



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2022 – 04:15 PM JST

PDB ID : 7XE1  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.30  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.30

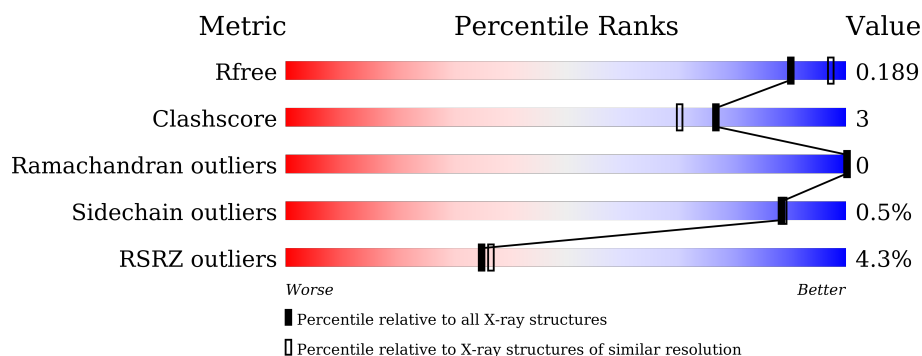
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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  $\geq 3$ , 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	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	B	793	<div> <div>5%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>

## 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.

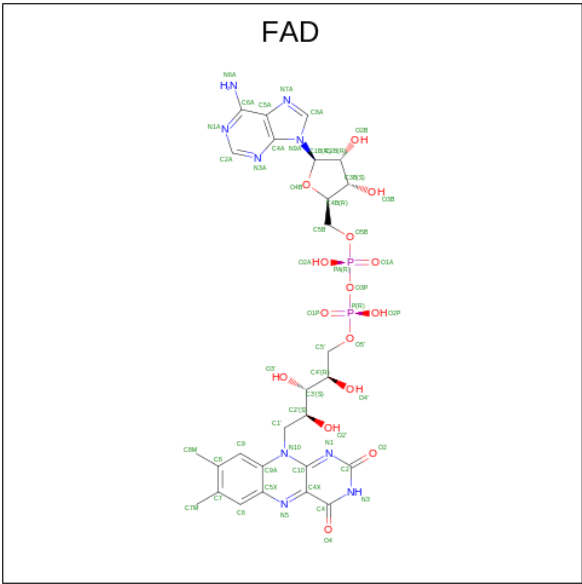
- Molecule 1 is a protein called Lysine-specific histone demethylase 1B.

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 (three-letter code: ZN) (formula: Zn).

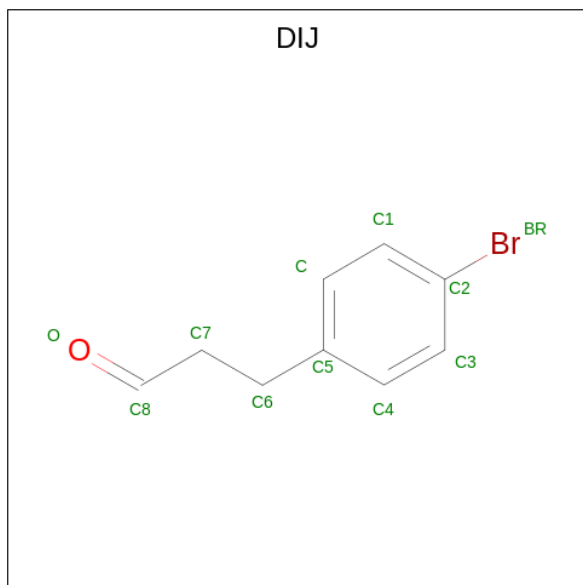
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



