



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:39 pm BST

PDB ID : 4ZOH
Title : Crystal structure of glyceraldehyde oxidoreductase
Authors : Nishimasu, H.; Fushinobu, S.; Wakagi, T.
Deposited on : 2015-05-06
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

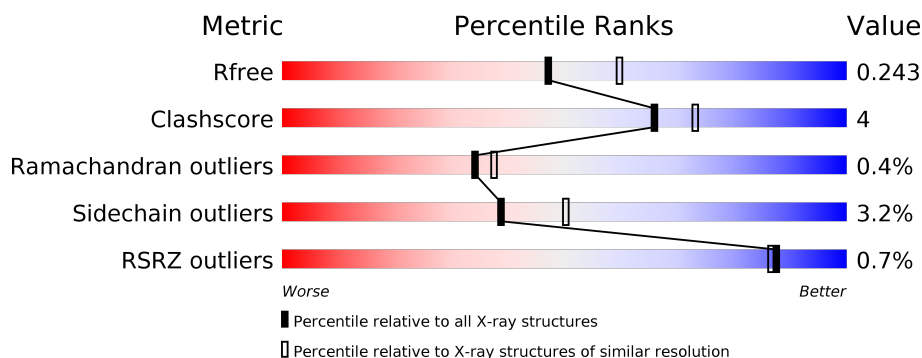
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	706	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 9% .. </div> </div>
2	B	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 10% .. </div> </div>
3	C	168	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 80%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 15% . . </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PEG	B	302	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 9598 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 Putative oxidoreductase molybdopterin-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5452	3502	902	1040	8			

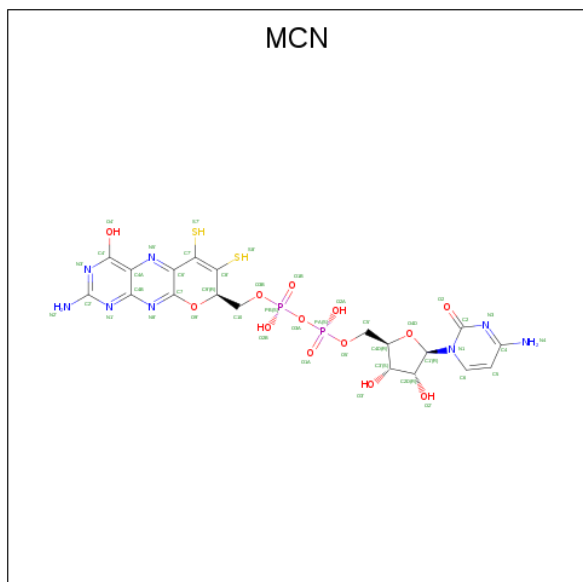
- Molecule 2 is a protein called Putative oxidoreductase FAD-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2122	1351	366	398	7			

- Molecule 3 is a protein called Putative oxidoreductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	161	Total	C	N	O	S	0	0	0
			1236	775	214	235	12			

- Molecule 4 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

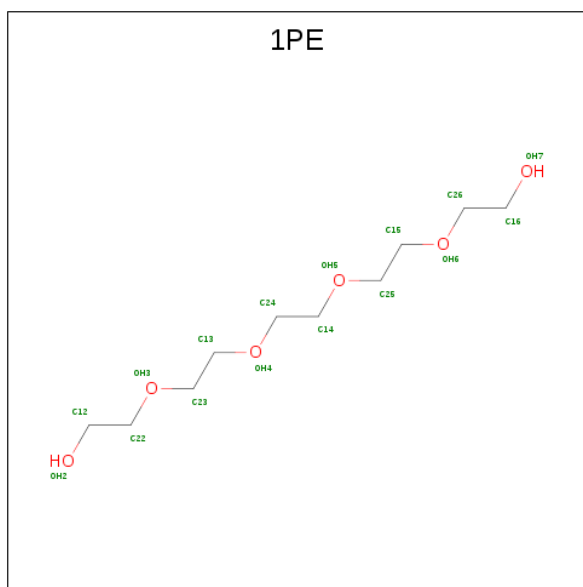


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			44	19	8	13	2	2	
									0
									0

- Molecule 5 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

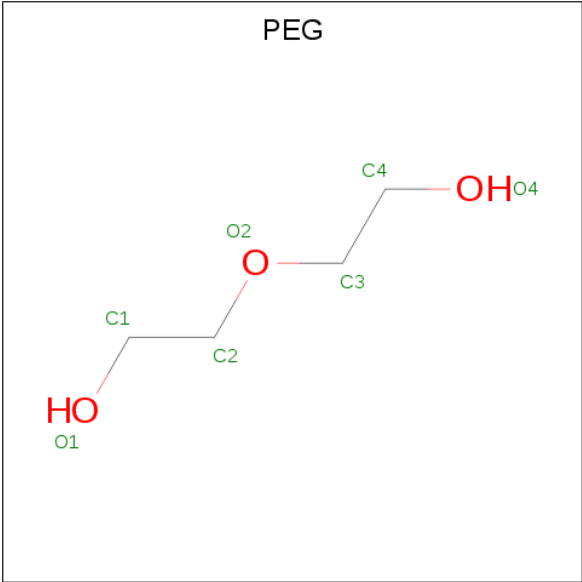
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo		
			1	1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



