



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 AM UTC

PDB ID : 2UXX / pdb_00002uxx
Title : Human LSD1 Histone Demethylase-CoREST in complex with an FAD- tranyl-
cypromine adduct
Authors : Yang, M.; Culhane, J.C.; Machius, M.; Cole, P.A.; Yu, H.
Deposited on : 2007-03-30
Resolution : 2.74 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

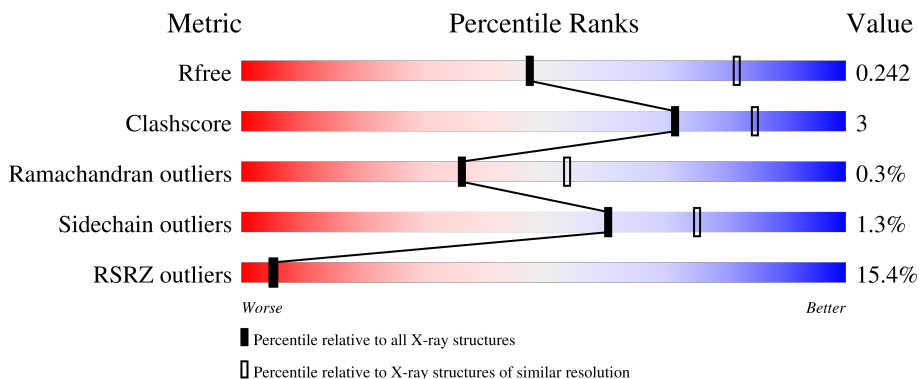
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	666	15% 89% 9%
2	B	235	9% 55% 43%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6379 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.

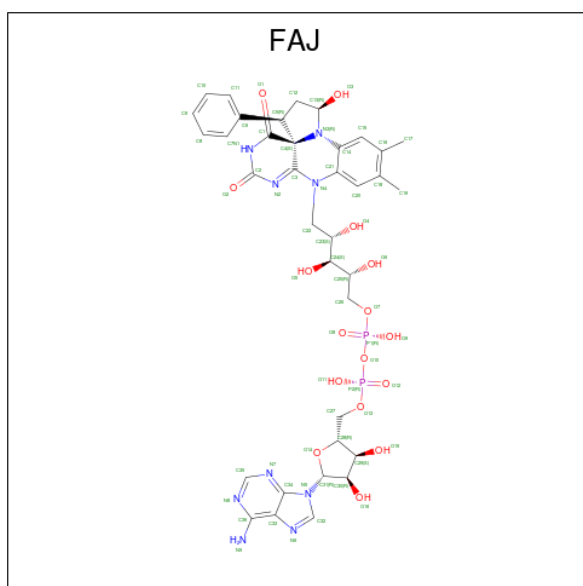
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	665	Total	C	N	O	S	0	0	0
			5209	3318	905	966	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1086	682	197	204	3			

- Molecule 3 is FAD-trans-2-Phenylcyclopropylamine Adduct (CCD ID: FAJ) (formula: $C_{36}H_{43}N_9O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			63	36	9	16	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.80Å 178.50Å 235.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.74 49.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.00-2.74) 97.5 (49.00-2.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.260 0.222 , 0.242	Depositor DCC
R_{free} test set	1529 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6379	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, FAJ

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	0.85	3/5323 (0.1%)	0.93	14/7221 (0.2%)
2	B	0.41	0/1102	0.84	0/1486
All	All	0.79	3/6425 (0.0%)	0.92	14/8707 (0.2%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	LYS	C-N	35.34	1.81	1.33
1	A	425	ASP	C-N	31.73	1.79	1.33
1	A	431	TRP	C-N	-25.93	0.95	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	TRP	O-C-N	18.87	145.31	122.48
1	A	431	TRP	CA-C-N	-13.04	98.32	121.14
1	A	431	TRP	C-N-CA	-13.04	98.32	121.14
1	A	424	LYS	O-C-N	-8.39	112.58	122.15
1	A	479	LEU	N-CA-C	-7.71	100.92	110.41
1	A	424	LYS	CA-C-N	6.48	130.97	120.60
1	A	424	LYS	C-N-CA	6.48	130.97	120.60
1	A	333	VAL	N-CA-C	5.61	116.02	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	VAL	N-CA-C	-5.48	100.53	108.36
1	A	287	GLY	N-CA-C	-5.36	104.37	112.41
1	A	805	ARG	N-CA-C	5.26	117.43	111.11
1	A	610	THR	N-CA-C	5.25	118.47	111.75
1	A	304	VAL	N-CA-C	5.21	115.62	108.12
1	A	551	HIS	N-CA-C	5.06	121.19	113.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	HIS	Mainchain