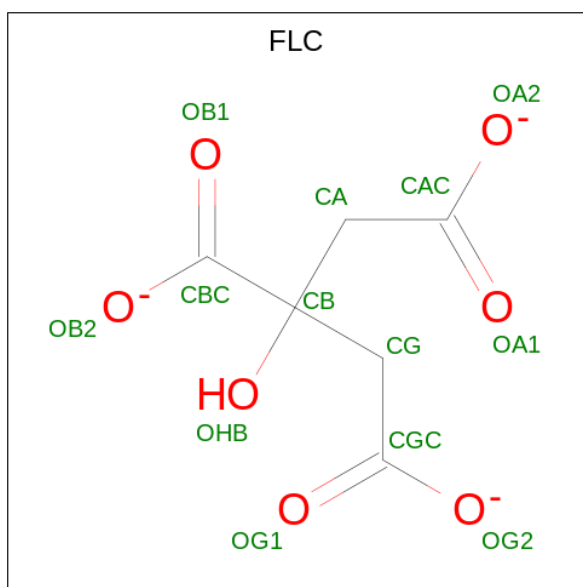
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 3-(4-bromophenyl)propanal (three-letter code: DIJ) (formula: C<sub>9</sub>H<sub>9</sub>BrO).



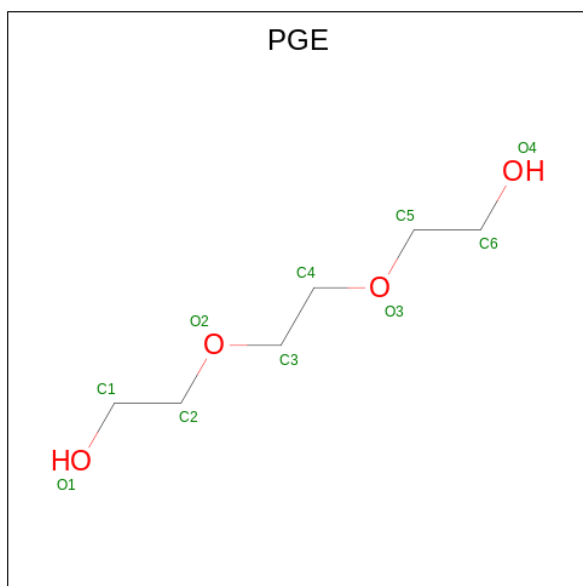
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	O	0	0
			11	1	9	1		
4	B	1	Total	Br	C	O	0	0
			11	1	9	1		

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: 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 (three-letter code: 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 (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



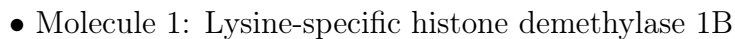
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

- 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		



- 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, $\alpha$ , $\beta$ , $\gamma$	144.12Å 170.76Å 202.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 2.07 48.39 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.75-2.07) 100.0 (48.39-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158+SVN	Depositor
R, $R_{free}$	0.164 , 0.192 0.160 , 0.189	Depositor DCC
$R_{free}$ test set	7547 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, FLC, ZN, DIJ, FAD, PGE, PEG

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	0.42	0/6155	0.58	0/8341
1	B	0.36	0/6071	0.55	0/8222
All	All	0.39	0/12226	0.57	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

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	34	0
1	B	5921	0	5828	38	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

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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	7	0
9	B	376	0	0	6	0
All	All	13150	0	11917	72	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 (72) 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: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: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:A:200:TRP:HD1	1:B:273:TYR:HH	1.52	0.54
1:B:306:MET:CE	1:B:344:ARG:HG3	2.39	0.53
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:380:TYR:OH	9:B:1002:HOH:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:O	1:A:171:MET:HG2	2.11	0.49
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: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: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: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:B:306:MET:HE3	1:B:344:ARG:HG3	2.01	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:48:LYS:HZ2	1:B:50:TYR:HE1	1.67	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
1:A:727:LYS:HG2	9:A:1467:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	92	93
1	B	641/676 (95%)	637 (99%)	4 (1%)	86	86
All	All	1291/1352 (96%)	1285 (100%)	6 (0%)	88	89