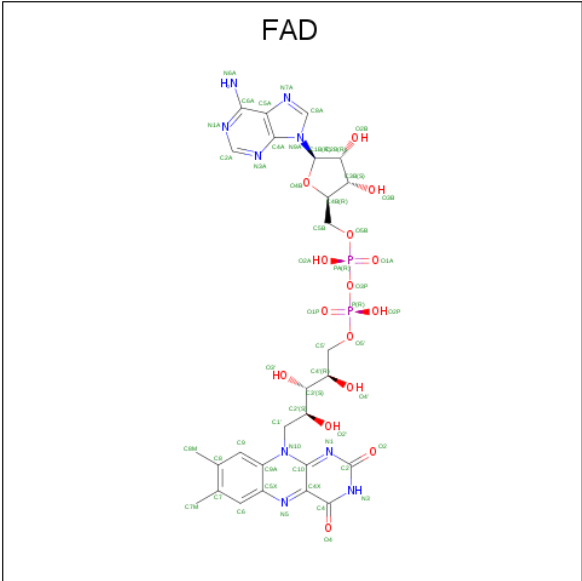
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O		
			16	10	6	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



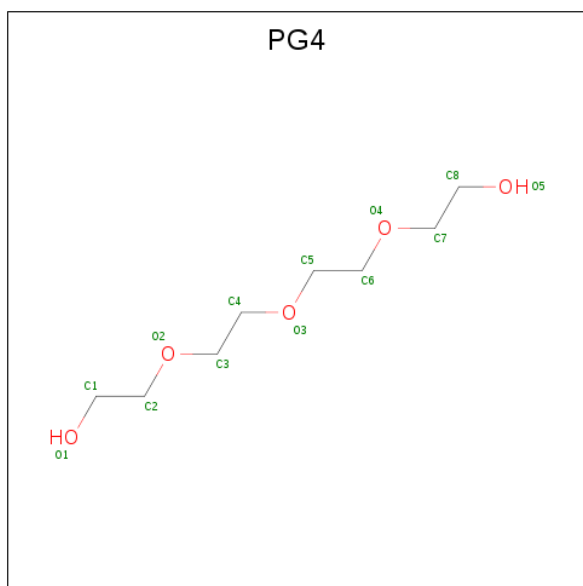
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



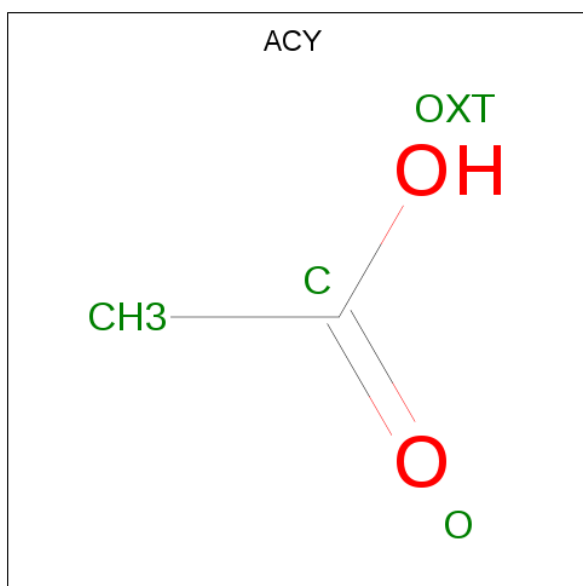
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	
			53	27	9	15	2	

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



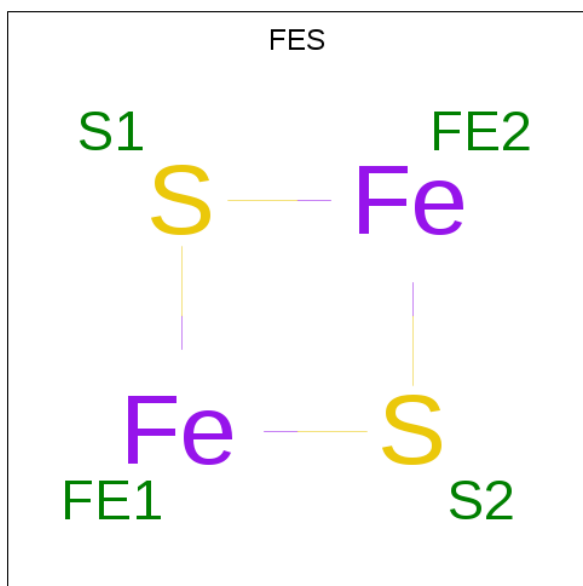
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O		
			13	8	5	0	0

- Molecule 10 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	Fe	S	0	0
			4	2	2		
11	C	1	Total	Fe	S	0	0
			4	2	2		

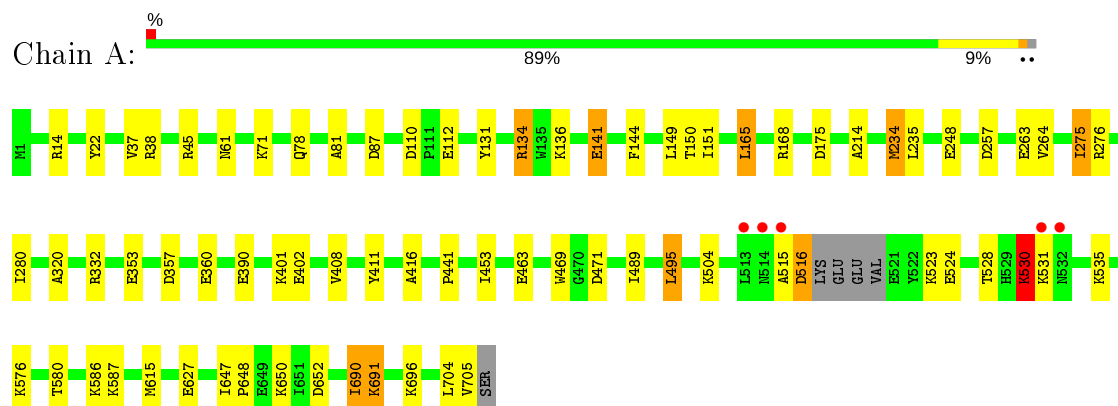
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	396	Total	O	0	0
			396	396		
12	B	126	Total	O	0	0
			126	126		
12	C	99	Total	O	0	0
			99	99		

