



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:10 AM UTC

PDB ID : 4Q72 / pdb_00004q72
Title : Crystal Structure of Bradyrhizobium japonicum Proline Utilization A (PutA) Mutant D779Y
Authors : Tanner, J.J.; Pemberton, T.A.; Luo, M.
Deposited on : 2014-04-23
Resolution : 2.30 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

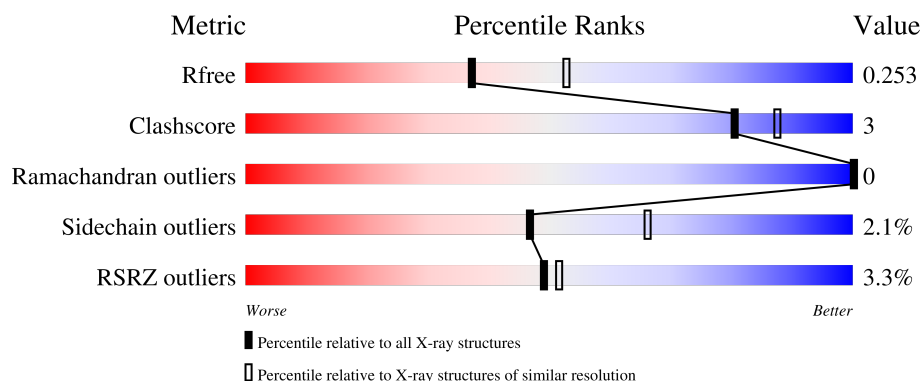
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

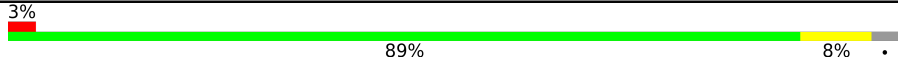
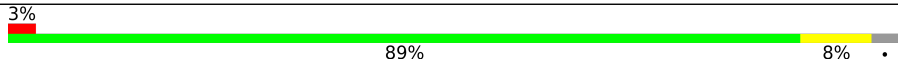
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1001	
1	B	1001	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14836 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.

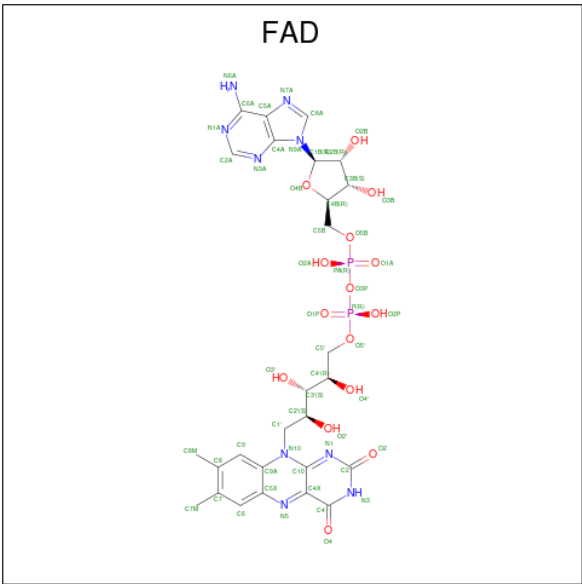
- Molecule 1 is a protein called Proline dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	971	7217	4562	1295	1337	23	0	0	0
1	B	969	7169	4533	1286	1327	23	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q89E26
A	0	HIS	-	expression tag	UNP Q89E26
A	779	TYR	ASP	engineered mutation	UNP Q89E26
B	-1	GLY	-	expression tag	UNP Q89E26
B	0	HIS	-	expression tag	UNP Q89E26
B	779	TYR	ASP	engineered mutation	UNP Q89E26

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

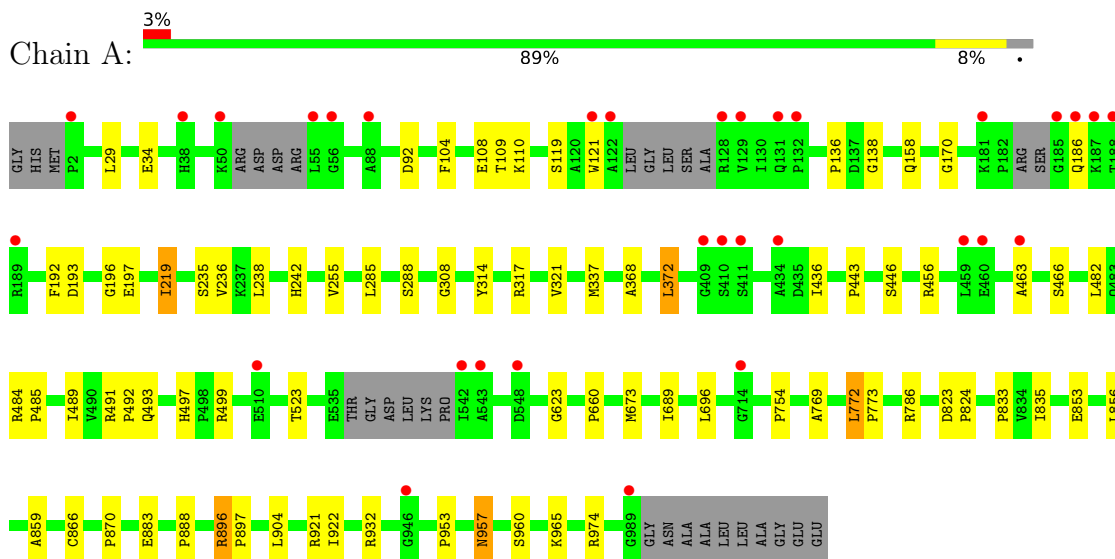
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	0
			186	186		
5	B	110	Total	O	0	0
			110	110		