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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	199	HIS
1	B	731	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 monosaccharides 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	$\# Z  > 2$
7	GOL	A	910	-	5,5,5	0.81	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	904	4	53,58,58	1.01	3 (5%)	68,89,89	1.30	9 (13%)
7	GOL	B	907	-	5,5,5	0.92	0	5,5,5	0.93	0
7	GOL	A	912	-	5,5,5	0.75	0	5,5,5	1.10	0
7	GOL	A	911	-	5,5,5	0.96	0	5,5,5	0.94	0
8	PEG	B	906	-	6,6,6	0.19	0	5,5,5	0.12	0
7	GOL	B	909	-	5,5,5	1.06	0	5,5,5	0.92	0
4	DIJ	B	905	3	11,11,11	0.30	0	13,13,13	0.40	0
7	GOL	A	908	-	5,5,5	0.78	0	5,5,5	1.27	1 (20%)
7	GOL	B	910	-	5,5,5	0.80	0	5,5,5	1.04	0
7	GOL	A	914	-	5,5,5	0.64	0	5,5,5	1.12	1 (20%)
7	GOL	A	913	-	5,5,5	0.69	0	5,5,5	1.03	0
7	GOL	A	915	-	5,5,5	0.75	0	5,5,5	1.36	1 (20%)
7	GOL	A	916	-	5,5,5	0.85	0	5,5,5	1.09	0
3	FAD	B	904	4	53,58,58	0.96	2 (3%)	68,89,89	1.28	8 (11%)
5	FLC	A	906	-	12,12,12	1.02	0	17,17,17	5.38	8 (47%)
7	GOL	A	909	-	5,5,5	0.72	0	5,5,5	1.13	0
6	PGE	A	907	-	9,9,9	0.51	0	8,8,8	0.43	0
7	GOL	B	908	-	5,5,5	0.61	0	5,5,5	1.18	1 (20%)
4	DIJ	A	905	3	11,11,11	0.27	0	13,13,13	0.39	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
7	GOL	A	910	-	-	2/4/4/4	-
3	FAD	A	904	4	-	2/30/50/50	0/6/6/6
7	GOL	B	907	-	-	0/4/4/4	-
7	GOL	A	912	-	-	2/4/4/4	-
7	GOL	A	911	-	-	0/4/4/4	-
8	PEG	B	906	-	-	1/4/4/4	-
7	GOL	B	909	-	-	4/4/4/4	-
4	DIJ	B	905	3	-	1/3/4/4	0/1/1/1
7	GOL	A	908	-	-	2/4/4/4	-
7	GOL	B	910	-	-	3/4/4/4	-
7	GOL	A	914	-	-	2/4/4/4	-
7	GOL	A	913	-	-	2/4/4/4	-
7	GOL	A	915	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	916	-	-	2/4/4/4	-
3	FAD	B	904	4	-	2/30/50/50	0/6/6/6
5	FLC	A	906	-	-	6/16/16/16	-
7	GOL	A	909	-	-	3/4/4/4	-
6	PGE	A	907	-	-	4/7/7/7	-
7	GOL	B	908	-	-	3/4/4/4	-
4	DIJ	A	905	3	-	1/3/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	904	FAD	C4X-N5	5.04	1.40	1.30
3	B	904	FAD	C4X-N5	4.79	1.40	1.30
3	A	904	FAD	C4X-C10	-2.32	1.37	1.44
3	B	904	FAD	C4X-C10	-2.11	1.37	1.44
3	A	904	FAD	C10-N1	2.07	1.37	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	906	FLC	OHB-CB-CBC	-12.51	91.30	108.86
5	A	906	FLC	OHB-CB-CG	-10.75	84.25	109.40
5	A	906	FLC	OHB-CB-CA	-10.18	85.57	109.40
5	A	906	FLC	OB2-CBC-CB	5.42	122.47	113.05
5	A	906	FLC	CA-CB-CBC	5.36	121.62	110.11
3	A	904	FAD	C9A-C5X-N5	-4.25	117.82	122.43
5	A	906	FLC	OB1-CBC-CB	-4.22	116.27	122.25
3	B	904	FAD	C9A-C5X-N5	-4.16	117.91	122.43
3	B	904	FAD	C4X-C10-N10	3.92	122.22	116.48
5	A	906	FLC	CG-CB-CA	3.90	119.33	109.16
5	A	906	FLC	CG-CB-CBC	3.80	118.27	110.11
3	A	904	FAD	C4X-C10-N10	3.74	121.95	116.48
3	B	904	FAD	C10-C4X-N5	-3.60	117.21	124.86
3	A	904	FAD	C10-C4X-N5	-3.56	117.30	124.86
3	B	904	FAD	C4-C4X-C10	3.32	122.37	116.79
3	A	904	FAD	C4-C4X-C10	3.20	122.17	116.79
3	B	904	FAD	C10-N1-C2	2.66	122.23	116.90
3	A	904	FAD	C10-N1-C2	2.56	122.01	116.90
7	A	908	GOL	C3-C2-C1	-2.45	102.17	111.70
3	B	904	FAD	C6-C5X-N5	2.44	122.78	118.51
3	A	904	FAD	C5A-C6A-N6A	2.38	123.97	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	FAD	O2P-P-O1P	2.33	123.75	112.24
3	B	904	FAD	C4X-C10-N1	-2.33	119.33	124.73
3	A	904	FAD	C6-C5X-N5	2.32	122.56	118.51
3	B	904	FAD	C5A-C6A-N6A	2.27	123.80	120.35
3	A	904	FAD	C4X-C10-N1	-2.26	119.49	124.73
7	A	915	GOL	O1-C1-C2	-2.19	99.68	110.20
7	A	914	GOL	C3-C2-C1	-2.04	103.77	111.70
7	B	908	GOL	C3-C2-C1	-2.01	103.89	111.70