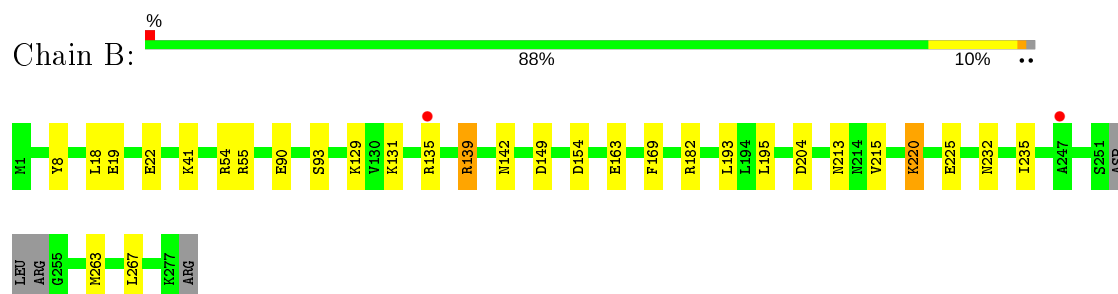
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

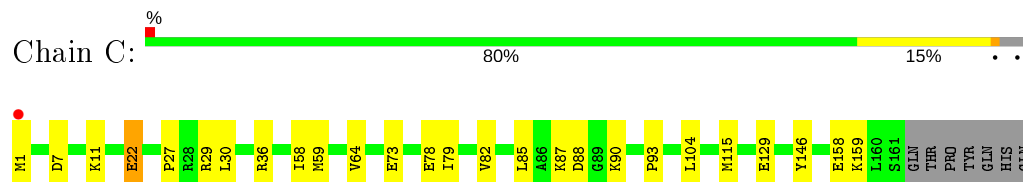
- Molecule 1: Putative oxidoreductase molybdopterin-binding subunit



- Molecule 2: Putative oxidoreductase FAD-binding subunit



- Molecule 3: Putative oxidoreductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	143.43 Å 143.43 Å 235.51 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.40 – 2.20 41.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.40-2.20) 99.9 (41.40-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.51 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.177 , 0.242 0.177 , 0.243	Depositor DCC
R_{free} test set	3679 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9598	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: MCN, MO, 1PE, PG4, FES, ACY, PEG, 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	1.04	3/5561 (0.1%)	1.00	15/7535 (0.2%)
2	B	0.85	0/2157	0.95	4/2911 (0.1%)
3	C	0.99	0/1254	1.06	4/1691 (0.2%)
All	All	0.99	3/8972 (0.0%)	1.00	23/12137 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	TYR	CE1-CZ	7.71	1.48	1.38
1	A	248	GLU	CD-OE2	5.30	1.31	1.25
1	A	411	TYR	CG-CD2	5.08	1.45	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	LEU	CB-CG-CD1	-8.41	96.70	111.00
3	C	29	ARG	NE-CZ-NH2	-8.06	116.27	120.30
3	C	36	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	B	149	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	14	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	C	36	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	257	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	691	LYS	N-CA-C	-6.33	93.92	111.00
2	B	204	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	45	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	276	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	690	ILE	N-CA-C	6.02	127.24	111.00
1	A	471	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	275	ILE	CB-CA-C	-5.93	99.73	111.60
1	A	165	LEU	CB-CG-CD2	5.84	120.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	175	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	87	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	182	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	168	ARG	NE-CZ-NH1	-5.23	117.69	120.30
2	B	267	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	495	LEU	CA-CB-CG	5.15	127.14	115.30
3	C	7	ASP	CB-CG-OD2	5.12	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5452	0	5516	41	0
2	B	2122	0	2194	20	0
3	C	1236	0	1250	15	0
4	A	44	0	17	1	0
5	A	1	0	0	0	0
6	A	16	0	22	1	0
7	A	7	0	10	0	0
7	B	14	0	20	4	0
7	C	7	0	10	1	0
8	B	53	0	31	0	0
9	B	13	0	18	0	0
10	B	4	0	3	0	0
11	C	8	0	0	0	0
12	A	396	0	0	7	0
12	B	126	0	0	0	0
12	C	99	0	0	1	0
All	All	9598	0	9091	73	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 4.