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	5209	0	5238	41	0
2	B	1086	0	1098	2	0
3	A	63	0	41	2	0
4	A	12	0	16	0	0
5	A	1	0	0	0	0
6	A	7	0	0	0	0
6	B	1	0	0	0	0
All	All	6379	0	6393	42	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 (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:C	1:A:426:GLU:N	1.79	1.39
1:A:424:LYS:C	1:A:425:ASP:N	1.81	1.37
1:A:427:GLN:O	1:A:431:TRP:CD1	2.18	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:O	1:A:431:TRP:HD1	1.64	0.78
1:A:695:TRP:HE1	1:A:706:LEU:HD11	1.54	0.71
1:A:801:GLU:HG2	1:A:809:ALA:H	1.54	0.70
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.74	0.68
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.78	0.64
1:A:801:GLU:CG	1:A:809:ALA:H	2.16	0.59
1:A:479:LEU:O	1:A:480:VAL:HB	2.05	0.57
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.38	0.54
1:A:360:CYS:SG	1:A:677:LEU:HD22	2.48	0.54
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.45	0.51
1:A:425:ASP:C	1:A:426:GLU:CA	2.79	0.50
1:A:415:VAL:O	1:A:419:GLN:HG2	2.12	0.50
1:A:677:LEU:HD23	1:A:693:LEU:HD11	1.94	0.49
1:A:801:GLU:CG	1:A:809:ALA:N	2.77	0.47
1:A:171:PRO:HB2	1:A:176:GLY:HA2	1.97	0.47
1:A:632:GLN:CD	1:A:758:ARG:HE	2.23	0.47
1:A:431:TRP:CE3	1:A:434:ILE:HD12	2.50	0.47
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.96	0.47
1:A:624:THR:HG22	1:A:799:ALA:HB3	1.96	0.47
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.49	0.46
1:A:458:LEU:HD12	1:A:490:LEU:HD12	1.98	0.46
1:A:463:LYS:O	1:A:467:GLU:HG3	2.16	0.45
1:A:425:ASP:CA	1:A:426:GLU:N	2.74	0.45
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.99	0.45
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.45
1:A:776:MET:HE2	1:A:802:HIS:HD2	1.82	0.44
1:A:174:VAL:HB	1:A:215:ASN:HB3	1.99	0.44
1:A:793:ILE:HD12	1:A:793:ILE:H	1.83	0.44
1:A:662:VAL:HB	1:A:705:ALA:HB3	2.00	0.43
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.92	0.43
1:A:335:THR:HG21	3:A:900:FAJ:H7	2.00	0.43
1:A:707:VAL:HG11	1:A:715:MET:HG3	2.01	0.43
1:A:388:ALA:HB1	2:B:316:LEU:HD11	1.99	0.43
1:A:820:ARG:NE	1:A:821:GLU:OE2	2.47	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.00	0.42
1:A:432:LYS:HA	1:A:435:VAL:HG22	2.02	0.42
1:A:801:GLU:HG2	1:A:809:ALA:N	2.27	0.41
3:A:900:FAJ:H5	3:A:900:FAJ:H10	1.87	0.41
1:A:501:GLN:O	1:A:505:GLU:HB2	2.21	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	663/666 (100%)	644 (97%)	17 (3%)	2 (0%)	36	54
2	B	132/235 (56%)	128 (97%)	4 (3%)	0	100	100
All	All	795/901 (88%)	772 (97%)	21 (3%)	2 (0%)	36	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLY
1	A	701	PRO

