



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:58 PM UTC

PDB ID : 6W4K / pdb_00006w4k
Title : Crystal structure of Lysine Specific Demethylase 1 (LSD1) with CC-90011
Authors : Hosfield, D.J.
Deposited on : 2020-03-11
Resolution : 2.93 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

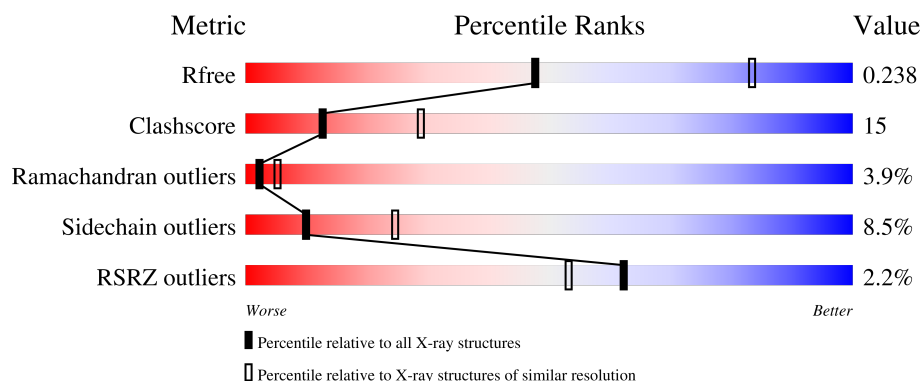
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

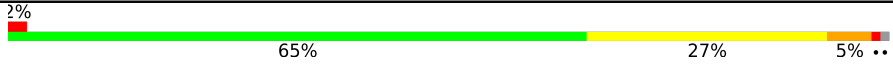
The reported resolution of this entry is 2.93 Å.

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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	659	
2	B	132	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6223 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.

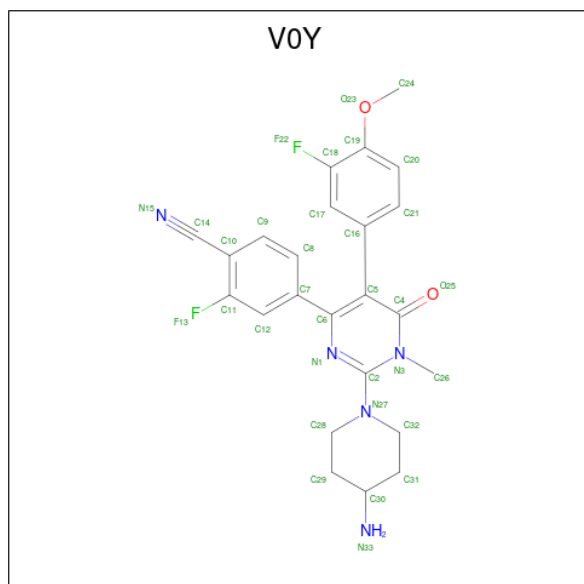
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5107	3254	888	946	19			

- Molecule 2 is a protein called REST corepressor 1.

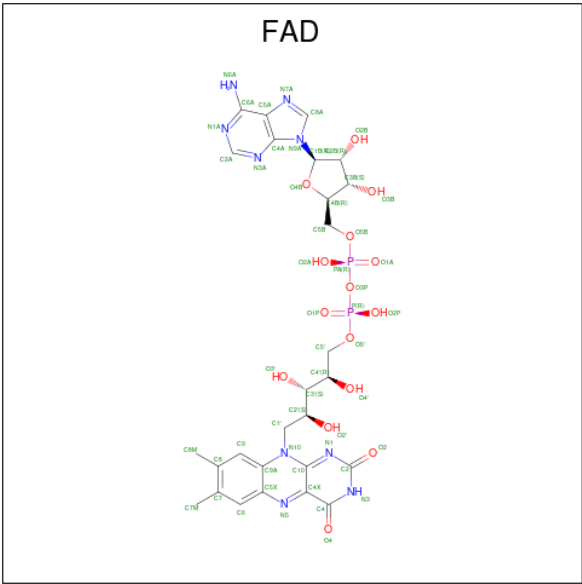
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			1008	632	181	192	3			

- Molecule 3 is 4-[2-(4-aminopiperidin-1-yl)-5-(3-fluoro-4-methoxyphenyl)-1-methyl-6-oxo-1,6-dihydropyrimidin-4-yl]-2-fluorobenzonitrile (CCD ID: V0Y) (formula: C₂₄H₂₃F₂N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			33	24	2	5	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