There are no chirality outliers.

All (44) torsion outliers are listed below:

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

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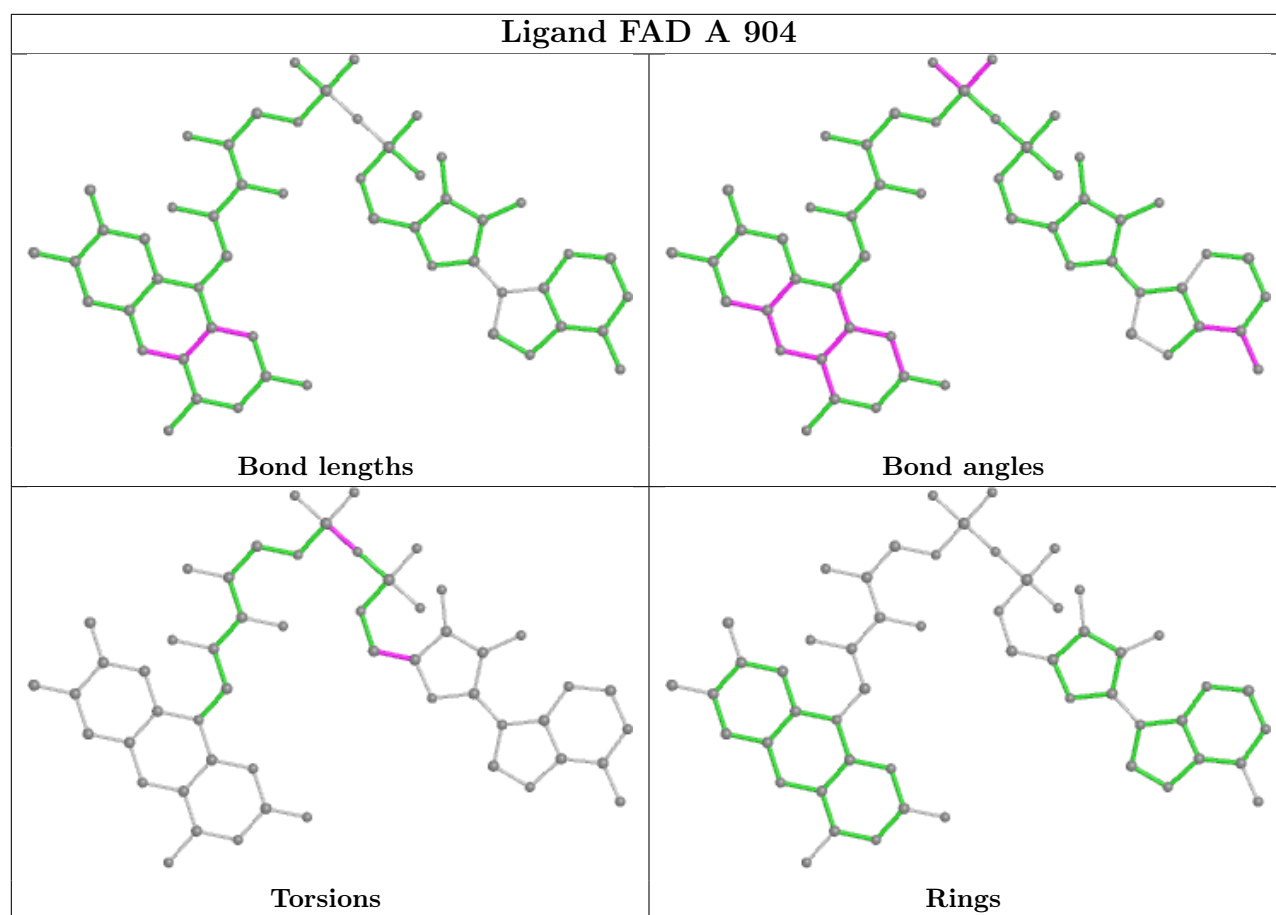
Mol	Chain	Res	Type	Atoms
7	B	910	GOL	O1-C1-C2-O2
7	B	910	GOL	O2-C2-C3-O3
6	A	907	PGE	C1-C2-O2-C3
5	A	906	FLC	CA-CB-CBC-OB1
7	A	910	GOL	O1-C1-C2-C3
7	B	908	GOL	C1-C2-C3-O3
3	A	904	FAD	O4B-C4B-C5B-O5B
7	A	909	GOL	O1-C1-C2-O2
3	B	904	FAD	O4B-C4B-C5B-O5B
4	A	905	DIJ	C4-C5-C6-C7
7	B	909	GOL	O1-C1-C2-C3
7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

