



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 4ZOH / pdb_00004zoh
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 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

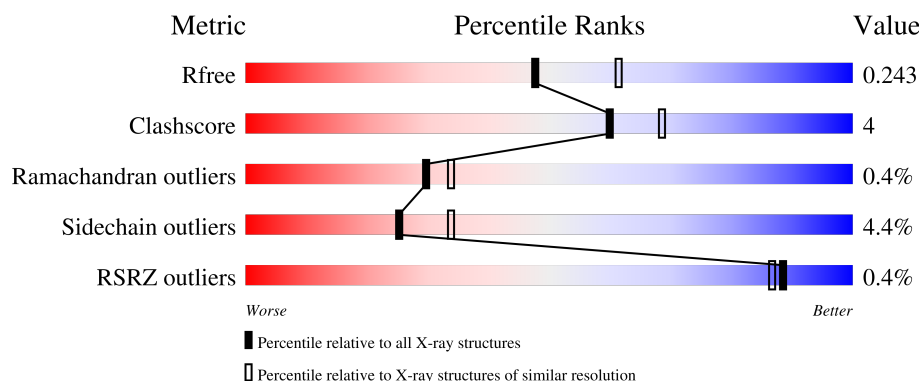
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	706	 84% 13% ..
2	B	278	 87% 11% ..
3	C	168	 79% 15% ..

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			

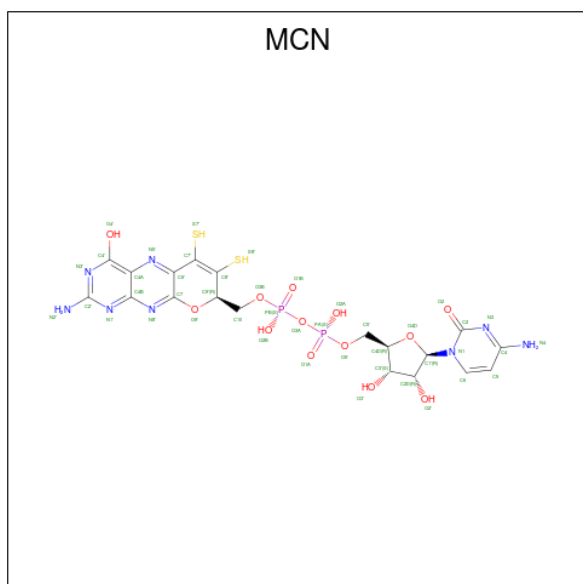
- Molecule 2 is a protein called Putative oxidoreductase FAD-binding subunit.

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 (CCD ID: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

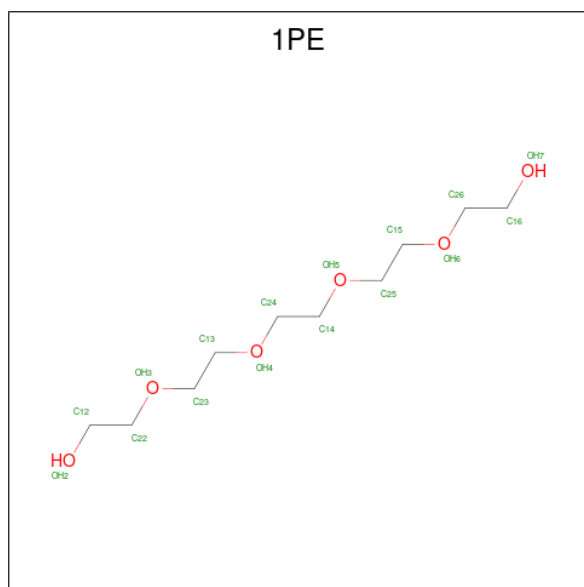


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			44	19	8	13	2	2	
									0
									0