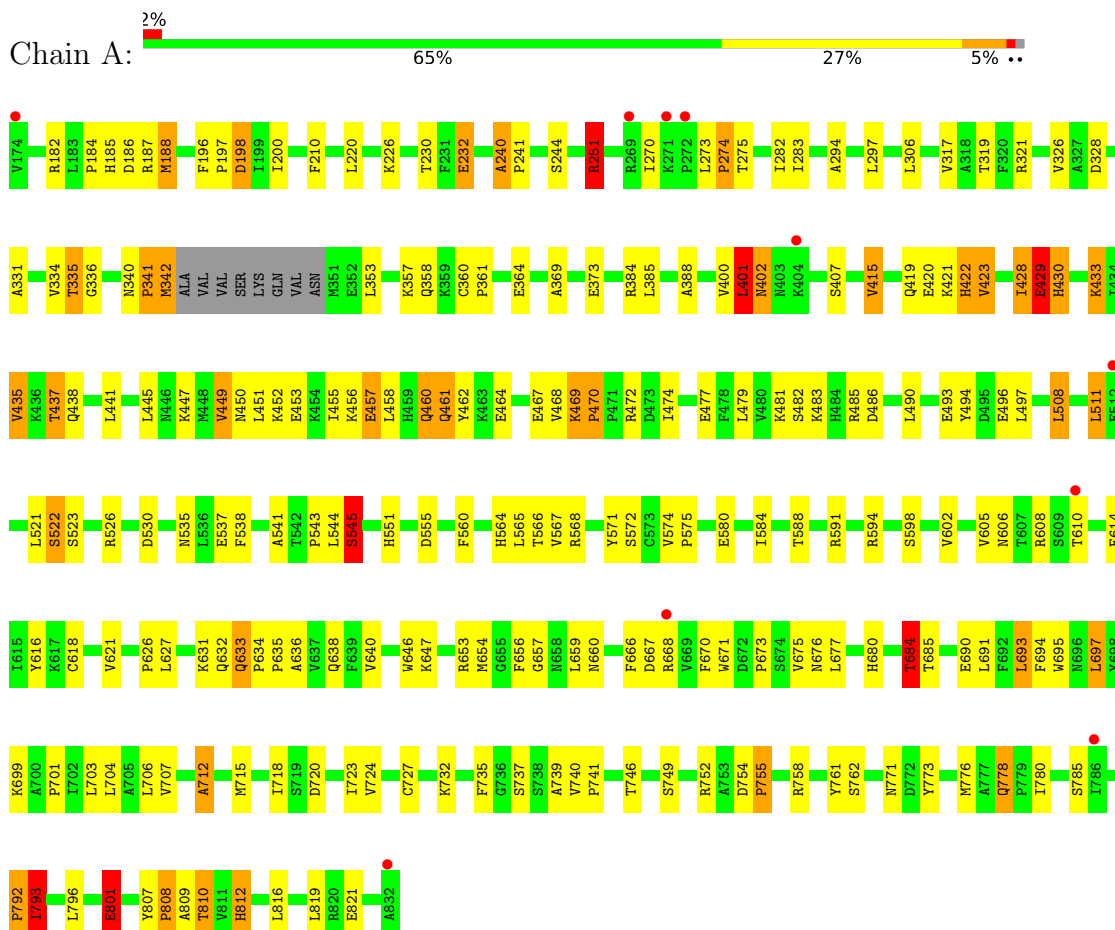
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		

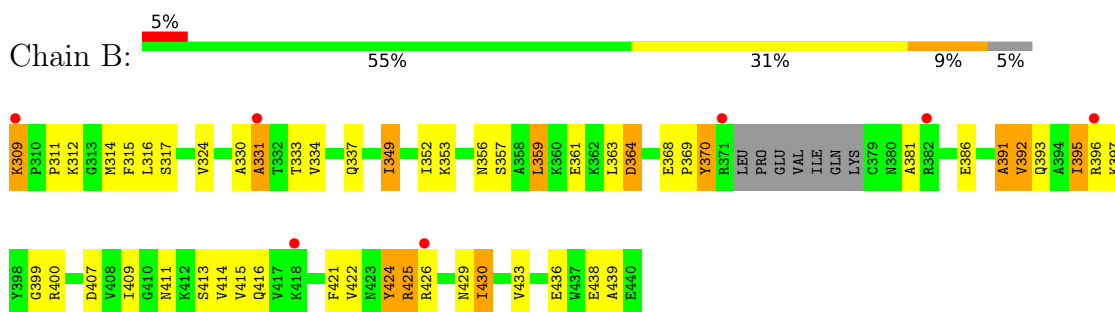
3 Residue-property plots

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



• Molecule 2: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.66Å 178.51Å 236.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.93 49.27 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.27-2.93) 99.5 (49.27-2.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.235 0.200 , 0.238	Depositor DCC
R_{free} test set	2723 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.3	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	0.95	EDS
Total number of atoms	6223	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 2.76% 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: FAD, V0Y

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	1.15	9/5218 (0.2%)	1.61	33/7077 (0.5%)
2	B	1.15	0/1021	1.66	9/1375 (0.7%)
All	All	1.15	9/6239 (0.1%)	1.62	42/8452 (0.5%)

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	3
2	B	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	PRO	C-O	-6.86	1.15	1.23
1	A	551	HIS	CE1-NE2	6.67	1.39	1.32
1	A	342	MET	C-O	6.39	1.36	1.23
1	A	618	CYS	C-O	6.13	1.31	1.23
1	A	819	LEU	C-O	5.90	1.31	1.24
1	A	188	MET	C-O	5.65	1.31	1.23
1	A	812	HIS	CE1-NE2	5.53	1.38	1.32
1	A	430	HIS	CE1-NE2	5.41	1.38	1.32
1	A	633	GLN	C-N	5.02	1.39	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	PRO	N-CA-C	9.36	122.11	110.70
1	A	555	ASP	CA-CB-CG	8.40	121.00	112.60
1	A	198	ASP	CA-CB-CG	-6.75	105.85	112.60
1	A	638	GLN	CB-CG-CD	-6.74	101.14	112.60
1	A	633	GLN	O-C-N	6.62	125.61	120.38
1	A	358	GLN	CB-CA-C	6.38	119.07	111.22
1	A	496	GLU	CB-CA-C	6.34	120.83	110.88
2	B	395	ILE	CA-C-O	-6.26	114.76	121.27
1	A	580	GLU	CB-CA-C	6.15	119.74	109.89
1	A	184	PRO	CA-C-O	-6.15	114.65	121.23
1	A	684	THR	CA-C-N	6.09	128.77	120.54
1	A	684	THR	C-N-CA	6.09	128.77	120.54
1	A	712	ALA	O-C-N	5.96	128.29	122.09
1	A	433	LYS	N-CA-C	-5.90	106.08	113.28
1	A	435	VAL	N-CA-CB	5.77	117.30	110.55
1	A	251	ARG	CG-CD-NE	5.76	124.67	112.00
1	A	635	PRO	CA-C-O	-5.75	114.78	121.34
2	B	424	TYR	CB-CA-C	5.71	121.01	110.56
1	A	423	VAL	CA-C-N	5.67	127.82	120.44
1	A	423	VAL	C-N-CA	5.67	127.82	120.44
1	A	752	ARG	N-CA-C	-5.66	105.09	112.23
1	A	810	THR	CA-CB-OG1	-5.59	101.22	109.60
1	A	808	PRO	N-CA-CB	5.45	108.09	103.35
1	A	373	GLU	CA-C-N	5.42	128.00	120.63
1	A	373	GLU	C-N-CA	5.42	128.00	120.63
1	A	545	SER	O-C-N	5.36	128.49	122.22
1	A	801	GLU	N-CA-CB	-5.35	101.45	110.49
1	A	251	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	B	353	LYS	N-CA-C	-5.31	105.62	112.68
2	B	393	GLN	CA-C-N	5.28	127.66	120.54
2	B	393	GLN	C-N-CA	5.28	127.66	120.54
2	B	407	ASP	CA-C-N	5.25	127.26	120.70
2	B	407	ASP	C-N-CA	5.25	127.26	120.70
1	A	477	GLU	N-CA-C	-5.21	105.68	111.36
2	B	386	GLU	CA-C-N	5.18	127.17	120.44
2	B	386	GLU	C-N-CA	5.18	127.17	120.44
1	A	653	ARG	CA-C-N	-5.09	113.36	122.07
1	A	653	ARG	C-N-CA	-5.09	113.36	122.07
1	A	819	LEU	O-C-N	5.08	127.50	122.12
1	A	712	ALA	CA-C-N	5.04	125.55	120.00
1	A	712	ALA	C-N-CA	5.04	125.55	120.00
1	A	523	SER	N-CA-C	-5.02	106.25	112.93

