



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:27 AM UTC

PDB ID : 7XE1 / pdb_00007xe1
Title : Crystal structure of LSD2 in complex with cis-4-Br-PCPA
Authors : Niwa, H.; Sato, S.; Umehara, T.
Deposited on : 2022-03-29
Resolution : 2.07 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

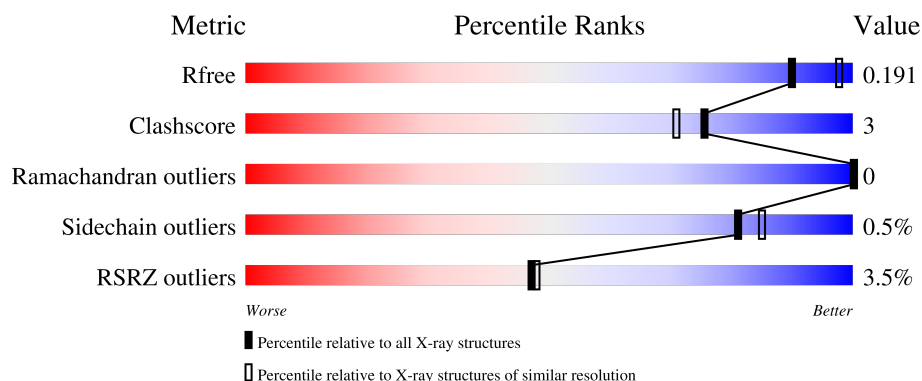
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

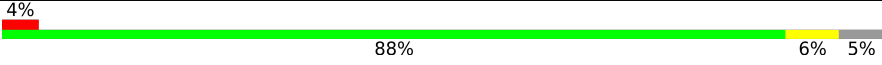
The reported resolution of this entry is 2.07 Å.

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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	793	
1	B	793	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13150 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.

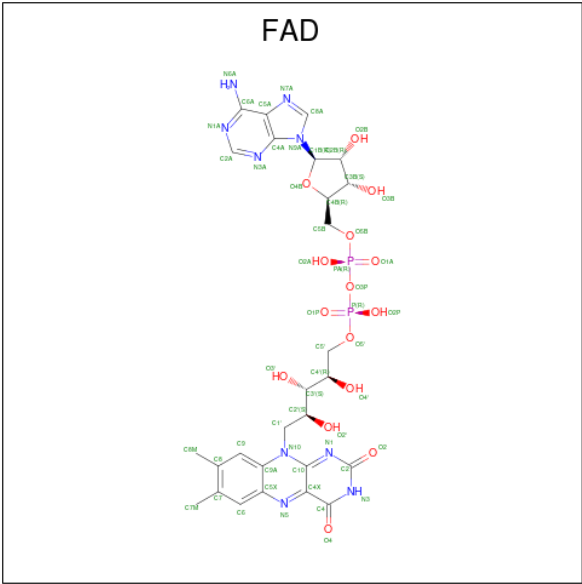
- Molecule 1 is a protein called Lysine-specific histone demethylase 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	8	0
			5983	3821	1017	1103	42			
1	B	740	Total	C	N	O	S	0	7	0
			5921	3783	1005	1092	41			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

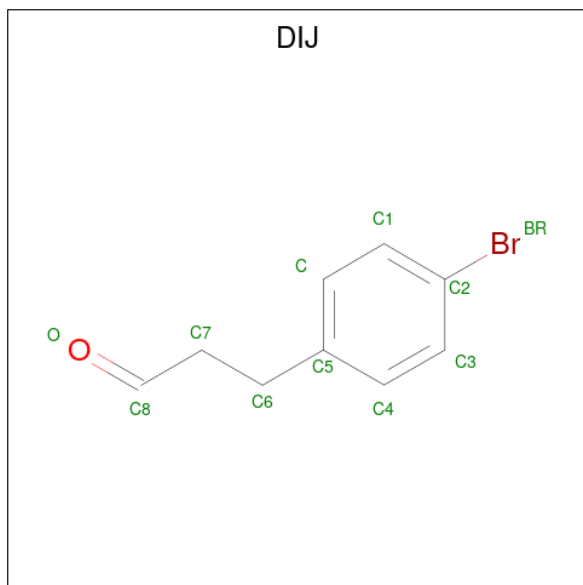
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 3-(4-bromophenyl)propanal (CCD ID: DIJ) (formula: C₉H₉BrO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	O	0	0
			11	1	9	1		
4	B	1	Total	Br	C	O	0	0
			11	1	9	1		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- 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	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
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		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

