



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:30 PM UTC

PDB ID : 6TUY / pdb_00006tuy
Title : Human LSD1/CoREST bound to the quinazoline inhibitor MC4106
Authors : Mattevi, A.; Marrocco, B.
Deposited on : 2020-01-08
Resolution : 2.60 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

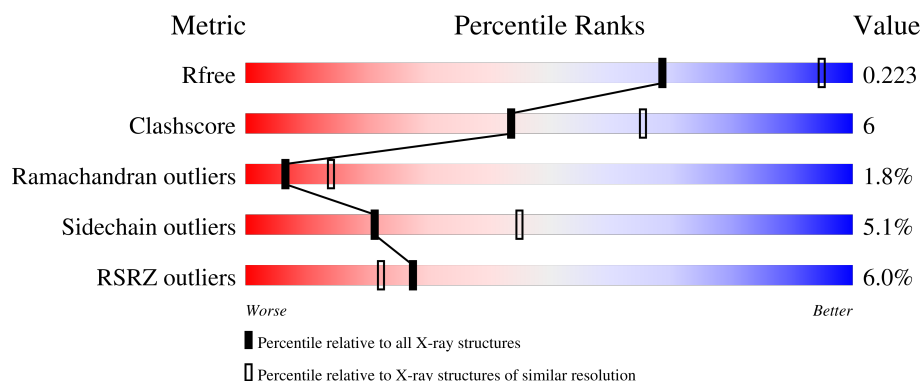
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	853	 4% 57% 19% • 22%
2	B	485	 3% 22% • • 72%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6536 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	667	Total	C	N	O	S	0	0	0
			5224	3329	907	968	20			

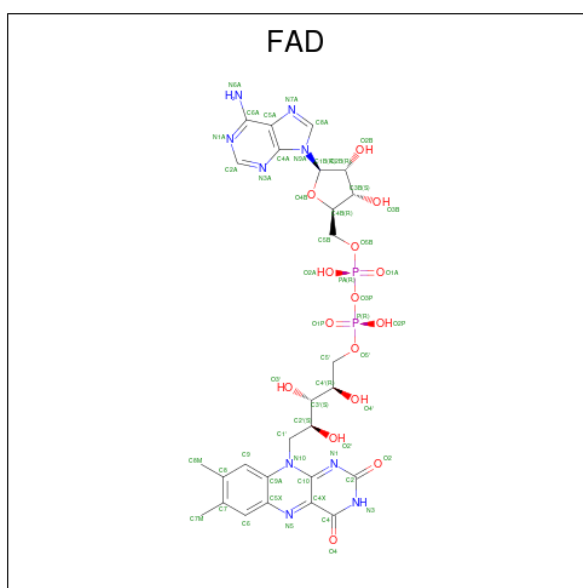
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	869	PRO	-	expression tag	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

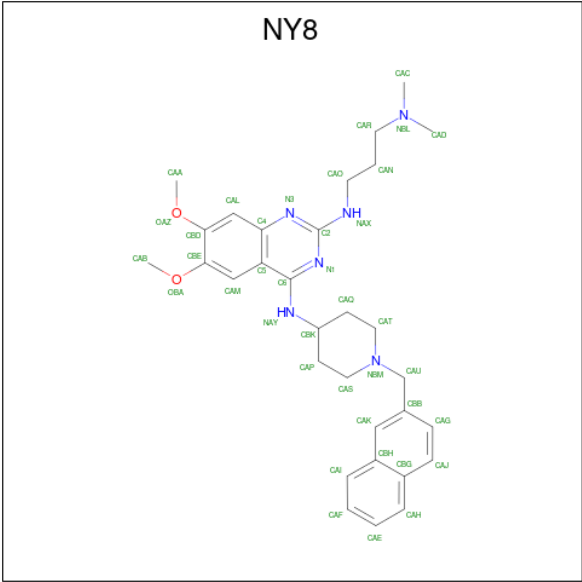
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1086	682	197	204	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is {N}2-[3-(dimethylamino)propyl]-6,7-dimethoxy- {N}4-[1-(naphthalen-2-ylmet hyl)piperidin-4-yl]quinazoline-2,4-diamine (CCD ID: NY8) (formula: C₃₁H₄₀N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			39	31	6	2			
4	A	1	Total	C	N	O		0	0
			39	31	6	2			
4	A	1	Total	C	N	O		0	0
			39	31	6	2			

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

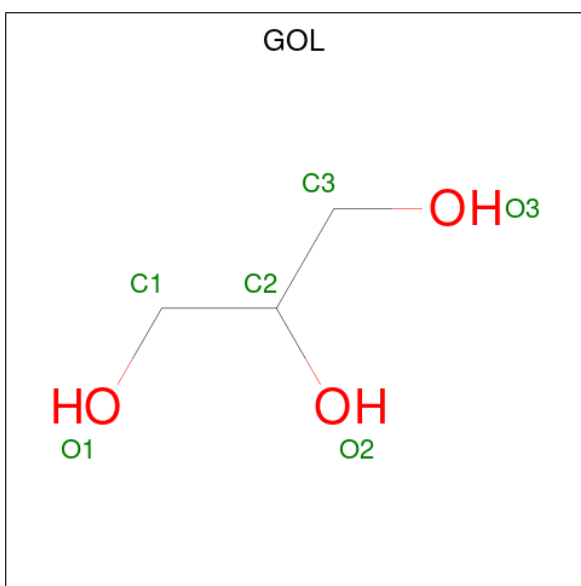


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

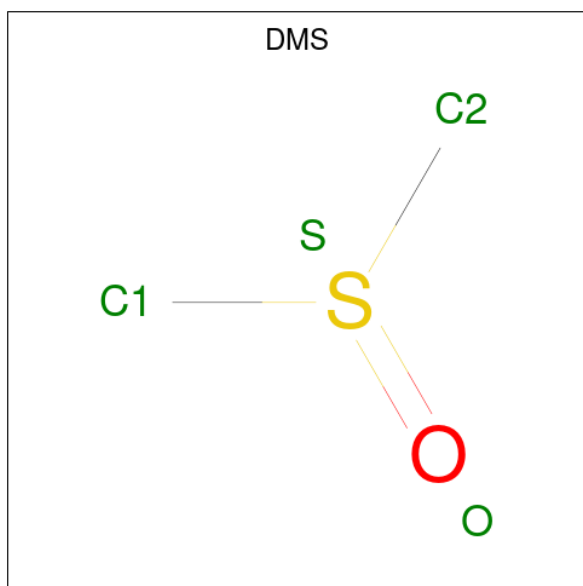
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	Cl	0	0
			5	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			4	2	1	1		