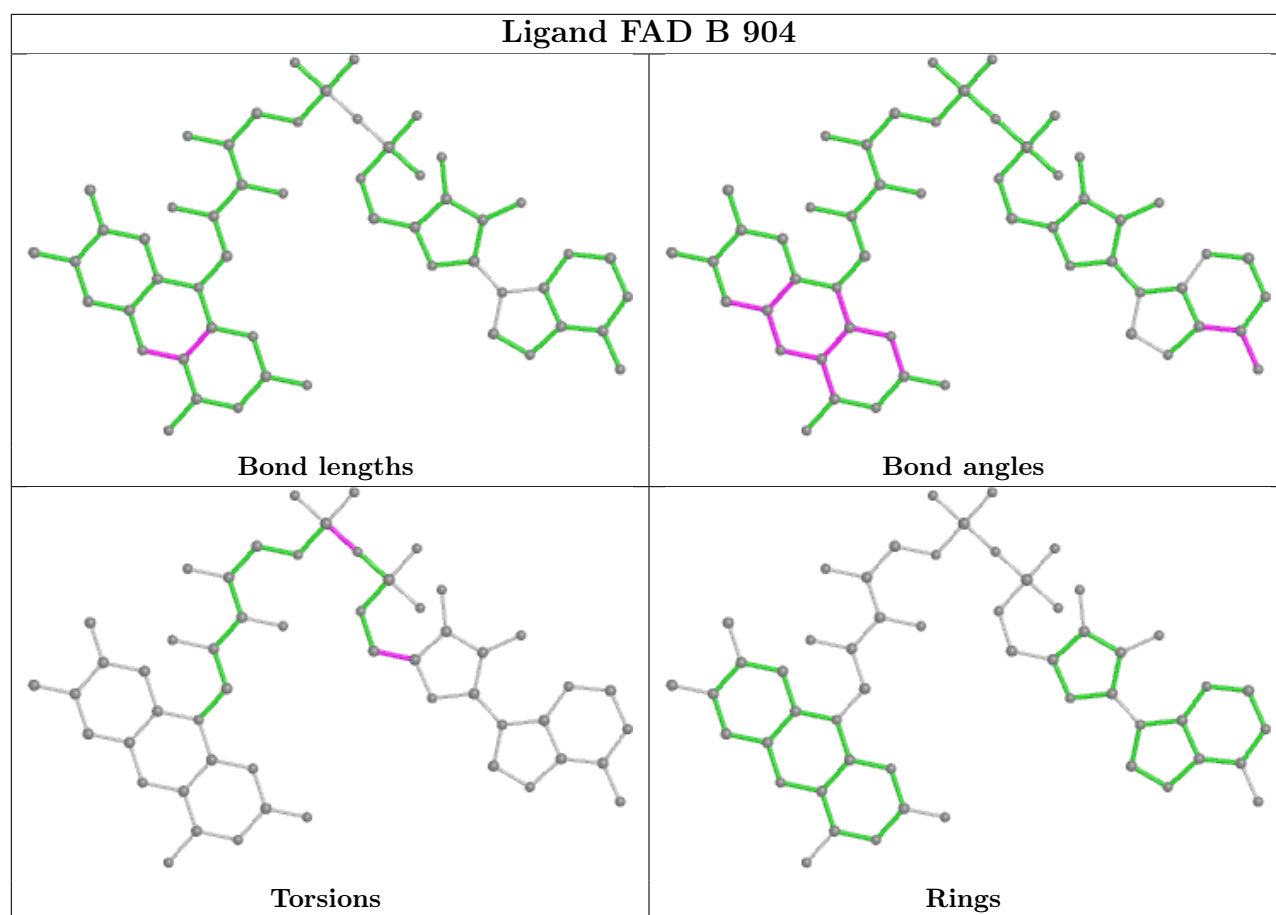
There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	907	GOL	2	0
7	A	912	GOL	1	0
7	A	911	GOL	1	0
8	B	906	PEG	1	0
7	A	908	GOL	1	0
7	A	914	GOL	1	0
7	A	913	GOL	1	0
6	A	907	PGE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	751/793 (94%)	-0.11	28 (3%)	41 43	22, 36, 69, 118	0
1	B	740/793 (93%)	-0.11	36 (4%)	29 30	30, 48, 89, 124	0
All	All	1491/1586 (94%)	-0.11	64 (4%)	35 36	22, 42, 84, 124	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	TYR	9.1
1	B	48	LYS	7.6
1	A	237	THR	6.9
1	B	78	TYR	5.8
1	B	372	ASP	5.6
1	A	236	SER	5.4
1	A	238	ASN	5.3
1	B	49	LYS	5.2
1	B	103	HIS	5.0
1	A	47	GLU	4.9
1	A	50	TYR	4.9
1	A	239	ARG	4.8
1	A	263	PRO	4.8
1	A	261	HIS	4.8
1	A	370	GLY	4.4
1	A	49	LYS	4.4
1	A	262	VAL	4.4
1	B	100	TYR	4.2
1	B	72	ARG	4.1
1	B	173	PRO	4.0