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	LYS	Peptide
1	A	697	LEU	Peptide
1	A	792	PRO	Peptide
2	B	438	GLU	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	5107	0	5135	152	0
2	B	1008	0	1012	46	0
3	A	33	0	0	1	0
4	A	53	0	31	3	0
5	A	22	0	0	6	0
All	All	6223	0	6178	188	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 15.

All (188) 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:437:THR:HG22	1:A:508:LEU:HD12	1.62	0.80
1:A:188:MET:HE3	1:A:210:PHE:CD2	2.17	0.78
1:A:633:GLN:NE2	1:A:634:PRO:CD	2.46	0.78
1:A:633:GLN:HG2	1:A:634:PRO:HD3	1.64	0.78
1:A:633:GLN:NE2	1:A:634:PRO:HD2	2.00	0.76
1:A:606:ASN:HD21	1:A:608:ARG:HH21	1.32	0.75
2:B:424:TYR:O	2:B:426:ARG:N	2.21	0.74
1:A:240:ALA:HB1	1:A:241:PRO:CD	2.18	0.73
1:A:762:SER:OG	1:A:801:GLU:OE2	2.04	0.72
2:B:369:PRO:C	2:B:370:TYR:CD1	2.69	0.71
1:A:437:THR:CG2	1:A:508:LEU:HD12	2.19	0.71
2:B:369:PRO:C	2:B:370:TYR:HD1	2.00	0.70
1:A:420:GLU:OE2	1:A:526:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1012:HOH:O	2:B:352:ILE:HD11	1.94	0.68
2:B:369:PRO:O	2:B:370:TYR:CD1	2.47	0.67
1:A:807:TYR:N	1:A:808:PRO:HD3	2.10	0.67
2:B:396:ARG:HD3	2:B:436:GLU:OE1	1.95	0.66
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.32	0.65
1:A:666:PHE:O	1:A:701:PRO:HG2	1.97	0.65
1:A:776:MET:HA	1:A:776:MET:HE3	1.80	0.63
1:A:633:GLN:CG	1:A:634:PRO:HD3	2.29	0.62
2:B:381:ALA:HA	2:B:416:GLN:HE22	1.63	0.62
1:A:693:LEU:HD12	1:A:694:PHE:N	2.15	0.62
1:A:538:PHE:CE1	1:A:706:LEU:HD23	2.36	0.60
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.32	0.60
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.32	0.59
1:A:331:ALA:HA	4:A:902:FAD:C4X	2.32	0.59
1:A:530:ASP:OD2	1:A:685:THR:HA	2.02	0.58
1:A:654:MET:HE1	1:A:773:TYR:CE1	2.37	0.58
1:A:415:VAL:HG22	2:B:316:LEU:HD21	1.84	0.58
2:B:422:VAL:O	2:B:425:ARG:HB2	2.03	0.58
1:A:438:GLN:HB3	1:A:508:LEU:HD11	1.85	0.58
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.86	0.58
1:A:633:GLN:NE2	1:A:634:PRO:HD3	2.18	0.58
1:A:684:THR:HG22	5:A:1021:HOH:O	2.04	0.58
1:A:633:GLN:CD	1:A:634:PRO:HD2	2.28	0.57
1:A:654:MET:HE1	1:A:773:TYR:CZ	2.40	0.57
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.87	0.57
1:A:198:ASP:HB2	1:A:251:ARG:HH22	1.70	0.57
1:A:240:ALA:HB1	1:A:241:PRO:HD2	1.87	0.57
1:A:660:ASN:HA	1:A:749:SER:OG	2.05	0.56
1:A:449:VAL:HG12	1:A:450:ASN:OD1	2.05	0.56
1:A:240:ALA:CB	1:A:241:PRO:CD	2.83	0.56
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.40	0.56
1:A:739:ALA:O	1:A:741:PRO:HD3	2.05	0.56
3:A:901:VOY:C28	3:A:901:VOY:C26	2.84	0.56
1:A:341:PRO:HG3	1:A:816:LEU:HD21	1.88	0.56
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.89	0.55
1:A:384:ARG:NH2	2:B:312:LYS:O	2.39	0.55
1:A:460:GLN:O	1:A:462:TYR:N	2.40	0.55
1:A:720:ASP:O	1:A:724:VAL:HG23	2.07	0.55
1:A:331:ALA:HA	4:A:902:FAD:N5	2.22	0.55
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.07	0.54
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TRP:CE3	1:A:697:LEU:HD21	2.42	0.54
1:A:187:ARG:HB2	1:A:187:ARG:NH1	2.21	0.54
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.90	0.54
1:A:633:GLN:CD	1:A:634:PRO:CD	2.81	0.54
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.43	0.53
1:A:240:ALA:HB1	1:A:241:PRO:HD3	1.89	0.53
1:A:401:LEU:O	1:A:402:ASN:HB2	2.08	0.53
1:A:319:THR:HB	1:A:572:SER:HB3	1.90	0.53
1:A:521:LEU:O	1:A:522:SER:O	2.26	0.53
1:A:467:GLU:O	1:A:469:LYS:HG3	2.08	0.53
2:B:413:SER:OG	2:B:415:VAL:HG12	2.09	0.53
1:A:479:LEU:O	1:A:483:LYS:HG2	2.09	0.52
1:A:447:LYS:HE3	1:A:497:LEU:HD21	1.90	0.52
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.91	0.52
1:A:485:ARG:HD2	5:A:1014:HOH:O	2.09	0.52
1:A:666:PHE:O	1:A:701:PRO:CG	2.58	0.52
1:A:807:TYR:N	1:A:808:PRO:CD	2.72	0.52
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.92	0.52
1:A:591:ARG:NH1	1:A:605:VAL:HG21	2.25	0.52
1:A:660:ASN:HA	1:A:749:SER:HG	1.75	0.51
1:A:538:PHE:CD1	1:A:706:LEU:HD23	2.46	0.51
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.93	0.51
2:B:361:GLU:O	2:B:364:ASP:HB2	2.11	0.50
2:B:426:ARG:HH11	2:B:426:ARG:HB2	1.77	0.50
1:A:456:LYS:HA	2:B:370:TYR:HE2	1.77	0.49
1:A:633:GLN:HE21	1:A:634:PRO:HD3	1.76	0.49
1:A:273:LEU:O	1:A:274:PRO:C	2.55	0.49
1:A:758:ARG:HD2	5:A:1013:HOH:O	2.12	0.49
2:B:426:ARG:HB3	2:B:426:ARG:NH1	2.28	0.49
1:A:732:LYS:HG2	1:A:740:VAL:HB	1.94	0.49
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.42	0.49
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.78	0.49
1:A:810:THR:HB	1:A:812:HIS:CE1	2.48	0.49
1:A:428:ILE:O	1:A:430:HIS:N	2.46	0.48
1:A:594:ARG:HA	1:A:640:VAL:O	2.14	0.48
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.96	0.48
2:B:368:GLU:HB2	2:B:369:PRO:HD3	1.95	0.48
1:A:627:LEU:HD21	1:A:654:MET:HG3	1.95	0.48
1:A:538:PHE:CE1	1:A:706:LEU:CD2	2.97	0.48