All (73) 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:528:THR:HG22	1:A:535:LYS:HG3	1.48	0.91
1:A:530:LYS:H	1:A:530:LYS:HD3	1.34	0.91
2:B:169:PHE:H	7:B:302:PEG:H21	1.35	0.90
3:C:85:LEU:HD11	3:C:115:MET:HE2	1.64	0.79
1:A:528:THR:CG2	1:A:535:LYS:HG3	2.12	0.78
2:B:169:PHE:N	7:B:302:PEG:H21	2.00	0.76
3:C:59:MET:HE3	3:C:64:VAL:HG21	1.70	0.73
3:C:85:LEU:HD11	3:C:115:MET:CE	2.18	0.72
1:A:234:MET:HE1	12:A:1214:HOH:O	1.90	0.72
2:B:41:LYS:HE3	12:C:313:HOH:O	1.92	0.69
1:A:690:ILE:HG21	1:A:704:LEU:HD22	1.77	0.66
1:A:576:LYS:HB2	1:A:586:LYS:HZ1	1.60	0.66
1:A:144:PHE:HE2	1:A:263:GLU:HG2	1.62	0.63
1:A:615:MET:HE1	1:A:648:PRO:HG3	1.82	0.61
1:A:453:ILE:HG23	1:A:495:LEU:HD13	1.83	0.60
2:B:139:ARG:NH2	2:B:154:ASP:OD2	2.34	0.60
2:B:232:ASN:ND2	2:B:235:ILE:HD11	2.16	0.59
1:A:390:GLU:HB3	12:A:1246:HOH:O	2.03	0.58
1:A:37:VAL:HB	1:A:81:ALA:HB3	1.86	0.57
2:B:41:LYS:HD3	3:C:30:LEU:HD11	1.86	0.57
1:A:463:GLU:HG3	12:A:1253:HOH:O	2.05	0.56
1:A:615:MET:HE3	1:A:648:PRO:HD3	1.88	0.54
1:A:615:MET:CE	1:A:648:PRO:HG3	2.37	0.54
3:C:85:LEU:CD1	3:C:115:MET:HE1	2.38	0.54
2:B:90:GLU:O	2:B:93:SER:HB2	2.07	0.53
3:C:93:PRO:HB3	3:C:159:LYS:HD3	1.89	0.53
1:A:528:THR:HG22	1:A:535:LYS:CG	2.31	0.53
1:A:144:PHE:CE2	1:A:263:GLU:HG2	2.41	0.52
3:C:82:VAL:HG23	3:C:115:MET:CE	2.39	0.52
1:A:576:LYS:HG3	1:A:586:LYS:HZ3	1.75	0.51
1:A:402:GLU:OE1	1:A:587:LYS:HE2	2.11	0.51
3:C:11:LYS:HE2	3:C:22:GLU:OE2	2.11	0.50
1:A:647:ILE:HD13	3:C:146:TYR:HB2	1.94	0.50
2:B:195:LEU:HD12	2:B:195:LEU:C	2.32	0.49
3:C:82:VAL:HA	3:C:115:MET:HE1	1.93	0.49
4:A:801:MCN:H5'1	4:A:801:MCN:H2'	1.68	0.48
1:A:523:LYS:HG2	1:A:524:GLU:HG3	1.94	0.48
2:B:169:PHE:HA	7:B:302:PEG:H21	1.96	0.48
1:A:516:ASP:OD1	1:A:516:ASP:N	2.48	0.47
2:B:193:LEU:HD21	2:B:195:LEU:HD23	1.95	0.47
1:A:141:GLU:HB2	12:A:1030:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:CG	1:A:280:ILE:HD13	2.44	0.46
2:B:169:PHE:CA	7:B:302:PEG:H21	2.45	0.46
1:A:112:GLU:HG3	1:A:280:ILE:HD13	1.97	0.46
2:B:55:ARG:HH12	7:C:203:PEG:H22	1.81	0.46
3:C:82:VAL:HG23	3:C:115:MET:HE1	1.97	0.45
1:A:515:ALA:C	1:A:516:ASP:OD1	2.55	0.45
3:C:58:ILE:O	3:C:79:ILE:HA	2.17	0.45
2:B:54:ARG:HD3	3:C:73:GLU:HG3	1.97	0.45
3:C:85:LEU:CD1	3:C:115:MET:CE	2.88	0.44
1:A:149:LEU:HD12	1:A:150:THR:H	1.83	0.43
1:A:134:ARG:HG2	1:A:136:LYS:HE3	2.00	0.43
1:A:416:ALA:HB1	1:A:489:ILE:HD11	2.00	0.43
2:B:220:LYS:HA	2:B:220:LYS:HE3	1.99	0.43
1:A:576:LYS:HB2	1:A:586:LYS:NZ	2.31	0.43
1:A:151:ILE:HD12	1:A:353:GLU:HG2	2.01	0.43
1:A:441:PRO:HD2	1:A:469:TRP:CD1	2.54	0.43
1:A:38:ARG:HA	1:A:78:GLN:O	2.19	0.42
6:A:803:1PE:H231	12:A:1112:HOH:O	2.18	0.42
1:A:264:VAL:HG23	1:A:275:ILE:HD13	2.02	0.42
1:A:615:MET:CE	1:A:648:PRO:CG	2.97	0.42
1:A:650:LYS:NZ	12:A:918:HOH:O	2.53	0.42
2:B:18:LEU:O	2:B:22:GLU:HG3	2.20	0.42
1:A:357:ASP:HB3	1:A:360:GLU:HB2	2.01	0.42
1:A:580:THR:HA	2:B:263:MET:SD	2.60	0.42
1:A:586:LYS:HG3	12:A:1049:HOH:O	2.20	0.42
2:B:129:LYS:NZ	2:B:142:ASN:OD1	2.53	0.42
2:B:8:TYR:HB2	3:C:27:PRO:HB3	2.03	0.41
1:A:615:MET:HB2	1:A:615:MET:HE2	1.64	0.41
1:A:131:TYR:HB3	1:A:320:ALA:HB3	2.03	0.40
2:B:213:ASN:HB2	2:B:215:VAL:O	2.21	0.40
1:A:650:LYS:HE3	1:A:652:ASP:OD1	2.21	0.40
2:B:131:LYS:HB3	2:B:163:GLU:HB3	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	697/706 (99%)	660 (95%)	33 (5%)	4 (1%)	25	26
2	B	270/278 (97%)	262 (97%)	8 (3%)	0	100	100
3	C	159/168 (95%)	155 (98%)	4 (2%)	0	100	100
All	All	1126/1152 (98%)	1077 (96%)	45 (4%)	4 (0%)	34	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	LYS
1	A	332	ARG
1	A	530	LYS
1	A	214	ALA