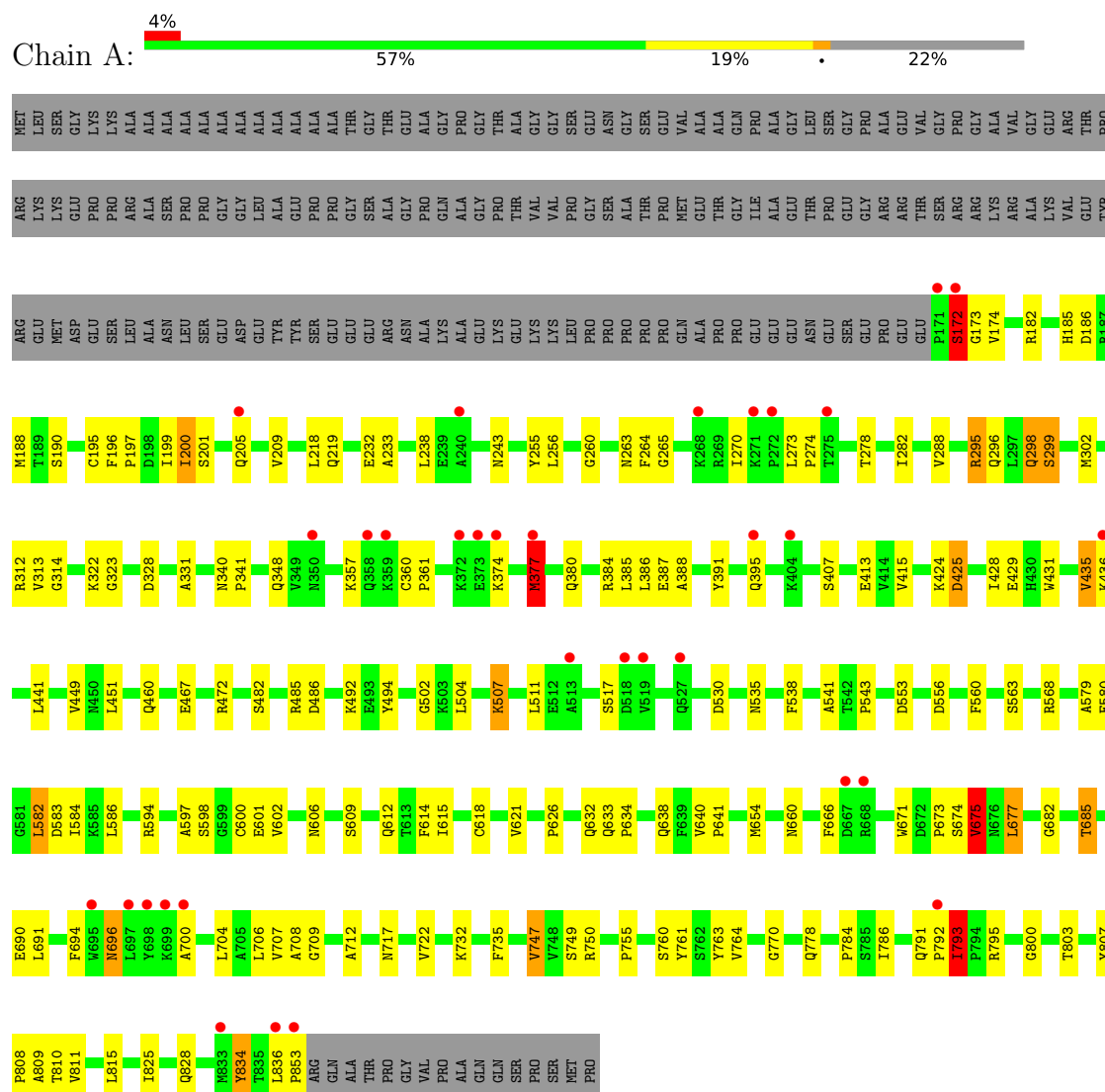
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	35	Total	O	0	0
			35	35		
9	B	1	Total	O	0	0
			1	1		

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	121.58Å 176.86Å 233.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.60 48.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.00-2.60) 99.5 (48.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.204 , 0.223 0.213 , 0.223	Depositor DCC
R_{free} test set	1478 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.4	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	0.96	EDS
Total number of atoms	6536	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: CL, GOL, NY8, PO4, DMS, 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	1.46	28/5339 (0.5%)	1.47	45/7244 (0.6%)
2	B	1.22	2/1102 (0.2%)	1.33	2/1486 (0.1%)
All	All	1.42	30/6441 (0.5%)	1.45	47/8730 (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	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	793	ILE	CA-C	9.55	1.62	1.52
1	A	597	ALA	C-O	-8.71	1.13	1.24
1	A	764	VAL	CA-C	-7.59	1.45	1.53
1	A	828	GLN	C-O	-7.21	1.15	1.24
1	A	586	LEU	C-O	-6.92	1.14	1.23
1	A	172	SER	CA-C	6.74	1.61	1.52
1	A	618	CYS	C-O	6.26	1.31	1.23
1	A	621	VAL	CA-C	6.16	1.60	1.52
1	A	263	ASN	C-O	6.16	1.30	1.23
1	A	314	GLY	N-CA	6.10	1.54	1.45
1	A	431	TRP	CA-C	6.02	1.60	1.52
1	A	472	ARG	CA-C	-5.82	1.45	1.52
1	A	600	CYS	C-O	5.69	1.30	1.23
1	A	582	LEU	C-O	-5.68	1.17	1.23
1	A	413	GLU	CD-OE2	5.68	1.36	1.25
2	B	375	VAL	CA-CB	5.65	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	795	ARG	CZ-NH2	-5.53	1.26	1.33
1	A	298	GLN	C-O	-5.50	1.17	1.24
1	A	708	ALA	C-O	-5.40	1.17	1.24
2	B	416	GLN	C-O	5.40	1.30	1.24
1	A	811	VAL	C-O	-5.32	1.17	1.24
1	A	825	ILE	C-O	-5.29	1.17	1.24
1	A	717	ASN	CA-C	5.28	1.61	1.52
1	A	172	SER	N-CA	5.24	1.52	1.46
1	A	791	GLN	C-O	5.15	1.31	1.24
1	A	763	TYR	N-CA	-5.05	1.40	1.46
1	A	288	VAL	N-CA	-5.04	1.40	1.46
1	A	348	GLN	C-O	-5.02	1.18	1.24
1	A	312	ARG	C-O	5.01	1.29	1.23
1	A	784	PRO	N-CA	5.00	1.52	1.47

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	GLN	CA-C-N	-14.55	105.15	119.85
1	A	791	GLN	C-N-CA	-14.55	105.15	119.85
1	A	360	CYS	CA-C-N	10.48	131.15	119.83
1	A	360	CYS	C-N-CA	10.48	131.15	119.83
1	A	313	VAL	N-CA-C	9.99	119.92	110.53
1	A	172	SER	N-CA-C	7.90	119.05	108.38
1	A	199	ILE	N-CA-C	7.78	117.84	110.53
1	A	299	SER	CA-CB-OG	7.56	126.22	111.10
1	A	328	ASP	N-CA-C	7.37	120.94	109.96
1	A	770	GLY	N-CA-C	-7.34	105.70	115.32
1	A	377	MET	N-CA-C	-6.70	103.08	111.11
1	A	677	LEU	N-CA-C	6.63	119.14	109.07
1	A	295	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	A	435	VAL	N-CA-CB	6.51	117.74	110.51
1	A	795	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	A	502	GLY	CA-C-N	6.44	129.15	120.65
1	A	502	GLY	C-N-CA	6.44	129.15	120.65
1	A	584	ILE	N-CA-C	6.43	117.18	108.17
1	A	195	CYS	N-CA-C	6.36	120.30	112.54
1	A	492	LYS	N-CA-C	-6.26	104.08	111.03
2	B	415	VAL	N-CA-C	-6.12	104.88	110.82
1	A	348	GLN	N-CA-C	6.02	117.64	111.14
1	A	791	GLN	N-CA-C	5.97	118.19	109.71
1	A	295	ARG	N-CA-C	-5.83	105.06	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ILE	N-CA-C	5.82	121.44	108.88
1	A	732	LYS	CA-CB-CG	5.80	125.71	114.10
1	A	717	ASN	N-CA-CB	-5.73	102.51	110.65
1	A	675	VAL	N-CA-C	5.63	115.97	107.75
1	A	700	ALA	CA-C-N	5.60	126.85	119.84
1	A	700	ALA	C-N-CA	5.60	126.85	119.84
1	A	377	MET	N-CA-CB	5.50	118.14	109.94
1	A	747	VAL	CB-CA-C	-5.49	102.04	110.50
1	A	786	ILE	CA-C-N	-5.48	114.32	119.85
1	A	786	ILE	C-N-CA	-5.48	114.32	119.85
1	A	460	GLN	N-CA-C	-5.39	105.32	111.14
1	A	361	PRO	CB-CA-C	-5.38	104.86	111.64
1	A	722	VAL	N-CA-C	5.37	116.00	110.36
1	A	201	SER	N-CA-C	-5.36	106.74	113.28
1	A	583	ASP	CA-C-N	-5.32	116.59	123.19
1	A	583	ASP	C-N-CA	-5.32	116.59	123.19
1	A	579	ALA	N-CA-C	5.27	119.34	113.01
1	A	696	ASN	CB-CA-C	5.26	118.84	109.38
2	B	382	ARG	N-CA-C	5.13	117.10	109.25
1	A	218	LEU	O-C-N	5.08	127.30	122.07
1	A	682	GLY	N-CA-C	-5.02	102.26	111.25
1	A	666	PHE	CA-C-N	5.02	129.17	121.19
1	A	666	PHE	C-N-CA	5.02	129.17	121.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	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	5224	0	5259	69	0
2	B	1086	0	1098	12	0
3	A	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	117	0	0	1	0
5	A	5	0	0	0	0
6	A	5	0	0	0	0
7	A	6	0	8	0	0
8	A	4	0	6	0	0
9	A	35	0	0	0	0
9	B	1	0	0	0	0
All	All	6536	0	6402	79	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 6.