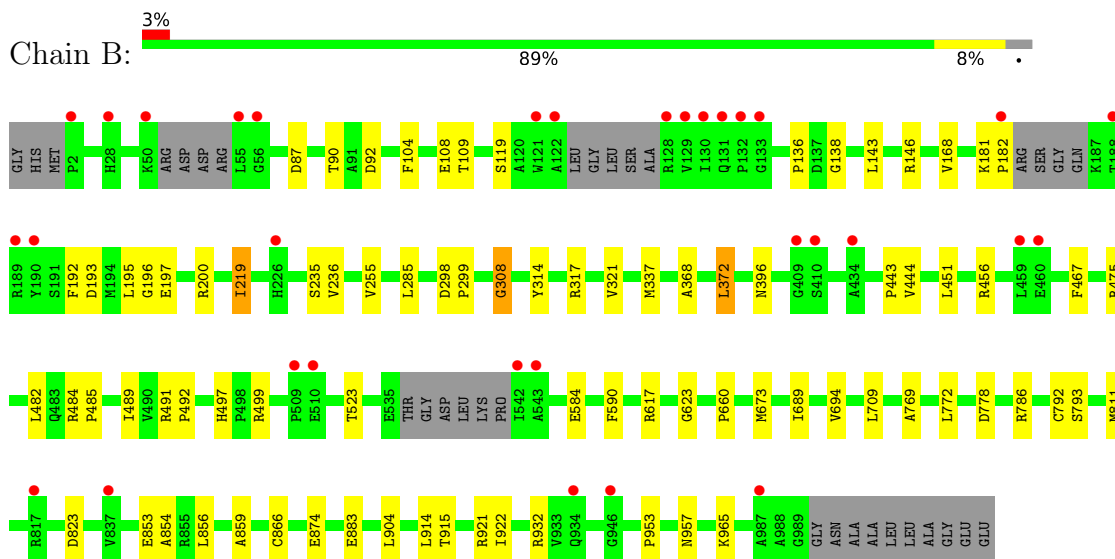
3 Residue-property plots [i](#)

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: Proline dehydrogenase



• Molecule 1: Proline dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.11Å 195.99Å 108.70Å 90.00° 121.44° 90.00°	Depositor
Resolution (Å)	31.99 – 2.30 31.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (31.99-2.30) 98.6 (31.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.215 , 0.251 0.218 , 0.253	Depositor DCC
R_{free} test set	6545 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14836	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.82% 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, FAD, SO4

