



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:08 PM UTC

PDB ID : 8JF5 / pdb_00008jf5
Title : Crystal structure of Lysine Specific Demethylase 1 (LSD1) with TAS1440
Authors : Fukushima, H.; Machida, T.; Yamashita, S.; Suzuki, T.
Deposited on : 2023-05-17
Resolution : 3.20 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

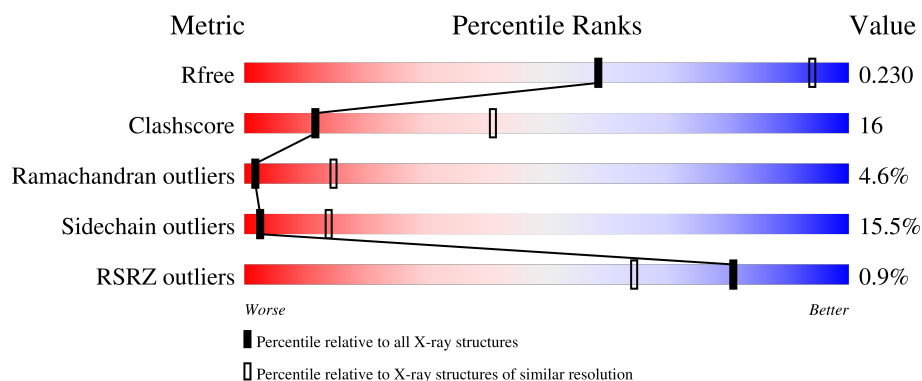
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	663	 61% 30% 7% .
2	B	135	 3% 46% 32% 17% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5956 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 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			4957	3165	853	919	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP O60341

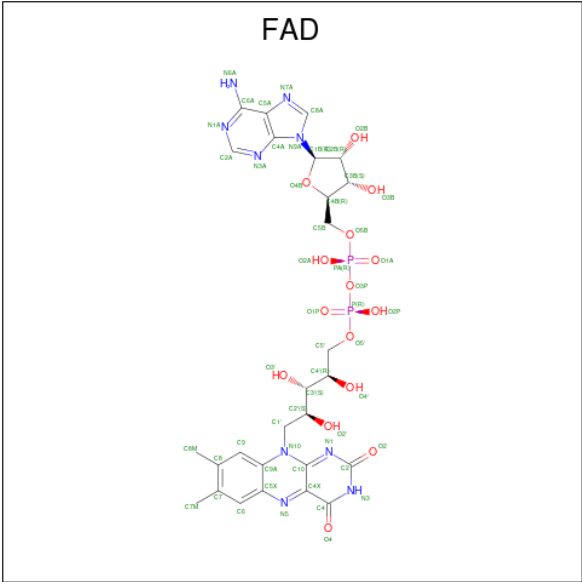
- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			899	563	159	174	3			

There are 2 discrepancies between the modelled and reference sequences:

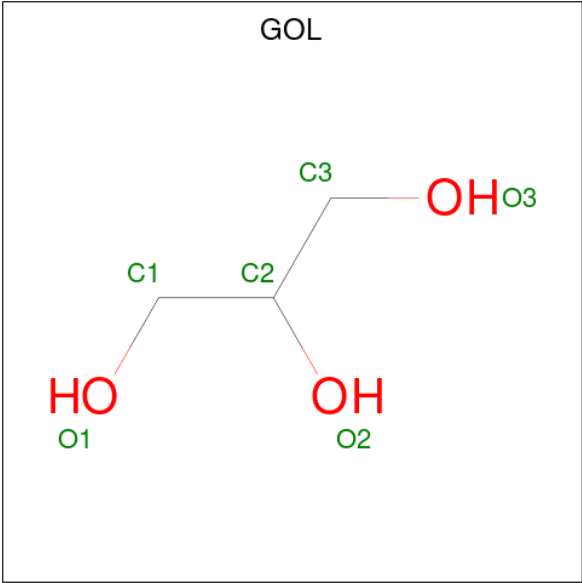
Chain	Residue	Modelled	Actual	Comment	Reference
B	306	MET	-	initiating methionine	UNP Q9UKL0
B	307	GLY	-	expression tag	UNP Q9UKL0

- 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
			53	27	9	15	2	

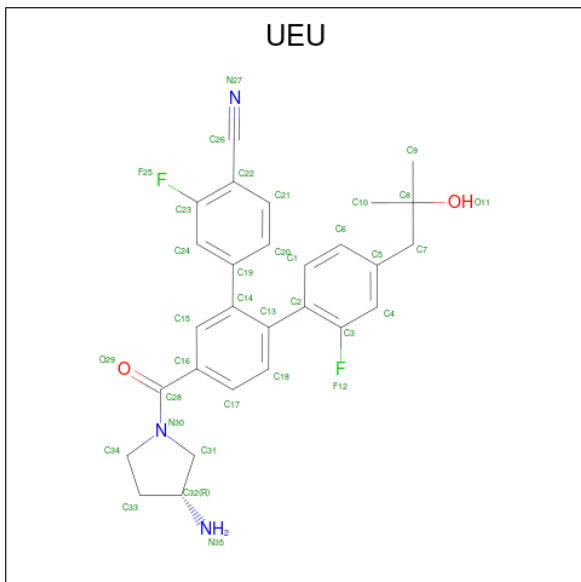
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 4-[5-[(3 {R})-3-azanylpyrrolidin-1-yl]carbonyl-2-[2-fluoranyl-4-(2-methyl-2-o

xidanyl-propyl)phenyl]phenyl]-2-fluoranyl-benzenecarbonitrile (CCD ID: UEU) (formula: C₂₈H₂₇F₂N₃O₂) (labeled as "Ligand of Interest" by depositor).