All (79) 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:380:GLN:HE21	1:A:384:ARG:HD2	1.49	0.77
1:A:296:GLN:O	1:A:299:SER:HB3	2.01	0.60
1:A:205:GLN:O	1:A:209:VAL:HG23	2.02	0.59
1:A:331:ALA:HA	3:A:901:FAD:N5	2.18	0.59
1:A:808:PRO:O	1:A:810:THR:HG23	2.03	0.57
1:A:196:PHE:N	1:A:197:PRO:HD3	2.19	0.57
1:A:380:GLN:NE2	1:A:384:ARG:HD2	2.19	0.56
1:A:485:ARG:C	1:A:485:ARG:HD3	2.31	0.56
2:B:417:VAL:O	2:B:420:PHE:HB3	2.07	0.54
1:A:675:VAL:O	1:A:696:ASN:ND2	2.41	0.53
1:A:485:ARG:HD3	1:A:486:ASP:N	2.24	0.53
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.53
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.45	0.52
1:A:196:PHE:N	1:A:197:PRO:CD	2.74	0.51
2:B:423:ASN:O	2:B:426:ARG:NH1	2.44	0.50
2:B:317:SER:HB3	2:B:320:ASP:OD2	2.11	0.50
1:A:260:GLY:O	1:A:264:PHE:CD2	2.65	0.50
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.47	0.50
2:B:413:SER:OG	2:B:416:GLN:HG3	2.12	0.49
2:B:350:GLN:HA	2:B:350:GLN:OE1	2.13	0.49
2:B:424:TYR:O	2:B:425:ARG:C	2.54	0.49
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.93	0.48
1:A:671:TRP:O	1:A:673:PRO:HD3	2.13	0.48
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.49	0.48
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.95	0.47
1:A:800:GLY:O	1:A:803:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLY:O	1:A:295:ARG:HD3	2.14	0.47
1:A:807:TYR:N	1:A:808:PRO:CD	2.78	0.47
1:A:424:LYS:O	1:A:425:ASP:C	2.58	0.47
1:A:660:ASN:OD1	1:A:749:SER:OG	2.31	0.47
1:A:386:LEU:O	1:A:387:GLU:C	2.58	0.47
2:B:401:ASP:C	2:B:401:ASP:OD1	2.58	0.46
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.50	0.46
1:A:632:GLN:O	1:A:633:GLN:NE2	2.47	0.46
1:A:612:GLN:HG2	1:A:614:PHE:CE1	2.51	0.46
1:A:535:ASN:O	1:A:538:PHE:HB3	2.16	0.45
2:B:428:PHE:O	2:B:429:ASN:C	2.60	0.45
1:A:760:SER:HB2	3:A:901:FAD:C8M	2.47	0.44
1:A:606:ASN:HD22	1:A:609:SER:HB3	1.82	0.44
1:A:690:GLU:O	1:A:691:LEU:C	2.61	0.44
1:A:834:TYR:C	1:A:834:TYR:CD1	2.95	0.44
1:A:530:ASP:OD2	1:A:685:THR:OG1	2.36	0.44
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.53	0.44
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.98	0.44
1:A:385:LEU:CD2	1:A:415:VAL:HG12	2.48	0.44
1:A:232:GLU:O	1:A:233:ALA:C	2.61	0.44
1:A:836:LEU:HA	1:A:853:PRO:HD2	1.93	0.44
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.48	0.43
1:A:435:VAL:HG23	1:A:436:LYS:N	2.33	0.43
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.53	0.43
1:A:188:MET:SD	1:A:200:ILE:HG13	2.58	0.43
1:A:278:THR:O	1:A:302:MET:HA	2.18	0.43
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.84	0.43
1:A:553:ASP:HB2	1:A:556:ASP:OD2	2.19	0.43
1:A:538:PHE:CE2	4:A:902:NY8:CAJ	3.01	0.43
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.01	0.43
1:A:594:ARG:HA	1:A:640:VAL:O	2.19	0.42
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.19	0.42
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.55	0.42
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.34	0.42
1:A:238:LEU:O	1:A:243:ASN:ND2	2.53	0.42
1:A:750:ARG:HH11	1:A:750:ARG:HG3	1.84	0.42
1:A:298:GLN:O	1:A:299:SER:C	2.62	0.41
1:A:172:SER:OG	1:A:173:GLY:N	2.54	0.41
1:A:385:LEU:HD23	1:A:415:VAL:CG1	2.51	0.41
1:A:654:MET:HB3	1:A:654:MET:HE2	1.72	0.41
1:A:594:ARG:HB2	1:A:601:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:NZ	1:A:377:MET:HE2	2.35	0.41
1:A:507:LYS:O	1:A:511:LEU:HG	2.20	0.41
1:A:633:GLN:HA	1:A:634:PRO:HA	1.94	0.41
1:A:273:LEU:O	1:A:274:PRO:C	2.64	0.41
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.51	0.40
2:B:325:SER:O	2:B:327:ASN:N	2.51	0.40
1:A:594:ARG:HD2	1:A:601:GLU:HG3	2.02	0.40
1:A:640:VAL:HA	1:A:641:PRO:HA	1.92	0.40
1:A:694:PHE:HA	1:A:704:LEU:O	2.21	0.40
1:A:322:LYS:O	1:A:323:GLY:C	2.64	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.99	0.40
2:B:379:CYS:HB3	2:B:416:GLN:NE2	2.37	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	665/853 (78%)	599 (90%)	58 (9%)	8 (1%)	10	23
2	B	132/485 (27%)	116 (88%)	10 (8%)	6 (4%)	2	2
All	All	797/1338 (60%)	715 (90%)	68 (8%)	14 (2%)	6	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	ILE
2	B	401	ASP
2	B	429	ASN
2	B	326	ALA
1	A	428	ILE
1	A	429	GLU

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Mol	Chain	Res	Type
1	A	507	LYS
1	A	834	TYR
2	B	379	CYS
1	A	541	ALA
2	B	369	PRO
1	A	425	ASP
1	A	709	GLY
2	B	375	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	567/700 (81%)	538 (95%)	29 (5%)	21	45
2	B	118/397 (30%)	112 (95%)	6 (5%)	21	45
All	All	685/1097 (62%)	650 (95%)	35 (5%)	21	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	190	SER
1	A	200	ILE
1	A	270	ILE
1	A	357	LYS
1	A	377	MET
1	A	407	SER
1	A	449	VAL
1	A	467	GLU
1	A	482	SER
1	A	517	SER
1	A	543	PRO
1	A	563	SER
1	A	568	ARG
1	A	580	GLU

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Mol	Chain	Res	Type
1	A	582	LEU
1	A	598	SER
1	A	615	ILE
1	A	626	PRO
1	A	638	GLN
1	A	674	SER
1	A	675	VAL
1	A	677	LEU
1	A	685	THR
1	A	747	VAL
1	A	755	PRO
1	A	778	GLN
1	A	793	ILE
1	A	815	LEU
2	B	317	SER
2	B	327	ASN
2	B	332	THR
2	B	357	SER
2	B	406	SER
2	B	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	259	HIS
1	A	298	GLN
1	A	358	GLN
1	A	380	GLN
1	A	395	GLN
1	A	410	GLN
1	A	551	HIS
1	A	680	HIS
1	A	771	ASN
1	A	806	ASN
2	B	388	GLN
2	B	416	GLN
2	B	419	ASN