1	A	372	ASP	3.7
1	B	51	ARG	3.7
1	B	235	THR	3.7
1	B	822	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	263	PRO	3.5
1	B	172	LYS	3.4
1	B	264	GLY	3.3
1	A	371	ALA	3.3
1	A	264	GLY	3.1
1	B	62	CYS	3.1
1	A	235	THR	3.1
1	B	382	ASN	3.0
1	A	382	ASN	3.0
1	A	103	HIS	2.9
1	B	81	ARG	2.9
1	A	79	THR	2.9
1	A	48	LYS	2.9
1	B	369	VAL	2.8
1	A	180	GLU	2.7
1	B	504	LEU	2.7
1	B	115	LYS	2.7
1	B	368	SER	2.7
1	A	500	ASP	2.6
1	B	56	ALA	2.5
1	A	72	ARG	2.4
1	B	156	GLU	2.4
1	A	505	GLN	2.4
1	A	504	LEU	2.3
1	B	80	SER	2.3
1	B	61	THR	2.3
1	A	75	LYS	2.3
1	B	79	THR	2.3
1	B	52	LYS	2.3
1	B	69	ALA	2.3
1	A	369	VAL	2.3
1	B	374	TYR	2.2
1	B	379	ASP	2.2
1	B	96	PHE	2.1
1	A	373	GLN	2.1
1	B	371	ALA	2.1
1	B	378	LYS	2.1
1	B	75	LYS	2.0
1	A	51	ARG	2.0
1	B	500	ASP	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](#)