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	565/566 (100%)	559 (99%)	6 (1%)	65	79
2	B	118/203 (58%)	115 (98%)	3 (2%)	42	63
All	All	683/769 (89%)	674 (99%)	9 (1%)	61	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	MET
1	A	475	THR
1	A	659	LEU
1	A	677	LEU

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	801	GLU
2	B	314	MET
2	B	368	GLU
2	B	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	535	ASN
1	A	564	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GOL	A	1838	-	5,5,5	0.36	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAJ	A	900	-	67,70,70	1.04	5 (7%)	91,109,109	1.59	15 (16%)
4	GOL	A	1837	-	5,5,5	0.37	0	5,5,5	0.33	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	GOL	A	1838	-	-	2/4/4/4	-
3	FAJ	A	900	-	-	6/38/106/106	0/8/8/8
4	GOL	A	1837	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAJ	C3-N2	3.51	1.41	1.31
3	A	900	FAJ	C33-N6	-2.99	1.33	1.39
3	A	900	FAJ	C1-N1	2.17	1.40	1.37
3	A	900	FAJ	C34-N5	-2.09	1.33	1.37
3	A	900	FAJ	C6-C5	2.01	1.54	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAJ	C1-C4-C3	-5.22	104.14	113.40
3	A	900	FAJ	C33-C34-N7	-5.02	119.81	126.72
3	A	900	FAJ	N8-C35-N7	-4.86	121.23	128.58
3	A	900	FAJ	C12-C5-C6	-4.52	107.80	116.60
3	A	900	FAJ	C35-N7-C34	3.58	120.57	111.83
3	A	900	FAJ	N7-C34-N5	3.47	133.08	127.17
3	A	900	FAJ	N5-C32-N6	-3.45	109.04	113.94
3	A	900	FAJ	C1-N1-C2	-2.99	120.91	125.42
3	A	900	FAJ	C33-N6-C32	2.81	107.86	103.45
3	A	900	FAJ	C34-C33-N6	-2.55	107.66	110.58
3	A	900	FAJ	C4-C1-N1	2.46	120.24	116.97
3	A	900	FAJ	C34-N5-C32	2.46	108.32	105.74
3	A	900	FAJ	C26-C25-C24	-2.22	108.02	112.22
3	A	900	FAJ	O14-C31-C30	-2.11	102.09	106.62
3	A	900	FAJ	C4-N3-C13	-2.08	107.41	109.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

