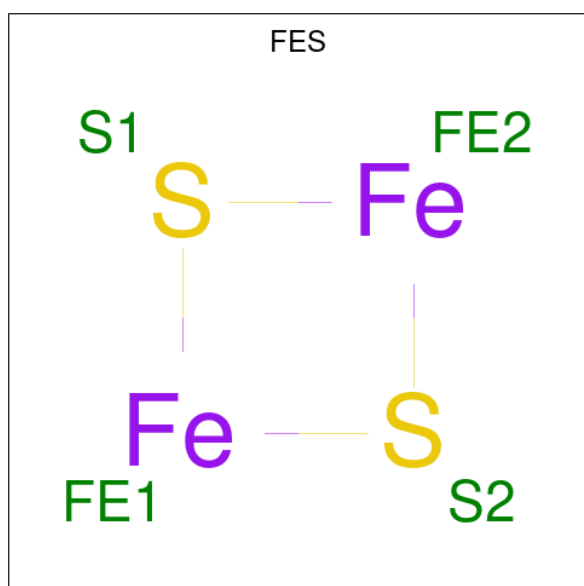
There are 9 unique types of molecules in this entry. The entry contains 21749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1286	Total	C	N	O	S	0	0	0
			9941	6301	1711	1866	63			
1	B	1286	Total	C	N	O	S	0	0	0
			9940	6301	1711	1865	63			

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

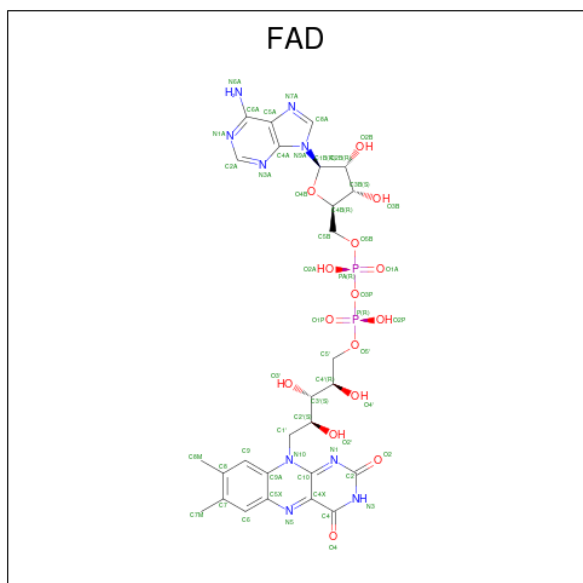


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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

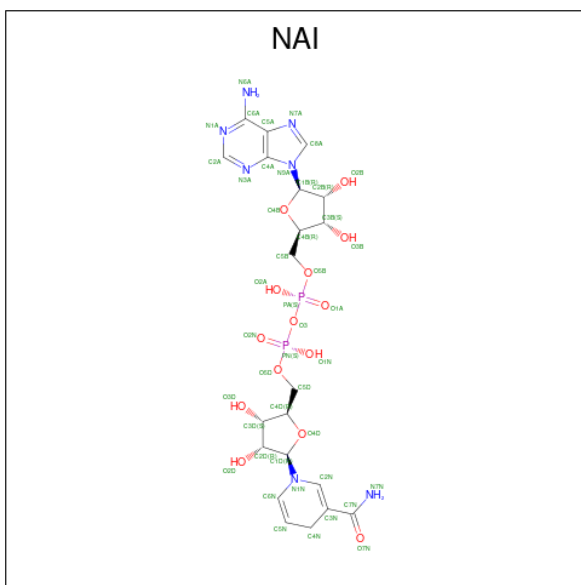
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



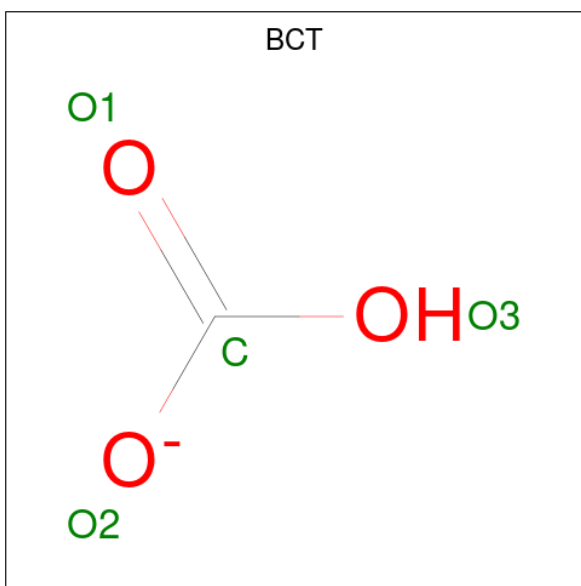
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).



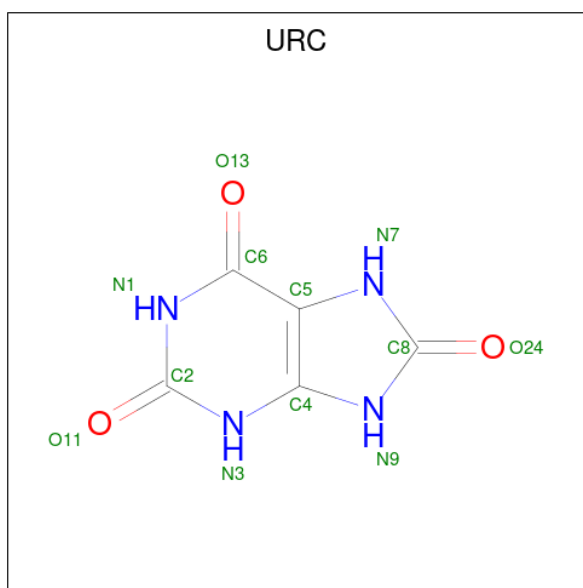
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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



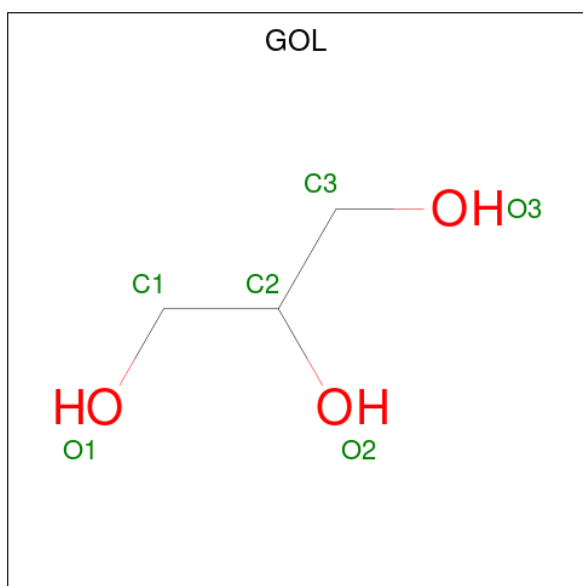
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	B	1	Total C O 4 1 3	0	0

- Molecule 7 is URIC ACID (CCD ID: URC) (formula: $C_5H_4N_4O_3$).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