- Molecule 5 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

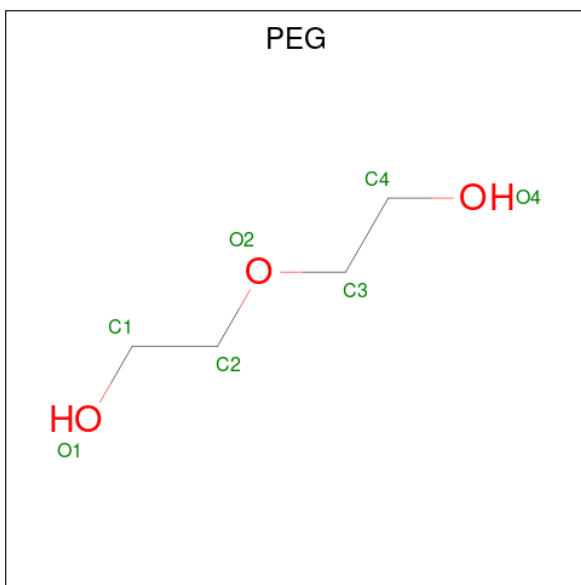
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo		
			1	1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



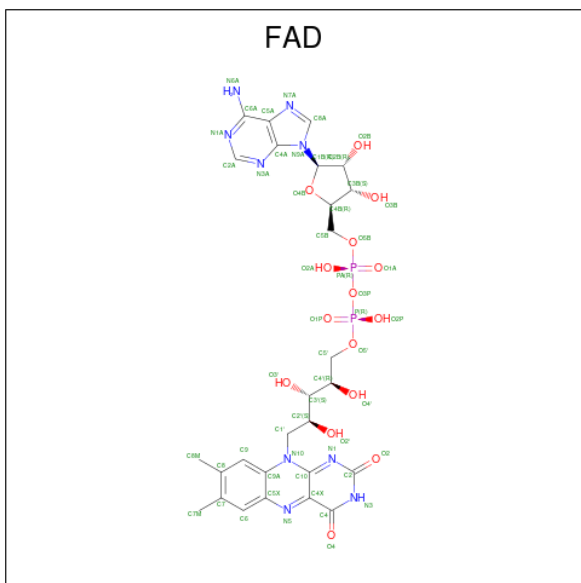
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O		
			16	10	6	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



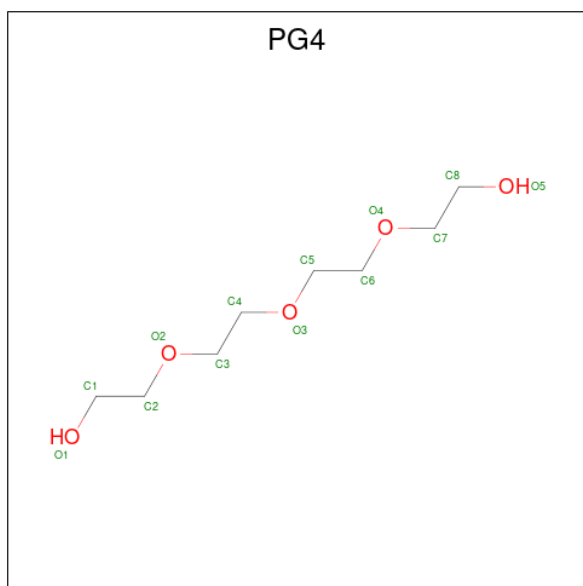
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



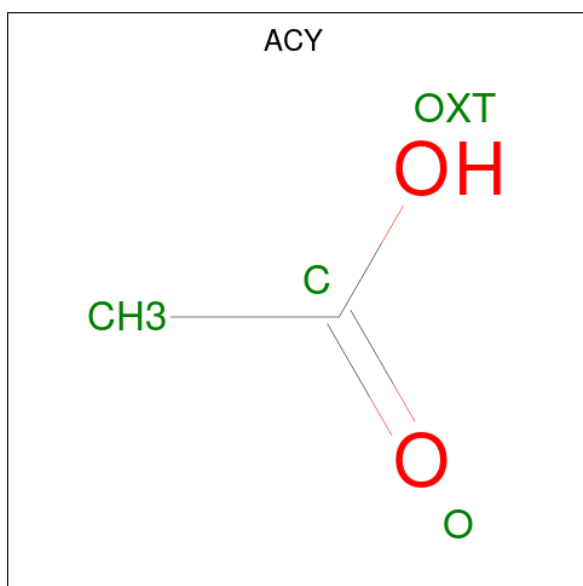
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