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 ⓘ

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	NY8	A	902	-	42,43,43	1.98	12 (28%)	58,59,59	2.53	21 (36%)
7	GOL	A	911	-	5,5,5	1.24	0	5,5,5	1.06	1 (20%)
3	FAD	A	901	-	58,58,58	1.74	13 (22%)	85,89,89	1.80	22 (25%)
5	PO4	A	905	-	4,4,4	0.67	0	6,6,6	1.20	1 (16%)
8	DMS	A	912	-	3,3,3	0.95	0	3,3,3	2.31	1 (33%)
4	NY8	A	904	-	42,43,43	1.73	9 (21%)	58,59,59	3.40	25 (43%)
4	NY8	A	903	-	42,43,43	1.75	10 (23%)	58,59,59	2.43	22 (37%)

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	NY8	A	902	-	-	8/19/41/41	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	911	-	-	4/4/4/4	-
3	FAD	A	901	-	-	3/34/50/50	0/6/6/6
4	NY8	A	904	-	-	11/19/41/41	0/5/5/5
4	NY8	A	903	-	-	5/19/41/41	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	FAD	PA-O3P	5.87	1.65	1.59
4	A	902	NY8	C6-C5	-5.63	1.37	1.44
4	A	904	NY8	CAU-CBB	-4.52	1.43	1.51
4	A	902	NY8	CAP-CAS	4.35	1.64	1.52
4	A	902	NY8	CAU-CBB	-4.27	1.43	1.51
4	A	903	NY8	CAL-CBD	4.13	1.44	1.36
4	A	904	NY8	CAL-CBD	3.99	1.43	1.36
4	A	903	NY8	CAU-CBB	-3.85	1.44	1.51
3	A	901	FAD	C5X-N5	-3.83	1.32	1.39
3	A	901	FAD	C5A-C4A	3.73	1.45	1.39
4	A	902	NY8	CAM-CBE	3.73	1.43	1.36
3	A	901	FAD	C9A-C5X	3.47	1.46	1.41
4	A	903	NY8	CAO-NAX	3.43	1.52	1.45
3	A	901	FAD	C8A-N7A	3.12	1.37	1.31
4	A	903	NY8	OAZ-CAA	3.05	1.51	1.42
3	A	901	FAD	C6-C7	-2.98	1.35	1.39
3	A	901	FAD	C8-C7	2.95	1.48	1.40
3	A	901	FAD	C4-N3	-2.94	1.33	1.38
3	A	901	FAD	C4A-N9A	-2.88	1.31	1.37
4	A	904	NY8	CAO-NAX	2.83	1.51	1.45
4	A	902	NY8	CAI-CBH	-2.79	1.35	1.42
4	A	903	NY8	CAK-CBB	2.79	1.43	1.37
4	A	903	NY8	CAF-CAI	2.73	1.42	1.36
4	A	903	NY8	OAZ-CBD	2.72	1.41	1.37
4	A	904	NY8	C6-N1	2.57	1.36	1.33
3	A	901	FAD	C2-N3	-2.55	1.33	1.39
4	A	902	NY8	CAQ-CAT	2.55	1.59	1.52
4	A	902	NY8	CAL-C4	-2.54	1.38	1.41
4	A	904	NY8	CAG-CBB	2.51	1.43	1.38
4	A	902	NY8	CAO-NAX	2.51	1.50	1.45
4	A	904	NY8	OBA-CBE	2.48	1.41	1.37
4	A	902	NY8	CAJ-CBG	-2.48	1.36	1.42
3	A	901	FAD	C5A-C6A	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	NY8	C6-C5	-2.38	1.41	1.44
3	A	901	FAD	C6-C5X	-2.34	1.36	1.40
4	A	902	NY8	CAQ-CBK	-2.30	1.46	1.52
4	A	902	NY8	CAU-NBM	2.20	1.51	1.47
3	A	901	FAD	C2A-N1A	2.17	1.37	1.33
4	A	904	NY8	OAZ-CBD	2.14	1.40	1.37
4	A	904	NY8	CAJ-CAG	2.12	1.41	1.36
4	A	903	NY8	CAJ-CAG	2.09	1.41	1.36
4	A	904	NY8	CAK-CBB	2.03	1.42	1.37
4	A	902	NY8	CAK-CBB	2.03	1.42	1.37
4	A	903	NY8	OBA-CBE	2.01	1.40	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	NY8	CAB-OBA-CBE	11.11	133.81	117.51
4	A	904	NY8	OBA-CBE-CAM	-7.98	115.05	125.16
4	A	904	NY8	CAA-OAZ-CBD	7.81	128.98	117.51
4	A	904	NY8	OBA-CBE-CBD	7.76	125.93	115.40
4	A	904	NY8	C6-C5-C4	7.53	120.31	115.86
4	A	903	NY8	C6-C5-C4	6.92	119.95	115.86
4	A	902	NY8	CBB-CAU-NBM	-6.33	100.20	113.15
4	A	904	NY8	C5-C4-N3	-6.17	116.27	122.80
4	A	903	NY8	NAX-C2-N3	5.68	126.95	117.16
4	A	902	NY8	C6-NAY-CBK	5.51	133.72	124.06
4	A	902	NY8	CAH-CBG-CBH	5.46	128.27	118.91
4	A	902	NY8	CAU-NBM-CAS	5.43	122.75	111.07
4	A	903	NY8	CAB-OBA-CBE	5.39	125.42	117.51
4	A	903	NY8	CAM-C5-C6	-5.12	120.68	124.84
4	A	904	NY8	C2-N3-C4	4.84	123.21	115.54
4	A	903	NY8	N3-C2-N1	-4.79	118.41	126.25
3	A	901	FAD	C5A-C4A-N3A	-4.69	120.27	126.72
4	A	904	NY8	NAX-C2-N3	4.63	125.14	117.16
3	A	901	FAD	C5'-C4'-C3'	-4.60	103.54	112.22
4	A	904	NY8	CAL-C4-N3	4.59	125.50	118.78
4	A	903	NY8	C5-C4-N3	-4.58	117.95	122.80
4	A	904	NY8	C6-NAY-CBK	4.55	132.03	124.06
3	A	901	FAD	N3A-C2A-N1A	-4.53	121.72	128.58
4	A	902	NY8	CAE-CAH-CBG	-4.50	114.23	120.48
4	A	904	NY8	N3-C2-N1	-4.42	119.01	126.25
4	A	902	NY8	CAC-NBL-CAR	-4.33	93.58	110.75
4	A	904	NY8	CAP-CBK-NAY	-4.08	104.20	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	NY8	CAQ-CBK-NAY	3.92	117.09	110.77
3	A	901	FAD	N3A-C4A-N9A	3.81	133.64	127.17
4	A	903	NY8	C2-N3-C4	3.71	121.43	115.54
4	A	902	NY8	CAU-CBB-CAG	-3.67	113.98	120.75
4	A	902	NY8	CAJ-CBG-CAH	-3.65	114.69	123.01
8	A	912	DMS	O-S-C1	3.63	124.67	106.49
3	A	901	FAD	C2A-N3A-C4A	3.62	120.68	111.83
4	A	902	NY8	CAK-CBH-CBG	3.60	123.95	118.96
4	A	902	NY8	OAZ-CBD-CAL	-3.59	120.61	125.16
3	A	901	FAD	O2P-P-O3P	-3.59	97.57	107.27
4	A	904	NY8	CAL-CBD-CBE	-3.58	116.67	120.06
3	A	901	FAD	O4-C4-C4X	-3.54	117.19	126.53
4	A	902	NY8	CAQ-CBK-NAY	3.45	116.33	110.77
4	A	902	NY8	N3-C2-N1	-3.44	120.62	126.25
4	A	902	NY8	CAD-NBL-CAC	3.39	118.41	109.72
4	A	903	NY8	C2-N1-C6	3.39	124.69	116.36
4	A	902	NY8	CAE-CAF-CAI	3.36	124.89	120.40
4	A	903	NY8	CAU-NBM-CAT	-3.35	103.87	111.07
4	A	902	NY8	CAU-CBB-CAK	3.31	129.14	121.43
4	A	903	NY8	CBB-CAU-NBM	3.20	119.69	113.15
4	A	902	NY8	CAD-NBL-CAR	-3.15	98.24	110.75
3	A	901	FAD	O5'-P-O1P	-3.15	96.44	108.94
4	A	904	NY8	CAS-CAP-CBK	-3.13	105.73	110.67
3	A	901	FAD	O2P-P-O1P	3.12	126.95	112.44
4	A	904	NY8	CBE-CAM-C5	3.10	125.93	120.59
4	A	903	NY8	CAL-C4-N3	3.07	123.28	118.78
4	A	902	NY8	OAZ-CBD-CBE	3.07	119.56	115.40
4	A	903	NY8	C5-C6-N1	-3.04	117.51	122.07
4	A	902	NY8	NAX-C2-N3	2.88	122.12	117.16
4	A	903	NY8	CAA-OAZ-CBD	2.73	121.52	117.51
4	A	904	NY8	CAM-C5-C6	-2.72	122.62	124.84
4	A	902	NY8	C2-N1-C6	2.69	122.97	116.36
3	A	901	FAD	C4X-C10-N1	-2.67	118.05	124.59
4	A	903	NY8	CAP-CBK-CAQ	2.64	115.37	110.80
3	A	901	FAD	O4B-C1B-C2B	-2.59	101.07	106.62
3	A	901	FAD	O2B-C2B-C3B	2.59	120.11	111.82
4	A	903	NY8	CAN-CAR-NBL	-2.51	107.22	113.71
4	A	903	NY8	CAO-NAX-C2	-2.48	119.53	123.82
5	A	905	PO4	O4-P-O2	2.47	115.61	107.91
4	A	904	NY8	CAF-CAE-CAH	2.47	123.71	120.40
4	A	903	NY8	CAN-CAO-NAX	2.42	118.02	111.46
4	A	904	NY8	CBD-CAL-C4	2.42	123.10	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	NY8	OAZ-CBD-CAL	2.40	128.19	125.16
3	A	901	FAD	O3'-C3'-C2'	2.40	114.38	108.93
3	A	901	FAD	N10-C10-N1	2.38	125.52	118.51
3	A	901	FAD	C4A-N9A-C8A	2.36	108.21	105.74
4	A	902	NY8	CAS-CAP-CBK	-2.36	106.95	110.67
4	A	904	NY8	CAC-NBL-CAR	2.34	120.02	110.75
4	A	903	NY8	CAT-CAQ-CBK	2.31	114.32	110.67
4	A	903	NY8	CAP-CBK-NAY	-2.30	107.07	110.77
4	A	902	NY8	CAI-CBH-CBG	-2.25	115.05	118.91
4	A	903	NY8	OBA-CBE-CBD	2.23	118.43	115.40
3	A	901	FAD	C2A-N1A-C6A	2.23	122.39	118.73
4	A	904	NY8	CAT-CAQ-CBK	-2.22	107.17	110.67
4	A	903	NY8	CAS-NBM-CAT	2.21	113.59	108.84
4	A	904	NY8	C2-N1-C6	2.16	121.66	116.36
3	A	901	FAD	C4X-C4-N3	2.14	118.71	113.25
3	A	901	FAD	C4'-C3'-C2'	-2.13	110.03	113.57
4	A	904	NY8	CAE-CAH-CBG	-2.11	117.56	120.48
4	A	903	NY8	OBA-CBE-CAM	-2.11	122.49	125.16
3	A	901	FAD	O4-C4-N3	2.10	124.06	120.11
3	A	901	FAD	C1'-C2'-C3'	-2.10	103.97	109.66
3	A	901	FAD	O4B-C4B-C5B	-2.09	102.65	109.33
4	A	904	NY8	NAY-C6-N1	2.08	122.53	118.56
3	A	901	FAD	C6-C5X-C9A	2.06	121.87	119.05
7	A	911	GOL	C3-C2-C1	2.02	119.21	111.80