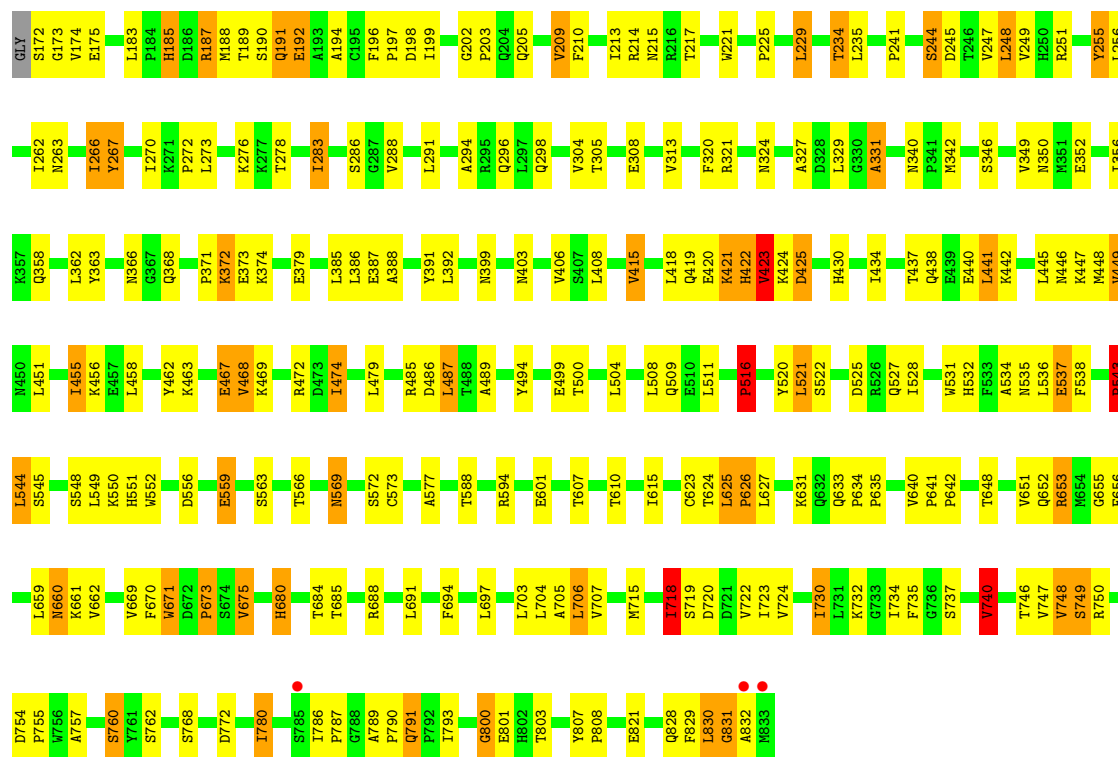
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			35	28	2	3	2		

3 Residue-property plots

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.

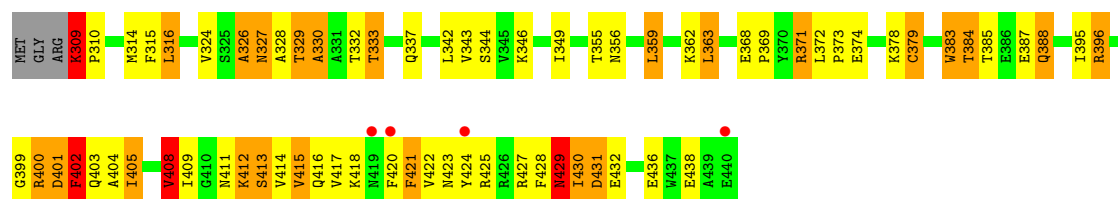
- Molecule 1: Lysine-specific histone demethylase 1A

Chain A: 



- Molecule 2: REST corepressor 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.77Å 179.12Å 235.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 3.20 49.13 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.13-3.20) 99.9 (49.13-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.230 0.198 , 0.230	Depositor DCC
R_{free} test set	2145 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	94.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5956	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: UEU, GOL, 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	1.29	12/5069 (0.2%)	1.45	40/6926 (0.6%)
2	B	1.61	13/910 (1.4%)	1.51	8/1248 (0.6%)
All	All	1.34	25/5979 (0.4%)	1.45	48/8174 (0.6%)

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
2	B	0	1
All	All	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	PRO	CA-C	-8.43	1.43	1.52
1	A	750	ARG	CA-C	8.11	1.63	1.53
1	A	760	SER	CA-C	-7.56	1.47	1.52
1	A	660	ASN	CA-C	6.83	1.60	1.52
2	B	424	TYR	CA-C	6.45	1.61	1.52
2	B	310	PRO	CA-C	-6.44	1.47	1.52
1	A	550	LYS	N-CA	6.28	1.54	1.46
2	B	417	VAL	N-CA	5.95	1.53	1.46
1	A	660	ASN	CA-CB	5.79	1.63	1.53
2	B	372	LEU	CA-C	5.79	1.60	1.52
1	A	748	VAL	CA-C	5.78	1.60	1.52
2	B	310	PRO	C-O	-5.62	1.20	1.24
2	B	326	ALA	N-CA	5.51	1.49	1.46
2	B	402	PHE	CA-C	5.49	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	PRO	C-O	-5.45	1.18	1.23
2	B	427	ARG	CA-C	5.42	1.59	1.52
1	A	740	VAL	N-CA	5.33	1.50	1.46
2	B	425	ARG	N-CA	5.27	1.52	1.46
2	B	383	TRP	CA-CB	5.21	1.59	1.52
2	B	438	GLU	CA-C	5.20	1.59	1.52
1	A	463	LYS	CA-C	5.18	1.59	1.52
1	A	623	CYS	CA-C	5.17	1.59	1.53
2	B	408	VAL	N-CA	5.16	1.52	1.46
2	B	423	ASN	N-CA	5.14	1.52	1.46
1	A	543	PRO	N-CA	-5.07	1.41	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	LEU	CA-C-N	14.16	134.33	119.89
1	A	625	LEU	C-N-CA	14.16	134.33	119.89
1	A	202	GLY	CA-C-N	9.77	129.86	119.90
1	A	202	GLY	C-N-CA	9.77	129.86	119.90
2	B	421	PHE	N-CA-C	-8.19	97.89	110.10
1	A	244	SER	N-CA-C	8.13	119.84	110.97
1	A	625	LEU	O-C-N	7.78	127.53	121.47
1	A	832	ALA	N-CA-C	7.27	119.28	111.36
1	A	192	GLU	N-CA-C	-7.24	102.57	111.40
2	B	310	PRO	CB-CA-C	-6.97	104.61	111.17
1	A	786	ILE	CA-C-N	-6.97	112.79	119.90
1	A	786	ILE	C-N-CA	-6.97	112.79	119.90
1	A	205	GLN	N-CA-C	-6.93	103.34	111.03
2	B	384	THR	CB-CA-C	-6.91	97.41	109.64
1	A	527	GLN	N-CA-C	6.86	118.84	111.36
1	A	670	PHE	N-CA-C	6.79	121.39	113.18
1	A	748	VAL	N-CA-C	6.60	123.07	109.34
1	A	831	GLY	N-CA-C	6.48	128.54	113.18
1	A	718	ILE	CB-CA-C	6.33	120.33	111.34
1	A	660	ASN	CB-CA-C	6.24	123.40	111.17
1	A	671	TRP	N-CA-C	-6.13	101.89	110.35
1	A	550	LYS	N-CA-CB	6.10	119.22	110.06
1	A	408	LEU	N-CA-C	-6.04	104.32	111.03
1	A	203	PRO	N-CA-C	5.95	120.55	111.15
2	B	309	LYS	CA-C-N	5.90	123.91	119.66
2	B	309	LYS	C-N-CA	5.90	123.91	119.66
1	A	800	GLY	N-CA-C	5.89	120.31	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ILE	N-CA-C	5.87	115.94	110.42
1	A	499	GLU	N-CA-C	-5.81	104.58	111.03
1	A	549	LEU	CA-C-O	-5.80	114.92	120.90
2	B	421	PHE	CB-CA-C	5.79	118.94	109.90
1	A	786	ILE	CB-CA-C	-5.79	104.19	110.85
1	A	266	ILE	N-CA-C	5.65	116.26	107.28
1	A	675	VAL	N-CA-C	5.60	116.16	107.99
1	A	768	SER	CA-CB-OG	5.58	122.26	111.10
1	A	656	PHE	N-CA-C	-5.57	100.11	109.07
1	A	780	ILE	N-CA-C	5.50	115.87	108.17
1	A	746	THR	N-CA-C	5.47	118.14	109.50
1	A	551	HIS	N-CA-C	5.38	121.68	113.61
1	A	791	GLN	CA-C-N	-5.27	115.34	120.98
1	A	791	GLN	C-N-CA	-5.27	115.34	120.98
1	A	327	ALA	N-CA-C	5.26	116.61	107.93
2	B	362	LYS	N-CA-C	5.22	118.75	112.38
1	A	283	ILE	CB-CA-C	-5.20	103.85	110.98
1	A	707	VAL	CB-CA-C	-5.11	103.08	110.63
2	B	420	PHE	N-CA-CB	5.10	117.41	110.01
1	A	653	ARG	N-CA-C	5.05	116.47	111.07
1	A	626	PRO	CB-CA-C	-5.03	104.96	111.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	SER	Peptide
2	B	412	LYS	Peptide