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	579/584 (99%)	563 (97%)	16 (3%)	43	56
2	B	230/234 (98%)	225 (98%)	5 (2%)	52	65
3	C	135/142 (95%)	126 (93%)	9 (7%)	16	18
All	All	944/960 (98%)	914 (97%)	30 (3%)	39	50

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	71	LYS
1	A	134	ARG
1	A	141	GLU
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	234	MET
1	A	235	LEU
1	A	401	LYS
1	A	408	VAL
1	A	504	LYS
1	A	516	ASP
1	A	530	LYS
1	A	627	GLU
1	A	691	LYS
1	A	696	LYS
1	A	705	VAL
2	B	19	GLU
2	B	135	ARG
2	B	139	ARG
2	B	220	LYS
2	B	225	GLU
3	C	1	MET
3	C	22	GLU
3	C	78	GLU
3	C	87	LYS
3	C	88	ASP
3	C	90	LYS
3	C	104	LEU
3	C	129	GLU
3	C	158	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
8	FAD	B	301	-	51,58,58	1.85	10 (19%)	60,89,89	1.76	7 (11%)
7	PEG	A	804	-	6,6,6	0.42	0	5,5,5	0.77	0
7	PEG	B	302	-	6,6,6	0.67	0	5,5,5	0.57	0
4	MCN	A	801	5	38,48,48	3.06	12 (31%)	40,74,74	2.25	12 (30%)
9	PG4	B	303	-	12,12,12	0.46	0	11,11,11	0.81	0
11	FES	C	201	3	0,4,4	0.00	-	-		
11	FES	C	202	3	0,4,4	0.00	-	-		
7	PEG	C	203	-	6,6,6	0.41	0	5,5,5	0.72	0
10	ACY	B	305	-	1,3,3	3.74	1 (100%)	0,3,3	0.00	-
6	1PE	A	803	-	15,15,15	1.11	0	14,14,14	1.16	0
7	PEG	B	304	-	6,6,6	0.55	0	5,5,5	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FAD	B	301	-	-	0/30/50/50	0/6/6/6
7	PEG	A	804	-	-	3/4/4/4	-
7	PEG	B	302	-	-	4/4/4/4	-
4	MCN	A	801	5	-	4/20/54/54	0/5/5/5
9	PG4	B	303	-	-	7/10/10/10	-
11	FES	C	201	3	-	-	0/1/1/1
11	FES	C	202	3	-	-	0/1/1/1
7	PEG	C	203	-	-	1/4/4/4	-
6	1PE	A	803	-	-	7/13/13/13	-
7	PEG	B	304	-	-	3/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	MCN	C6'-N5'	9.83	1.46	1.32
4	A	801	MCN	C6'-C7	9.05	1.56	1.43
4	A	801	MCN	C7-N8'	7.91	1.50	1.30
8	B	301	FAD	O4B-C1B	6.99	1.50	1.41
4	A	801	MCN	O9'-C7	5.15	1.41	1.35
4	A	801	MCN	C2'-N3'	4.76	1.43	1.35
8	B	301	FAD	C5X-N5	4.73	1.43	1.35
10	B	305	ACY	CH3-C	3.74	1.53	1.48
8	B	301	FAD	C5B-C4B	3.73	1.63	1.51
8	B	301	FAD	C10-N1	3.64	1.37	1.33
4	A	801	MCN	O5'-C5'	-3.49	1.31	1.44
8	B	301	FAD	C4X-N5	3.40	1.38	1.33
8	B	301	FAD	C2B-C1B	-2.82	1.49	1.53
4	A	801	MCN	C6-N1	2.42	1.38	1.35
4	A	801	MCN	C4-N3	2.41	1.39	1.35
8	B	301	FAD	C8M-C8	2.36	1.55	1.51
8	B	301	FAD	C9A-N10	2.33	1.41	1.38
8	B	301	FAD	C4A-N3A	2.18	1.38	1.35
8	B	301	FAD	C5'-C4'	2.16	1.54	1.51
4	A	801	MCN	O4D-C4D	2.13	1.49	1.45
4	A	801	MCN	C4'-N3'	2.12	1.41	1.36
4	A	801	MCN	C4A-N5'	2.12	1.41	1.37
4	A	801	MCN	C3'-C4D	-2.08	1.47	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	301	FAD	C4-N3-C2	6.66	120.76	115.14
4	A	801	MCN	C7-N8'-C4B	6.56	122.19	116.61
8	B	301	FAD	N3A-C2A-N1A	-5.87	119.51	128.68
4	A	801	MCN	C5'-C4D-C3'	-5.60	94.21	115.18
4	A	801	MCN	O9'-C7-N8'	-5.06	109.03	115.30
8	B	301	FAD	C1'-N10-C9A	5.05	122.27	118.29
4	A	801	MCN	N1'-C2'-N3'	-3.32	122.80	127.22
4	A	801	MCN	PB-O3A-PA	-3.30	121.51	132.83
8	B	301	FAD	C4X-C4-N3	-3.26	118.98	123.43
4	A	801	MCN	C2'-N1'-C4B	3.25	119.07	115.36
4	A	801	MCN	C4B-C4A-N5'	-3.23	118.51	122.41
4	A	801	MCN	C6'-N5'-C4A	2.95	123.39	117.26
8	B	301	FAD	C1B-N9A-C4A	-2.88	121.58	126.64
4	A	801	MCN	O5'-PA-O1A	2.67	119.51	109.07
8	B	301	FAD	C9A-N10-C10	-2.49	118.65	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	MCN	O4D-C4D-C5'	2.42	117.34	109.37
4	A	801	MCN	O4'-C4'-C4A	2.35	124.06	119.67
4	A	801	MCN	O2A-PA-O5'	-2.31	97.01	107.75
8	B	301	FAD	C4X-C10-N10	2.03	122.39	120.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