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	0.57	0/7359	0.83	8/10013 (0.1%)
1	B	0.53	0/7309	0.82	5/9949 (0.1%)
All	All	0.55	0/14668	0.83	13/19962 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	GLY	N-CA-C	6.39	118.84	111.36
1	B	196	GLY	N-CA-C	6.33	118.77	111.36
1	B	823	ASP	CA-C-N	5.90	126.32	119.47
1	B	823	ASP	C-N-CA	5.90	126.32	119.47
1	A	823	ASP	CA-C-N	5.80	126.19	119.47
1	A	823	ASP	C-N-CA	5.80	126.19	119.47
1	A	896	ARG	CA-C-N	5.62	125.72	119.32
1	A	896	ARG	C-N-CA	5.62	125.72	119.32
1	B	195	LEU	N-CA-C	5.44	117.97	111.71
1	B	308	GLY	N-CA-C	5.31	118.89	111.19
1	A	835	ILE	N-CA-C	5.16	115.37	110.42
1	A	242	HIS	CA-C-N	5.08	124.69	119.56
1	A	242	HIS	C-N-CA	5.08	124.69	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	7217	0	7155	37	0
1	B	7169	0	7083	37	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	18	0	24	0	0
4	A	15	0	0	0	0
4	B	15	0	0	1	0
5	A	186	0	0	1	0
5	B	110	0	0	0	0
All	All	14836	0	14324	75	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 (75) 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:491:ARG:HD2	1:B:492:PRO:HD2	1.65	0.77
1:A:491:ARG:HD2	1:A:492:PRO:HD2	1.69	0.73
1:B:197:GLU:OE1	1:B:456:ARG:NH1	2.33	0.61
1:B:623:GLY:HA3	1:B:673:MET:HE2	1.85	0.58
1:A:197:GLU:OE1	1:A:456:ARG:NH1	2.38	0.56
1:B:475:ARG:NH2	4:B:1003:SO4:O2	2.38	0.55
1:A:158:GLN:NE2	5:A:2186:HOH:O	2.29	0.55
1:A:108:GLU:HG3	1:A:921:ARG:HH11	1.72	0.55
1:A:623:GLY:HA3	1:A:673:MET:HE2	1.88	0.54
1:B:482:LEU:O	1:B:484:ARG:NH1	2.40	0.53
1:A:138:GLY:HA2	1:A:922:ILE:HG23	1.92	0.52
1:B:108:GLU:HG3	1:B:921:ARG:HH11	1.74	0.51
1:A:463:ALA:O	1:A:466:SER:HB3	2.11	0.51
1:A:772:LEU:HD12	1:A:773:PRO:HD2	1.93	0.51
1:A:482:LEU:O	1:A:484:ARG:NH1	2.44	0.51
1:A:192:PHE:CE2	1:A:219:ILE:HG12	2.47	0.50
1:A:308:GLY:HA3	1:A:337:MET:O	2.12	0.50
1:B:168:VAL:HB	1:B:444:VAL:HG22	1.94	0.50
1:A:368:ALA:HB3	1:A:489:ILE:HD11	1.94	0.49
1:A:870:PRO:HA	1:A:888:PRO:O	2.13	0.49
1:B:694:VAL:HG21	1:B:709:LEU:HD13	1.93	0.49
1:B:138:GLY:HA2	1:B:922:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:PRO:HB2	1:B:965:LYS:HD3	1.94	0.48
1:B:660:PRO:HB2	1:B:689:ILE:HG21	1.96	0.48
1:A:372:LEU:HD23	1:A:485:PRO:HB2	1.95	0.48
1:B:192:PHE:CE2	1:B:219:ILE:HG12	2.49	0.48
1:A:824:PRO:HG3	1:A:833:PRO:HD2	1.94	0.48
1:A:491:ARG:HE	1:A:493:GLN:HB3	1.79	0.48
1:B:792:CYS:O	1:B:914:LEU:HD23	2.14	0.47
1:B:200:ARG:NH1	1:B:778:ASP:OD2	2.37	0.47
1:A:856:LEU:HD11	1:A:859:ALA:HB2	1.98	0.46
1:A:29:LEU:HB2	1:A:34:GLU:OE2	2.16	0.45
1:A:957:ASN:O	1:A:960:SER:HB2	2.17	0.45
1:A:108:GLU:HG3	1:A:921:ARG:NH1	2.32	0.45
1:B:109:THR:HG23	1:B:769:ALA:HB3	1.98	0.45
1:B:497:HIS:CE1	1:B:499:ARG:HB2	2.52	0.45
1:A:497:HIS:HE1	1:A:499:ARG:HB2	1.82	0.44
1:B:372:LEU:HD23	1:B:485:PRO:HB2	2.00	0.44
1:A:109:THR:HG23	1:A:769:ALA:HB3	1.99	0.44
1:B:368:ALA:HB3	1:B:489:ILE:HD11	1.99	0.44
1:A:238:LEU:HD12	1:A:288:SER:HB2	1.99	0.44
1:A:497:HIS:CE1	1:A:499:ARG:HB2	2.52	0.44
1:B:451:LEU:HB3	1:B:772:LEU:HD13	2.00	0.44
1:B:590:PHE:HD2	1:B:689:ILE:HD11	1.83	0.44
1:B:856:LEU:HD11	1:B:859:ALA:HB2	1.99	0.44
1:B:285:LEU:HD23	1:B:317:ARG:CZ	2.47	0.44
1:B:854:ALA:HB1	1:B:874:GLU:O	2.17	0.44
1:B:396:ASN:HA	1:B:467:PHE:CD2	2.53	0.43
1:B:811:MET:HE2	1:B:811:MET:HB2	1.90	0.43
1:B:317:ARG:O	1:B:321:VAL:HG23	2.19	0.43
1:A:170:GLY:O	1:A:446:SER:HA	2.18	0.43
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.82	0.43
1:A:754:PRO:HB3	1:A:974:ARG:NH2	2.34	0.42
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.90	0.42
1:A:660:PRO:HB2	1:A:689:ILE:HG21	2.01	0.42
1:A:104:PHE:CE2	1:A:136:PRO:HA	2.54	0.42
1:A:193:ASP:O	1:A:443:PRO:HA	2.20	0.42
1:B:87:ASP:HB3	1:B:90:THR:OG1	2.20	0.42
1:B:193:ASP:O	1:B:443:PRO:HA	2.20	0.41
1:A:896:ARG:HA	1:A:897:PRO:HD3	1.88	0.41
1:B:584:GLU:OE2	1:B:617:ARG:NH2	2.44	0.41
1:B:793:SER:HB2	1:B:915:THR:HG21	2.02	0.41
1:A:285:LEU:HD23	1:A:317:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:O	1:A:321:VAL:HG23	2.21	0.41
1:B:104:PHE:CE2	1:B:136:PRO:HA	2.56	0.41
1:B:904:LEU:HD13	1:B:932:ARG:HG2	2.02	0.41
2:A:2001:FAD:H4'	2:A:2001:FAD:H1'1	1.91	0.41
1:B:181:LYS:HA	1:B:182:PRO:HD3	1.93	0.41
1:B:298:ASP:HA	1:B:299:PRO:HD3	1.89	0.41
1:A:110:LYS:HB3	1:A:121:TRP:HE3	1.86	0.40
1:A:696:LEU:HD23	1:A:696:LEU:C	2.47	0.40
1:A:953:PRO:HB2	1:A:965:LYS:HD3	2.03	0.40
1:B:308:GLY:HA3	1:B:337:MET:O	2.20	0.40
1:A:904:LEU:HD13	1:A:932:ARG:HG2	2.02	0.40
1:B:146:ARG:HH21	1:B:146:ARG:HD3	1.76	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	961/1001 (96%)	940 (98%)	21 (2%)	0	100	100
1	B	959/1001 (96%)	941 (98%)	18 (2%)	0	100	100
All	All	1920/2002 (96%)	1881 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	706/758 (93%)	690 (98%)	16 (2%)	44	63
1	B	695/758 (92%)	681 (98%)	14 (2%)	48	67
All	All	1401/1516 (92%)	1371 (98%)	30 (2%)	47	66