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	4957	0	4750	154	1
2	B	899	0	780	41	0
3	A	53	0	31	5	0
4	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	35	0	0	1	0
All	All	5956	0	5577	183	1

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 16.

All (183) 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:198:ASP:OD1	1:A:199:ILE:HG13	1.78	0.83
2:B:428:PHE:O	2:B:430:ILE:N	2.16	0.77
1:A:213:ILE:HD13	1:A:248:LEU:HD21	1.70	0.73
1:A:660:ASN:HA	1:A:749:SER:CB	2.18	0.73
1:A:217:THR:HG23	1:A:234:THR:HG21	1.69	0.73
1:A:363:TYR:HD2	1:A:734:ILE:CB	2.04	0.70
1:A:366:ASN:OD1	1:A:368:GLN:N	2.26	0.68
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.23	0.68
1:A:308:GLU:OE1	3:A:901:FAD:O3B	2.13	0.67
1:A:448:MET:HE3	2:B:363:LEU:HD12	1.77	0.66
1:A:331:ALA:HA	3:A:901:FAD:N5	2.12	0.64
1:A:732:LYS:CE	1:A:740:VAL:HG22	2.27	0.64
2:B:396:ARG:HH11	2:B:396:ARG:CG	2.10	0.64
1:A:535:ASN:OD1	5:A:904:UEU:O11	2.15	0.64
1:A:458:LEU:HD23	1:A:487:LEU:HD12	1.80	0.64
1:A:363:TYR:CD2	1:A:734:ILE:CB	2.81	0.64
2:B:399:GLY:O	2:B:401:ASP:N	2.31	0.63
2:B:400:ARG:O	2:B:402:PHE:N	2.31	0.63
1:A:538:PHE:CZ	1:A:706:LEU:HD12	2.34	0.63
1:A:449:VAL:HG23	2:B:363:LEU:HD21	1.79	0.62
1:A:536:LEU:HD23	1:A:544:LEU:HD11	1.83	0.61
1:A:372:LYS:O	1:A:374:LYS:N	2.34	0.60
1:A:199:ILE:HD11	1:A:248:LEU:HD12	1.83	0.60
1:A:520:TYR:CE2	1:A:521:LEU:HD23	2.36	0.60
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.37	0.59
1:A:188:MET:HE3	1:A:210:PHE:CD2	2.38	0.59
1:A:196:PHE:N	1:A:197:PRO:CD	2.66	0.59
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.33	0.59
1:A:371:PRO:O	1:A:372:LYS:O	2.20	0.59
1:A:627:LEU:O	1:A:631:LYS:HG3	2.02	0.59
1:A:362:LEU:C	1:A:363:TYR:HD1	2.10	0.59
1:A:420:GLU:O	1:A:423:VAL:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:C	1:A:441:LEU:HD23	2.29	0.58
1:A:485:ARG:NH1	1:A:489:ALA:HB2	2.19	0.58
2:B:401:ASP:O	2:B:403:GLN:N	2.37	0.57
1:A:340:ASN:OD1	1:A:342:MET:N	2.33	0.57
1:A:371:PRO:C	1:A:372:LYS:O	2.45	0.57
1:A:421:LYS:O	1:A:423:VAL:N	2.37	0.57
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.86	0.56
2:B:396:ARG:HH11	2:B:396:ARG:HG3	1.71	0.56
1:A:537:GLU:OE2	1:A:544:LEU:HD23	2.05	0.56
2:B:401:ASP:O	2:B:402:PHE:C	2.49	0.56
1:A:241:PRO:O	1:A:244:SER:OG	2.24	0.55
1:A:732:LYS:HD2	1:A:737:SER:HA	1.89	0.55
1:A:209:VAL:HG22	1:A:213:ILE:HD11	1.87	0.55
1:A:425:ASP:N	1:A:425:ASP:OD1	2.38	0.55
2:B:396:ARG:CG	2:B:396:ARG:NH1	2.70	0.54
1:A:520:TYR:CD2	1:A:521:LEU:HD23	2.42	0.54
1:A:263:ASN:C	1:A:267:TYR:HE2	2.16	0.53
1:A:422:HIS:O	1:A:423:VAL:C	2.52	0.53
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.91	0.53
1:A:829:PHE:O	1:A:830:LEU:HD23	2.09	0.53
1:A:594:ARG:HA	1:A:640:VAL:O	2.09	0.53
1:A:748:VAL:O	1:A:749:SER:C	2.52	0.53
1:A:807:TYR:N	1:A:808:PRO:HD3	2.24	0.53
1:A:660:ASN:CA	1:A:749:SER:CB	2.86	0.53
2:B:418:LYS:O	2:B:421:PHE:O	2.27	0.53
1:A:441:LEU:CD2	2:B:356:ASN:ND2	2.72	0.52
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.92	0.52
1:A:732:LYS:HD3	1:A:740:VAL:HG22	1.91	0.52
1:A:659:LEU:C	1:A:659:LEU:HD12	2.35	0.52
1:A:720:ASP:O	1:A:724:VAL:HG23	2.11	0.51
1:A:248:LEU:C	1:A:248:LEU:HD23	2.35	0.51
1:A:331:ALA:H	3:A:901:FAD:C6	2.23	0.51
1:A:661:LYS:H	1:A:749:SER:CB	2.23	0.51
1:A:718:ILE:HG22	1:A:723:ILE:CG1	2.42	0.50
2:B:368:GLU:N	2:B:369:PRO:HD2	2.25	0.50
1:A:385:LEU:O	1:A:388:ALA:HB3	2.11	0.50
1:A:352:GLU:CB	1:A:569:ASN:HD21	2.24	0.50
1:A:660:ASN:CB	1:A:749:SER:CB	2.90	0.50
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.42	0.49
1:A:418:LEU:CD2	2:B:324:VAL:HG21	2.42	0.49
1:A:286:SER:CB	1:A:313:VAL:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HZ2	1:A:525:ASP:CB	2.25	0.49
1:A:641:PRO:HB2	1:A:642:PRO:HD2	1.93	0.49
1:A:420:GLU:C	1:A:421:LYS:O	2.51	0.49
2:B:342:LEU:HD21	2:B:346:LYS:HD2	1.94	0.49
2:B:408:VAL:HG12	2:B:409:ILE:N	2.27	0.49
1:A:468:VAL:HG12	1:A:468:VAL:O	2.12	0.49
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.95	0.48
1:A:437:THR:O	1:A:438:GLN:C	2.55	0.48
1:A:641:PRO:HB2	1:A:642:PRO:CD	2.42	0.48
1:A:386:LEU:O	1:A:387:GLU:C	2.55	0.48
1:A:706:LEU:N	1:A:706:LEU:HD23	2.28	0.48
1:A:229:LEU:HD21	1:A:234:THR:HG23	1.96	0.48
2:B:388:GLN:HG2	2:B:428:PHE:CZ	2.48	0.48
1:A:192:GLU:HG2	1:A:255:TYR:CZ	2.50	0.47
1:A:732:LYS:HE2	1:A:740:VAL:HG22	1.95	0.47
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.96	0.47