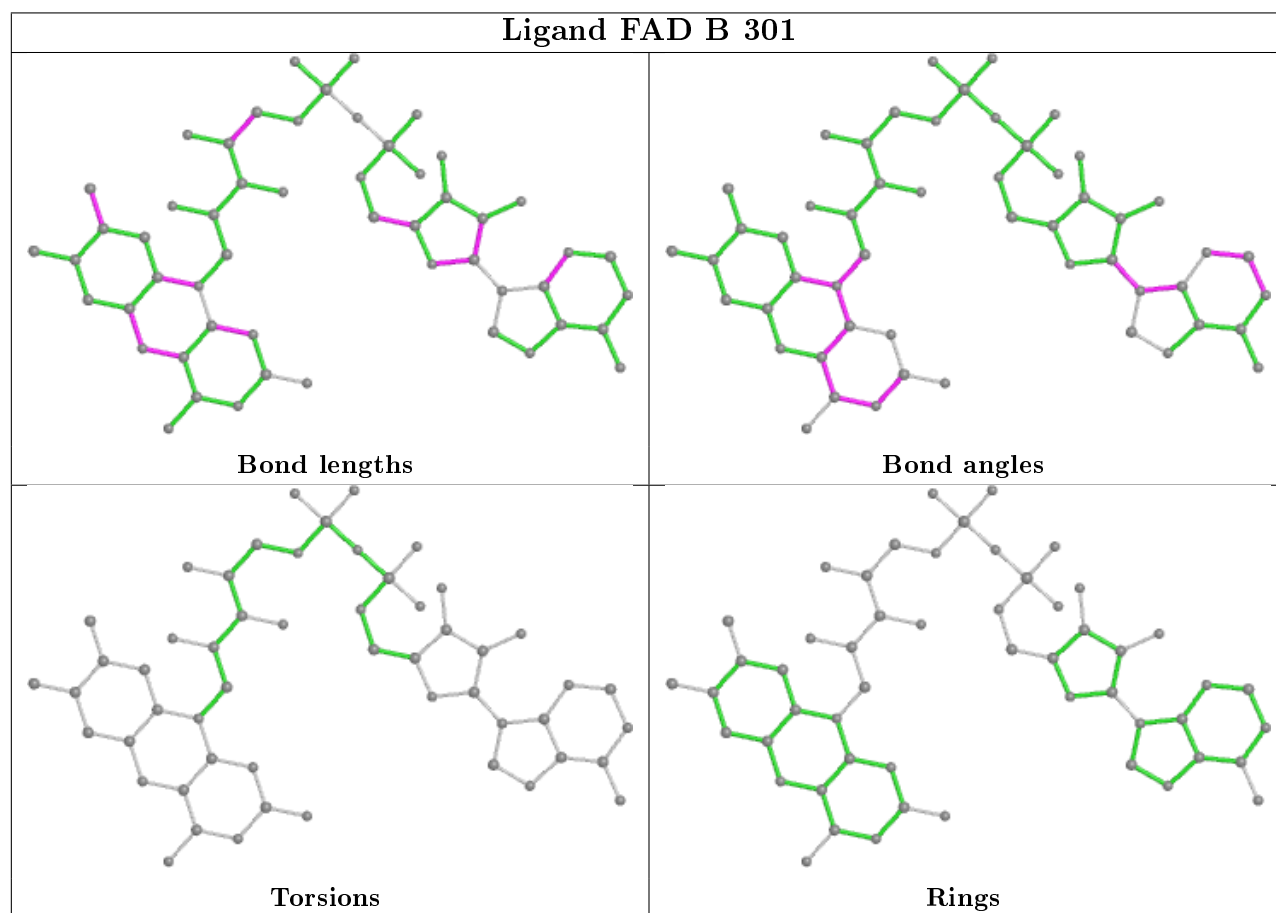
Mol	Chain	Res	Type	Atoms
4	A	801	MCN	C5'-O5'-PA-O1A
9	B	303	PG4	O3-C5-C6-O4
6	A	803	1PE	OH4-C13-C23-OH3
7	B	302	PEG	O1-C1-C2-O2
6	A	803	1PE	OH2-C12-C22-OH3
7	B	304	PEG	O1-C1-C2-O2
7	A	804	PEG	O1-C1-C2-O2
6	A	803	1PE	OH7-C16-C26-OH6
7	B	304	PEG	O2-C3-C4-O4
7	B	302	PEG	O2-C3-C4-O4
9	B	303	PG4	O4-C7-C8-O5
6	A	803	1PE	C25-C15-OH6-C26
9	B	303	PG4	O2-C3-C4-O3
9	B	303	PG4	C5-C6-O4-C7
6	A	803	1PE	C13-C23-OH3-C22
7	B	304	PEG	C1-C2-O2-C3
4	A	801	MCN	C5'-O5'-PA-O3A
7	A	804	PEG	O2-C3-C4-O4
4	A	801	MCN	C5'-O5'-PA-O2A
7	B	302	PEG	C4-C3-O2-C2
6	A	803	1PE	C23-C13-OH4-C24
9	B	303	PG4	C3-C4-O3-C5
7	C	203	PEG	C1-C2-O2-C3
9	B	303	PG4	O1-C1-C2-O2
6	A	803	1PE	OH6-C15-C25-OH5
7	A	804	PEG	C4-C3-O2-C2
9	B	303	PG4	C1-C2-O2-C3
7	B	302	PEG	C1-C2-O2-C3
4	A	801	MCN	C10-O3B-PB-O2B