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	119	SER
1	A	186	GLN
1	A	219	ILE
1	A	235	SER
1	A	236	VAL
1	A	255	VAL
1	A	314	TYR
1	A	372	LEU
1	A	523	THR
1	A	772	LEU
1	A	786	ARG
1	A	853	GLU
1	A	866	CYS
1	A	883	GLU
1	A	957	ASN
1	B	92	ASP
1	B	119	SER
1	B	219	ILE
1	B	235	SER
1	B	236	VAL
1	B	255	VAL
1	B	314	TYR
1	B	372	LEU
1	B	523	THR
1	B	786	ARG
1	B	853	GLU
1	B	866	CYS
1	B	883	GLU
1	B	957	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	274	ASN
1	A	391	GLN
1	A	433	HIS
1	A	461	ASN
1	A	589	HIS
1	A	957	ASN
1	A	970	HIS
1	B	106	HIS
1	B	107	HIS
1	B	274	ASN
1	B	391	GLN
1	B	957	ASN
1	B	970	HIS

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](#)

11 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	$\# Z > 2$
2	FAD	B	1001	-	58,58,58	2.35	16 (27%)	85,89,89	1.94	21 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	2007	-	4,4,4	0.26	0	6,6,6	0.50	0
2	FAD	A	2001	-	58,58,58	2.27	15 (25%)	85,89,89	1.92	20 (23%)
4	SO4	A	2005	-	4,4,4	0.25	0	6,6,6	0.20	0
4	SO4	B	1003	-	4,4,4	0.22	0	6,6,6	0.14	0
3	GOL	A	2003	-	5,5,5	0.34	0	5,5,5	0.70	0
4	SO4	B	1004	-	4,4,4	0.22	0	6,6,6	0.09	0
3	GOL	A	2002	-	5,5,5	0.42	0	5,5,5	0.16	0
4	SO4	A	2006	-	4,4,4	0.19	0	6,6,6	0.28	0
4	SO4	B	1002	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	A	2004	-	5,5,5	0.36	0	5,5,5	0.78	0