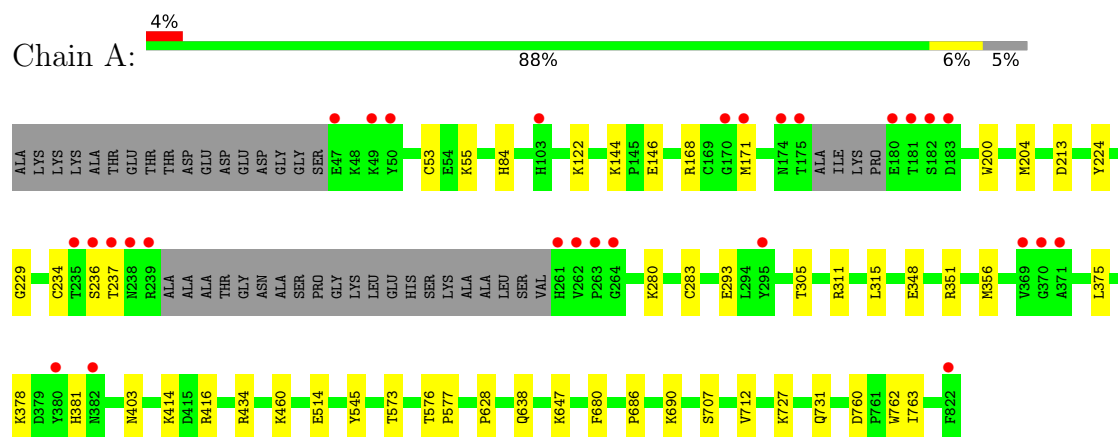
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	628	Total	O	0	0
			628	628		
9	B	376	Total	O	0	0
			376	376		

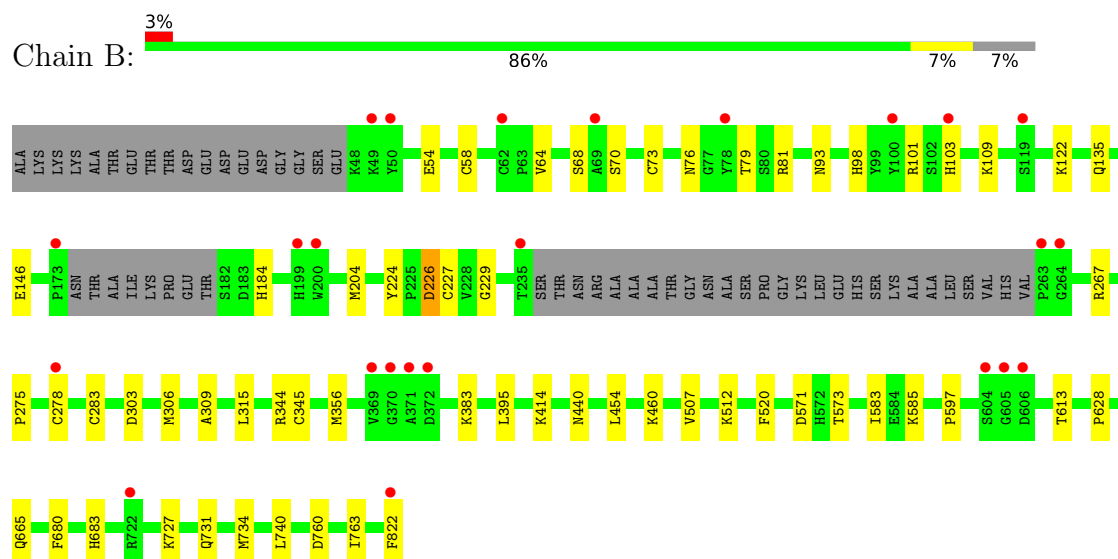
3 Residue-property plots [i](#)

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: Lysine-specific histone demethylase 1B



- Molecule 1: Lysine-specific histone demethylase 1B



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	144.12Å 170.76Å 202.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 2.07 46.75 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.75-2.07) 100.0 (46.75-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158+SVN	Depositor
R, R_{free}	0.164 , 0.192 0.163 , 0.191	Depositor DCC
R_{free} test set	7547 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13150	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: PEG, GOL, PGE, ZN, DIJ, FLC, 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	0.33	0/6155	0.50	0/8341
1	B	0.27	0/6071	0.44	0/8222
All	All	0.30	0/12226	0.47	0/16563

There are no bond length outliers.

There are no bond angle outliers.