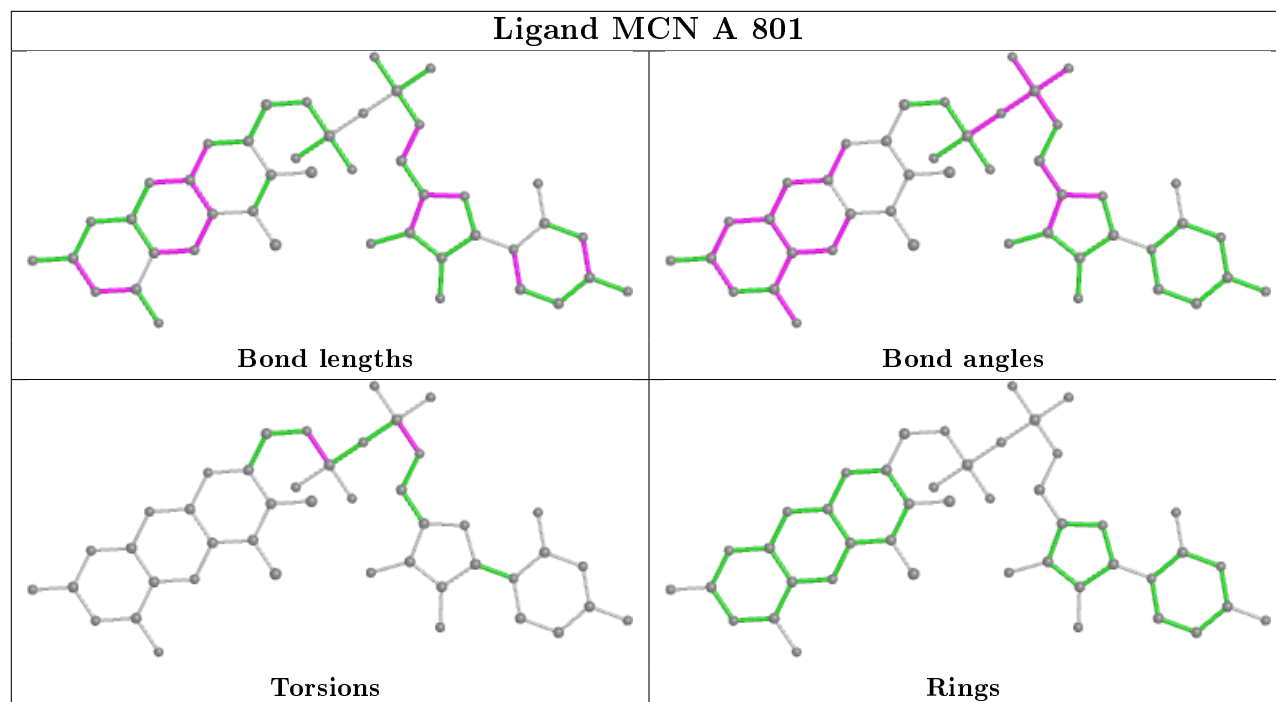
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	PEG	4	0
4	A	801	MCN	1	0
7	C	203	PEG	1	0
6	A	803	1PE	1	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	701/706 (99%)	-0.57	5 (0%) 87 86	15, 28, 50, 80	0
2	B	274/278 (98%)	-0.43	2 (0%) 87 86	22, 35, 58, 88	0
3	C	161/168 (95%)	-0.35	1 (0%) 89 88	17, 25, 52, 77	0
All	All	1136/1152 (98%)	-0.51	8 (0%) 87 86	15, 29, 53, 88	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	135	ARG	3.1
1	A	531	LYS	2.8
1	A	513	LEU	2.5
1	A	515	ALA	2.1
3	C	1	MET	2.1
1	A	514	ASN	2.0
1	A	532	ASN	2.0
2	B	247	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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,