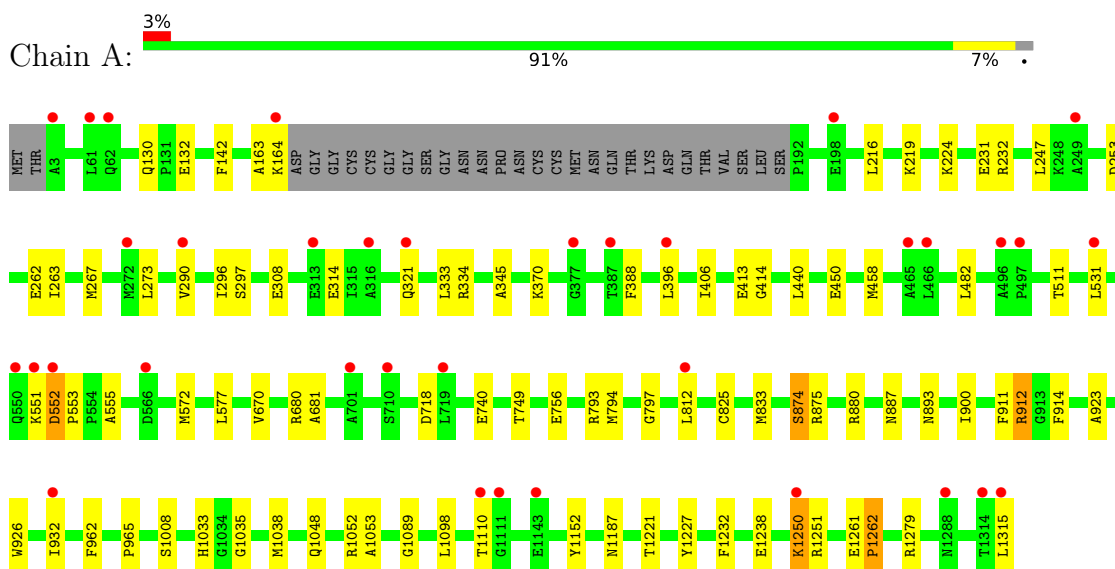
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	698	Total	O	0	0
			698	698		
9	B	914	Total	O	0	0
			914	914		

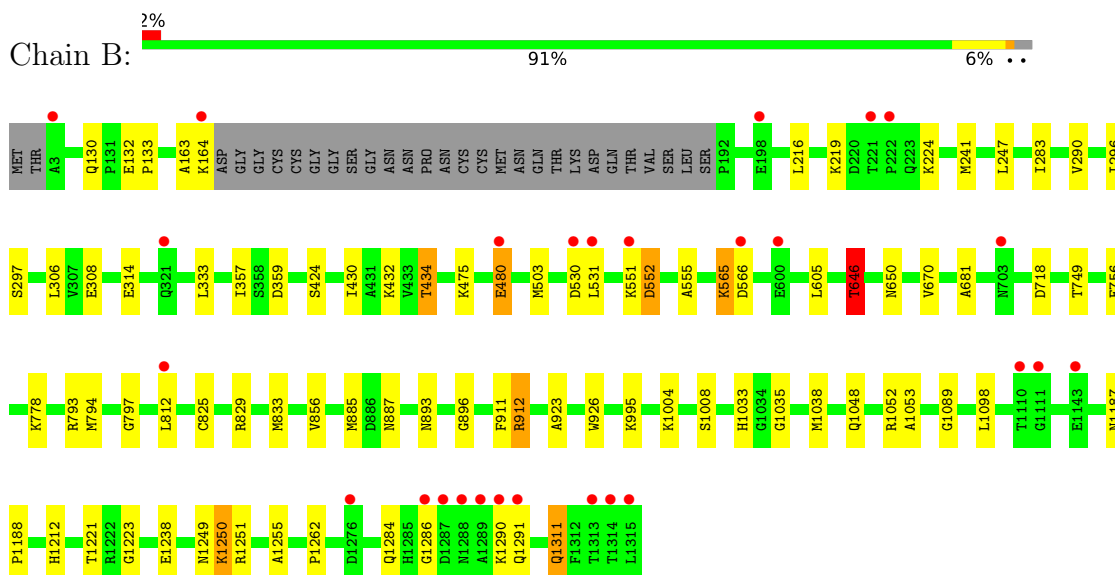
3 Residue-property plots [i](#)

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

• Molecule 1: Xanthine dehydrogenase/oxidase



• Molecule 1: Xanthine dehydrogenase/oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.46Å 137.64Å 222.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.41 – 1.99 42.41 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.41-1.99) 94.7 (42.41-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.219 0.180 , 0.216	Depositor DCC
R_{free} test set	9850 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21749	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BCT, NAI, URC, CA, FES, FAD

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	0.53	0/10151	0.77	2/13736 (0.0%)
1	B	0.58	0/10150	0.77	2/13734 (0.0%)
All	All	0.56	0/20301	0.77	4/27470 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1262	PRO	N-CA-C	6.55	118.70	110.70
1	A	1262	PRO	N-CA-C	6.19	118.25	110.70
1	A	874	SER	N-CA-C	5.74	118.28	111.33
1	B	646	THR	CB-CA-C	-5.68	99.12	110.42

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	9941	0	9948	53	0
1	B	9940	0	9948	65	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	53	0	31	2	0
4	B	53	0	31	0	0
5	A	44	0	27	0	0
5	B	44	0	27	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	12	0	4	0	0
7	B	12	0	4	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	698	0	0	2	0
9	B	914	0	0	6	0
All	All	21749	0	20036	115	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 3.