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
2	FAD	B	1001	-	-	8/34/50/50	0/6/6/6
2	FAD	A	2001	-	-	6/34/50/50	0/6/6/6
3	GOL	A	2003	-	-	2/4/4/4	-
3	GOL	A	2002	-	-	4/4/4/4	-
3	GOL	A	2004	-	-	0/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	FAD	PA-O3P	-8.68	1.50	1.59
2	A	2001	FAD	PA-O3P	-8.42	1.50	1.59
2	B	1001	FAD	O4-C4	7.33	1.37	1.23
2	A	2001	FAD	O4-C4	6.66	1.36	1.23
2	B	1001	FAD	O2-C2	6.37	1.37	1.24
2	A	2001	FAD	O2-C2	6.27	1.36	1.24
2	B	1001	FAD	C4X-N5	4.10	1.39	1.30
2	A	2001	FAD	P-O3P	4.02	1.63	1.59
2	A	2001	FAD	C4X-N5	3.97	1.39	1.30
2	B	1001	FAD	P-O3P	3.95	1.63	1.59
2	B	1001	FAD	C6A-N6A	3.93	1.44	1.34
2	A	2001	FAD	C6A-N6A	3.51	1.43	1.34
2	B	1001	FAD	C2-N1	3.29	1.44	1.36
2	A	2001	FAD	C2-N1	2.76	1.42	1.36
2	A	2001	FAD	O4B-C4B	-2.73	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	PA-O5B	-2.71	1.48	1.59
2	B	1001	FAD	C10-N1	2.69	1.38	1.33
2	B	1001	FAD	O4B-C4B	-2.61	1.39	1.45
2	B	1001	FAD	PA-O5B	-2.60	1.49	1.59
2	A	2001	FAD	O2'-C2'	-2.58	1.37	1.43
2	A	2001	FAD	PA-O2A	-2.51	1.43	1.55
2	B	1001	FAD	O2'-C2'	-2.42	1.38	1.43
2	A	2001	FAD	C10-N1	2.35	1.38	1.33
2	B	1001	FAD	PA-O2A	-2.33	1.44	1.55
2	A	2001	FAD	O3'-C3'	-2.32	1.37	1.43
2	B	1001	FAD	O4'-C4'	-2.29	1.38	1.43
2	A	2001	FAD	C4A-N9A	2.28	1.42	1.37
2	A	2001	FAD	O4'-C4'	-2.22	1.38	1.43
2	B	1001	FAD	O3'-C3'	-2.21	1.37	1.43
2	B	1001	FAD	C4A-N9A	2.20	1.42	1.37
2	B	1001	FAD	O2B-C2B	-2.07	1.37	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	FAD	O2P-P-O3P	-6.55	89.56	107.27
2	A	2001	FAD	N3A-C2A-N1A	-6.20	119.19	128.58
2	B	1001	FAD	N3A-C2A-N1A	-5.97	119.54	128.58
2	A	2001	FAD	C5A-C4A-N3A	-5.70	118.86	126.72
2	B	1001	FAD	C5A-C4A-N3A	-5.69	118.88	126.72
2	A	2001	FAD	O2P-P-O3P	-4.92	93.96	107.27
2	A	2001	FAD	C2A-N3A-C4A	4.42	122.62	111.83
2	B	1001	FAD	N3A-C4A-N9A	4.36	134.59	127.17
2	B	1001	FAD	C2A-N3A-C4A	4.20	122.08	111.83
2	A	2001	FAD	N3A-C4A-N9A	4.19	134.30	127.17
2	B	1001	FAD	O3P-P-O1P	4.14	123.17	110.70
2	A	2001	FAD	C5A-N7A-C8A	4.05	109.81	103.45
2	B	1001	FAD	C5A-N7A-C8A	3.69	109.24	103.45
2	A	2001	FAD	C4-C4X-N5	3.65	123.24	118.21
2	A	2001	FAD	O3P-P-O1P	3.42	120.98	110.70
2	A	2001	FAD	N9A-C8A-N7A	-3.23	109.35	113.94
2	B	1001	FAD	C4-C4X-N5	3.12	122.52	118.21
2	A	2001	FAD	C4X-C4-N3	3.11	121.18	113.25
2	A	2001	FAD	O4-C4-C4X	-3.05	118.49	126.53
2	A	2001	FAD	C4A-C5A-N7A	-3.03	107.11	110.58
2	B	1001	FAD	O4-C4-C4X	-3.00	118.61	126.53
2	B	1001	FAD	N9A-C8A-N7A	-2.98	109.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	FAD	C4X-C4-N3	2.96	120.78	113.25
2	A	2001	FAD	C4-N3-C2	-2.95	120.40	125.64
2	B	1001	FAD	C4-N3-C2	-2.91	120.47	125.64
2	B	1001	FAD	O2A-PA-O5B	-2.80	94.89	107.57
2	B	1001	FAD	C4A-C5A-N7A	-2.65	107.56	110.58
2	A	2001	FAD	O2A-PA-O5B	-2.64	95.61	107.57
2	A	2001	FAD	O2-C2-N1	-2.60	117.48	121.80
2	B	1001	FAD	O5B-PA-O1A	2.50	118.86	108.94
2	A	2001	FAD	O5'-P-O1P	2.43	118.58	108.94
2	A	2001	FAD	C4X-C10-N10	2.41	119.92	116.48
2	B	1001	FAD	C5X-C9A-N10	2.36	120.10	117.97
2	B	1001	FAD	O2A-PA-O3P	-2.36	100.90	107.27
2	A	2001	FAD	O5B-PA-O1A	2.32	118.12	108.94
2	B	1001	FAD	C10-N1-C2	2.21	121.64	116.85
2	A	2001	FAD	C10-N1-C2	2.20	121.62	116.85
2	A	2001	FAD	O2-C2-N3	2.18	122.77	118.58
2	B	1001	FAD	O5'-P-O1P	2.14	117.40	108.94
2	B	1001	FAD	C10-C4X-N5	-2.05	120.62	124.81
2	B	1001	FAD	O2-C2-N1	-2.02	118.44	121.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	P-O3P-PA-O5B
2	A	2001	FAD	N10-C1'-C2'-O2'
2	A	2001	FAD	N10-C1'-C2'-C3'
2	A	2001	FAD	C1'-C2'-C3'-C4'
2	B	1001	FAD	P-O3P-PA-O5B
2	B	1001	FAD	N10-C1'-C2'-O2'
2	B	1001	FAD	N10-C1'-C2'-C3'
2	B	1001	FAD	C1'-C2'-C3'-C4'
3	A	2002	GOL	C1-C2-C3-O3
3	A	2002	GOL	O2-C2-C3-O3
3	A	2002	GOL	O1-C1-C2-C3
3	A	2002	GOL	O1-C1-C2-O2
3	A	2003	GOL	O1-C1-C2-O2
2	B	1001	FAD	C1'-C2'-C3'-O3'
2	A	2001	FAD	C3B-C4B-C5B-O5B
3	A	2003	GOL	O1-C1-C2-C3
2	A	2001	FAD	O2'-C2'-C3'-C4'
2	B	1001	FAD	O2'-C2'-C3'-O3'