1:A:335:THR:HG22	1:A:335:THR:O	2.15	0.47
1:A:632:GLN:OE1	1:A:636:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:GLN:HE21	1:A:634:PRO:CD	2.23	0.47
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.96	0.47
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.49	0.47
1:A:792:PRO:HA	1:A:793:ILE:HD12	1.97	0.47
1:A:441:LEU:HD23	2:B:356:ASN:ND2	2.29	0.47
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.97	0.47
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.96	0.47
1:A:690:GLU:O	1:A:691:LEU:C	2.58	0.46
2:B:309:LYS:HE2	2:B:309:LYS:N	2.30	0.46
1:A:188:MET:HE3	1:A:210:PHE:CG	2.50	0.46
1:A:470:PRO:O	1:A:472:ARG:N	2.48	0.46
1:A:776:MET:HE3	1:A:776:MET:CA	2.44	0.46
1:A:792:PRO:CA	1:A:793:ILE:HD12	2.46	0.46
1:A:187:ARG:CB	1:A:187:ARG:CZ	2.93	0.46
1:A:754:ASP:OD1	1:A:754:ASP:C	2.59	0.46
2:B:426:ARG:HH11	2:B:426:ARG:CB	2.28	0.46
1:A:449:VAL:HG23	2:B:363:LEU:HD23	1.97	0.46
1:A:455:ILE:HG22	2:B:370:TYR:HD2	1.80	0.46
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.96	0.46
1:A:385:LEU:O	1:A:388:ALA:HB3	2.15	0.46
1:A:724:VAL:HG11	1:A:746:THR:HG21	1.97	0.46
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.49	0.45
1:A:198:ASP:HB2	1:A:251:ARG:NH2	2.29	0.45
1:A:694:PHE:HA	1:A:704:LEU:O	2.16	0.45
1:A:407:SER:CB	1:A:545:SER:O	2.65	0.45
1:A:568:ARG:HH21	1:A:699:LYS:HD2	1.81	0.45
1:A:670:PHE:C	1:A:670:PHE:CD1	2.95	0.45
2:B:411:ASN:O	2:B:411:ASN:CG	2.58	0.45
1:A:564:HIS:N	1:A:564:HIS:CD2	2.84	0.45
1:A:419:GLN:HE22	2:B:315:PHE:H	1.66	0.44
1:A:428:ILE:HG22	1:A:429:GLU:N	2.32	0.44
1:A:541:ALA:O	1:A:657:GLY:HA3	2.16	0.44
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.99	0.44
1:A:451:LEU:HD21	1:A:493:GLU:HG2	2.00	0.44
1:A:633:GLN:CD	1:A:633:GLN:H	2.25	0.44
2:B:324:VAL:O	2:B:324:VAL:HG22	2.18	0.44
2:B:352:ILE:O	2:B:352:ILE:HG22	2.17	0.44
1:A:328:ASP:HB3	5:A:1002:HOH:O	2.17	0.44
1:A:574:VAL:HB	1:A:575:PRO:HD3	2.00	0.44
2:B:359:LEU:HD23	2:B:359:LEU:N	2.32	0.44
1:A:627:LEU:CD2	1:A:654:MET:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG13	1:A:571:TYR:HB3	1.99	0.43
1:A:422:HIS:CD2	1:A:422:HIS:C	2.96	0.43
1:A:511:LEU:HD23	1:A:511:LEU:N	2.33	0.43
2:B:369:PRO:HG2	2:B:370:TYR:HE1	1.83	0.43
1:A:187:ARG:CZ	1:A:187:ARG:HB3	2.49	0.43
1:A:400:VAL:HG12	1:A:401:LEU:N	2.34	0.43
1:A:407:SER:HB3	1:A:545:SER:O	2.18	0.43
2:B:413:SER:OG	2:B:416:GLN:HG3	2.19	0.43
1:A:240:ALA:CB	1:A:241:PRO:HD2	2.47	0.42
1:A:353:LEU:HD13	1:A:565:LEU:HD12	2.01	0.42
1:A:627:LEU:HG	1:A:631:LYS:HD2	2.02	0.42
1:A:633:GLN:CG	1:A:634:PRO:CD	2.95	0.42
1:A:677:LEU:HD12	1:A:693:LEU:HD11	2.01	0.42
2:B:426:ARG:HB3	2:B:426:ARG:CZ	2.49	0.42
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.86	0.42
1:A:821:GLU:OE1	1:A:821:GLU:HA	2.15	0.42
2:B:330:ALA:O	2:B:331:ALA:C	2.62	0.42
1:A:334:VAL:O	1:A:336:GLY:N	2.49	0.42
1:A:455:ILE:HG22	2:B:370:TYR:CD2	2.53	0.42
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.53	0.42
1:A:282:ILE:O	1:A:621:VAL:HA	2.20	0.42
1:A:321:ARG:HG2	1:A:326:VAL:HG22	2.02	0.42
1:A:196:PHE:N	1:A:197:PRO:CD	2.82	0.42
1:A:656:PHE:CE1	1:A:761:TYR:HA	2.55	0.42
1:A:778:GLN:HG3	5:A:1019:HOH:O	2.19	0.42
1:A:460:GLN:O	1:A:461:GLN:C	2.63	0.41
1:A:796:LEU:HD12	1:A:796:LEU:HA	1.87	0.41
2:B:391:ALA:O	2:B:392:VAL:C	2.63	0.41
2:B:426:ARG:NH1	2:B:426:ARG:CB	2.83	0.41
1:A:754:ASP:OD1	1:A:755:PRO:HD2	2.19	0.41
2:B:334:VAL:HA	2:B:337:GLN:NE2	2.35	0.41
2:B:421:PHE:O	2:B:425:ARG:HG3	2.20	0.41
1:A:360:CYS:HA	1:A:361:PRO:HD2	1.92	0.41
1:A:460:GLN:HE21	1:A:464:GLU:HG3	1.86	0.41
1:A:481:LYS:O	1:A:482:SER:C	2.63	0.41
1:A:626:PRO:HD3	4:A:902:FAD:H51A	2.03	0.41
1:A:660:ASN:CA	1:A:749:SER:OG	2.69	0.41
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.55	0.41
1:A:187:ARG:HB2	1:A:187:ARG:HH11	1.84	0.41
1:A:230:THR:HG23	1:A:270:ILE:HD12	2.03	0.41
1:A:230:THR:OG1	1:A:232:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:PRO:O	1:A:810:THR:HG23	2.20	0.41
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.93	0.41
1:A:671:TRP:O	1:A:673:PRO:HD3	2.21	0.41
2:B:311:PRO:HG2	2:B:314:MET:CG	2.50	0.41
1:A:614:PHE:HB3	1:A:616:TYR:CE1	2.56	0.40
2:B:391:ALA:CB	2:B:409:ILE:HD11	2.51	0.40
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.02	0.40
1:A:422:HIS:O	1:A:422:HIS:CG	2.72	0.40
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.61	0.40
1:A:198:ASP:CB	1:A:251:ARG:HH22	2.34	0.40
1:A:437:THR:HG22	1:A:508:LEU:CD1	2.43	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	647/659 (98%)	542 (84%)	82 (13%)	23 (4%)	2	6
2	B	121/132 (92%)	96 (79%)	18 (15%)	7 (6%)	1	2
All	All	768/791 (97%)	638 (83%)	100 (13%)	30 (4%)	2	5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	THR
1	A	522	SER
1	A	610	THR
1	A	793	ILE
2	B	331	ALA
2	B	425	ARG
2	B	439	ALA