2:B:326:ALA:O	2:B:327:ASN:C	2.56	0.47
1:A:671:TRP:O	1:A:673:PRO:HD3	2.14	0.47
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.47	0.47
1:A:468:VAL:O	1:A:472:ARG:NH1	2.48	0.47
2:B:315:PHE:C	2:B:316:LEU:HG	2.39	0.47
1:A:446:ASN:O	1:A:447:LYS:C	2.58	0.47
1:A:719:SER:OG	1:A:722:VAL:HG23	2.14	0.47
1:A:385:LEU:CD2	1:A:415:VAL:HG12	2.44	0.47
1:A:680:HIS:ND1	1:A:680:HIS:C	2.73	0.47
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.48	0.46
1:A:732:LYS:CD	1:A:740:VAL:HG22	2.46	0.46
2:B:388:GLN:HG2	2:B:428:PHE:CE2	2.51	0.46
2:B:330:ALA:HA	2:B:333:THR:HB	1.98	0.46
1:A:706:LEU:N	1:A:706:LEU:CD2	2.79	0.46
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.51	0.46
1:A:653:ARG:HH11	1:A:772:ASP:CG	2.23	0.46
2:B:411:ASN:O	2:B:411:ASN:ND2	2.49	0.46
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.97	0.46
1:A:760:SER:HA	3:A:901:FAD:HM81	1.98	0.46
1:A:800:GLY:O	1:A:803:THR:OG1	2.25	0.45
1:A:187:ARG:HB3	1:A:187:ARG:NH2	2.32	0.45
1:A:245:ASP:OD1	1:A:247:VAL:HG12	2.15	0.45
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.82	0.45
1:A:422:HIS:O	1:A:424:LYS:N	2.50	0.45
2:B:413:SER:C	2:B:415:VAL:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:CE1	1:A:256:LEU:HD23	2.52	0.45
1:A:442:LYS:CE	2:B:355:THR:HG21	2.47	0.45
1:A:448:MET:HE3	2:B:363:LEU:CD1	2.45	0.45
2:B:414:VAL:O	2:B:418:LYS:CB	2.64	0.45
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.99	0.45
1:A:633:GLN:HA	1:A:634:PRO:C	2.41	0.45
1:A:286:SER:O	1:A:291:LEU:HD11	2.17	0.45
1:A:437:THR:O	1:A:440:GLU:N	2.44	0.44
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.99	0.44
1:A:685:THR:O	1:A:688:ARG:HG2	2.17	0.44
1:A:566:THR:HB	1:A:697:LEU:HD12	2.00	0.44
1:A:680:HIS:CD2	1:A:730:ILE:HG21	2.53	0.44
1:A:821:GLU:OE2	1:A:821:GLU:HA	2.18	0.44
2:B:412:LYS:O	2:B:416:GLN:CB	2.65	0.44
1:A:175:GLU:CB	1:A:185:HIS:CD2	3.01	0.44
1:A:399:ASN:C	1:A:406:VAL:HG23	2.43	0.44
2:B:378:LYS:O	2:B:379:CYS:O	2.36	0.44
1:A:320:PHE:HB2	1:A:329:LEU:HD11	1.98	0.43
1:A:651:VAL:O	1:A:652:GLN:C	2.60	0.43
1:A:434:ILE:HG21	2:B:349:ILE:HD12	2.00	0.43
1:A:694:PHE:HA	1:A:704:LEU:O	2.18	0.43
1:A:624:THR:O	1:A:625:LEU:C	2.60	0.43
2:B:359:LEU:HD23	2:B:359:LEU:N	2.33	0.43
1:A:270:ILE:O	1:A:272:PRO:HD3	2.18	0.43
1:A:198:ASP:OD1	1:A:199:ILE:N	2.52	0.43
1:A:754:ASP:OD1	1:A:754:ASP:C	2.61	0.43
1:A:659:LEU:HD12	1:A:660:ASN:N	2.34	0.43
2:B:404:ALA:O	2:B:405:ILE:C	2.62	0.43
1:A:421:LYS:O	1:A:422:HIS:C	2.61	0.42
2:B:432:GLU:O	2:B:436:GLU:HG2	2.19	0.42
1:A:525:ASP:O	1:A:528:ILE:N	2.52	0.42
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.19	0.42
1:A:467:GLU:O	1:A:469:LYS:N	2.53	0.42
2:B:396:ARG:NH1	2:B:396:ARG:HG2	2.34	0.42
1:A:187:ARG:HB3	1:A:187:ARG:HH21	1.84	0.42
1:A:263:ASN:C	1:A:267:TYR:CE2	2.95	0.42
1:A:455:ILE:O	1:A:456:LYS:C	2.62	0.42
2:B:327:ASN:C	2:B:329:THR:H	2.27	0.42
1:A:494:TYR:CD1	1:A:494:TYR:C	2.97	0.42
1:A:349:VAL:O	1:A:349:VAL:HG12	2.19	0.42
1:A:391:TYR:O	1:A:392:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LYS:N	1:A:749:SER:CB	2.83	0.42
1:A:462:TYR:CD1	1:A:462:TYR:C	2.97	0.41
1:A:485:ARG:HH12	1:A:489:ALA:HB2	1.85	0.41
1:A:548:SER:O	1:A:552:TRP:HB3	2.20	0.41
1:A:680:HIS:NE2	1:A:730:ILE:HG21	2.34	0.41
1:A:209:VAL:O	1:A:210:PHE:C	2.64	0.41
1:A:509:GLN:HA	1:A:509:GLN:OE1	2.21	0.41
1:A:485:ARG:HD3	1:A:486:ASP:OD1	2.21	0.41
1:A:537:GLU:OE2	1:A:543:PRO:HA	2.20	0.41
1:A:556:ASP:O	1:A:559:GLU:HG2	2.20	0.41
1:A:191:GLN:HA	1:A:194:ALA:HB2	2.02	0.41
2:B:429:ASN:O	2:B:431:ASP:N	2.54	0.41
1:A:196:PHE:N	1:A:197:PRO:HD3	2.36	0.41
1:A:248:LEU:HD23	1:A:249:VAL:N	2.34	0.41
1:A:441:LEU:HD22	2:B:356:ASN:ND2	2.36	0.41
1:A:531:TRP:CE3	1:A:531:TRP:C	2.99	0.41
1:A:691:LEU:HD12	1:A:691:LEU:N	2.36	0.41
1:A:209:VAL:CG2	1:A:213:ILE:HD11	2.49	0.41
1:A:391:TYR:HE2	2:B:309:LYS:HB3	1.86	0.41
1:A:430:HIS:CD2	1:A:516:PRO:HD2	2.56	0.41
1:A:419:GLN:NE2	2:B:314:MET:HA	2.36	0.41
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.86	0.40
1:A:379:GLU:HG2	1:A:532:HIS:NE2	2.36	0.40
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.82	0.40
1:A:321:ARG:NH2	1:A:572:SER:OG	2.52	0.40
1:A:655:GLY:O	1:A:762:SER:HA	2.21	0.40
1:A:828:GLN:HB3	1:A:829:PHE:CD2	2.57	0.40
1:A:288:VAL:HA	1:A:291:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:GLU:OE2	1:A:601:GLU:OE2[2_455]	1.77	0.43