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	5983	0	5894	35	0
1	B	5921	0	5828	37	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	11	0	0	0	0
4	B	11	0	0	0	0
5	A	13	0	5	0	0
6	A	10	0	14	2	0
7	A	54	0	72	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	24	0	32	2	0
8	B	7	0	10	1	0
9	A	628	0	0	8	0
9	B	376	0	0	5	0
All	All	13150	0	11917	73	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 (73) 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:306:MET:HE1	1:B:344:ARG:HG3	1.52	0.89
1:B:79:THR:HG21	1:B:93:ASN:H	1.43	0.83
1:B:303:ASP:OD1	9:B:1001:HOH:O	2.05	0.74
1:A:638[B]:GLN:NE2	9:A:1002:HOH:O	2.22	0.73
1:A:638[B]:GLN:NE2	9:A:1004:HOH:O	2.23	0.71
1:B:64:VAL:HG23	1:B:76:ASN:HB3	1.76	0.67
1:B:665:GLN:NE2	9:B:1004:HOH:O	2.31	0.64
1:A:234[A]:CYS:HB3	1:A:237:THR:HB	1.80	0.62
1:B:122:LYS:HD2	1:B:227:CYS:SG	2.40	0.62
1:A:434:ARG:NH1	9:A:1006:HOH:O	2.26	0.61
1:B:414:LYS:NZ	1:B:760:ASP:OD2	2.34	0.60
1:B:70:SER:HB3	1:B:98:HIS:HB2	1.84	0.59
1:B:734:MET:HG3	7:B:907:GOL:H2	1.84	0.59
1:B:306:MET:HE3	1:B:345:CYS:HA	1.86	0.58
1:A:514[B]:GLU:HG2	7:A:914:GOL:HO3	1.68	0.58
1:A:762:TRP:CH2	7:A:908:GOL:H11	2.40	0.56
1:A:224:TYR:H	6:A:907:PGE:H62	1.72	0.55
7:A:913:GOL:O3	9:A:1001:HOH:O	2.18	0.55
1:B:109:LYS:NZ	1:B:135:GLN:OE1	2.38	0.53
1:B:731:GLN:HG2	7:B:907:GOL:O3	2.10	0.52
1:A:144:LYS:HE2	1:A:146:GLU:OE2	2.11	0.50
1:A:686:PRO:HG2	1:A:690:LYS:HD2	1.92	0.50
1:B:226:ASP:OD1	1:B:226:ASP:N	2.41	0.50
1:B:229:GLY:HA3	1:B:309:ALA:HB2	1.94	0.50
1:B:727:LYS:HE2	1:B:731:GLN:NE2	2.27	0.50
1:A:293:GLU:OE2	1:A:311:ARG:HD3	2.12	0.49
1:A:416[B]:ARG:NH2	9:A:1022:HOH:O	2.46	0.49
1:B:278:CYS:SG	9:B:1008:HOH:O	2.60	0.49
1:A:168:ARG:O	1:A:171:MET:HG2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:HG3	9:A:1467:HOH:O	2.13	0.49
1:B:101:ARG:HB3	1:B:103:HIS:CE1	2.49	0.48
1:A:545:TYR:CD1	1:A:712:VAL:HG11	2.49	0.48
1:A:146:GLU:OE1	1:A:146:GLU:N	2.45	0.48
1:A:647:LYS:NZ	9:A:1024:HOH:O	2.48	0.47
1:B:146:GLU:OE1	1:B:146:GLU:N	2.34	0.47
7:A:911:GOL:O2	1:B:122:LYS:HD3	2.15	0.47
1:A:545:TYR:CE1	1:A:712:VAL:HG11	2.50	0.46
1:B:520:PHE:CD1	8:B:906:PEG:H31	2.51	0.46
1:B:597:PRO:HG2	1:B:613:THR:OG1	2.16	0.46
1:B:628:PRO:HG2	1:B:763:ILE:HA	1.98	0.46
1:A:55:LYS:HD3	1:B:224:TYR:CZ	2.51	0.45
1:B:58:CYS:HA	1:B:204:MET:HE2	1.98	0.45
1:A:460:LYS:HA	1:A:573:THR:HG22	1.99	0.45
1:A:234[B]:CYS:HB2	1:A:237:THR:HB	1.99	0.44
1:A:229:GLY:HA2	1:A:305:THR:HG23	1.98	0.44
1:A:628:PRO:HG2	1:A:763:ILE:HA	1.99	0.44
1:B:54:GLU:OE1	1:B:81:ARG:NH1	2.50	0.43
1:B:315:LEU:HG	1:B:356:MET:HE1	1.99	0.43
1:B:454:LEU:HD21	1:B:585:LYS:HG2	2.01	0.43
1:A:378:LYS:HD3	1:A:381:HIS:ND1	2.33	0.43
1:B:507:VAL:HG21	1:B:512:LYS:HD3	2.01	0.43
1:A:53:CYS:SG	1:A:84:HIS:HB2	2.59	0.43
1:A:200:TRP:CG	1:B:275:PRO:HA	2.54	0.42
1:B:683:HIS:CD2	1:B:740:LEU:HD21	2.54	0.42
1:A:280:LYS:HE3	1:A:283:CYS:SG	2.59	0.42
1:B:267:ARG:NH2	1:B:571:ASP:OD2	2.52	0.42
1:A:122:LYS:HE3	1:A:224:TYR:CE2	2.55	0.41
1:A:315:LEU:HG	1:A:356:MET:HE1	2.02	0.41
7:A:912:GOL:H11	9:B:1081:HOH:O	2.20	0.41
1:B:184:HIS:HD2	9:B:1350:HOH:O	2.02	0.41
1:A:576[B]:THR:OG1	1:A:577:PRO:HD3	2.21	0.41
1:A:348:GLU:OE2	1:A:351:ARG:HD3	2.21	0.41
1:B:727:LYS:O	1:B:731:GLN:HG3	2.21	0.41
1:A:414:LYS:NZ	1:A:760:ASP:OD2	2.48	0.41
6:A:907:PGE:H32	6:A:907:PGE:H5	1.88	0.41
1:B:68:SER:HA	1:B:73:CYS:SG	2.61	0.41
1:B:460:LYS:HA	1:B:573:THR:HG22	2.02	0.41
1:A:375:LEU:HD12	1:A:403:ASN:HB3	2.03	0.41
1:B:395:LEU:HD12	1:B:583:ILE:HD12	2.03	0.40
1:A:213:ASP:OD1	1:A:236:SER:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LYS:HG2	9:A:1467:HOH:O	2.21	0.40
1:B:383:LYS:HE2	1:B:822:PHE:HB2	2.03	0.40
1:A:200:TRP:O	1:A:204:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	753/793 (95%)	738 (98%)	15 (2%)	0	100	100
1	B	741/793 (93%)	723 (98%)	18 (2%)	0	100	100
All	All	1494/1586 (94%)	1461 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/676 (96%)	648 (100%)	2 (0%)	86	89
1	B	641/676 (95%)	637 (99%)	4 (1%)	78	82
All	All	1291/1352 (96%)	1285 (100%)	6 (0%)	81	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	680	PHE
1	A	707	SER
1	B	226	ASP
1	B	283	CYS
1	B	440	ASN
1	B	680	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	135	GLN
1	A	152	GLN
1	A	199	HIS
1	A	274	GLN
1	A	347	GLN
1	B	141	GLN
1	B	731	GLN
1	B	744	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 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	DIJ	A	905	3	10,11,11	0.21	0	13,13,13	0.34	0
7	GOL	A	910	-	5,5,5	0.84	0	5,5,5	1.01	0
7	GOL	A	916	-	5,5,5	0.89	0	5,5,5	1.18	0
7	GOL	A	908	-	5,5,5	0.79	0	5,5,5	1.37	1 (20%)
4	DIJ	B	905	3	10,11,11	0.24	0	13,13,13	0.36	0
7	GOL	A	911	-	5,5,5	1.01	0	5,5,5	1.02	0
7	GOL	B	908	-	5,5,5	0.62	0	5,5,5	1.28	1 (20%)
7	GOL	B	910	-	5,5,5	0.83	0	5,5,5	1.12	0
3	FAD	A	904	4	58,58,58	0.87	3 (5%)	85,89,89	1.15	8 (9%)
3	FAD	B	904	4	58,58,58	0.82	3 (5%)	85,89,89	1.14	7 (8%)
7	GOL	A	912	-	5,5,5	0.79	0	5,5,5	1.18	0
5	FLC	A	906	-	12,12,12	1.03	0	17,17,17	5.34	8 (47%)
7	GOL	A	913	-	5,5,5	0.71	0	5,5,5	1.11	0
7	GOL	A	914	-	5,5,5	0.66	0	5,5,5	1.20	1 (20%)
7	GOL	A	909	-	5,5,5	0.74	0	5,5,5	1.22	0
6	PGE	A	907	-	9,9,9	0.51	0	8,8,8	0.43	0
7	GOL	A	915	-	5,5,5	0.77	0	5,5,5	1.47	1 (20%)
7	GOL	B	907	-	5,5,5	0.95	0	5,5,5	1.00	0
7	GOL	B	909	-	5,5,5	1.12	1 (20%)	5,5,5	0.99	0
8	PEG	B	906	-	6,6,6	0.19	0	5,5,5	0.12	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
4	DIJ	A	905	3	-	1/4/4/4	0/1/1/1
7	GOL	A	910	-	-	1/4/4/4	-
7	GOL	A	916	-	-	2/4/4/4	-
7	GOL	A	908	-	-	2/4/4/4	-
4	DIJ	B	905	3	-	1/4/4/4	0/1/1/1
7	GOL	A	911	-	-	0/4/4/4	-
7	GOL	B	908	-	-	2/4/4/4	-
7	GOL	B	910	-	-	2/4/4/4	-
3	FAD	A	904	4	-	2/34/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	904	4	-	2/34/50/50	0/6/6/6
7	GOL	A	912	-	-	2/4/4/4	-
5	FLC	A	906	-	-	6/16/16/16	-
7	GOL	A	913	-	-	2/4/4/4	-
7	GOL	A	914	-	-	2/4/4/4	-
7	GOL	A	909	-	-	3/4/4/4	-
6	PGE	A	907	-	-	4/7/7/7	-
7	GOL	A	915	-	-	2/4/4/4	-
7	GOL	B	907	-	-	0/4/4/4	-
7	GOL	B	909	-	-	3/4/4/4	-
8	PEG	B	906	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	904	FAD	C4X-N5	4.54	1.40	1.30
3	B	904	FAD	C4X-N5	4.31	1.40	1.30
3	A	904	FAD	C4X-C10	-2.35	1.37	1.44
3	B	904	FAD	C4X-C10	-2.13	1.37	1.44
3	A	904	FAD	C10-N1	2.09	1.37	1.33
7	B	909	GOL	C1-C2	2.06	1.59	1.51
3	B	904	FAD	C5X-N5	2.01	1.43	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	906	FLC	OHB-CB-CBC	-12.45	91.30	108.96
5	A	906	FLC	OHB-CB-CG	-11.02	84.25	109.38
5	A	906	FLC	OHB-CB-CA	-10.44	85.57	109.38
5	A	906	FLC	CA-CB-CBC	5.24	121.62	110.03
5	A	906	FLC	OB2-CBC-CB	4.86	122.47	113.14
3	A	904	FAD	C9A-C5X-N5	-4.37	117.82	122.45
3	B	904	FAD	C9A-C5X-N5	-4.28	117.91	122.45
3	B	904	FAD	C4X-C10-N10	4.01	122.22	116.48
5	A	906	FLC	CG-CB-CA	3.90	119.33	109.31
3	A	904	FAD	C4X-C10-N10	3.82	121.95	116.48
3	B	904	FAD	C10-C4X-N5	-3.72	117.21	124.81
5	A	906	FLC	CG-CB-CBC	3.72	118.27	110.03
3	A	904	FAD	C10-C4X-N5	-3.68	117.30	124.81
3	B	904	FAD	C4-C4X-C10	3.17	122.37	116.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	FAD	C4-C4X-C10	3.05	122.17	116.93
5	A	906	FLC	OB1-CBC-CB	-3.00	116.27	122.09
7	A	908	GOL	C3-C2-C1	-2.62	102.17	111.80
3	B	904	FAD	C6-C5X-N5	2.61	122.78	118.44
3	B	904	FAD	C10-N1-C2	2.49	122.23	116.85
3	A	904	FAD	C6-C5X-N5	2.48	122.56	118.44
3	A	904	FAD	O2P-P-O1P	2.43	123.75	112.44
3	A	904	FAD	C10-N1-C2	2.39	122.01	116.85
7	A	915	GOL	O1-C1-C2	-2.37	99.68	110.38
7	A	914	GOL	C3-C2-C1	-2.19	103.77	111.80
7	B	908	GOL	C3-C2-C1	-2.16	103.89	111.80
3	B	904	FAD	C4X-C10-N1	-2.14	119.33	124.59
3	A	904	FAD	C4X-C10-N1	-2.08	119.49	124.59