All (115) 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:B:1089:GLY:HA3	9:B:4609:HOH:O	1.06	1.22
1:A:1089:GLY:HA3	9:A:3449:HOH:O	1.02	1.17
1:B:749:THR:HB	1:B:812:LEU:HD12	1.37	1.02
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.44	0.99
1:B:1311:GLN:HE21	1:B:1311:GLN:H	1.16	0.93
1:B:565:LYS:HD3	1:B:565:LYS:H	1.36	0.91
1:B:646:THR:HG23	9:B:4276:HOH:O	1.71	0.90
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.56	0.87
1:B:565:LYS:H	1:B:565:LYS:CD	1.93	0.81
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.67	0.76
1:B:565:LYS:HD3	1:B:565:LYS:N	2.00	0.76
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.70	0.74
1:A:749:THR:HB	1:A:812:LEU:HD12	1.72	0.71
1:B:130:GLN:HE21	1:B:132:GLU:H	1.37	0.71
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.71	0.70
1:B:551:LYS:O	1:B:552:ASP:HB2	1.92	0.69
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.93	0.66
1:B:359:ASP:OD2	1:B:434:THR:HG21	1.95	0.66
1:A:232:ARG:NH1	1:A:273:LEU:HD13	2.11	0.65
1:B:718:ASP:H	1:B:893:ASN:HD22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:ARG:HD2	1:B:833:MET:HE2	1.81	0.63
1:A:130:GLN:HE21	1:A:132:GLU:H	1.47	0.62
1:A:749:THR:HB	1:A:812:LEU:CD1	2.29	0.62
1:B:290:VAL:HG22	1:B:297:SER:HB2	1.81	0.62
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.30	0.61
1:B:749:THR:HB	1:B:812:LEU:CD1	2.24	0.60
1:B:829:ARG:HG3	1:B:833:MET:HE3	1.84	0.60
1:A:718:ASP:H	1:A:893:ASN:HD22	1.51	0.59
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.85	0.59
1:B:812:LEU:HD21	1:B:825:CYS:CB	2.33	0.58
1:B:359:ASP:OD2	1:B:434:THR:CG2	2.52	0.57
1:B:1250:LYS:HG3	9:B:4316:HOH:O	2.05	0.57
1:A:740:GLU:HG2	1:A:833:MET:HE3	1.85	0.57
1:B:718:ASP:H	1:B:893:ASN:ND2	2.03	0.56
1:A:232:ARG:HH11	1:A:273:LEU:HD13	1.71	0.55
1:A:718:ASP:H	1:A:893:ASN:ND2	2.04	0.55
1:B:1311:GLN:H	1:B:1311:GLN:NE2	1.96	0.55
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.53	0.55
1:B:359:ASP:HA	1:B:434:THR:HG21	1.87	0.55
1:B:605:LEU:HD13	1:B:812:LEU:HD23	1.89	0.55
1:A:794:MET:HE3	1:A:1038:MET:HB3	1.90	0.54
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.91	0.52
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.90	0.52
1:B:833:MET:CE	1:B:1223:GLY:HA2	2.40	0.52
1:B:432:LYS:HE2	1:B:503:MET:SD	2.50	0.52
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.91	0.52
1:B:216:LEU:O	1:B:219:LYS:HG3	2.09	0.52
1:A:216:LEU:O	1:A:219:LYS:HG3	2.10	0.52
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.59	0.51
1:A:345:ALA:HB1	4:A:3004:FAD:H4'	1.92	0.51
1:B:224:LYS:H	1:B:224:LYS:HD2	1.76	0.50
1:B:1033:HIS:CD2	1:B:1035:GLY:H	2.29	0.50
1:B:475:LYS:HD3	1:B:480:GLU:OE2	2.12	0.50
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.60	0.49
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.76	0.49
1:B:1221:THR:HG22	9:B:4952:HOH:O	2.13	0.49
1:B:794:MET:HE3	1:B:1038:MET:HB3	1.95	0.49
1:A:458:MET:HE2	1:A:511:THR:HG21	1.95	0.49
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.27	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:A:932:ILE:HD11	9:A:3689:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:MET:HE2	1:A:577:LEU:HD13	1.95	0.48
1:A:911:PHE:O	1:A:912:ARG:C	2.57	0.47
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.14	0.47
1:A:263:ILE:HG22	1:A:267:MET:HE2	1.96	0.47
1:A:875:ARG:HG2	1:A:900:ILE:HD13	1.97	0.47
1:B:1048:GLN:HE22	1:B:1187:ASN:HB2	1.80	0.47
1:A:932:ILE:HD13	1:A:1279:ARG:NH2	2.30	0.46
1:A:1048:GLN:HE22	1:A:1187:ASN:HB2	1.80	0.46
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.39	0.46
1:B:308:GLU:HG3	1:B:333:LEU:HD13	1.97	0.46
1:A:756:GLU:CD	1:B:793:ARG:HH12	2.23	0.46
1:B:296:ILE:HD11	1:B:314:GLU:HG3	1.96	0.46
1:A:756:GLU:OE2	1:B:793:ARG:NH1	2.42	0.45
1:A:308:GLU:HG3	1:A:333:LEU:HD13	1.98	0.45
1:A:321:GLN:HE21	1:A:414:GLY:H	1.63	0.45
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.61	0.45
1:A:163:ALA:O	1:A:164:LYS:HB2	2.17	0.45
1:B:911:PHE:O	1:B:912:ARG:C	2.59	0.45
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.46	0.45
1:A:1152:TYR:HB3	1:A:1251:ARG:HD2	1.98	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.45
1:B:1250:LYS:HD2	1:B:1251:ARG:N	2.32	0.44
1:B:164:LYS:HD3	9:B:4891:HOH:O	2.17	0.44
1:B:1212:HIS:HD2	9:B:4967:HOH:O	2.00	0.44
1:B:1250:LYS:HD2	1:B:1251:ARG:H	1.81	0.44
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.51	0.44
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.53	0.44
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.36	0.44
1:B:833:MET:HE1	1:B:1223:GLY:HA2	1.98	0.44
1:B:424:SER:OG	1:B:432:LYS:NZ	2.51	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.18	0.43
1:B:357:ILE:HD13	1:B:430:ILE:HG23	2.00	0.43
1:A:388:PHE:HA	1:A:396:LEU:HG	2.00	0.43
1:A:440:LEU:HB3	1:A:450:GLU:HB2	2.00	0.43
1:A:1250:LYS:HD3	1:A:1251:ARG:N	2.34	0.43
1:B:749:THR:O	1:B:812:LEU:HD13	2.19	0.43
1:A:262:GLU:HB2	4:A:3004:FAD:H52A	2.01	0.43
1:B:555:ALA:HB3	1:B:1238:GLU:HG2	1.99	0.43
1:B:565:LYS:H	1:B:565:LYS:CE	2.32	0.43
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.19	0.42
1:A:880:ARG:HD2	1:A:914:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.50	0.42
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.50	0.42
1:B:885:MET:SD	1:B:896:GLY:HA3	2.59	0.42
1:A:142:PHE:HB3	1:A:1232:PHE:CE1	2.55	0.41
1:A:334:ARG:HH21	1:A:551:LYS:NZ	2.18	0.41
1:B:833:MET:HE3	1:B:1223:GLY:HA2	2.02	0.41
1:B:1311:GLN:HE21	1:B:1311:GLN:N	1.98	0.41
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.54	0.41
1:B:1187:ASN:HA	1:B:1188:PRO:HD2	1.94	0.41
1:B:133:PRO:O	1:B:163:ALA:HA	2.21	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.40
1:A:793:ARG:HH12	1:B:756:GLU:CD	2.30	0.40
1:A:552:ASP:HA	1:A:553:PRO:HD3	1.86	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	1282/1315 (98%)	1245 (97%)	32 (2%)	5 (0%)	30	27
1	B	1282/1315 (98%)	1245 (97%)	30 (2%)	7 (0%)	24	21
All	All	2564/2630 (98%)	2490 (97%)	62 (2%)	12 (0%)	24	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY

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Mol	Chain	Res	Type
1	B	552	ASP
1	B	797	GLY
1	B	1290	LYS
1	A	552	ASP
1	A	887	ASN
1	B	887	ASN
1	B	1286	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1085/1109 (98%)	1074 (99%)	11 (1%)	68	75
1	B	1085/1109 (98%)	1070 (99%)	15 (1%)	59	66
All	All	2170/2218 (98%)	2144 (99%)	26 (1%)	63	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	A	247	LEU
1	A	253	ASP
1	A	370	LYS
1	A	406	ILE
1	A	482	LEU
1	A	531	LEU
1	A	1052	ARG
1	A	1110	THR
1	A	1250	LYS
1	A	1315	LEU
1	B	247	LEU
1	B	306	LEU
1	B	434	THR
1	B	480	GLU
1	B	530	ASP

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Mol	Chain	Res	Type
1	B	531	LEU
1	B	565	LYS
1	B	566	ASP
1	B	646	THR
1	B	856	VAL
1	B	1004	LYS
1	B	1052	ARG
1	B	1250	LYS
1	B	1291	GLN
1	B	1311	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	81	HIS
1	A	130	GLN
1	A	145	ASN
1	A	250	GLN
1	A	260	ASN
1	A	321	GLN
1	A	449	GLN
1	A	583	ASN
1	A	585	GLN
1	A	699	GLN
1	A	705	ASN
1	A	728	ASN
1	A	869	ASN
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1173	ASN
1	A	1194	GLN
1	A	1220	HIS
1	A	1294	GLN
1	B	130	GLN
1	B	145	ASN
1	B	250	GLN
1	B	472	GLN
1	B	583	ASN
1	B	585	GLN
1	B	705	ASN