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	660/663 (100%)	564 (86%)	76 (12%)	20 (3%)	3	23
2	B	130/135 (96%)	93 (72%)	21 (16%)	16 (12%)	0	1
All	All	790/798 (99%)	657 (83%)	97 (12%)	36 (5%)	2	15

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	276	LYS
1	A	358	GLN
1	A	372	LYS
1	A	421	LYS
1	A	422	HIS
1	A	468	VAL
1	A	749	SER
1	A	831	GLY
2	B	379	CYS
2	B	400	ARG
2	B	401	ASP
2	B	415	VAL
2	B	429	ASN
1	A	423	VAL
1	A	516	PRO
2	B	374	GLU
2	B	402	PHE
1	A	373	GLU
1	A	500	THR
1	A	715	MET
2	B	327	ASN
2	B	422	VAL
1	A	173	GLY
1	A	331	ALA

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Mol	Chain	Res	Type
1	A	757	ALA
2	B	330	ALA
2	B	333	THR
2	B	413	SER
1	A	573	CYS
2	B	328	ALA
2	B	430	ILE
2	B	431	ASP
1	A	791	GLN
2	B	373	PRO
1	A	669	VAL

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	500/562 (89%)	431 (86%)	69 (14%)	3	18
2	B	74/118 (63%)	54 (73%)	20 (27%)	0	2
All	All	574/680 (84%)	485 (84%)	89 (16%)	2	14

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	174	VAL
1	A	183	LEU
1	A	185	HIS
1	A	187	ARG
1	A	189	THR
1	A	209	VAL
1	A	225	PRO
1	A	229	LEU
1	A	234	THR
1	A	235	LEU
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	255	TYR
1	A	267	TYR
1	A	273	LEU
1	A	278	THR
1	A	296	GLN
1	A	298	GLN
1	A	304	VAL
1	A	305	THR
1	A	324	ASN
1	A	346	SER
1	A	350	ASN
1	A	356	ILE
1	A	403	ASN
1	A	415	VAL
1	A	423	VAL
1	A	425	ASP
1	A	441	LEU
1	A	445	LEU
1	A	449	VAL
1	A	467	GLU
1	A	474	ILE
1	A	479	LEU
1	A	487	LEU
1	A	504	LEU
1	A	511	LEU
1	A	516	PRO
1	A	521	LEU
1	A	522	SER
1	A	537	GLU
1	A	543	PRO
1	A	544	LEU
1	A	545	SER
1	A	559	GLU
1	A	563	SER
1	A	569	ASN
1	A	588	THR
1	A	607	THR
1	A	610	THR
1	A	615	ILE
1	A	626	PRO
1	A	648	THR
1	A	673	PRO

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Mol	Chain	Res	Type
1	A	675	VAL
1	A	680	HIS
1	A	684	THR
1	A	703	LEU
1	A	706	LEU
1	A	718	ILE
1	A	730	ILE
1	A	740	VAL
1	A	747	VAL
1	A	755	PRO
1	A	780	ILE
1	A	787	PRO
1	A	793	ILE
1	A	801	GLU
1	A	830	LEU
2	B	309	LYS
2	B	316	LEU
2	B	329	THR
2	B	332	THR
2	B	337	GLN
2	B	343	VAL
2	B	344	SER
2	B	359	LEU
2	B	363	LEU
2	B	371	ARG
2	B	383	TRP
2	B	384	THR
2	B	385	THR
2	B	387	GLU
2	B	388	GLN
2	B	395	ILE
2	B	396	ARG
2	B	405	ILE
2	B	408	VAL
2	B	429	ASN

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	185	HIS
1	A	219	GLN
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	430	HIS
1	A	460	GLN
1	A	535	ASN
1	A	658	ASN
1	A	812	HIS
2	B	388	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
4	GOL	A	902	-	5,5,5	0.66	0	5,5,5	0.69	0
5	UEU	A	904	-	37,38,38	1.94	6 (16%)	52,56,56	2.92	25 (48%)
4	GOL	A	903	-	5,5,5	1.24	0	5,5,5	1.31	1 (20%)
3	FAD	A	901	-	58,58,58	1.85	13 (22%)	85,89,89	2.23	33 (38%)

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	902	-	-	4/4/4/4	-
5	UEU	A	904	-	-	7/22/32/32	0/4/4/4
4	GOL	A	903	-	-	3/4/4/4	-
3	FAD	A	901	-	-	2/34/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	UEU	C22-C26	-8.99	1.31	1.44
3	A	901	FAD	P-O3P	5.79	1.65	1.59
3	A	901	FAD	C5X-N5	-4.72	1.30	1.39
3	A	901	FAD	C5A-C4A	4.65	1.47	1.39
3	A	901	FAD	C9A-C5X	4.19	1.47	1.41
3	A	901	FAD	PA-O3P	3.73	1.63	1.59
3	A	901	FAD	C5A-N7A	-3.10	1.33	1.39
3	A	901	FAD	C4-N3	-2.98	1.33	1.38
5	A	904	UEU	C13-C14	-2.88	1.36	1.41
5	A	904	UEU	C33-C32	-2.71	1.49	1.53
3	A	901	FAD	C4A-N9A	-2.58	1.32	1.37
5	A	904	UEU	C17-C16	-2.53	1.35	1.39
3	A	901	FAD	C8-C7	2.48	1.46	1.40
3	A	901	FAD	C2A-N1A	2.46	1.38	1.33
3	A	901	FAD	C2-N3	-2.40	1.33	1.39
5	A	904	UEU	O29-C28	2.34	1.27	1.22
5	A	904	UEU	C24-C23	2.26	1.41	1.37
3	A	901	FAD	C2'-C3'	-2.15	1.49	1.53
3	A	901	FAD	C8A-N7A	2.07	1.35	1.31