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Mol	Chain	Res	Type
1	A	232	GLU
1	A	240	ALA
1	A	244	SER
1	A	275	THR
1	A	364	GLU
1	A	402	ASN
1	A	428	ILE
1	A	429	GLU
1	A	460	GLN
1	A	461	GLN
1	A	468	VAL
1	A	801	GLU
2	B	391	ALA
2	B	399	GLY
1	A	274	PRO
1	A	341	PRO
1	A	369	ALA
2	B	429	ASN
1	A	401	LEU
1	A	457	GLU
1	A	486	ASP
1	A	737	SER
2	B	392	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	553/560 (99%)	509 (92%)	44 (8%)	11	27
2	B	109/116 (94%)	97 (89%)	12 (11%)	6	17
All	All	662/676 (98%)	606 (92%)	56 (8%)	10	24

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ILE
1	A	220	LEU
1	A	226	LYS
1	A	251	ARG
1	A	342	MET
1	A	357	LYS
1	A	401	LEU
1	A	415	VAL
1	A	421	LYS
1	A	422	HIS
1	A	423	VAL
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	445	LEU
1	A	449	VAL
1	A	452	LYS
1	A	453	GLU
1	A	457	GLU
1	A	458	LEU
1	A	474	ILE
1	A	490	LEU
1	A	508	LEU
1	A	511	LEU
1	A	535	ASN
1	A	543	PRO
1	A	545	SER
1	A	567	VAL
1	A	588	THR
1	A	598	SER
1	A	659	LEU
1	A	667	ASP
1	A	668	ARG
1	A	675	VAL
1	A	676	ASN
1	A	680	HIS
1	A	684	THR
1	A	693	LEU
1	A	703	LEU
1	A	755	PRO
1	A	771	ASN
1	A	778	GLN
1	A	785	SER

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Mol	Chain	Res	Type
1	A	793	ILE
2	B	309	LYS
2	B	317	SER
2	B	333	THR
2	B	349	ILE
2	B	357	SER
2	B	359	LEU
2	B	364	ASP
2	B	370	TYR
2	B	397	LYS
2	B	400	ARG
2	B	414	VAL
2	B	430	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	237	GLN
1	A	395	GLN
1	A	402	ASN
1	A	422	HIS
1	A	430	HIS
1	A	460	GLN
1	A	564	HIS
1	A	633	GLN
1	A	638	GLN
1	A	680	HIS
1	A	771	ASN
1	A	778	GLN
1	A	806	ASN
1	A	812	HIS
1	A	828	GLN
2	B	411	ASN
2	B	416	GLN