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Mol	Chain	Res	Type
1	B	869	ASN
1	B	893	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1173	ASN
1	B	1220	HIS
1	B	1284	GLN
1	B	1285	HIS
1	B	1288	ASN
1	B	1311	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](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
8	GOL	A	3008	-	5,5,5	0.35	0	5,5,5	0.47	0
2	FES	B	4002	1	0,4,4	-	-	-		
2	FES	A	3001	1	0,4,4	-	-	-		
6	BCT	A	3006	-	3,3,3	0.55	0	2,3,3	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	URC	A	3007	-	13,13,13	3.47	2 (15%)	17,19,19	2.54	6 (35%)
6	BCT	B	4006	-	3,3,3	0.54	0	2,3,3	0.39	0
8	GOL	B	4008	-	5,5,5	0.34	0	5,5,5	0.74	0
4	FAD	A	3004	-	58,58,58	1.16	5 (8%)	85,89,89	1.55	14 (16%)
2	FES	B	4001	1	0,4,4	-	-	-	-	-
7	URC	B	4007	-	13,13,13	3.33	2 (15%)	17,19,19	2.70	8 (47%)
5	NAI	B	4005	-	47,48,48	1.35	6 (12%)	64,73,73	1.55	11 (17%)
2	FES	A	3002	1	0,4,4	-	-	-	-	-
5	NAI	A	3005	-	47,48,48	1.38	7 (14%)	64,73,73	1.74	13 (20%)
4	FAD	B	4004	-	58,58,58	1.10	7 (12%)	85,89,89	1.56	15 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	3008	-	-	0/4/4/4	-
2	FES	B	4002	1	-	-	0/1/1/1
2	FES	A	3001	1	-	-	0/1/1/1
7	URC	A	3007	-	-	-	0/2/2/2
8	GOL	B	4008	-	-	3/4/4/4	-
4	FAD	A	3004	-	-	5/34/50/50	0/6/6/6
2	FES	B	4001	1	-	-	0/1/1/1
7	URC	B	4007	-	-	-	0/2/2/2
5	NAI	B	4005	-	-	5/29/72/72	0/5/5/5
2	FES	A	3002	1	-	-	0/1/1/1
5	NAI	A	3005	-	-	3/29/72/72	0/5/5/5
4	FAD	B	4004	-	-	5/34/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3007	URC	O24-C8	11.75	1.48	1.23
7	B	4007	URC	O24-C8	11.27	1.47	1.23
5	A	3005	NAI	C4N-C3N	-5.40	1.39	1.50
5	B	4005	NAI	C4N-C3N	-5.20	1.40	1.50
4	A	3004	FAD	C4X-N5	3.74	1.38	1.30
5	A	3005	NAI	C4N-C5N	-3.62	1.39	1.49
4	B	4004	FAD	C4X-N5	3.44	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4005	NAI	C4N-C5N	-3.25	1.40	1.49
4	A	3004	FAD	PA-O3P	2.86	1.62	1.59
4	A	3004	FAD	C10-N1	2.71	1.38	1.33
4	A	3004	FAD	C2A-N3A	2.70	1.38	1.33
4	B	4004	FAD	PA-O3P	2.68	1.62	1.59
4	A	3004	FAD	C2A-N1A	2.63	1.38	1.33
5	A	3005	NAI	PA-O3	2.55	1.62	1.59
4	B	4004	FAD	C2A-N1A	2.50	1.38	1.33
4	B	4004	FAD	C10-N1	2.44	1.38	1.33
5	B	4005	NAI	PN-O3	2.29	1.62	1.59
5	B	4005	NAI	C6N-N1N	2.25	1.42	1.37
5	B	4005	NAI	C6N-C5N	2.25	1.39	1.33
4	B	4004	FAD	C8A-N7A	2.25	1.36	1.31
5	A	3005	NAI	C6N-N1N	2.24	1.42	1.37
4	B	4004	FAD	C5A-N7A	-2.23	1.35	1.39
7	B	4007	URC	C5-C6	2.23	1.48	1.41
7	A	3007	URC	C5-C6	2.22	1.48	1.41
5	A	3005	NAI	C5A-N7A	-2.20	1.35	1.39
5	A	3005	NAI	C8A-N7A	2.16	1.35	1.31
4	B	4004	FAD	C2A-N3A	2.09	1.37	1.33
5	A	3005	NAI	C6N-C5N	2.09	1.39	1.33
5	B	4005	NAI	PA-O3	2.07	1.61	1.59