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	UEU	C10-C8-C7	9.17	121.12	111.21
5	A	904	UEU	C13-C2-C3	-7.13	116.00	122.45
5	A	904	UEU	C9-C8-C7	-6.92	103.74	111.21
5	A	904	UEU	C33-C34-N30	-6.82	94.17	102.93
3	A	901	FAD	N3A-C4A-N9A	5.72	136.89	127.17
5	A	904	UEU	C7-C5-C4	-5.47	113.44	120.35
3	A	901	FAD	N6A-C6A-N1A	5.46	130.54	118.38
3	A	901	FAD	O4'-C4'-C3'	5.46	122.02	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	C4A-N9A-C8A	4.82	110.80	105.74
3	A	901	FAD	C5A-C6A-N6A	-4.60	111.89	123.29
3	A	901	FAD	C5A-C4A-N3A	-4.55	120.44	126.72
3	A	901	FAD	C5'-C4'-C3'	-4.37	103.98	112.22
5	A	904	UEU	C19-C24-C23	-4.30	116.21	119.61
5	A	904	UEU	C20-C19-C14	-4.22	113.91	120.91
3	A	901	FAD	O5'-P-O1P	-3.69	94.30	108.94
3	A	901	FAD	O2'-C2'-C3'	-3.66	100.68	109.25
5	A	904	UEU	C1-C2-C3	3.60	121.91	116.20
5	A	904	UEU	C8-C7-C5	-3.42	110.58	114.95
3	A	901	FAD	O2A-PA-O1A	3.40	128.27	112.44
3	A	901	FAD	C6-C5X-C9A	3.38	123.69	119.05
3	A	901	FAD	C4X-C10-N1	-3.24	116.64	124.59
5	A	904	UEU	C15-C16-C28	3.21	127.27	120.13
5	A	904	UEU	C6-C5-C4	2.99	122.67	118.55
3	A	901	FAD	O5B-PA-O1A	-2.97	97.16	108.94
3	A	901	FAD	O4-C4-C4X	-2.95	118.74	126.53
3	A	901	FAD	O3'-C3'-C2'	-2.91	102.32	108.93
3	A	901	FAD	C5A-C4A-N9A	-2.89	102.67	105.81
5	A	904	UEU	F25-C23-C22	-2.79	112.72	118.02
5	A	904	UEU	C17-C16-C28	-2.71	113.32	120.28
5	A	904	UEU	F25-C23-C24	2.68	123.99	118.64
3	A	901	FAD	C2A-N3A-C4A	2.68	118.37	111.83
3	A	901	FAD	C10-N1-C2	2.67	122.62	116.85
5	A	904	UEU	O11-C8-C9	-2.66	99.70	107.99
3	A	901	FAD	N3A-C2A-N1A	-2.61	124.63	128.58
3	A	901	FAD	C4-N3-C2	-2.56	121.09	125.64
5	A	904	UEU	C24-C19-C14	2.51	124.82	120.61
3	A	901	FAD	C4X-C4-N3	2.48	119.56	113.25
5	A	904	UEU	C1-C6-C5	-2.42	117.82	121.00
3	A	901	FAD	C9A-N10-C10	-2.38	117.12	120.75
3	A	901	FAD	C9-C9A-C5X	-2.36	115.85	120.03
5	A	904	UEU	C4-C3-C2	-2.34	119.84	123.59
3	A	901	FAD	C5X-N5-C4X	2.33	121.86	118.09
3	A	901	FAD	P-O5'-C5'	-2.32	108.05	121.35
3	A	901	FAD	C9-C9A-N10	2.31	124.97	121.85
3	A	901	FAD	C4B-O4B-C1B	-2.28	104.44	109.47
5	A	904	UEU	C20-C19-C24	2.20	121.26	118.23
4	A	903	GOL	O3-C3-C2	2.17	120.14	110.38
5	A	904	UEU	C17-C18-C13	2.16	124.06	120.33
5	A	904	UEU	C2-C13-C14	2.15	126.83	123.72
3	A	901	FAD	O2P-P-O1P	2.14	122.41	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	UEU	C16-C28-N30	-2.12	116.01	118.66
3	A	901	FAD	C1'-N10-C9A	2.08	124.68	120.63
3	A	901	FAD	N9A-C8A-N7A	-2.08	110.99	113.94
5	A	904	UEU	C9-C8-C10	2.06	115.23	110.63
3	A	901	FAD	N10-C10-N1	2.05	124.55	118.51
5	A	904	UEU	C18-C17-C16	-2.05	118.61	120.80
3	A	901	FAD	O2P-P-O3P	-2.04	101.75	107.27
3	A	901	FAD	C9A-C5X-N5	-2.02	120.31	122.45
5	A	904	UEU	C7-C5-C6	2.00	123.75	121.06

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FAD	PA-O3P-P-O5'
4	A	902	GOL	O1-C1-C2-C3
4	A	903	GOL	O1-C1-C2-C3
5	A	904	UEU	O29-C28-N30-C34
5	A	904	UEU	O29-C28-N30-C31
5	A	904	UEU	C16-C28-N30-C34
5	A	904	UEU	C16-C28-N30-C31
5	A	904	UEU	C5-C7-C8-O11
5	A	904	UEU	C5-C7-C8-C10
5	A	904	UEU	C5-C7-C8-C9
4	A	902	GOL	C1-C2-C3-O3
4	A	903	GOL	O1-C1-C2-O2
4	A	902	GOL	O1-C1-C2-O2
4	A	902	GOL	O2-C2-C3-O3
4	A	903	GOL	O2-C2-C3-O3
3	A	901	FAD	P-O3P-PA-O2A