5.3.3 RNA ⓘ

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](#)

2 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	$\# Z > 2$
3	V0Y	A	901	-	35,36,36	2.31	10 (28%)	49,52,52	3.22	22 (44%)
4	FAD	A	902	-	58,58,58	0.66	1 (1%)	85,89,89	0.87	2 (2%)

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
3	V0Y	A	901	-	-	2/16/26/26	0/4/4/4
4	FAD	A	902	-	-	13/34/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	V0Y	C10-C14	-9.03	1.31	1.44
3	A	901	V0Y	C32-N27	-4.30	1.39	1.47
3	A	901	V0Y	C30-N33	-3.75	1.34	1.46
3	A	901	V0Y	C2-N1	3.31	1.36	1.31
3	A	901	V0Y	C28-N27	-3.09	1.41	1.47
3	A	901	V0Y	C20-C19	-2.74	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	V0Y	C17-C18	2.72	1.42	1.37
3	A	901	V0Y	C5-C4	-2.52	1.38	1.45
3	A	901	V0Y	C16-C5	2.35	1.54	1.49
3	A	901	V0Y	C2-N27	2.29	1.44	1.37
4	A	902	FAD	C4X-C4	-2.03	1.37	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	V0Y	O23-C19-C18	14.87	126.95	116.27
3	A	901	V0Y	O23-C19-C20	-6.38	113.55	124.30
3	A	901	V0Y	C11-C10-C14	-4.99	116.50	120.41
3	A	901	V0Y	C8-C7-C6	-4.93	112.67	120.74
3	A	901	V0Y	C17-C16-C5	4.48	128.37	120.17
3	A	901	V0Y	C21-C16-C17	-4.17	114.42	119.25
3	A	901	V0Y	C2-N3-C4	4.08	122.51	120.79
3	A	901	V0Y	N27-C2-N1	3.83	125.78	118.89
3	A	901	V0Y	C10-C14-N15	-3.62	171.94	177.90
3	A	901	V0Y	C17-C18-C19	-3.57	118.05	122.86
3	A	901	V0Y	C12-C7-C6	3.49	127.62	120.51
4	A	902	FAD	O3P-PA-O1A	-2.81	102.24	110.70
3	A	901	V0Y	C16-C17-C18	2.80	122.88	119.07
3	A	901	V0Y	C5-C4-N3	2.73	119.87	115.46
4	A	902	FAD	O2P-P-O1P	2.65	124.78	112.44
3	A	901	V0Y	C20-C21-C16	2.58	123.55	120.80
3	A	901	V0Y	F13-C11-C12	2.44	123.51	118.64
3	A	901	V0Y	O25-C4-C5	-2.43	119.50	124.73
3	A	901	V0Y	C21-C16-C5	-2.30	117.18	120.79
3	A	901	V0Y	F13-C11-C10	-2.28	113.70	118.02
3	A	901	V0Y	C24-O23-C19	-2.27	114.18	117.51
3	A	901	V0Y	C9-C10-C14	2.24	123.25	119.36
3	A	901	V0Y	C9-C10-C11	2.13	120.11	117.59
3	A	901	V0Y	C8-C9-C10	-2.03	118.17	120.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	V0Y	C18-C19-O23-C24
4	A	902	FAD	C5B-O5B-PA-O1A
4	A	902	FAD	O4'-C4'-C5'-O5'
4	A	902	FAD	C5'-O5'-P-O2P

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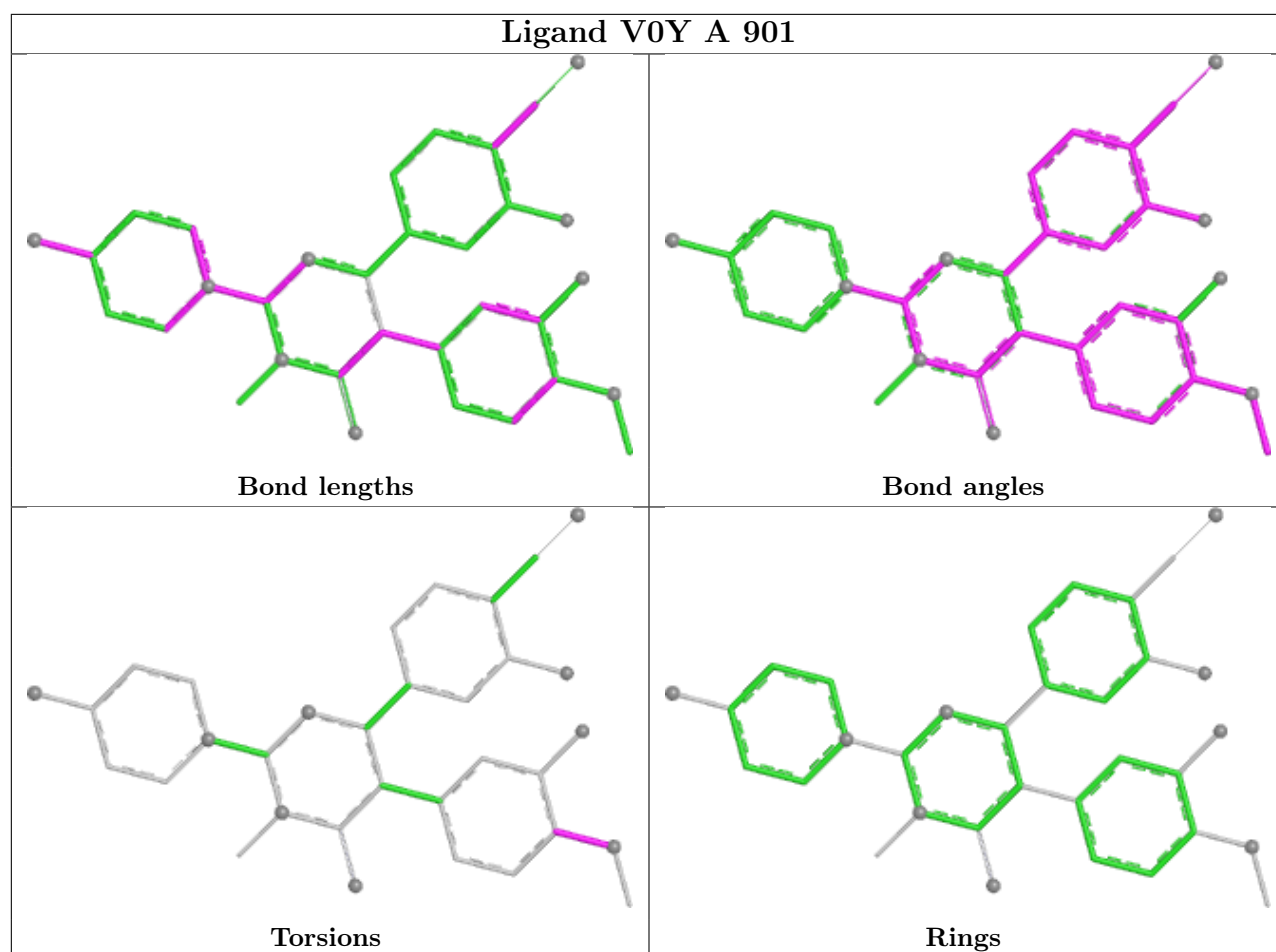
Mol	Chain	Res	Type	Atoms
3	A	901	V0Y	C20-C19-O23-C24
4	A	902	FAD	C2'-C3'-C4'-O4'
4	A	902	FAD	C3'-C4'-C5'-O5'
4	A	902	FAD	C2'-C3'-C4'-C5'
4	A	902	FAD	C5B-O5B-PA-O2A
4	A	902	FAD	C5B-O5B-PA-O3P
4	A	902	FAD	C5'-O5'-P-O1P
4	A	902	FAD	C5'-O5'-P-O3P
4	A	902	FAD	O3'-C3'-C4'-O4'
4	A	902	FAD	O3'-C3'-C4'-C5'
4	A	902	FAD	O4B-C4B-C5B-O5B