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	909	GOL	C1-C2-C3-O3
7	A	912	GOL	O2-C2-C3-O3
7	A	913	GOL	O1-C1-C2-C3
7	A	915	GOL	O1-C1-C2-C3
7	A	916	GOL	C1-C2-C3-O3
7	B	909	GOL	C1-C2-C3-O3
5	A	906	FLC	OHB-CB-CG-CGC
7	B	909	GOL	O2-C2-C3-O3
5	A	906	FLC	CAC-CA-CB-CBC
7	A	908	GOL	O1-C1-C2-C3
7	A	912	GOL	C1-C2-C3-O3
7	A	914	GOL	C1-C2-C3-O3
7	A	909	GOL	O2-C2-C3-O3
7	A	916	GOL	O2-C2-C3-O3
6	A	907	PGE	O3-C5-C6-O4
5	A	906	FLC	CBC-CB-CG-CGC
7	A	908	GOL	O1-C1-C2-O2
7	A	913	GOL	O1-C1-C2-O2
7	A	914	GOL	O2-C2-C3-O3
7	A	915	GOL	O1-C1-C2-O2
5	A	906	FLC	CA-CB-CBC-OB2
3	A	904	FAD	PA-O3P-P-O5'
3	B	904	FAD	PA-O3P-P-O5'
6	A	907	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