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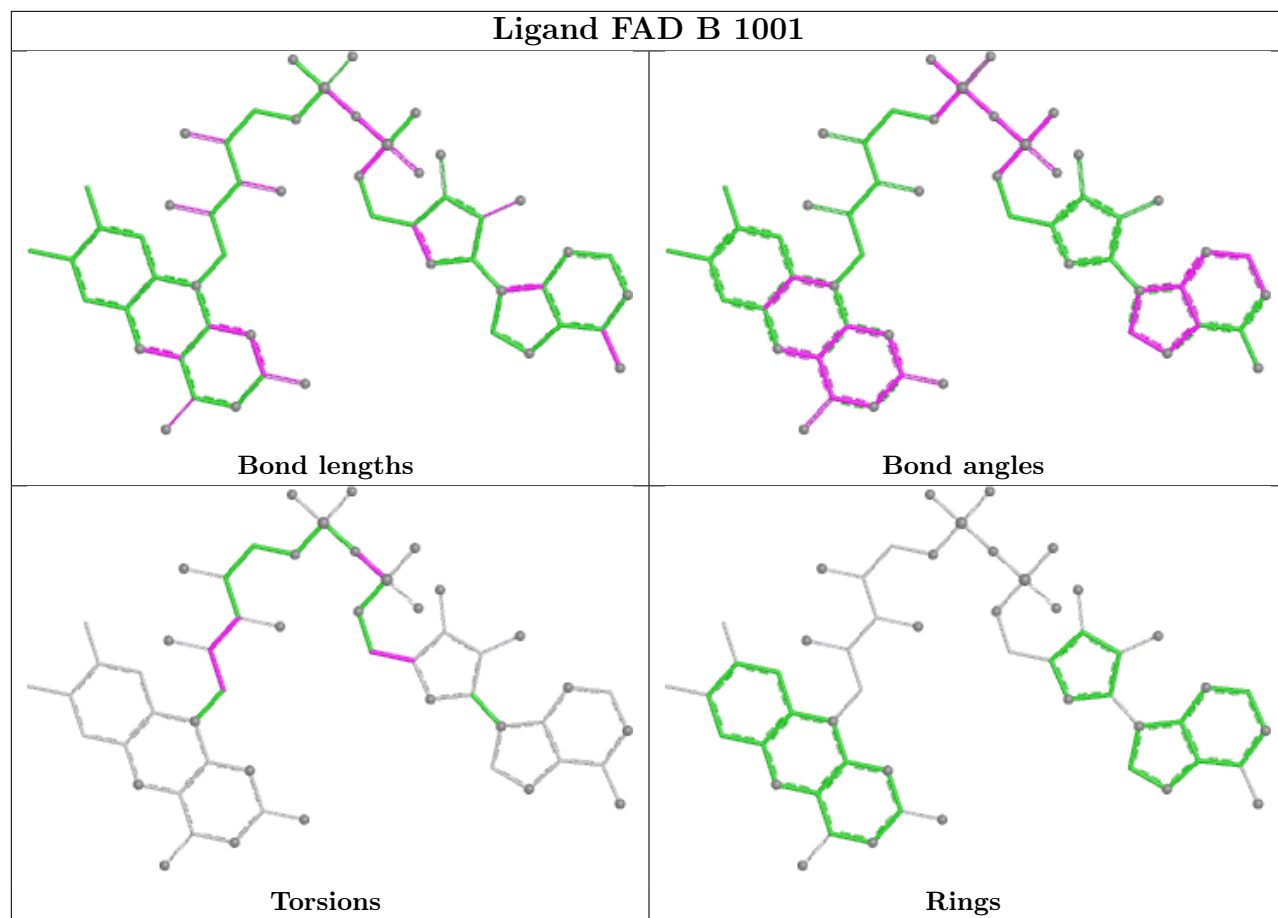
Mol	Chain	Res	Type	Atoms
2	B	1001	FAD	O2'-C2'-C3'-C4'
2	B	1001	FAD	C3B-C4B-C5B-O5B