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NY8	C5-C6-NAY-CBK
4	A	902	NY8	N1-C6-NAY-CBK
4	A	902	NY8	CAQ-CBK-NAY-C6
4	A	902	NY8	CBB-CAU-NBM-CAS
4	A	904	NY8	C5-C6-NAY-CBK
4	A	904	NY8	N1-C6-NAY-CBK
4	A	904	NY8	N1-C2-NAX-CAO
4	A	904	NY8	N3-C2-NAX-CAO
4	A	904	NY8	CAQ-CBK-NAY-C6
7	A	911	GOL	C1-C2-C3-O3
4	A	902	NY8	CBB-CAU-NBM-CAT
4	A	904	NY8	CAM-CBE-OBA-CAB
4	A	904	NY8	CBD-CBE-OBA-CAB

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Mol	Chain	Res	Type	Atoms
4	A	903	NY8	CBB-CAU-NBM-CAS
4	A	904	NY8	CAN-CAR-NBL-CAC
4	A	904	NY8	CAN-CAR-NBL-CAD
4	A	903	NY8	CAL-CBD-OAZ-CAA
7	A	911	GOL	O1-C1-C2-C3
4	A	903	NY8	CBE-CBD-OAZ-CAA
7	A	911	GOL	O2-C2-C3-O3
4	A	904	NY8	CBE-CBD-OAZ-CAA
4	A	903	NY8	CBB-CAU-NBM-CAT
4	A	902	NY8	CBE-CBD-OAZ-CAA
4	A	904	NY8	CAL-CBD-OAZ-CAA
3	A	901	FAD	C2'-C3'-C4'-C5'
3	A	901	FAD	C2'-C3'-C4'-O4'
4	A	903	NY8	CAO-CAN-CAR-NBL
4	A	902	NY8	CAL-CBD-OAZ-CAA
7	A	911	GOL	O1-C1-C2-O2
4	A	902	NY8	CAO-CAN-CAR-NBL
3	A	901	FAD	C2B-C1B-N9A-C8A

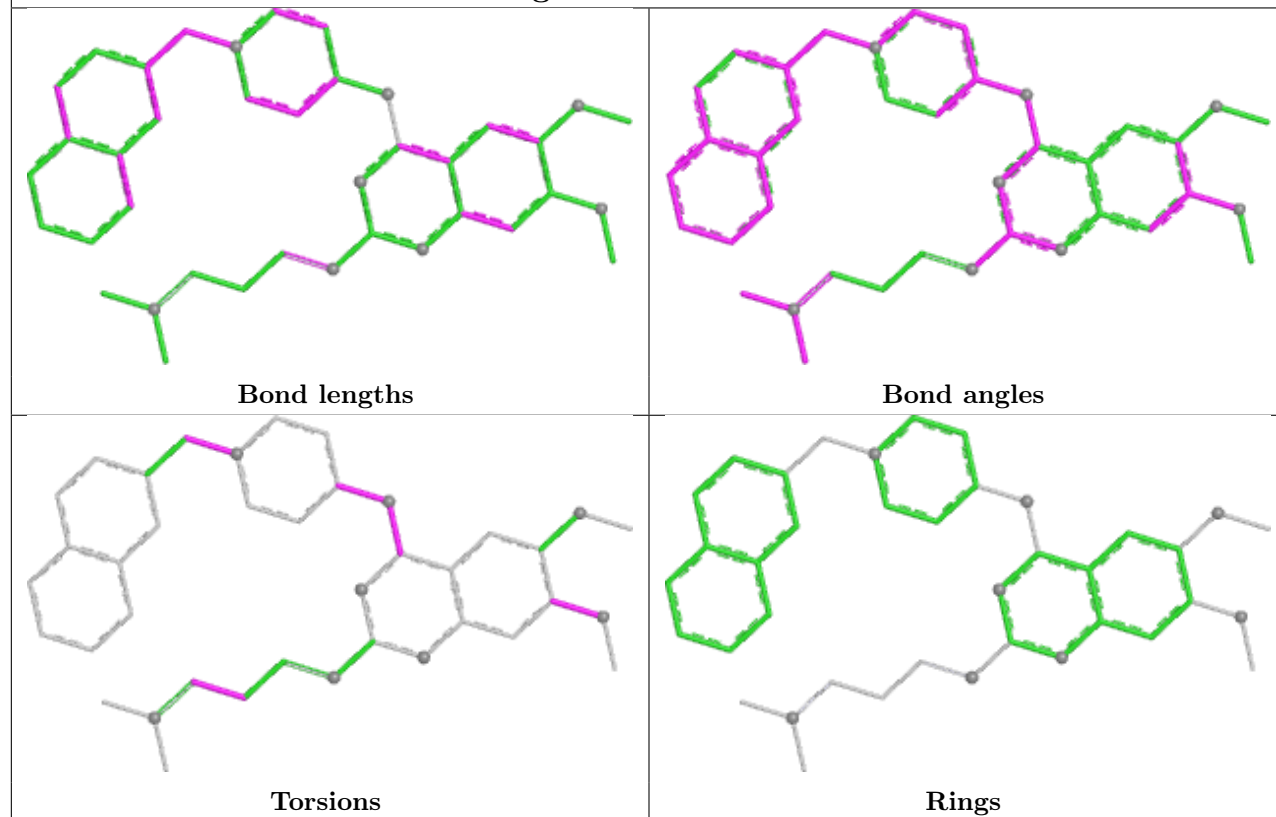
There are no ring outliers.