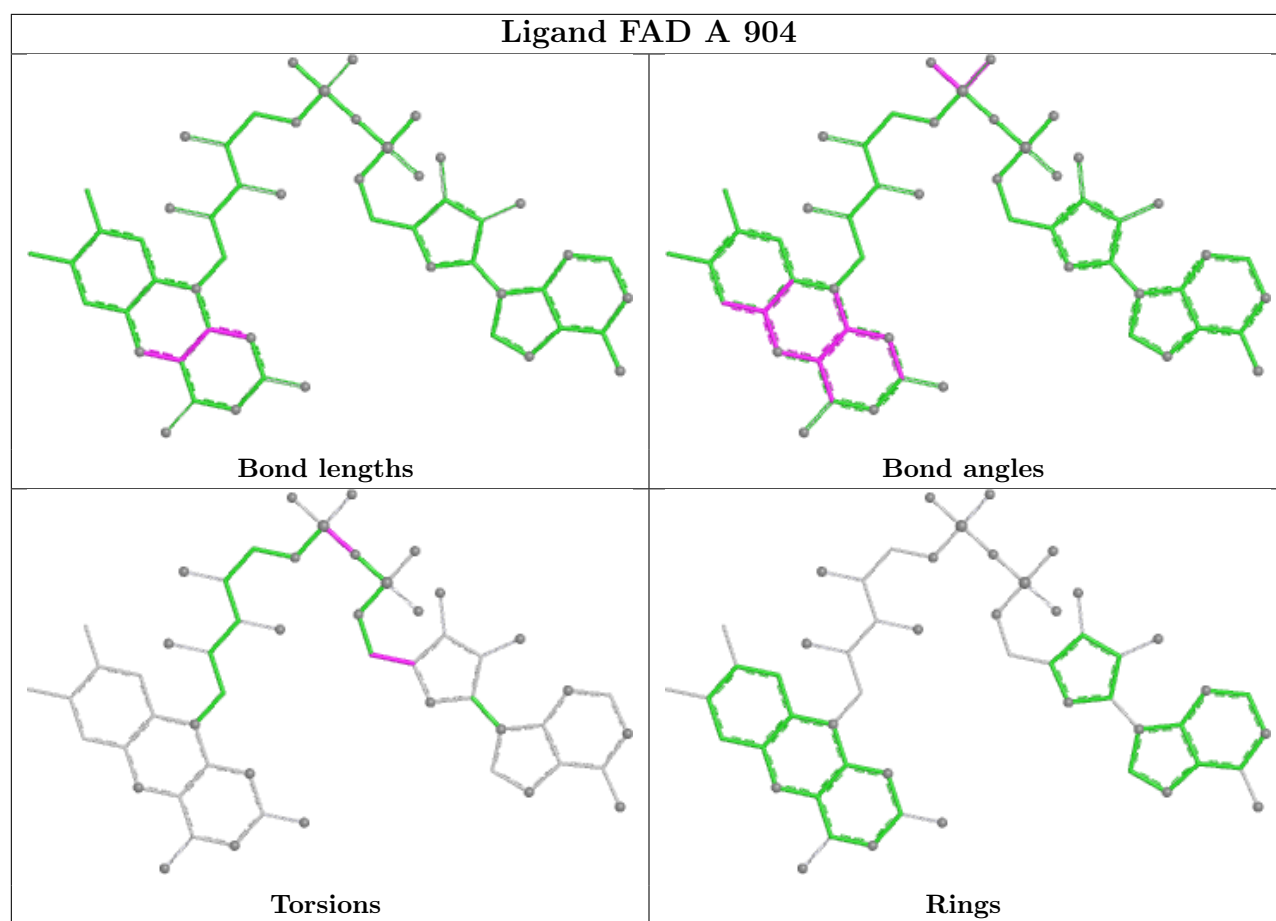
Mol	Chain	Res	Type	Atoms
7	A	910	GOL	O1-C1-C2-O2
7	B	908	GOL	O1-C1-C2-O2
7	B	908	GOL	O2-C2-C3-O3
7	B	909	GOL	O1-C1-C2-O2
7	B	910	GOL	O1-C1-C2-O2
7	B	910	GOL	O2-C2-C3-O3
5	A	906	FLC	CAC-CA-CB-CG
5	A	906	FLC	CA-CB-CBC-OB1
6	A	907	PGE	C1-C2-O2-C3
7	A	909	GOL	O1-C1-C2-O2
4	A	905	DIJ	C4-C5-C6-C7
4	B	905	DIJ	C4-C5-C6-C7
6	A	907	PGE	O2-C3-C4-O3
8	B	906	PEG	C1-C2-O2-C3
3	B	904	FAD	P-O3P-PA-O2A
3	A	904	FAD	O4B-C4B-C5B-O5B