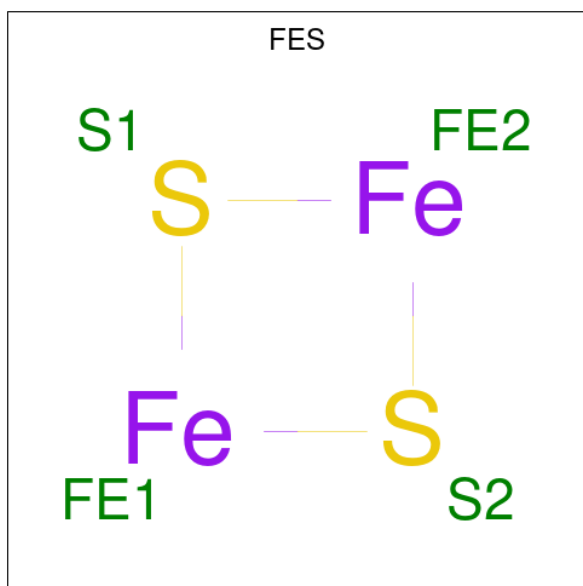
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is ACETIC ACID (CCD ID: 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 (CCD ID: FES) (formula: Fe_2S_2).



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		

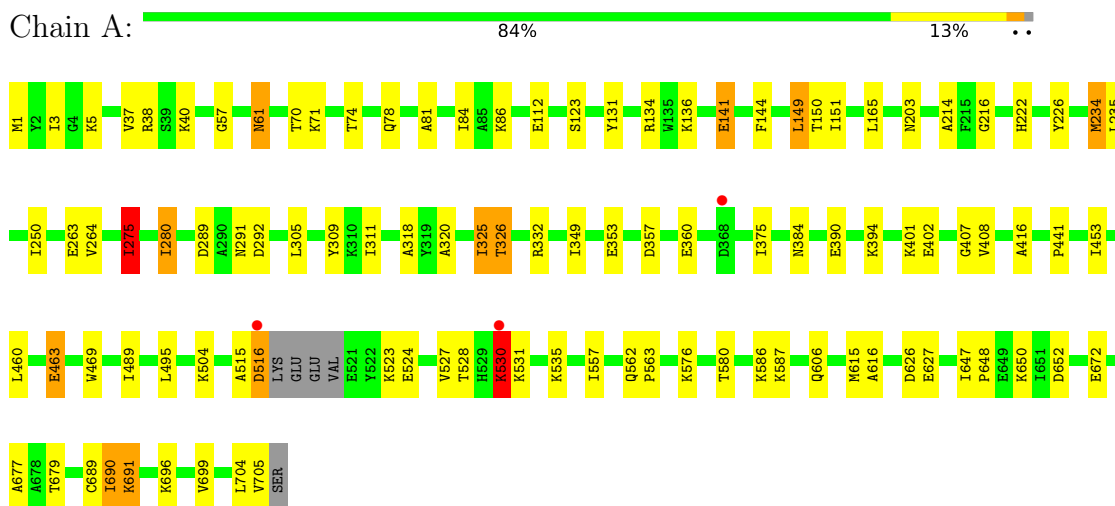
- Molecule 12 is water.

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		

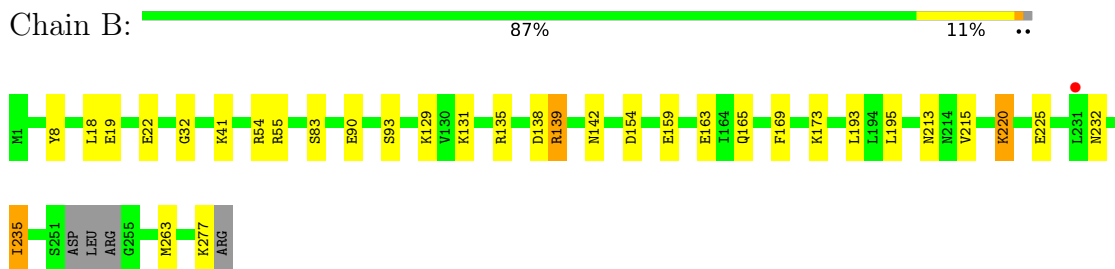
3 Residue-property plots

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.