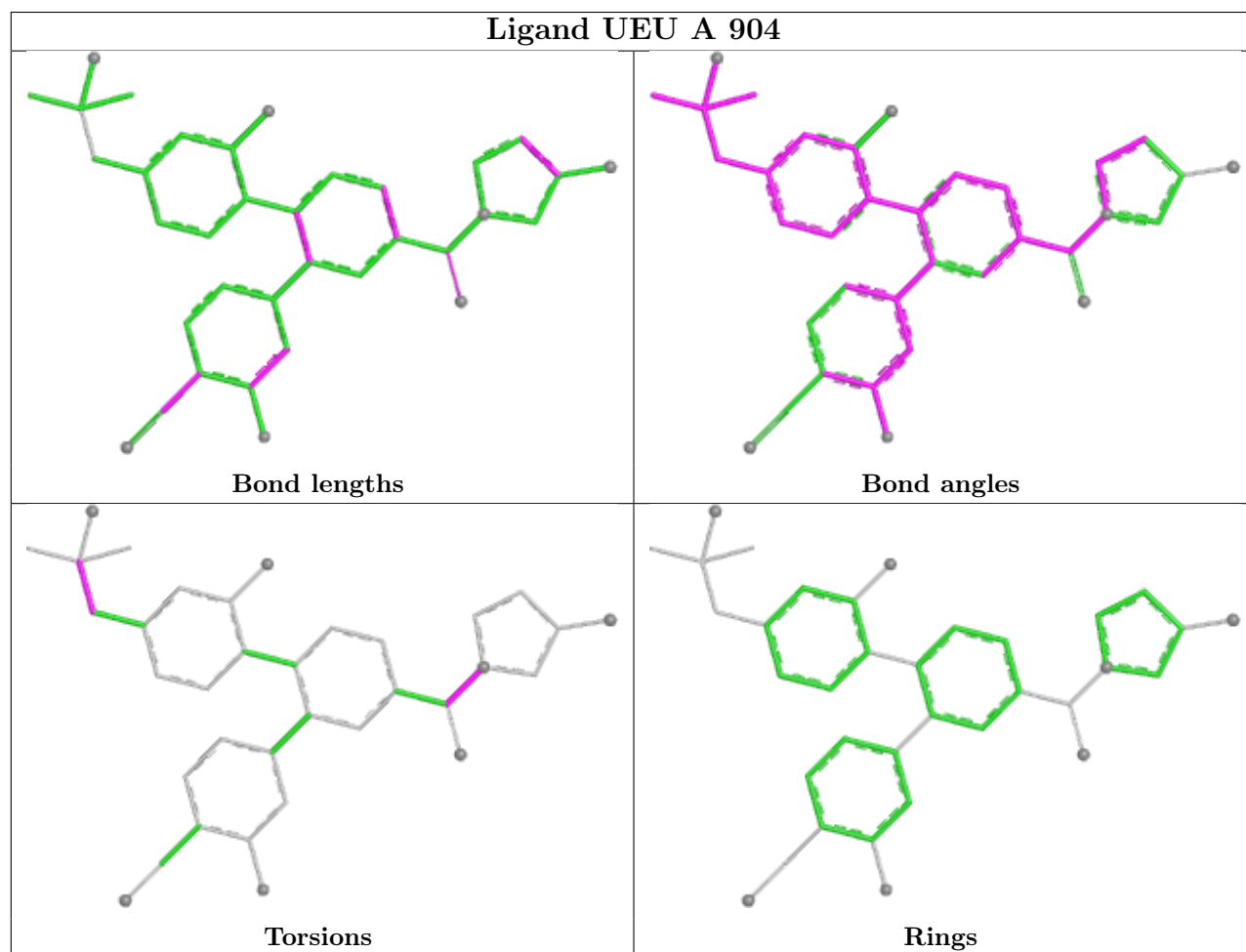
There are no ring outliers.

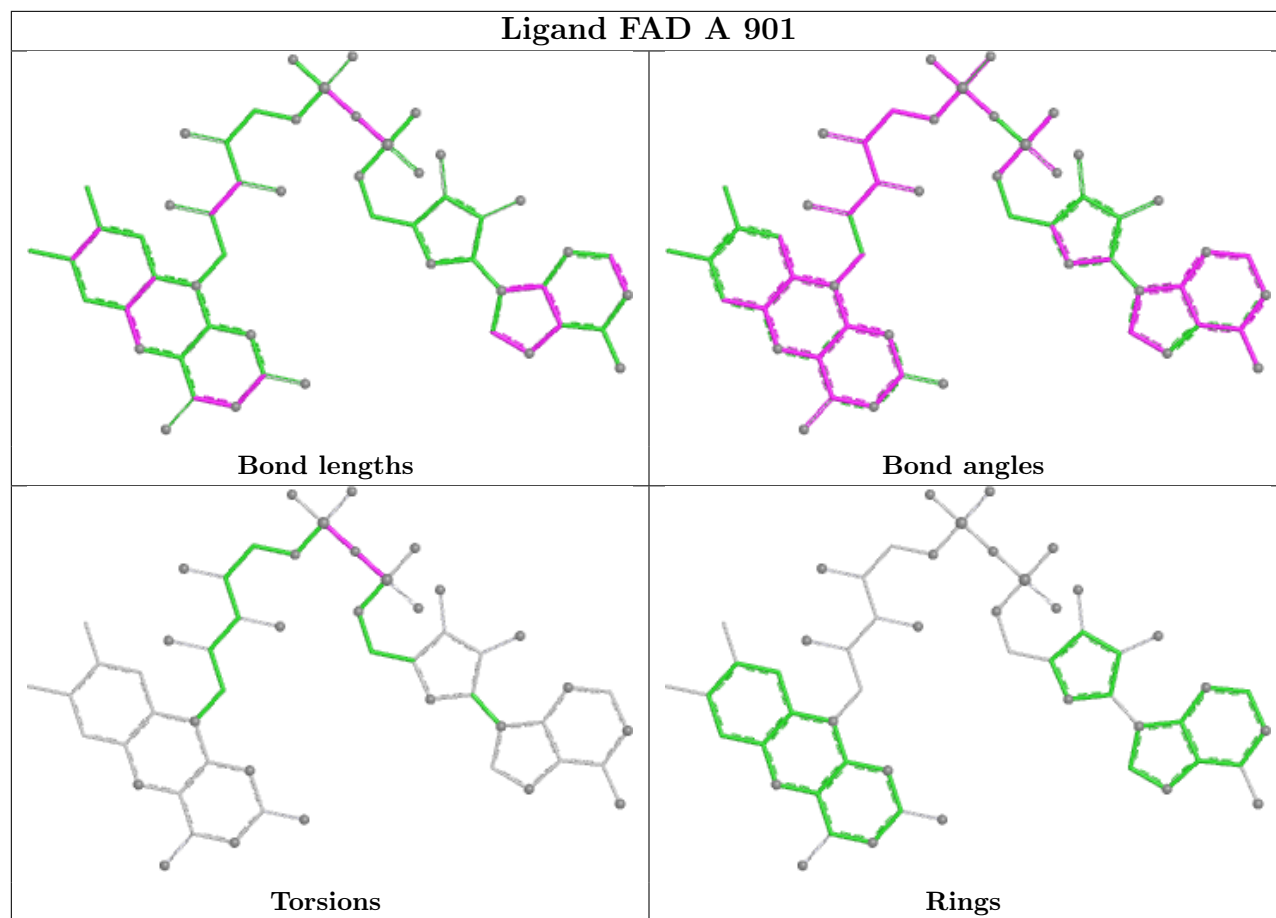
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	UEU	1	0
3	A	901	FAD	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	662/663 (99%)	-0.36	3 (0%)	87 76	50, 91, 127, 174	0
2	B	132/135 (97%)	0.17	4 (3%)	52 33	90, 122, 163, 177	0
All	All	794/798 (99%)	-0.27	7 (0%)	81 64	50, 96, 140, 177	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	833	MET	4.4
2	B	424	TYR	3.8
2	B	440	GLU	3.8
1	A	785	SER	3.2
1	A	832	ALA	3.0
2	B	420	PHE	2.7
2	B	419	ASN	2.2

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](#)