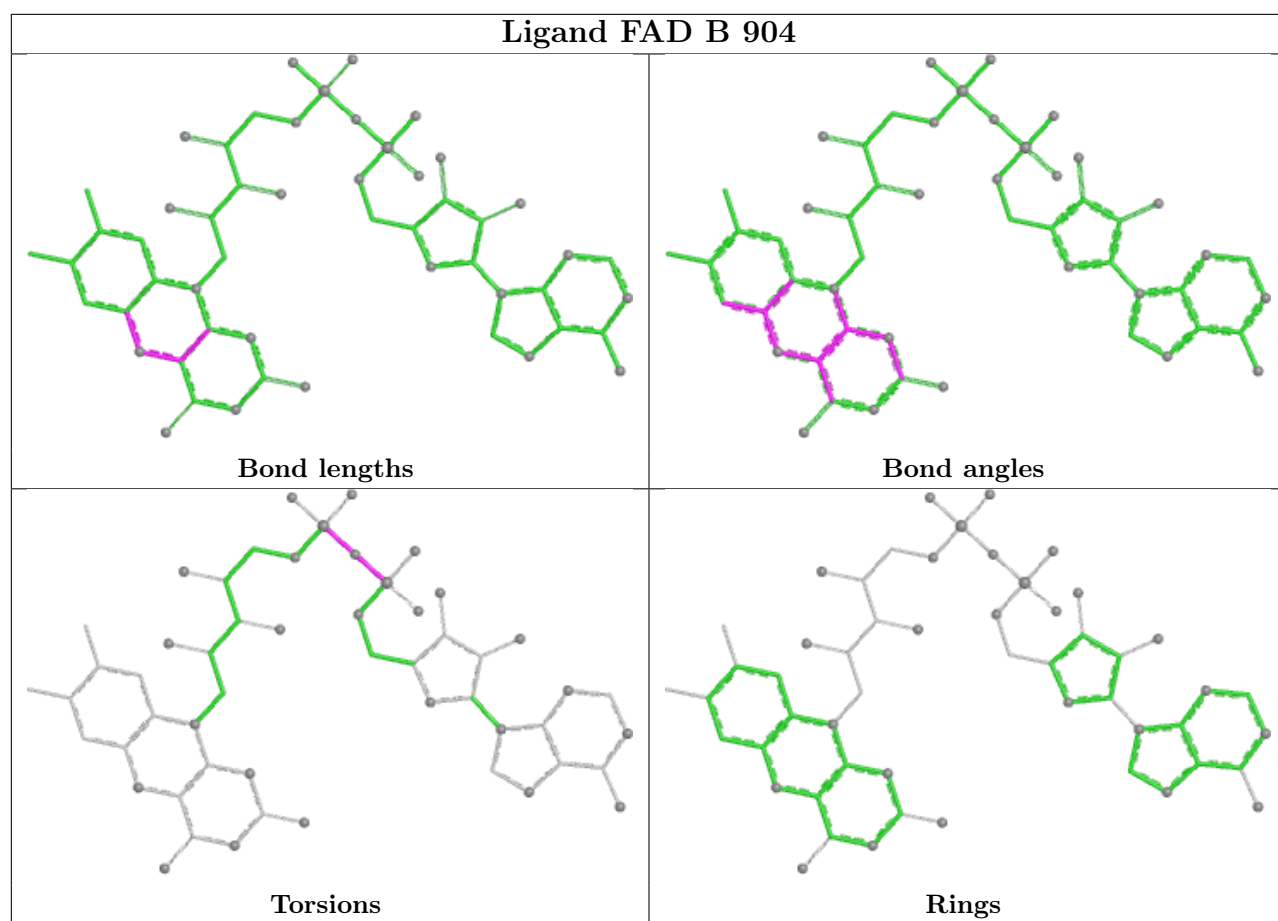
There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	908	GOL	1	0
7	A	911	GOL	1	0
7	A	912	GOL	1	0
7	A	913	GOL	1	0
7	A	914	GOL	1	0
6	A	907	PGE	2	0
7	B	907	GOL	2	0
8	B	906	PEG	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	751/793 (94%)	-0.30	28 (3%)	45 46	18, 36, 69, 118	8 (1%)
1	B	740/793 (93%)	0.06	24 (3%)	50 50	23, 48, 89, 124	7 (0%)
All	All	1491/1586 (94%)	-0.12	52 (3%)	47 48	18, 42, 84, 124	15 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	605[A]	GLY	7.1
1	B	173	PRO	6.2
1	A	237	THR	5.6
1	B	606[A]	ASP	4.8
1	A	175	THR	4.5
1	A	181	THR	3.9
1	B	263	PRO	3.9
1	A	180	GLU	3.7
1	A	263	PRO	3.7
1	B	103	HIS	3.6
1	B	822	PHE	3.6
1	A	262	VAL	3.5
1	A	236	SER	3.4
1	A	239	ARG	3.3
1	B	235	THR	3.3
1	B	50	TYR	3.1
1	B	78	TYR	3.0
1	B	278	CYS	3.0
1	A	183	ASP	3.0
1	A	370	GLY	2.9
1	A	380	TYR	2.9
1	A	174	ASN	2.8
1	B	49	LYS	2.8
1	A	171	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	2.6
1	A	371	ALA	2.6
1	A	49	LYS	2.6
1	A	235	THR	2.6
1	A	264	GLY	2.6
1	B	369	VAL	2.5
1	B	100	TYR	2.5
1	A	182	SER	2.5
1	B	370	GLY	2.5
1	B	371	ALA	2.5
1	A	295	TYR	2.4
1	A	261	HIS	2.4
1	B	372	ASP	2.4
1	B	62	CYS	2.4
1	A	50	TYR	2.3
1	A	238	ASN	2.3
1	A	382	ASN	2.3
1	A	170	GLY	2.3
1	B	604[A]	SER	2.3
1	A	369	VAL	2.2
1	B	119	SER	2.2
1	B	722	ARG	2.1
1	A	103	HIS	2.1
1	B	69	ALA	2.1
1	A	47	GLU	2.1
1	A	822	PHE	2.1
1	B	199	HIS	2.0
1	B	200	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