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4007	URC	N7-C8-N9	6.53	116.47	107.22
7	A	3007	URC	N7-C8-N9	6.04	115.77	107.22
4	B	4004	FAD	N3A-C2A-N1A	-5.90	119.65	128.58
4	A	3004	FAD	N3A-C2A-N1A	-5.81	119.79	128.58
5	A	3005	NAI	C5A-C4A-N3A	-5.31	119.41	126.72
5	B	4005	NAI	N3A-C2A-N1A	-4.98	121.04	128.58
5	A	3005	NAI	N3A-C2A-N1A	-4.87	121.20	128.58
5	B	4005	NAI	C5A-C4A-N3A	-4.84	120.05	126.72
7	B	4007	URC	C5-N7-C8	-4.66	102.81	108.82
4	A	3004	FAD	C5A-C4A-N3A	-4.33	120.75	126.72
7	A	3007	URC	C5-N7-C8	-4.29	103.29	108.82
5	A	3005	NAI	O4D-C1D-N1N	4.23	116.14	108.08
4	B	4004	FAD	N9A-C8A-N7A	-4.06	108.17	113.94
4	A	3004	FAD	N9A-C8A-N7A	-4.04	108.20	113.94
4	B	4004	FAD	C5A-C4A-N3A	-4.03	121.17	126.72
7	A	3007	URC	N3-C2-N1	3.89	121.86	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4007	URC	N3-C2-N1	3.85	121.79	115.74
5	A	3005	NAI	C6N-N1N-C2N	-3.64	115.42	119.32
4	A	3004	FAD	C5A-N7A-C8A	3.54	109.01	103.45
5	A	3005	NAI	N3A-C4A-N9A	3.52	133.16	127.17
5	A	3005	NAI	C2A-N3A-C4A	3.49	120.37	111.83
5	A	3005	NAI	N9A-C8A-N7A	-3.49	108.98	113.94
5	A	3005	NAI	C1D-N1N-C6N	-3.49	113.40	120.77
4	A	3004	FAD	C2A-N3A-C4A	3.43	120.22	111.83
4	B	4004	FAD	C5A-N7A-C8A	3.30	108.64	103.45
5	B	4005	NAI	N9A-C8A-N7A	-3.28	109.28	113.94
4	B	4004	FAD	C2A-N3A-C4A	3.26	119.78	111.83
5	B	4005	NAI	N3A-C4A-N9A	3.24	132.68	127.17
7	B	4007	URC	C6-N1-C2	-3.20	121.96	126.37
5	B	4005	NAI	C2A-N3A-C4A	3.20	119.64	111.83
7	A	3007	URC	C6-N1-C2	-3.05	122.16	126.37
4	A	3004	FAD	N3A-C4A-N9A	3.02	132.31	127.17
7	B	4007	URC	O13-C6-C5	-2.87	120.34	127.26
4	B	4004	FAD	C4-N3-C2	-2.83	120.61	125.64
4	A	3004	FAD	O2A-PA-O3P	2.83	114.92	107.27
4	B	4004	FAD	C4X-C10-N10	2.83	120.53	116.48
5	B	4005	NAI	C6N-N1N-C2N	-2.81	116.31	119.32
4	A	3004	FAD	C4X-C10-N10	2.77	120.44	116.48
5	A	3005	NAI	C5A-N7A-C8A	2.76	107.79	103.45
5	A	3005	NAI	C4A-C5A-N7A	-2.74	107.44	110.58
7	A	3007	URC	O13-C6-C5	-2.74	120.66	127.26
4	B	4004	FAD	N3A-C4A-N9A	2.70	131.76	127.17
4	B	4004	FAD	C10-C4X-N5	-2.65	119.39	124.81
5	B	4005	NAI	C1D-N1N-C6N	-2.64	115.19	120.77
5	B	4005	NAI	O4D-C1D-N1N	2.59	113.03	108.08
5	B	4005	NAI	C4A-N9A-C8A	2.58	108.45	105.74
5	B	4005	NAI	C4A-C5A-N7A	-2.52	107.70	110.58
4	A	3004	FAD	C4-N3-C2	-2.50	121.21	125.64
5	A	3005	NAI	C4A-N9A-C8A	2.48	108.34	105.74
5	B	4005	NAI	C5A-N7A-C8A	2.45	107.30	103.45
4	A	3004	FAD	C10-C4X-N5	-2.45	119.81	124.81
4	A	3004	FAD	C4X-C4-N3	2.36	119.25	113.25
4	A	3004	FAD	C4A-C5A-N7A	-2.35	107.90	110.58
4	B	4004	FAD	O2A-PA-O3P	2.33	113.57	107.27
4	B	4004	FAD	C4X-C4-N3	2.32	119.17	113.25
5	A	3005	NAI	C1D-N1N-C2N	-2.32	117.32	121.14
4	A	3004	FAD	C5X-C9A-N10	2.14	119.90	117.97
4	B	4004	FAD	C4X-C10-N1	-2.13	119.36	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4007	URC	O24-C8-N7	-2.13	121.70	125.56
4	A	3004	FAD	C4A-N9A-C8A	2.11	107.95	105.74
4	B	4004	FAD	C4A-C5A-N7A	-2.06	108.22	110.58
7	B	4007	URC	O24-C8-N9	-2.05	121.83	125.56
4	B	4004	FAD	C4A-N9A-C8A	2.05	107.89	105.74
5	A	3005	NAI	O2A-PA-O1A	2.04	121.92	112.44
7	B	4007	URC	O11-C2-N3	-2.03	118.25	121.86
7	A	3007	URC	O24-C8-N9	-2.03	121.87	125.56
4	B	4004	FAD	C9A-C5X-N5	-2.02	120.31	122.45

There are no chirality outliers.

All (21) torsion outliers are listed below:

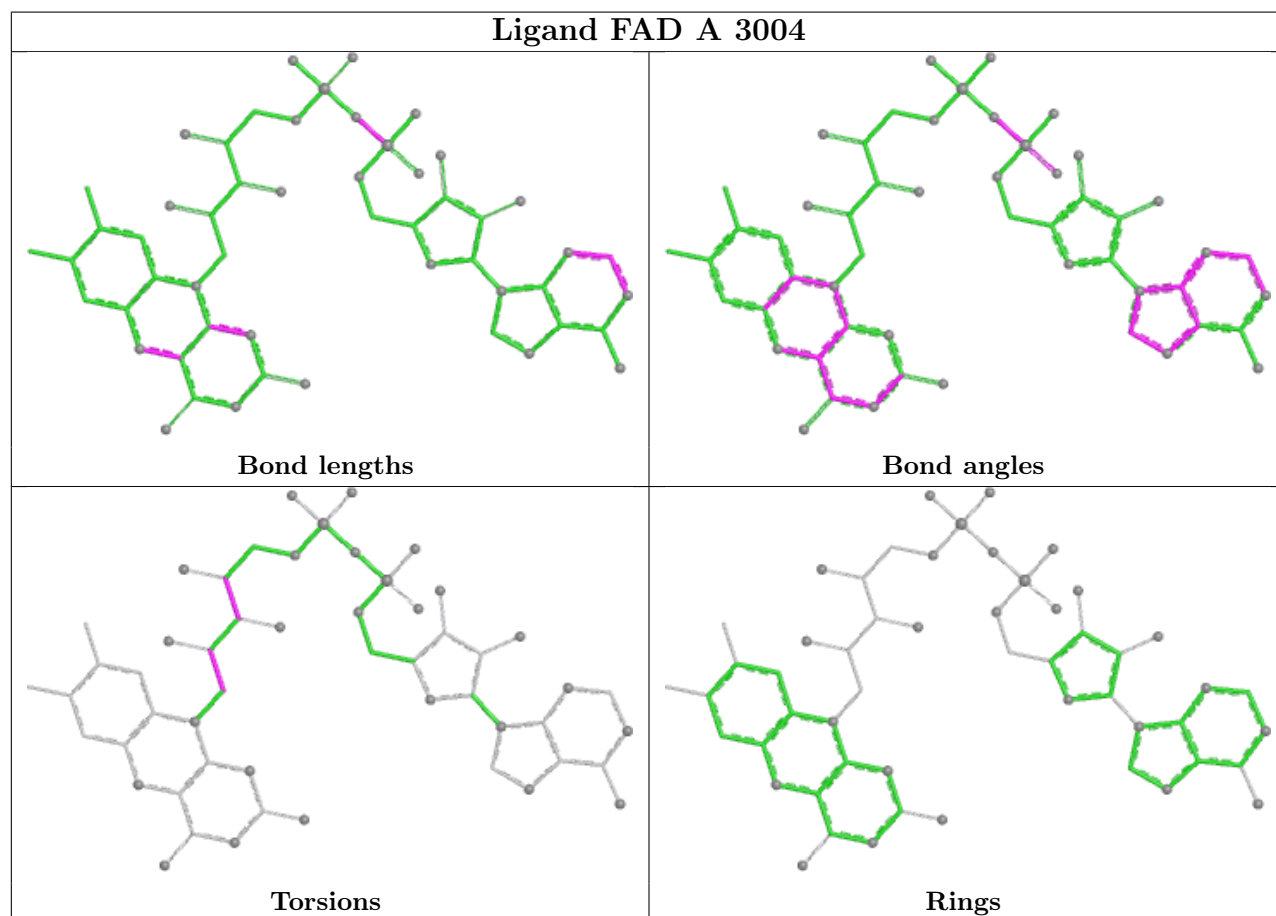
Mol	Chain	Res	Type	Atoms
4	A	3004	FAD	N10-C1'-C2'-O2'
4	A	3004	FAD	N10-C1'-C2'-C3'
4	B	4004	FAD	N10-C1'-C2'-O2'
4	B	4004	FAD	N10-C1'-C2'-C3'
8	B	4008	GOL	O1-C1-C2-C3
5	B	4005	NAI	C2D-C1D-N1N-C6N
5	A	3005	NAI	C2D-C1D-N1N-C6N
8	B	4008	GOL	O1-C1-C2-O2
8	B	4008	GOL	O2-C2-C3-O3
4	A	3004	FAD	C2'-C3'-C4'-O4'
4	B	4004	FAD	C2'-C3'-C4'-O4'
5	B	4005	NAI	O4D-C1D-N1N-C6N
4	B	4004	FAD	C5B-O5B-PA-O1A
5	A	3005	NAI	O4D-C1D-N1N-C6N
5	B	4005	NAI	O4D-C4D-C5D-O5D
5	A	3005	NAI	C2N-C3N-C7N-N7N
5	B	4005	NAI	C2N-C3N-C7N-N7N
4	A	3004	FAD	C2'-C3'-C4'-C5'
4	B	4004	FAD	O3'-C3'-C4'-O4'
4	A	3004	FAD	O3'-C3'-C4'-O4'
5	B	4005	NAI	C3D-C4D-C5D-O5D