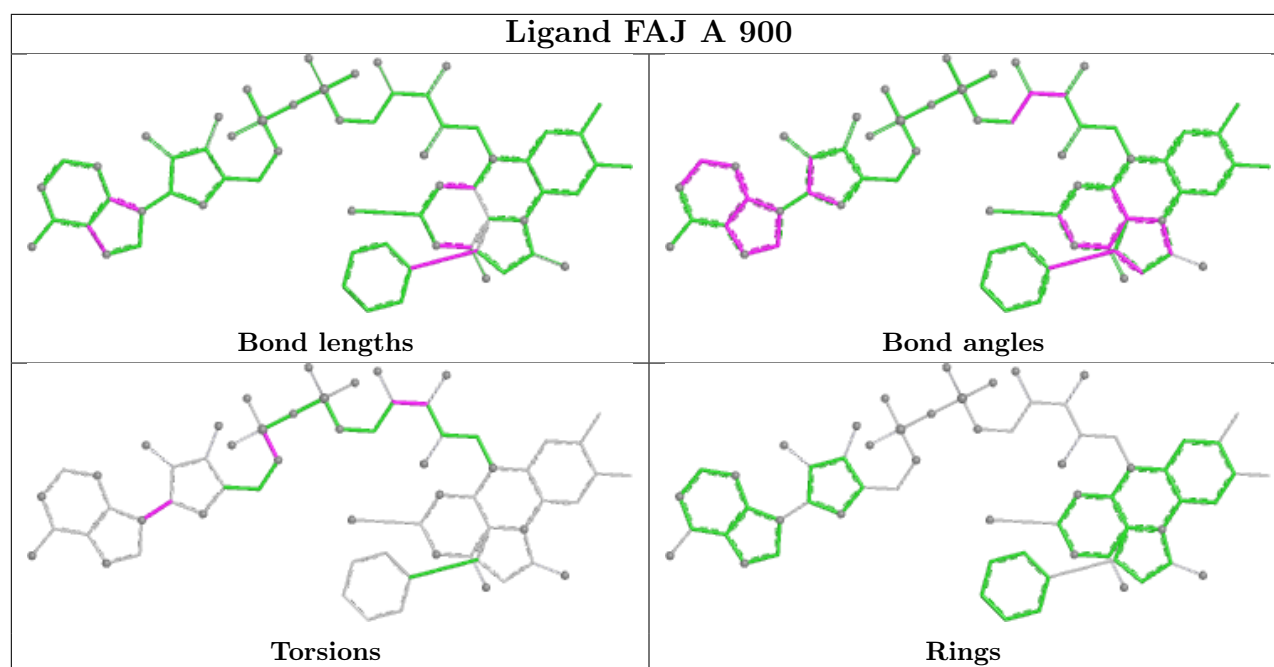
Mol	Chain	Res	Type	Atoms
3	A	900	FAJ	C27-O13-P2-O11
4	A	1838	GOL	O1-C1-C2-C3
4	A	1838	GOL	O1-C1-C2-O2
3	A	900	FAJ	C23-C24-C25-O6
3	A	900	FAJ	C23-C24-C25-C26
3	A	900	FAJ	O5-C24-C25-C26
3	A	900	FAJ	O5-C24-C25-O6
3	A	900	FAJ	C30-C31-N5-C32

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAJ	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	424:LYS	C	425:ASP	N	1.81
1	A	425:ASP	C	426:GLU	N	1.79
1	A	431:TRP	C	432:LYS	N	0.95