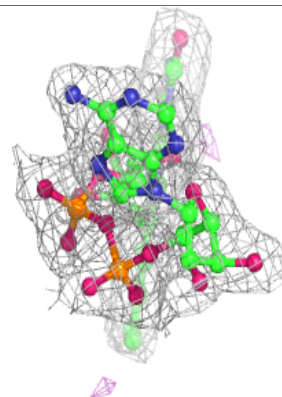
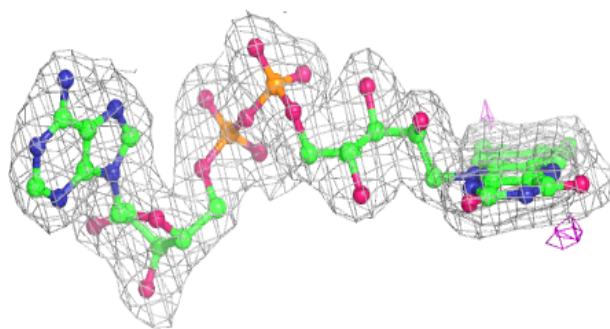
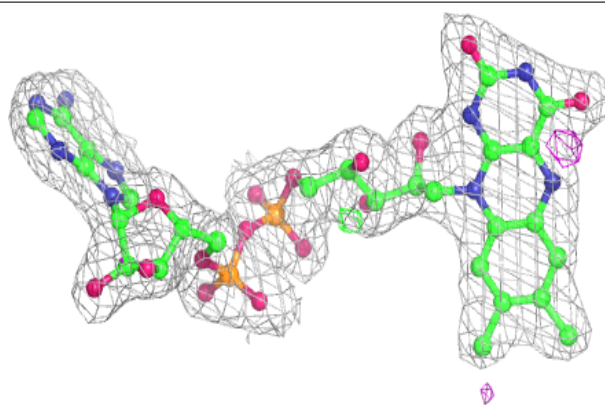
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

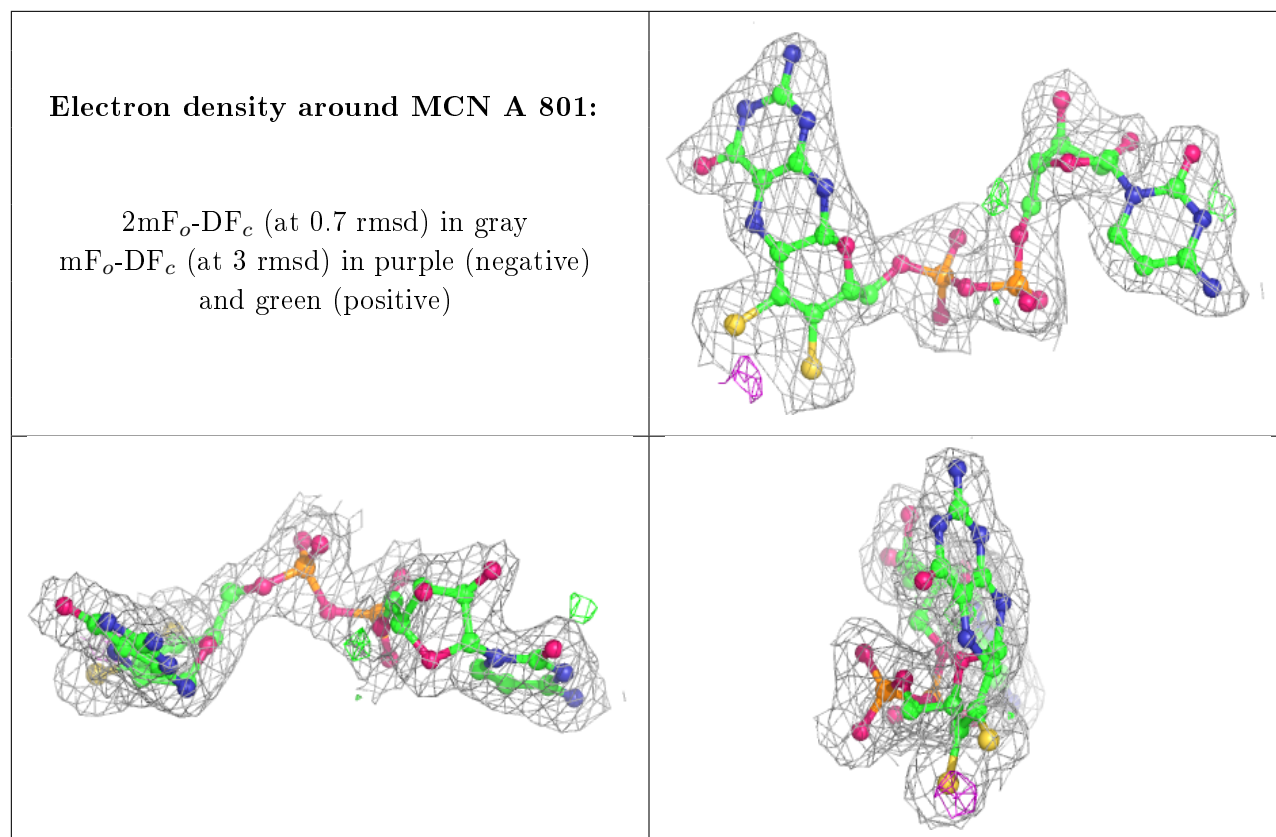
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PEG	B	304	7/7	0.81	0.19	46,51,57,59	0
6	1PE	A	803	16/16	0.83	0.24	43,47,51,52	0
7	PEG	B	302	7/7	0.85	0.17	43,50,61,66	0
7	PEG	A	804	7/7	0.87	0.11	47,51,60,60	0
7	PEG	C	203	7/7	0.90	0.13	39,43,49,50	0
9	PG4	B	303	13/13	0.93	0.11	44,47,56,58	0
10	ACY	B	305	4/4	0.95	0.11	35,36,36,37	0
8	FAD	B	301	53/53	0.97	0.10	21,27,32,36	0
4	MCN	A	801	44/44	0.98	0.12	19,24,27,34	0
11	FES	C	201	4/4	0.99	0.11	20,21,21,23	0
11	FES	C	202	4/4	1.00	0.09	21,21,22,23	0
5	MO	A	802	1/1	1.00	0.05	29,29,29,29	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 FAD B 301:

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.