2 monomers are involved in 4 short contacts:

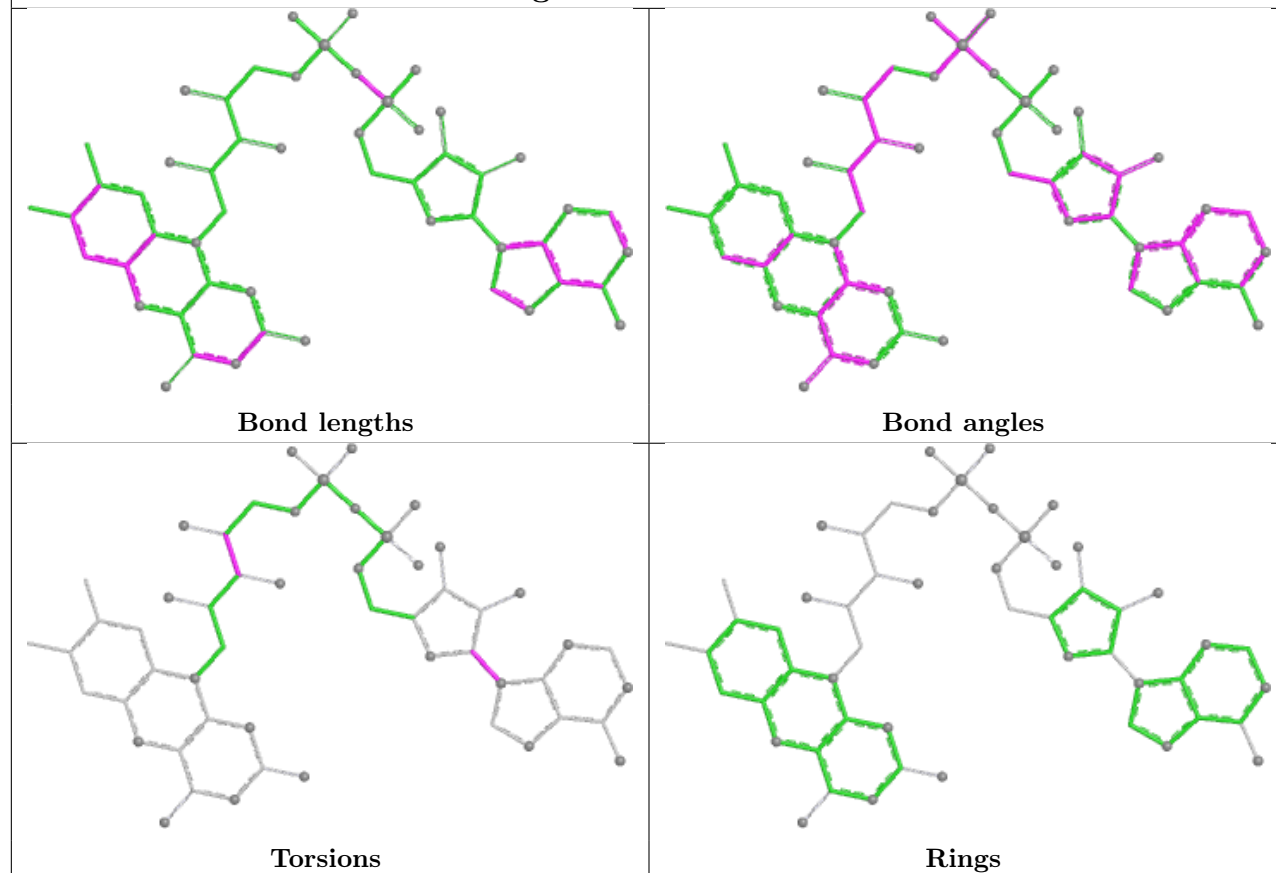
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	NY8	1	0
3	A	901	FAD	3	0

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.