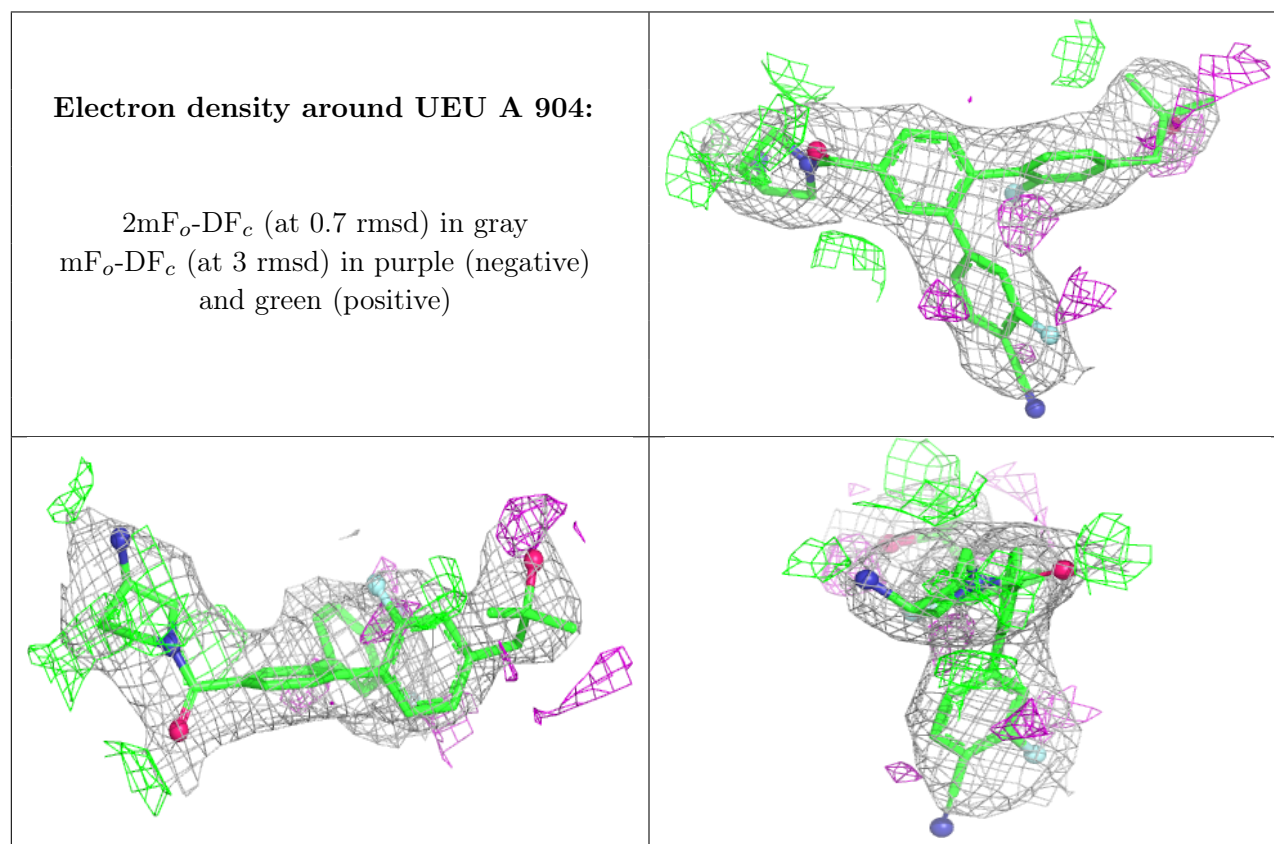
There are no oligosaccharides in this entry.

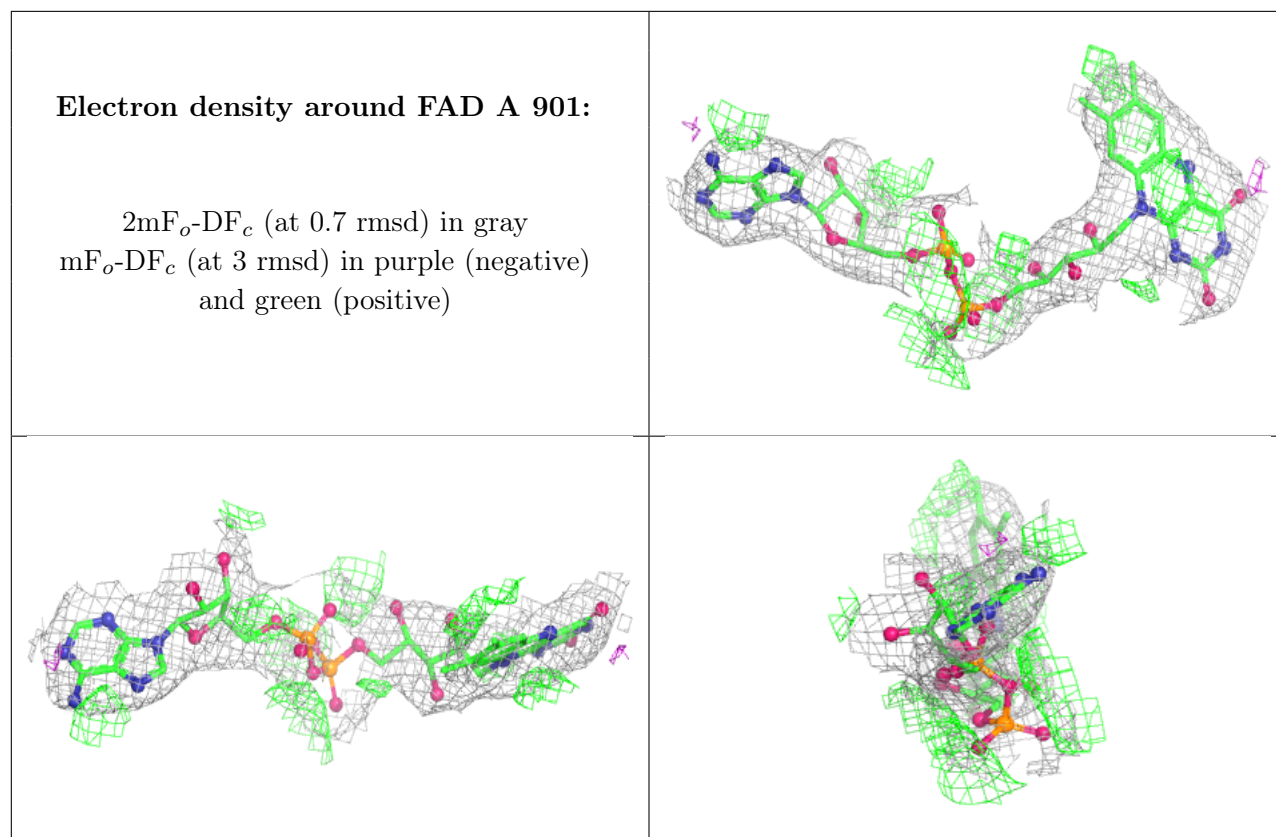
6.4 Ligands [i](#)

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	GOL	A	903	6/6	0.91	0.19	80,102,109,124	0
5	UEU	A	904	35/35	0.95	0.12	56,78,93,104	0
4	GOL	A	902	6/6	0.96	0.13	72,88,95,98	0
3	FAD	A	901	53/53	0.98	0.07	51,69,92,96	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.