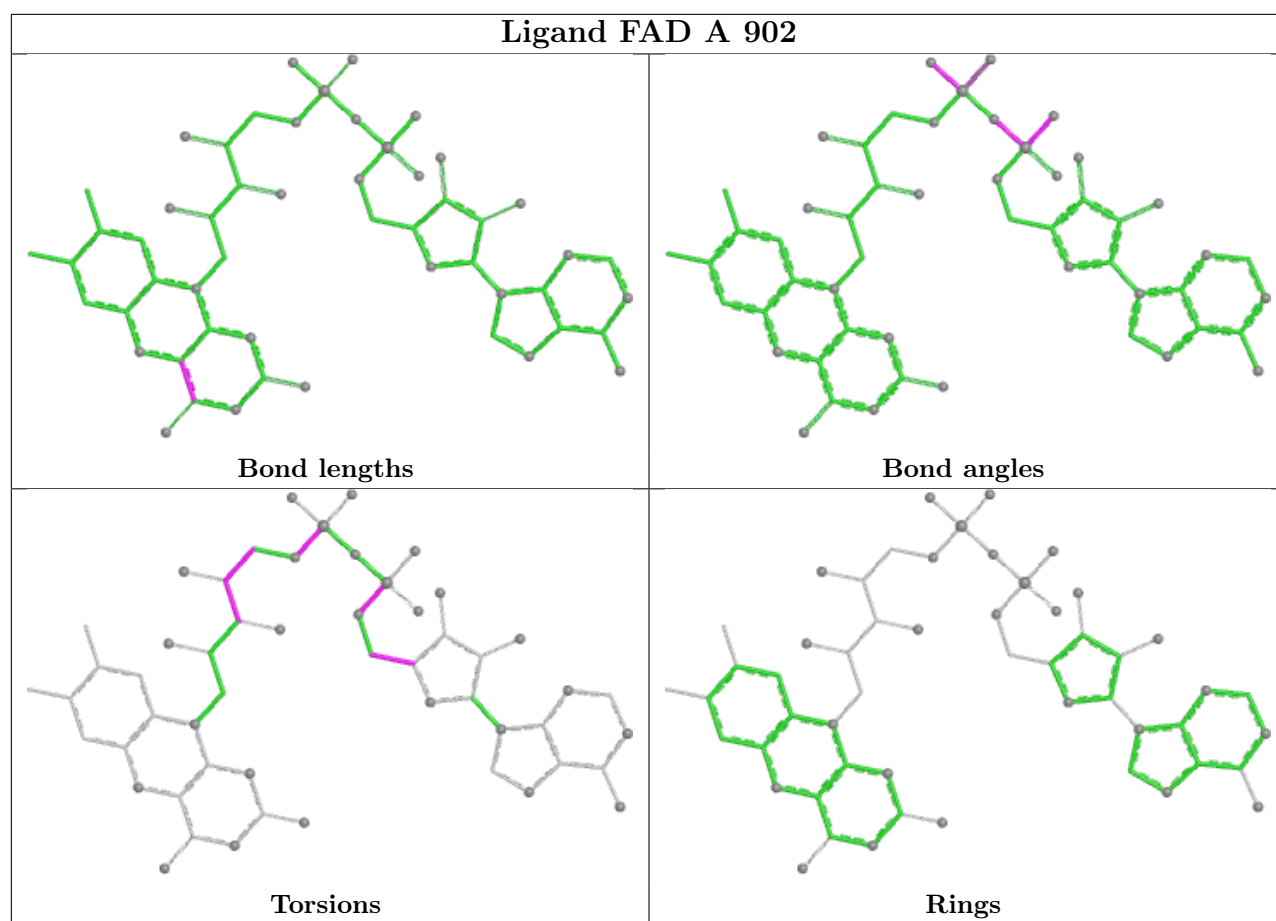
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	V0Y	1	0
4	A	902	FAD	3	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	651/659 (98%)	-0.11	10 (1%) 72 65	57, 89, 134, 165	0
2	B	125/132 (94%)	0.38	7 (5%) 30 24	88, 120, 142, 179	0
All	All	776/791 (98%)	-0.03	17 (2%) 62 53	57, 95, 136, 179	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	832	ALA	5.8
1	A	174	VAL	4.1
2	B	371	ARG	3.6
2	B	382	ARG	3.5
2	B	309	LYS	3.5
2	B	331	ALA	3.5
1	A	269	ARG	3.3
1	A	668	ARG	3.3
2	B	418	LYS	3.0
1	A	786	ILE	2.9
2	B	396	ARG	2.7
2	B	426	ARG	2.4
1	A	272	PRO	2.4
1	A	271	LYS	2.4
1	A	512	GLU	2.4
1	A	610	THR	2.4
1	A	404	LYS	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](#)