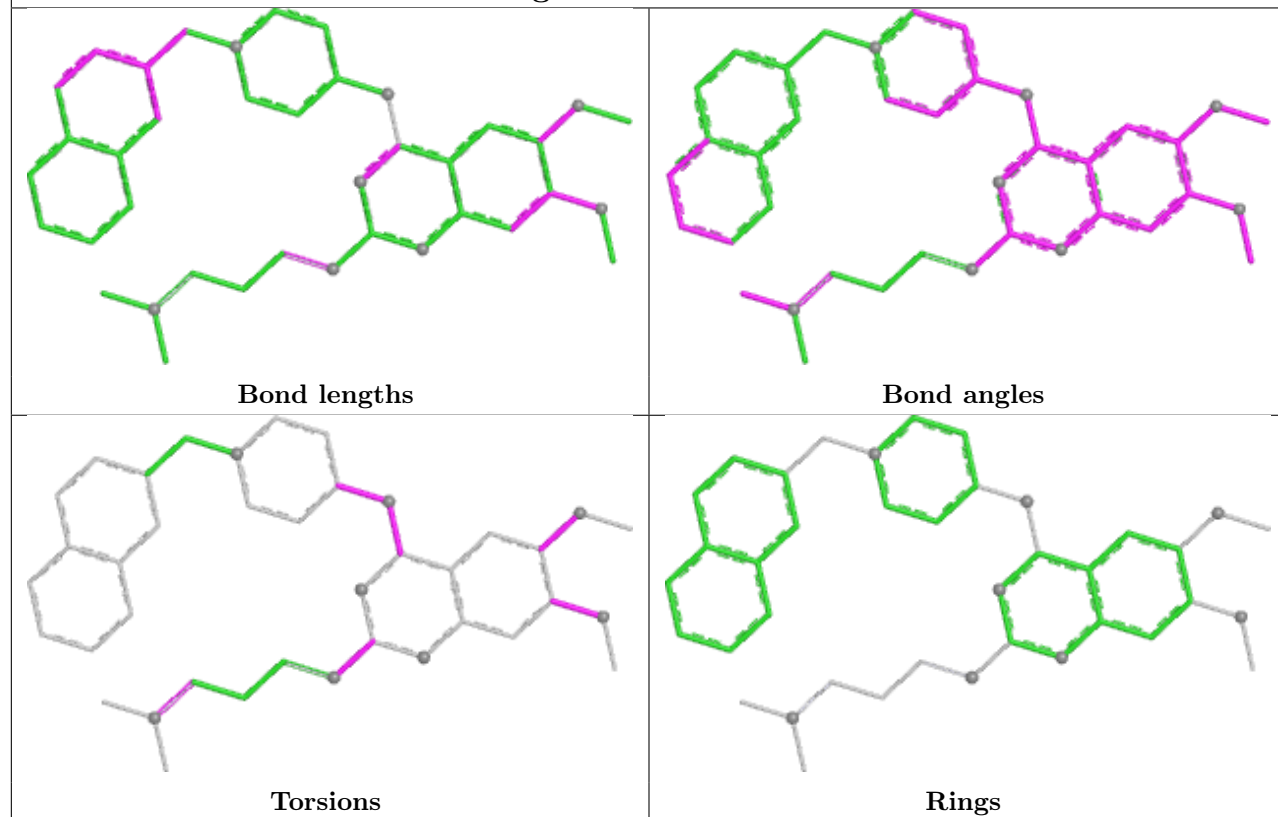
Ligand NY8 A 902



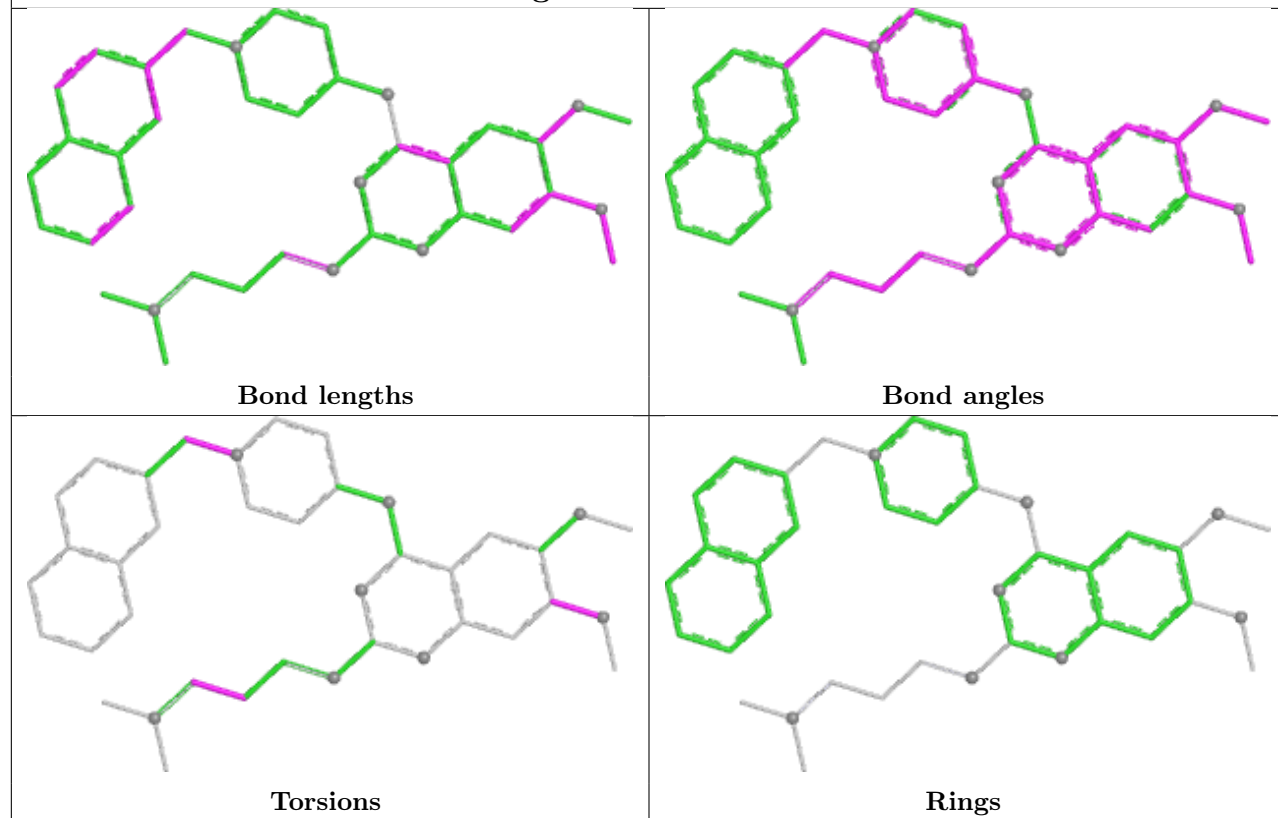
Ligand FAD A 901



Ligand NY8 A 904



Ligand NY8 A 903



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	667/853 (78%)	0.04	33 (4%) 35 29	43, 74, 112, 147	0
2	B	134/485 (27%)	0.75	15 (11%) 10 8	71, 105, 132, 161	0
All	All	801/1338 (59%)	0.15	48 (5%) 27 22	43, 79, 122, 161	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	375	VAL	7.6
1	A	853	PRO	7.1
2	B	376	ILE	5.8
1	A	171	PRO	5.7
1	A	519	VAL	4.8
1	A	699	LYS	4.6
1	A	833	MET	4.3
1	A	668	ARG	4.2
1	A	667	ASP	3.9
2	B	308	ARG	3.8
2	B	309	LYS	3.8
1	A	359	LYS	3.5
2	B	426	ARG	3.4
2	B	312	LYS	3.2
1	A	275	THR	3.1
1	A	836	LEU	3.1
1	A	372	LYS	3.1
1	A	172	SER	2.9
1	A	350	ASN	2.9
1	A	377	MET	2.9
1	A	358	GLN	2.9
1	A	271	LYS	2.8
1	A	374	LYS	2.8
2	B	381	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	441	HIS	2.8
1	A	697	LEU	2.7
2	B	374	GLU	2.6
1	A	240	ALA	2.6
1	A	436	LYS	2.5
1	A	700	ALA	2.5
1	A	698	TYR	2.4
1	A	395	GLN	2.4
1	A	373	GLU	2.3
2	B	382	ARG	2.3
1	A	527	GLN	2.3
1	A	695	TRP	2.3
1	A	513	ALA	2.3
2	B	340	MET	2.3
1	A	792	PRO	2.2
1	A	518	ASP	2.2
1	A	205	GLN	2.2
2	B	313	GLY	2.2
2	B	329	THR	2.1
2	B	427	ARG	2.1
1	A	272	PRO	2.1
1	A	268	LYS	2.1
1	A	404	LYS	2.1
2	B	318	GLN	2.1

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](#)

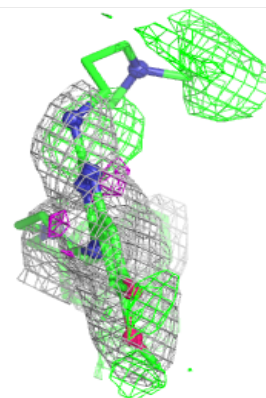
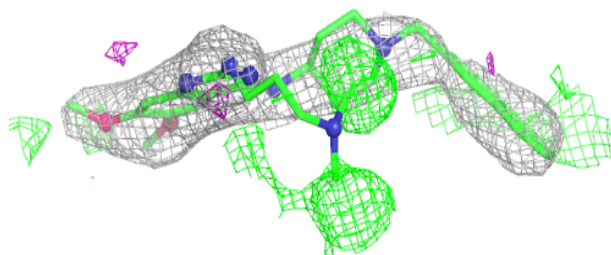
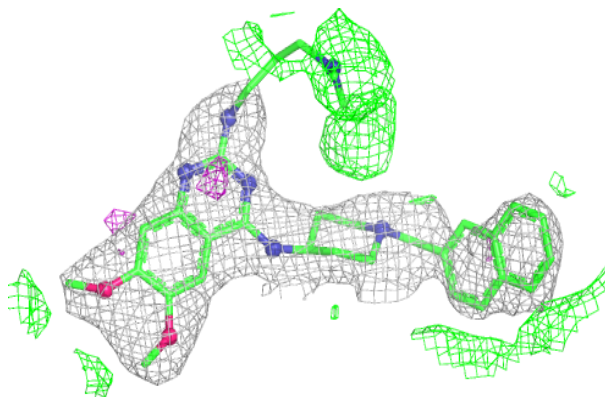
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NY8	A	904	39/39	0.86	0.32	86,133,164,174	0
7	GOL	A	911	6/6	0.86	0.21	79,96,97,104	0
5	PO4	A	905	5/5	0.88	0.12	85,93,103,109	0
6	CL	A	910	1/1	0.89	0.17	87,87,87,87	0
6	CL	A	907	1/1	0.91	0.24	86,86,86,86	0
4	NY8	A	903	39/39	0.93	0.18	76,94,117,122	0
8	DMS	A	912	4/4	0.94	0.17	70,77,81,82	0
6	CL	A	908	1/1	0.96	0.15	89,89,89,89	0
6	CL	A	906	1/1	0.96	0.08	80,80,80,80	0
4	NY8	A	902	39/39	0.97	0.10	46,79,101,123	0
6	CL	A	909	1/1	0.98	0.09	78,78,78,78	0
3	FAD	A	901	53/53	0.98	0.06	37,52,70,79	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.