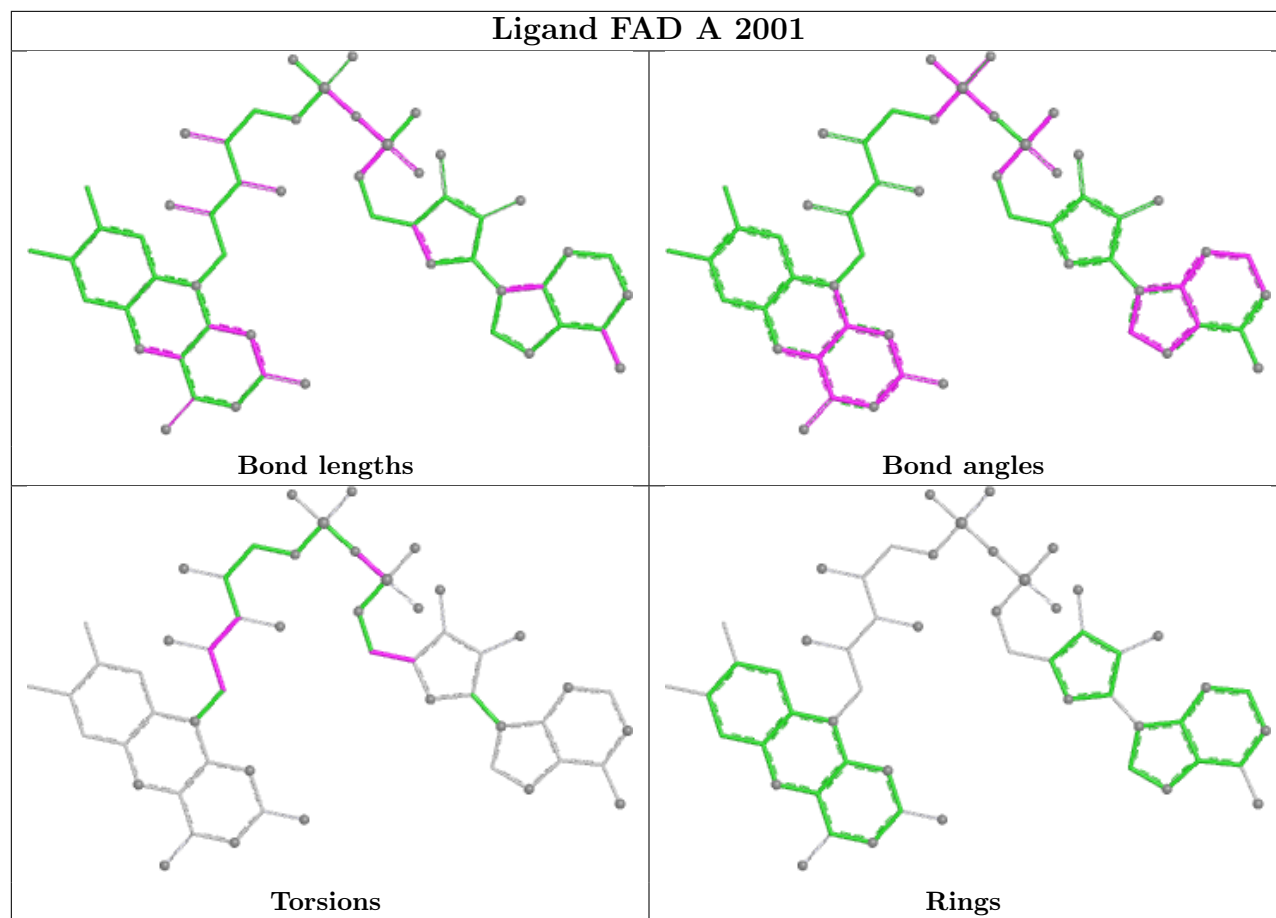
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	FAD	1	0
4	B	1003	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	971/1001 (97%)	0.01	32 (3%) 49 51	20, 34, 57, 84	0
1	B	969/1001 (96%)	0.12	32 (3%) 49 51	26, 39, 61, 85	0
All	All	1940/2002 (96%)	0.06	64 (3%) 49 51	20, 37, 59, 85	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	6.9
1	A	55	LEU	5.3
1	B	129	VAL	5.0
1	A	129	VAL	4.9
1	B	409	GLY	4.0
1	B	189	ARG	4.0
1	B	131	GLN	3.8
1	A	185	GLY	3.8
1	B	434	ALA	3.8
1	A	409	GLY	3.8
1	A	460	GLU	3.7
1	A	122	ALA	3.6
1	A	131	GLN	3.4
1	A	188	THR	3.4
1	B	460	GLU	3.2
1	B	122	ALA	3.1
1	B	188	THR	3.0
1	A	121	TRP	2.8
1	B	190	TYR	2.8
1	B	132	PRO	2.7
1	A	186	GLN	2.7
1	B	133	GLY	2.7
1	B	946	GLY	2.7
1	B	410	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	543	ALA	2.7
1	A	542	ILE	2.6
1	B	2	PRO	2.6
1	A	459	LEU	2.6
1	B	128	ARG	2.6
1	B	56	GLY	2.5
1	A	189	ARG	2.4
1	B	509	PRO	2.4
1	B	50	LYS	2.4
1	A	434	ALA	2.4
1	A	128	ARG	2.4
1	B	817	ARG	2.4
1	A	510	GLU	2.3
1	A	181	LYS	2.3
1	A	56	GLY	2.3
1	B	510	GLU	2.3
1	A	132	PRO	2.3
1	B	28	HIS	2.3
1	A	946	GLY	2.2
1	A	88	ALA	2.2
1	A	410	SER	2.2
1	A	50	LYS	2.2
1	B	121	TRP	2.2
1	B	459	LEU	2.2
1	B	542	ILE	2.2
1	A	463	ALA	2.2
1	A	548	ASP	2.1
1	B	182	PRO	2.1
1	B	543	ALA	2.1
1	A	411	SER	2.1
1	B	130	ILE	2.1
1	B	934	GLN	2.1
1	A	2	PRO	2.1
1	B	987	ALA	2.0
1	B	837	VAL	2.0
1	A	714	GLY	2.0
1	A	989	GLY	2.0
1	A	187	LYS	2.0
1	A	38	HIS	2.0
1	B	226	HIS	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](#)