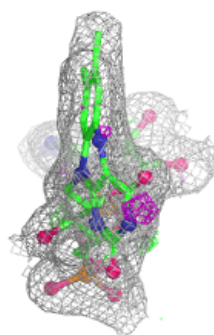
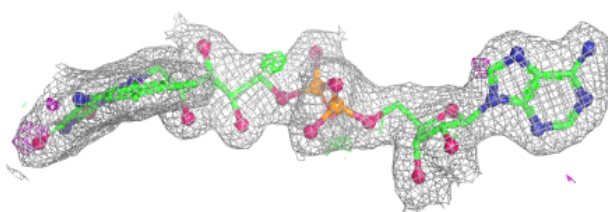
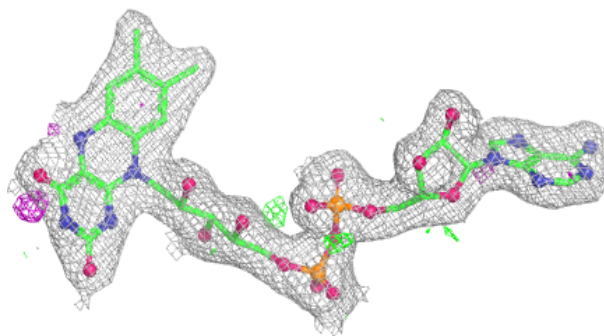
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	910	6/6	0.77	0.18	68,72,73,74	0
7	GOL	B	908	6/6	0.79	0.20	61,66,68,70	0
7	GOL	A	915	6/6	0.81	0.18	50,54,62,64	0
7	GOL	B	907	6/6	0.82	0.17	64,66,70,70	0
7	GOL	A	916	6/6	0.83	0.15	57,57,62,65	0
7	GOL	A	910	6/6	0.84	0.16	53,57,60,64	0
6	PGE	A	907	10/10	0.85	0.13	56,61,63,72	0
8	PEG	B	906	7/7	0.85	0.16	54,57,62,65	0
7	GOL	B	909	6/6	0.88	0.12	51,55,57,66	0
7	GOL	A	914	6/6	0.89	0.13	50,52,55,56	0
7	GOL	A	912	6/6	0.90	0.15	50,52,52,54	0
7	GOL	A	913	6/6	0.91	0.13	50,59,60,63	0
5	FLC	A	906	13/13	0.91	0.10	46,58,64,67	0
7	GOL	A	908	6/6	0.91	0.12	45,49,52,53	0
7	GOL	A	909	6/6	0.93	0.10	45,48,56,58	0
4	DIJ	A	905	11/11	0.94	0.12	28,31,35,54	11
7	GOL	A	911	6/6	0.94	0.13	40,42,45,49	0
4	DIJ	B	905	11/11	0.95	0.13	39,41,47,57	11
2	ZN	B	903	1/1	0.98	0.05	73,73,73,73	0
3	FAD	B	904	53/53	0.98	0.06	27,35,38,39	0
3	FAD	A	904	53/53	0.99	0.04	19,23,27,30	0
2	ZN	A	903	1/1	0.99	0.03	45,45,45,45	0
2	ZN	B	901	1/1	0.99	0.03	42,42,42,42	0
2	ZN	B	902	1/1	0.99	0.03	59,59,59,59	0
2	ZN	A	901	1/1	0.99	0.02	40,40,40,40	0
2	ZN	A	902	1/1	1.00	0.01	36,36,36,36	0