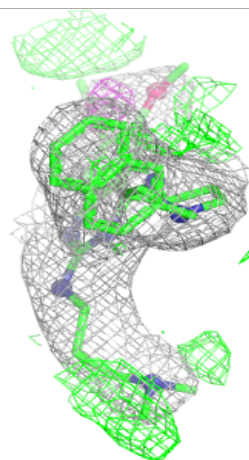
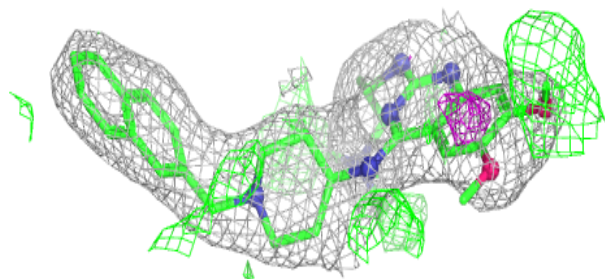
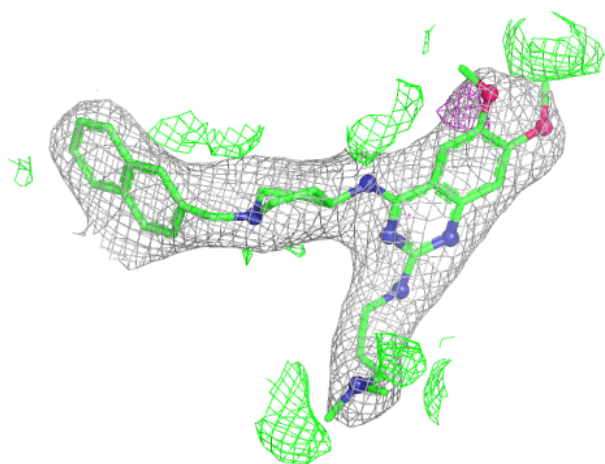
Electron density around NY8 A 904:

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



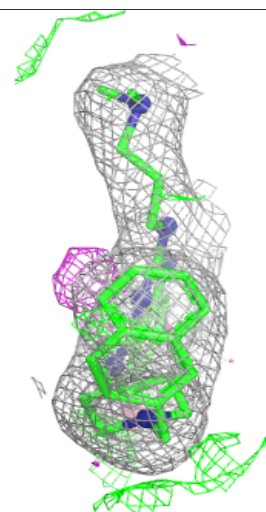
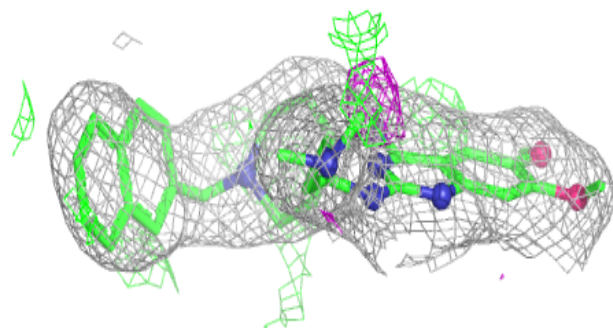
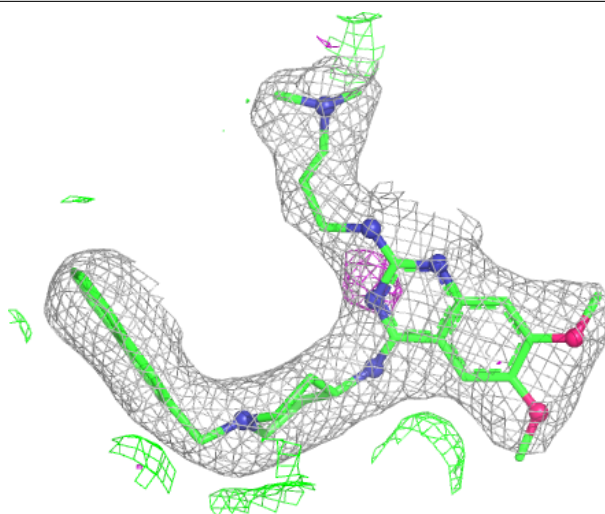
Electron density around NY8 A 903:

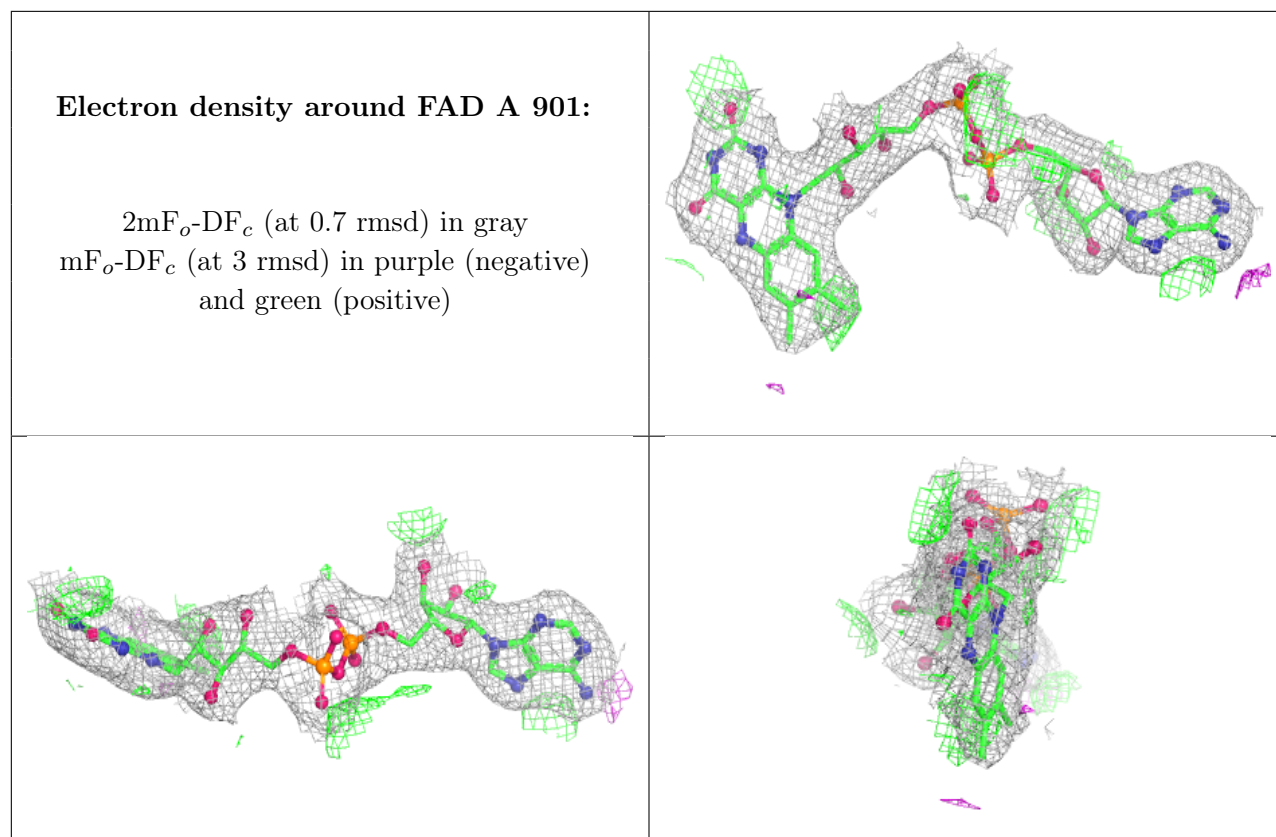
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NY8 A 902:

$2mF_o-DF_c$ (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.