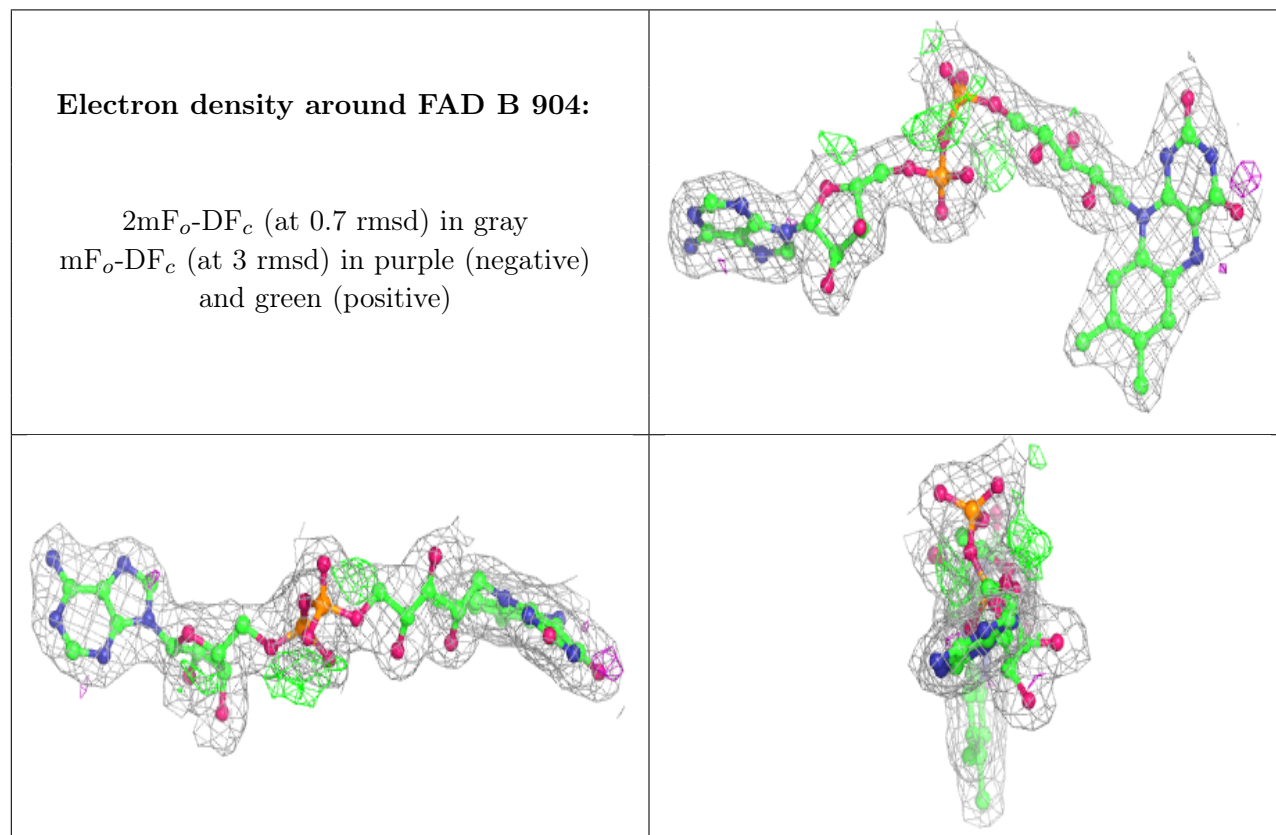
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