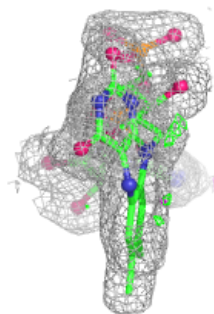
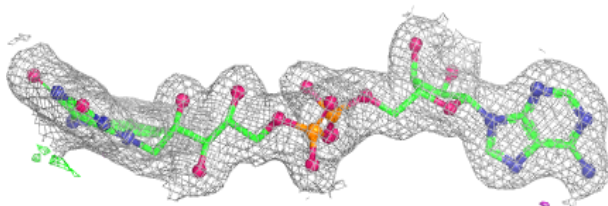
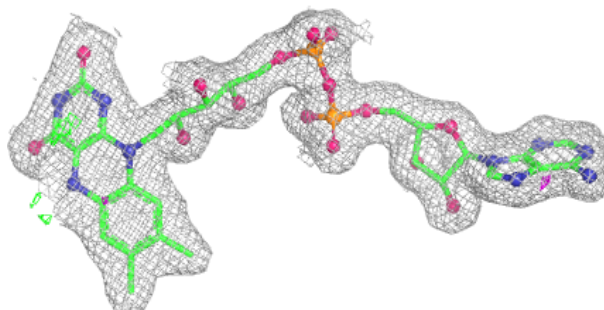
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 904:

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

**Electron density around FAD A 904:**

$2mF_o-DF_c$ (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.