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	665/666 (99%)	1.17	101 (15%) 5 5	70, 100, 117, 125	0
2	B	134/235 (57%)	1.27	22 (16%) 4 5	77, 98, 117, 126	0
All	All	799/901 (88%)	1.19	123 (15%) 5 5	70, 99, 118, 126	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	835	THR	6.8
1	A	171	PRO	6.5
2	B	376	ILE	5.8
1	A	834	TYR	4.9
1	A	698	TYR	4.8
1	A	480	VAL	4.8
1	A	786	ILE	4.7
2	B	375	VAL	4.7
2	B	378	LYS	4.4
1	A	431	TRP	4.3
1	A	833	MET	4.3
1	A	832	ALA	4.3
1	A	174	VAL	4.2
2	B	308	ARG	4.1
1	A	828	GLN	4.0
1	A	377	MET	3.9
1	A	188	MET	3.6
1	A	481	LYS	3.6
1	A	332	MET	3.6
1	A	518	ASP	3.5
2	B	441	HIS	3.5
2	B	328	ALA	3.5
1	A	240	ALA	3.5
1	A	275	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	793	ILE	3.4
2	B	377	GLN	3.2
1	A	785	SER	3.2
1	A	475	THR	3.1
1	A	200	ILE	3.1
1	A	270	ILE	3.0
1	A	273	LEU	3.0
1	A	829	PHE	3.0
1	A	787	PRO	3.0
1	A	717	ASN	3.0
1	A	790	PRO	2.9
1	A	413	GLU	2.9
1	A	667	ASP	2.9
1	A	258	ARG	2.8
1	A	744	LYS	2.8
1	A	189	THR	2.8
1	A	472	ARG	2.8
1	A	645	GLU	2.8
1	A	506	GLU	2.8
1	A	242	TYR	2.8
1	A	194	ALA	2.7
1	A	425	ASP	2.7
1	A	274	PRO	2.7
2	B	338	LEU	2.7
1	A	233	ALA	2.7
1	A	398	PHE	2.7
2	B	350	GLN	2.7
2	B	374	GLU	2.7
1	A	198	ASP	2.6
2	B	399	GLY	2.6
1	A	247	VAL	2.6
1	A	272	PRO	2.6
1	A	438	GLN	2.6
1	A	610	THR	2.5
1	A	683	SER	2.5
1	A	235	LEU	2.5
1	A	191	GLN	2.5
2	B	371	ARG	2.5
1	A	232	GLU	2.5
1	A	210	PHE	2.5
1	A	201	SER	2.5
1	A	276	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	503	LYS	2.5
2	B	382	ARG	2.5
1	A	430	HIS	2.5
2	B	334	VAL	2.5
1	A	791	GLN	2.4
1	A	193	ALA	2.4
1	A	771	ASN	2.4
1	A	611	SER	2.4
2	B	402	PHE	2.4
2	B	309	LYS	2.4
1	A	784	PRO	2.4
1	A	435	VAL	2.4
1	A	468	VAL	2.4
1	A	795	ARG	2.4
1	A	255	TYR	2.3
1	A	830	LEU	2.3
1	A	185	HIS	2.3
1	A	770	GLY	2.3
1	A	519	VAL	2.3
1	A	777	ALA	2.3
1	A	230	THR	2.3
1	A	299	SER	2.3
1	A	269	ARG	2.3
1	A	252	VAL	2.3
1	A	502	GLY	2.3
2	B	368	GLU	2.2
1	A	668	ARG	2.2
1	A	190	SER	2.2
1	A	478	PHE	2.2
1	A	822	ALA	2.2
2	B	312	LYS	2.2
1	A	612	GLN	2.2
1	A	336	GLY	2.2
1	A	476	ALA	2.2
1	A	739	ALA	2.2
1	A	380	GLN	2.2
1	A	632	GLN	2.2
1	A	260	GLY	2.2
2	B	381	ALA	2.2
1	A	477	GLU	2.2
1	A	363	TYR	2.2
1	A	555	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	465	ALA	2.1
1	A	278	THR	2.1
1	A	563	SER	2.1
1	A	335	THR	2.1
2	B	362	LYS	2.1
1	A	652	GLN	2.1
1	A	788	GLY	2.1
1	A	510	GLU	2.1
1	A	229	LEU	2.0
1	A	373	GLU	2.0
1	A	347	LYS	2.0
2	B	437	TRP	2.0
1	A	634	PRO	2.0
2	B	434	LEU	2.0
1	A	325	TYR	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](#)

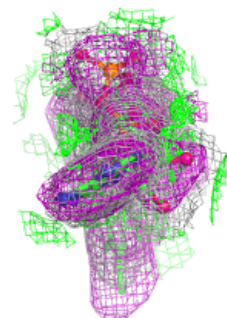
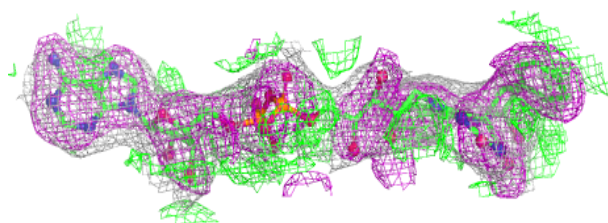
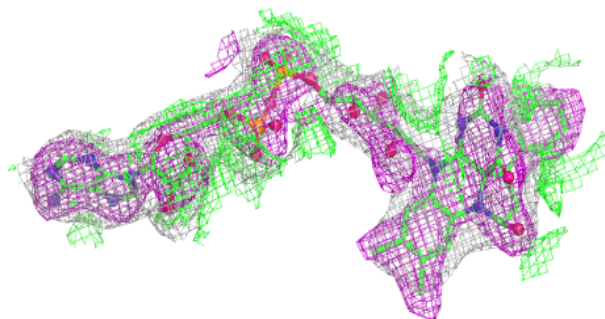
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	CL	A	1840	1/1	0.88	0.18	109,109,109,109	0
4	GOL	A	1838	6/6	0.89	0.24	133,134,134,134	0
3	FAJ	A	900	63/63	0.92	0.16	58,67,74,74	0
4	GOL	A	1837	6/6	0.95	0.18	83,84,85,85	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 FAJ A 900:

$2mF_o-DF_c$ (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.