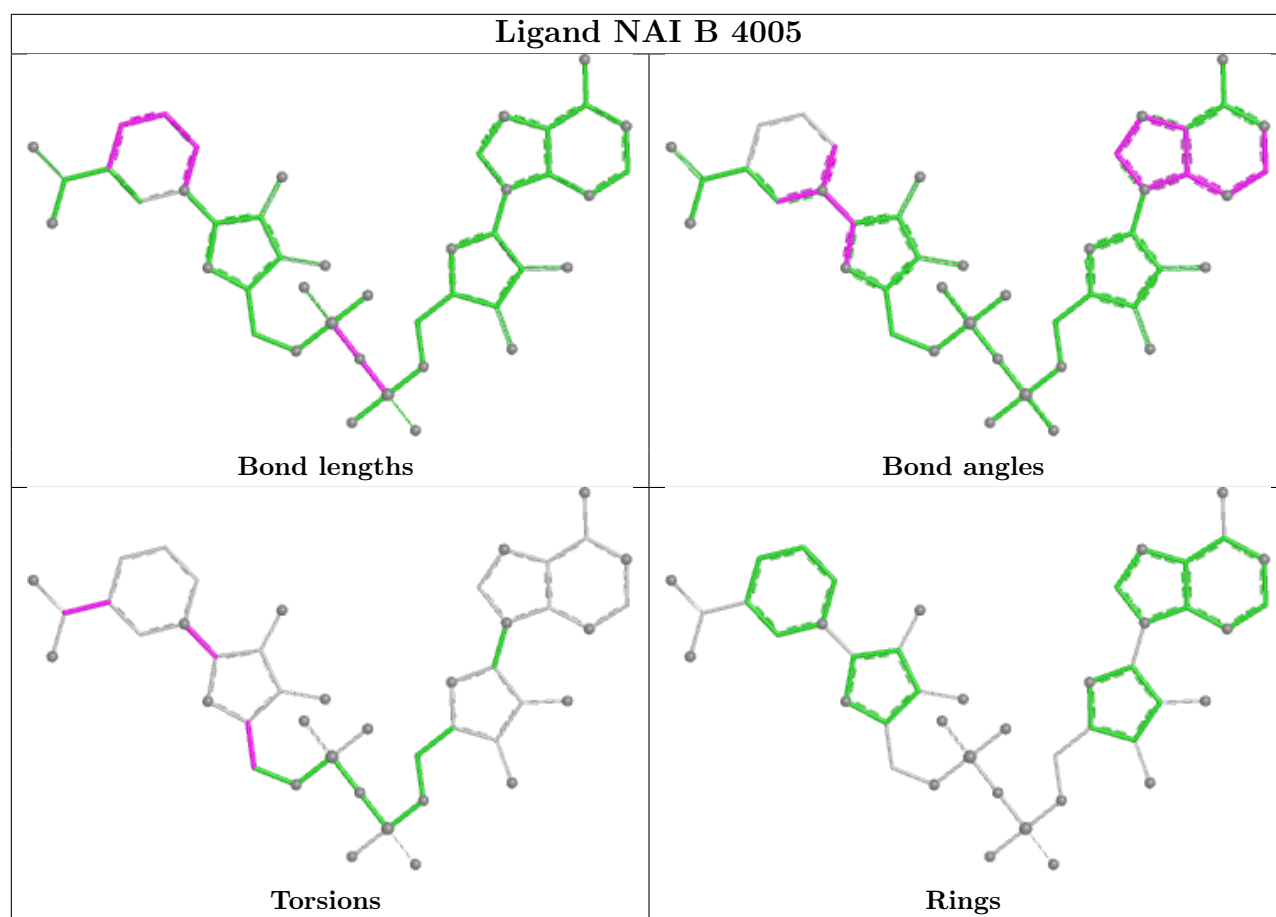
There are no ring outliers.

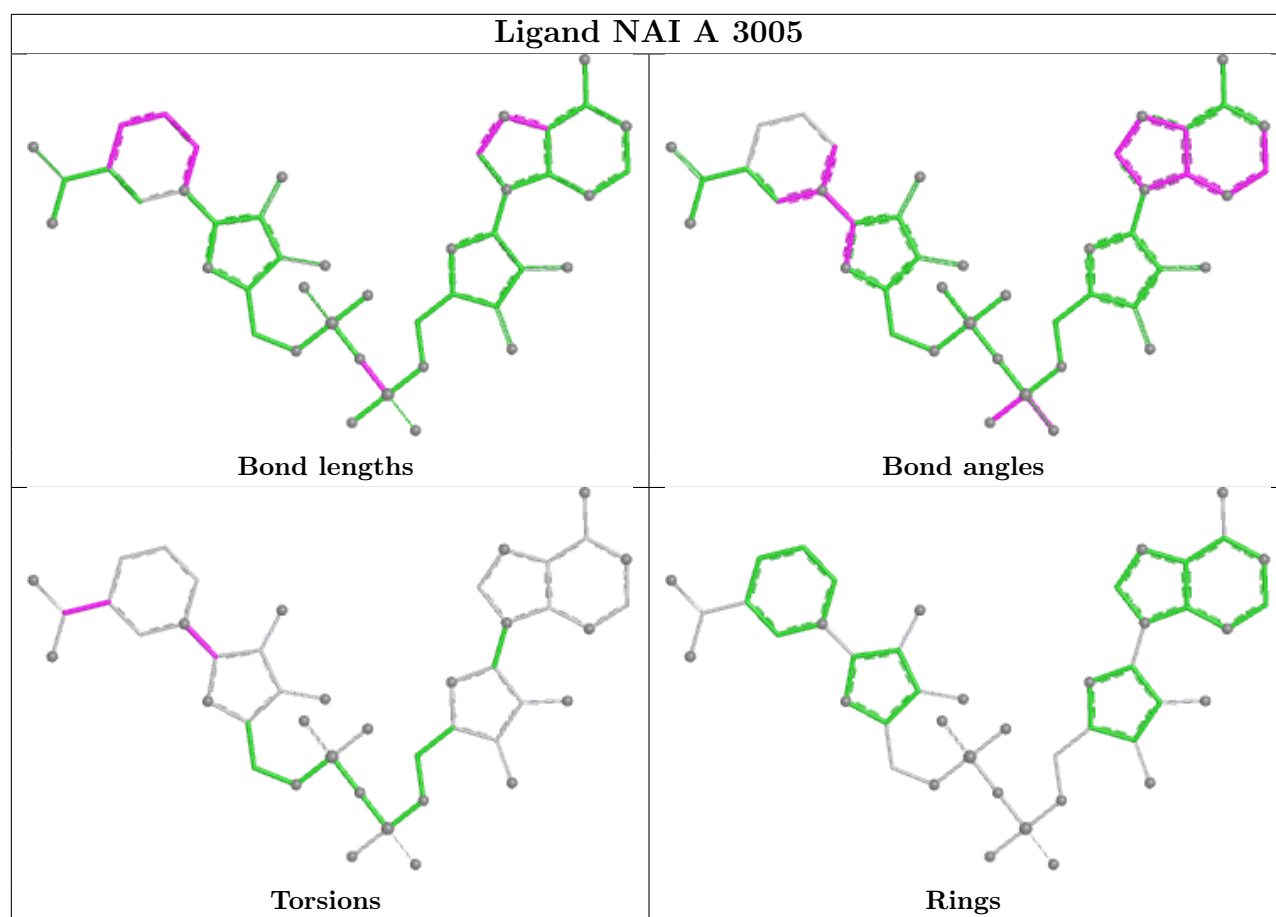
1 monomer is involved in 2 short contacts:

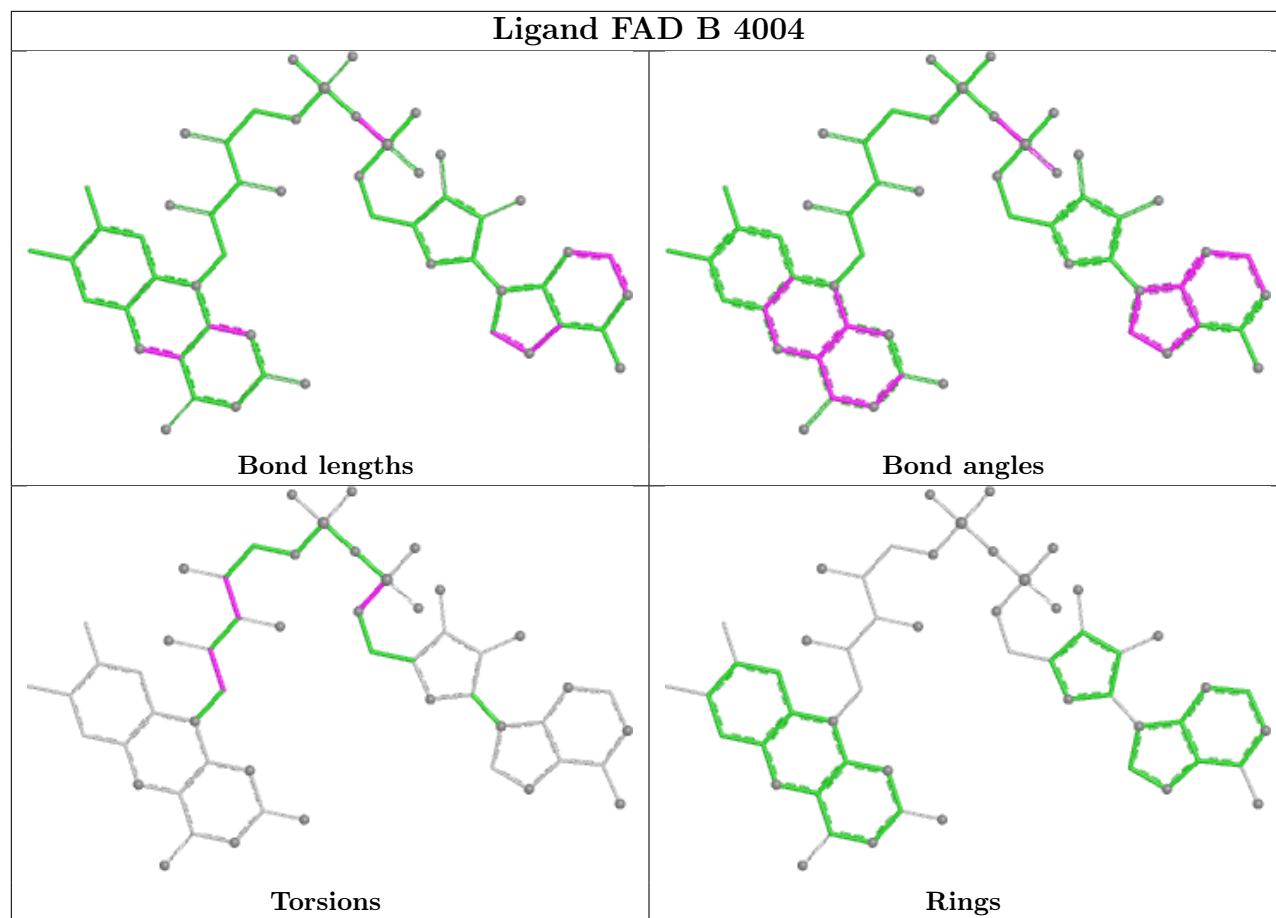
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3004	FAD	2	0

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 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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1286/1315 (97%)	0.18	35 (2%) 56 55	14, 25, 40, 48	0
1	B	1286/1315 (97%)	-0.11	27 (2%) 63 63	11, 19, 32, 49	0
All	All	2572/2630 (97%)	0.04	62 (2%) 59 59	11, 22, 38, 49	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1315	LEU	10.8
1	B	1289	ALA	10.2
1	B	1286	GLY	9.7
1	A	1315	LEU	7.4
1	B	1288	ASN	5.7
1	B	3	ALA	5.6
1	B	1287	ASP	5.5
1	A	551	LYS	5.3
1	B	1314	THR	5.3
1	A	3	ALA	5.1
1	B	1290	LYS	4.9
1	A	1111	GLY	4.5
1	B	1111	GLY	4.3
1	A	396	LEU	4.2
1	B	566	ASP	3.6
1	B	551	LYS	3.5
1	A	61	LEU	3.5
1	A	1110	THR	3.4
1	A	812	LEU	3.4
1	A	377	GLY	3.3
1	B	703	ASN	3.2
1	A	1250	LYS	3.2
1	A	466	LEU	3.1
1	A	272	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	719	LEU	3.0
1	B	480	GLU	2.9
1	B	164	LYS	2.9
1	A	566	ASP	2.9
1	B	198	GLU	2.9
1	A	1288	ASN	2.9
1	B	530	ASP	2.9
1	B	221	THR	2.8
1	A	701	ALA	2.7
1	A	198	GLU	2.6
1	A	552	ASP	2.6
1	A	290	VAL	2.6
1	A	387	THR	2.5
1	A	550	GLN	2.5
1	A	164	LYS	2.5
1	A	313	GLU	2.5
1	B	1110	THR	2.5
1	A	321	GLN	2.4
1	A	531	LEU	2.4
1	A	497	PRO	2.4
1	B	321	GLN	2.4
1	B	600	GLU	2.3
1	B	222	PRO	2.3
1	A	1143	GLU	2.3
1	B	1143	GLU	2.3
1	A	932	ILE	2.2
1	A	465	ALA	2.2
1	A	710	SER	2.1
1	A	249	ALA	2.1
1	B	1313	THR	2.1
1	B	812	LEU	2.1
1	B	1276	ASP	2.1
1	A	1314	THR	2.1
1	B	1291	GLN	2.1
1	B	531	LEU	2.1
1	A	316	ALA	2.1
1	A	496	ALA	2.1
1	A	62	GLN	2.0