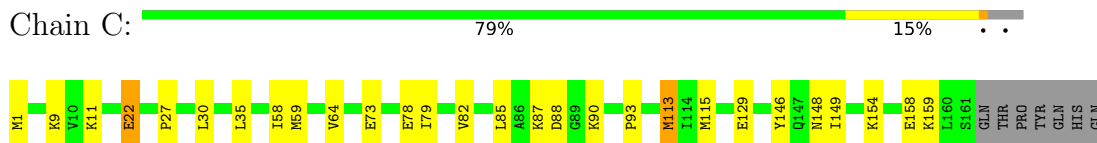
• Molecule 1: Putative oxidoreductase molybdopterin-binding subunit



• 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	143.43Å 143.43Å 235.51Å 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 2.20Å)	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)	0.34 , 43.7	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	0.96	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, 1PE, PEG, ACY, PG4, FES, MO, MCN

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	1.34	16/5561 (0.3%)	1.27	27/7535 (0.4%)
2	B	1.13	1/2157 (0.0%)	1.19	4/2911 (0.1%)
3	C	1.32	1/1254 (0.1%)	1.28	3/1691 (0.2%)
All	All	1.29	18/8972 (0.2%)	1.25	34/12137 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	563	PRO	CA-C	7.31	1.58	1.52
1	A	325	ILE	C-O	6.54	1.31	1.23
1	A	292	ASP	CA-C	6.27	1.60	1.52
1	A	384	ASN	CA-C	-6.21	1.46	1.53
1	A	289	ASP	N-CA	6.09	1.53	1.46
1	A	407	GLY	CA-C	-5.94	1.46	1.51
1	A	123	SER	N-CA	5.82	1.53	1.46
1	A	318	ALA	N-CA	5.63	1.53	1.46
3	C	35	LEU	C-O	5.47	1.30	1.24
1	A	5	LYS	C-O	5.42	1.31	1.24
1	A	61	ASN	CA-C	5.32	1.59	1.52
1	A	222	HIS	N-CA	-5.31	1.37	1.45
2	B	165	GLN	N-CA	5.20	1.52	1.46
1	A	616	ALA	CA-C	5.18	1.59	1.52
1	A	291	ASN	CA-C	-5.14	1.46	1.52
1	A	226	TYR	N-CA	5.12	1.52	1.46
1	A	606	GLN	N-CA	5.08	1.52	1.46
1	A	216	GLY	C-O	-5.02	1.17	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	ILE	N-CA-C	17.95	127.24	111.81
1	A	689	CYS	CA-C-N	-7.55	113.44	122.35
1	A	689	CYS	C-N-CA	-7.55	113.44	122.35
1	A	305	LEU	CA-C-N	-7.23	112.35	119.87
1	A	305	LEU	C-N-CA	-7.23	112.35	119.87
1	A	557	ILE	N-CA-C	-6.62	98.84	108.11
1	A	275	ILE	CB-CA-C	-6.35	99.73	110.71
1	A	311	ILE	CA-C-N	-6.25	114.97	122.35
1	A	311	ILE	C-N-CA	-6.25	114.97	122.35
1	A	691	LYS	N-CA-C	-6.10	93.92	111.00
1	A	460	LEU	CA-C-N	-6.08	113.50	119.76
1	A	460	LEU	C-N-CA	-6.08	113.50	119.76
1	A	74	THR	N-CA-C	5.89	120.48	112.88
1	A	672	GLU	CA-C-N	5.88	128.48	120.54
1	A	672	GLU	C-N-CA	5.88	128.48	120.54
1	A	326	THR	CA-C-N	-5.82	113.77	119.76
1	A	326	THR	C-N-CA	-5.82	113.77	119.76
1	A	562	GLN	CA-C-N	-5.78	114.43	120.38
1	A	562	GLN	C-N-CA	-5.78	114.43	120.38
2	B	83	SER	N-CA-C	5.61	119.43	112.59
1	A	690	ILE	CB-CA-C	-5.60	105.11	111.55
2	B	159	GLU	N-CA-C	5.53	118.56	109.72
3	C	154	LYS	N-CA-C	-5.37	105.34	111.14
1	A	677	ALA	N-CA-C	5.35	117.19	111.36
2	B	32	GLY	N-CA-C	-5.32	108.35	115.32
3	C	148	ASN	N-CA-C	5.27	117.77	111.71
3	C	113	MET	N-CA-C	-5.18	105.72	111.36
1	A	527	VAL	CB-CA-C	5.16	118.26	110.63
1	A	349	ILE	N-CA-C	-5.13	105.54	110.72
1	A	309	TYR	N-CA-C	5.11	118.45	110.32
2	B	138	ASP	N-CA-C	5.06	117.74	109.59
1	A	280	ILE	N-CA-C	5.04	115.11	107.80
1	A	679	THR	CA-C-N	-5.01	113.88	119.19
1	A	679	THR	C-N-CA	-5.01	113.88	119.19