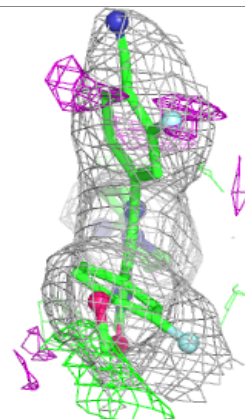
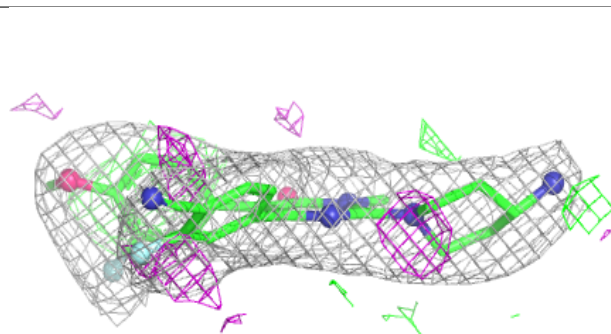
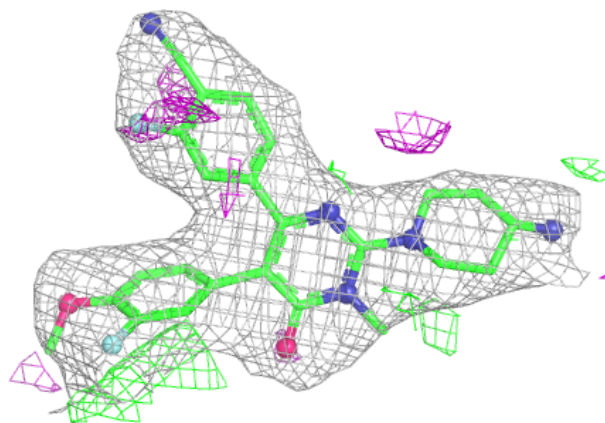
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

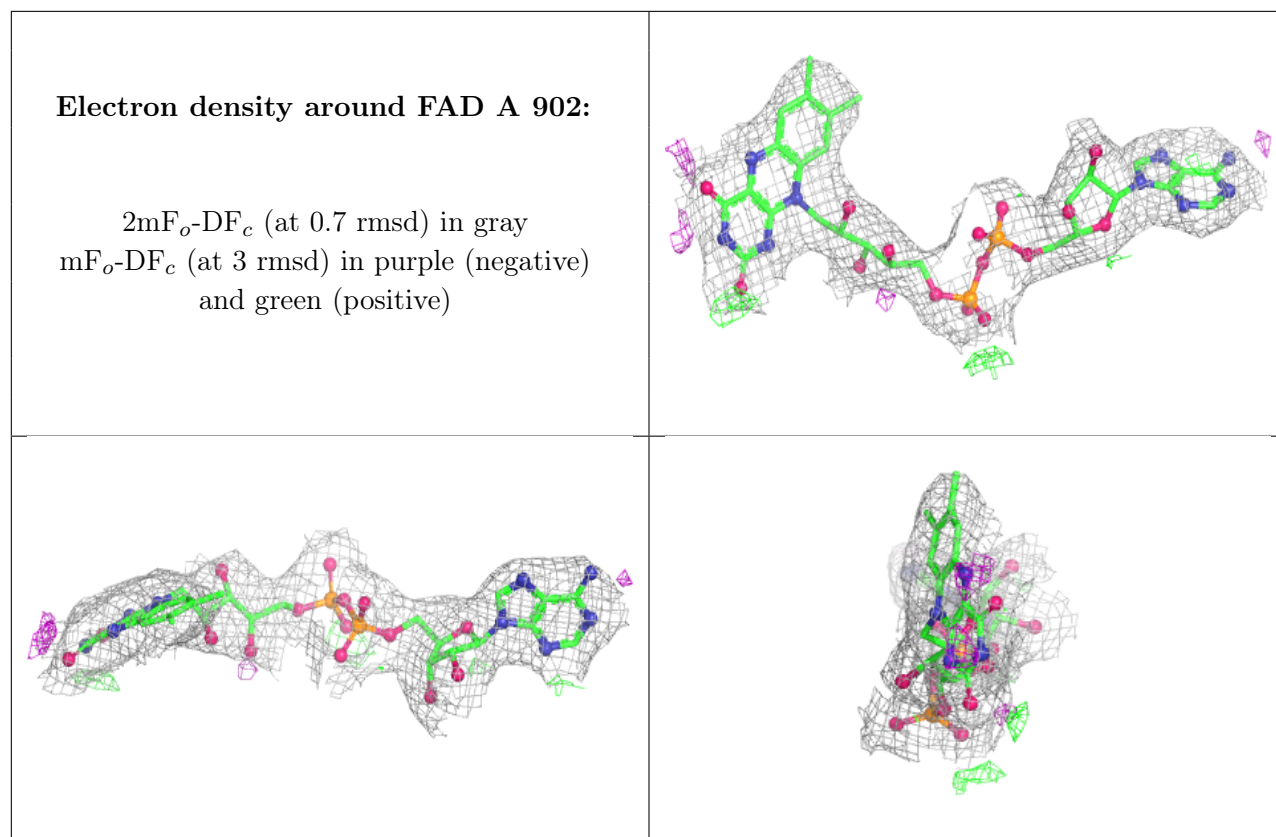
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	V0Y	A	901	33/33	0.97	0.09	51,73,92,106	0
4	FAD	A	902	53/53	0.99	0.05	52,66,84,89	0

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 V0Y A 901:

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.