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

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 ⓘ

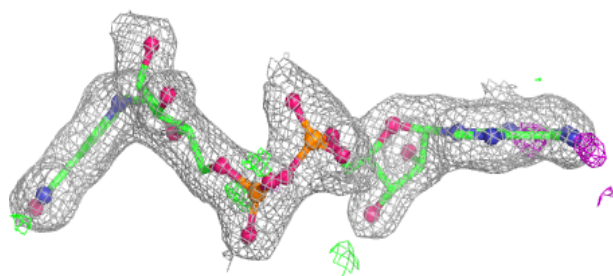
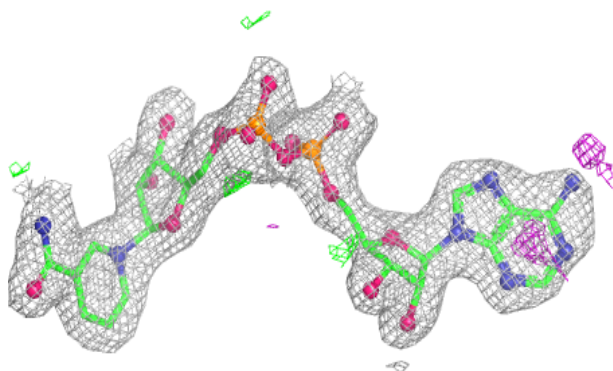
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	GOL	B	4008	6/6	0.91	0.08	21,24,25,25	0
8	GOL	A	3008	6/6	0.92	0.10	24,25,26,26	0
5	NAI	A	3005	44/44	0.94	0.08	25,31,35,36	0
7	URC	A	3007	12/12	0.95	0.06	23,23,24,24	0
4	FAD	A	3004	53/53	0.96	0.07	22,23,25,26	0
5	NAI	B	4005	44/44	0.97	0.05	17,21,23,24	0
2	FES	A	3001	4/4	0.97	0.11	26,26,26,28	0
7	URC	B	4007	12/12	0.97	0.05	19,20,20,20	0
4	FAD	B	4004	53/53	0.97	0.06	12,14,15,17	0
2	FES	B	4001	4/4	0.97	0.11	23,24,24,25	0
3	CA	A	3003	1/1	0.98	0.09	26,26,26,26	0
6	BCT	A	3006	4/4	0.98	0.05	22,22,22,22	0
2	FES	A	3002	4/4	0.99	0.04	17,18,18,19	0
6	BCT	B	4006	4/4	0.99	0.03	17,17,17,18	0
2	FES	B	4002	4/4	1.00	0.02	12,13,13,14	0
3	CA	B	4003	1/1	1.00	0.05	19,19,19,19	0

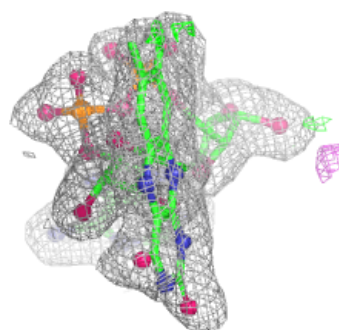
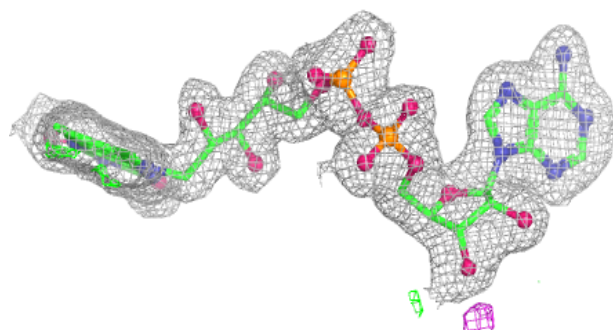
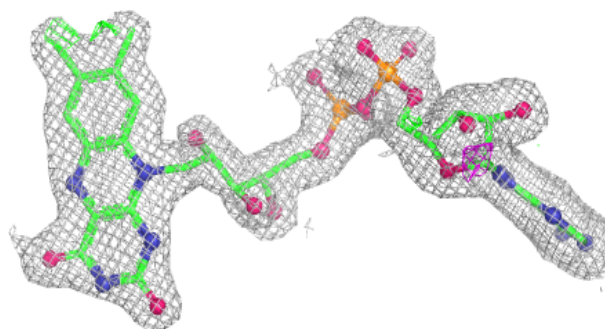
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI A 3005:

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

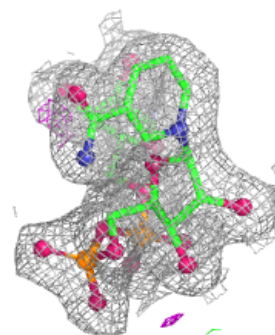
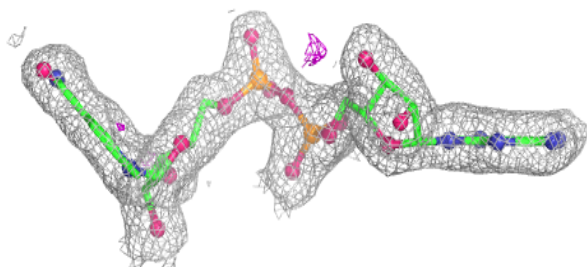
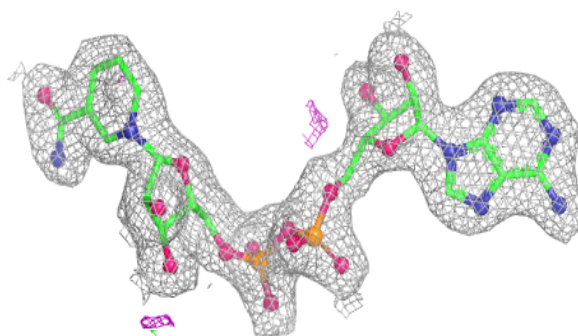
**Electron density around FAD A 3004:**

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

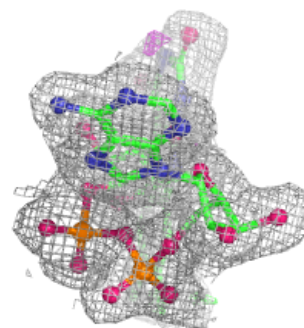
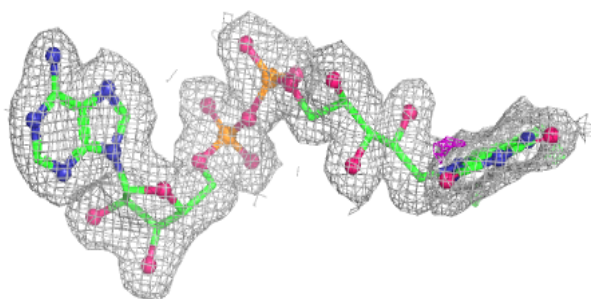
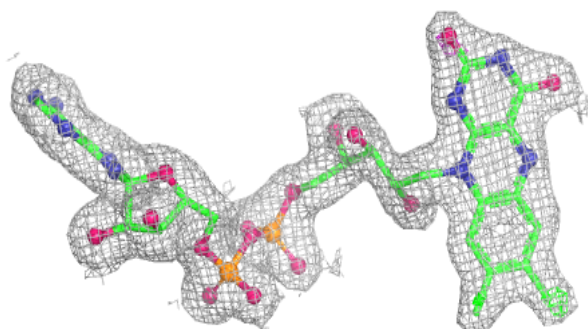


Electron density around NAI B 4005:

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

**Electron density around FAD B 4004:**

$2mF_o-DF_c$ (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.