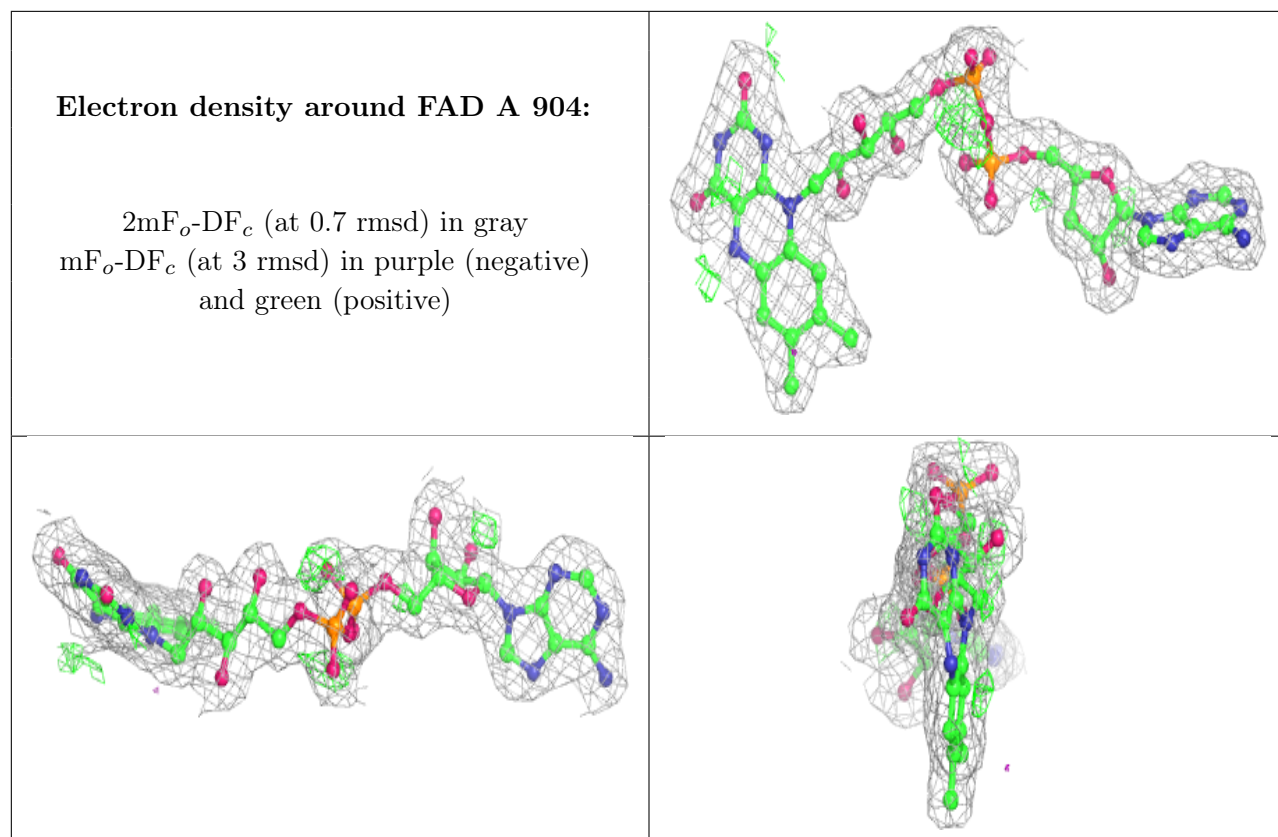
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	B	908	6/6	0.76	0.26	61,66,68,70	0
7	GOL	A	916	6/6	0.82	0.17	57,57,62,65	0
6	PGE	A	907	10/10	0.82	0.14	56,61,63,72	0
7	GOL	B	907	6/6	0.84	0.29	64,66,70,70	0
7	GOL	B	910	6/6	0.87	0.23	68,72,73,74	0
8	PEG	B	906	7/7	0.87	0.29	54,57,62,65	0
7	GOL	A	910	6/6	0.89	0.16	53,57,60,64	0
7	GOL	B	909	6/6	0.89	0.20	51,55,57,66	0
5	FLC	A	906	13/13	0.90	0.15	46,58,64,67	0
7	GOL	A	913	6/6	0.90	0.23	50,59,60,63	0
7	GOL	A	914	6/6	0.90	0.14	50,52,55,56	0
4	DIJ	A	905	11/11	0.91	0.16	28,31,35,54	11
7	GOL	A	912	6/6	0.91	0.11	50,52,52,54	0
7	GOL	A	908	6/6	0.92	0.12	45,49,52,53	0
7	GOL	A	915	6/6	0.92	0.16	50,54,62,64	0
4	DIJ	B	905	11/11	0.94	0.12	39,41,47,57	11
7	GOL	A	911	6/6	0.95	0.10	40,42,45,49	0
2	ZN	B	903	1/1	0.97	0.09	73,73,73,73	0
7	GOL	A	909	6/6	0.97	0.09	45,48,56,58	0
2	ZN	A	903	1/1	0.98	0.07	45,45,45,45	0
3	FAD	B	904	53/53	0.98	0.08	27,35,38,39	0
3	FAD	A	904	53/53	0.99	0.13	19,23,27,30	0
2	ZN	B	901	1/1	0.99	0.10	42,42,42,42	0
2	ZN	B	902	1/1	0.99	0.06	59,59,59,59	0
2	ZN	A	901	1/1	0.99	0.11	40,40,40,40	0
2	ZN	A	902	1/1	1.00	0.11	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.