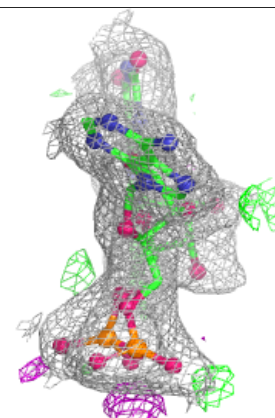
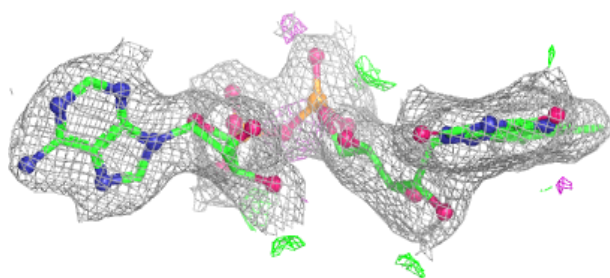
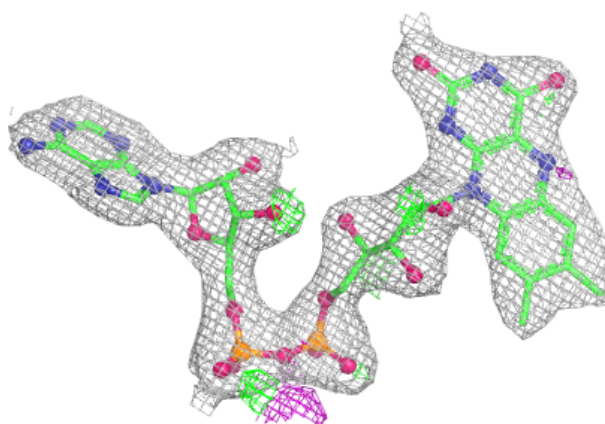
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	2005	5/5	0.78	0.14	82,82,86,87	0
4	SO4	B	1003	5/5	0.80	0.11	84,85,90,92	0
3	GOL	A	2002	6/6	0.85	0.17	51,53,53,53	0
3	GOL	A	2004	6/6	0.89	0.12	32,43,46,48	0
3	GOL	A	2003	6/6	0.92	0.12	42,46,48,50	0
4	SO4	B	1004	5/5	0.93	0.14	58,60,64,68	0
4	SO4	A	2006	5/5	0.94	0.12	48,52,59,63	0
4	SO4	A	2007	5/5	0.96	0.10	45,48,53,53	0
4	SO4	B	1002	5/5	0.96	0.09	57,61,65,67	0
2	FAD	B	1001	53/53	0.97	0.07	20,32,41,42	0
2	FAD	A	2001	53/53	0.97	0.06	17,23,31,44	0

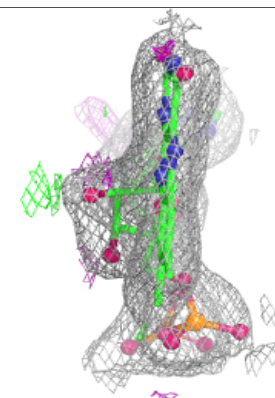
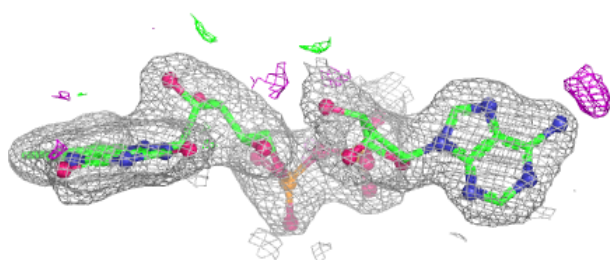
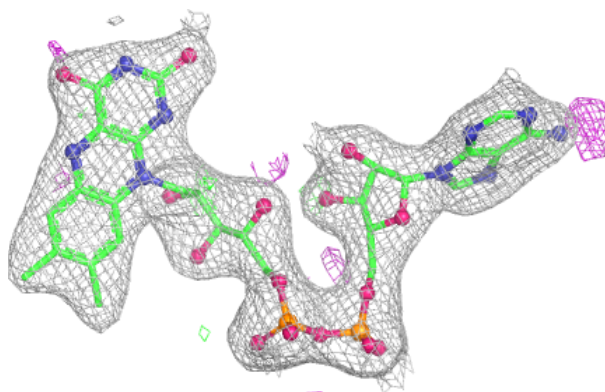
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1001:

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

**Electron density around FAD A 2001:**

$2mF_o-DF_c$ (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.