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	45	0
2	B	2122	0	2194	21	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	1	0
12	C	99	0	0	1	0
All	All	9598	0	9091	78	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 (78) 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)
3:C:85:LEU:HD11	3:C:115:MET:HE1	1.38	1.06
1:A:528:THR:HG22	1:A:535:LYS:HG3	1.48	0.91
1:A:530:LYS:HD3	1:A:530:LYS:H	1.34	0.91
3:C:85:LEU:CD1	3:C:115:MET:HE1	1.99	0.91
2:B:169:PHE:H	7:B:302:PEG:H21	1.35	0.90
1:A:615:MET:HE1	1:A:648:PRO:CG	2.03	0.89
1:A:615:MET:HE1	1:A:648:PRO:HG3	1.58	0.83
3:C:82:VAL:HG23	3:C:115:MET:HE3	1.63	0.81
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:85:LEU:HD11	3:C:115:MET:CE	2.18	0.72
3:C:59:MET:HE3	3:C:64:VAL:HG21	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:615:MET:HE1	1:A:648:PRO:CD	2.33	0.58
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
2:B:195:LEU:C	2:B:195:LEU:HD12	2.32	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:615:MET:HE1	1:A:648:PRO:HD3	1.90	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
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
1:A:515:ALA:C	1:A:516:ASP:OD1	2.55	0.50
1:A:1:MET:HE2	1:A:3:ILE:O	2.12	0.50
1:A:615:MET:CE	1:A:648:PRO:HG3	2.37	0.49
4:A:801:MCN:H2'	4:A:801:MCN:H5'1	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
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:CE	2.39	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:115:MET:HA	3:C:115:MET:HE2	1.99	0.45
1:A:626:ASP:OD1	1:A:626:ASP:C	2.60	0.44
3:C:113:MET:HE3	3:C:149:ILE:HD13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLY:C	1:A:70:THR:HG22	2.43	0.43
1:A:416:ALA:HB1	1:A:489:ILE:HD11	2.00	0.43
2:B:220:LYS:HE3	2:B:220:LYS:HA	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: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:131:TYR:HB3	1:A:320:ALA:HB3	2.03	0.40
1:A:325:ILE:O	1:A:326:THR:C	2.64	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
2:B:277:LYS:C	12:B:410:HOH:O	2.63	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%)	21	23
2	B	270/278 (97%)	262 (97%)	8 (3%)	0	100	100
3	C	159/168 (95%)	155 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1126/1152 (98%)	1077 (96%)	45 (4%)	4 (0%)	30 34

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%)	553 (96%)	26 (4%)	24 33
2	B	230/234 (98%)	223 (97%)	7 (3%)	36 49
3	C	135/142 (95%)	126 (93%)	9 (7%)	15 17
All	All	944/960 (98%)	902 (96%)	42 (4%)	25 34

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	61	ASN
1	A	71	LYS
1	A	84	ILE
1	A	86	LYS
1	A	141	GLU
1	A	149	LEU
1	A	165	LEU
1	A	203	ASN
1	A	234	MET
1	A	235	LEU
1	A	250	ILE

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	375	ILE
1	A	394	LYS
1	A	401	LYS
1	A	408	VAL
1	A	463	GLU
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	699	VAL
1	A	705	VAL
2	B	19	GLU
2	B	135	ARG
2	B	139	ARG
2	B	173	LYS
2	B	220	LYS
2	B	225	GLU
2	B	235	ILE
3	C	1	MET
3	C	9	LYS
3	C	22	GLU
3	C	78	GLU
3	C	87	LYS
3	C	88	ASP
3	C	90	LYS
3	C	129	GLU
3	C	158	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	606	GLN
2	B	213	ASN

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](#)

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	$\# Z > 2$
7	PEG	A	804	-	6,6,6	0.43	0	5,5,5	0.76	0
9	PG4	B	303	-	12,12,12	0.47	0	11,11,11	0.80	0
11	FES	C	201	3	0,4,4	-	-	-		
11	FES	C	202	3	0,4,4	-	-	-		
7	PEG	C	203	-	6,6,6	0.42	0	5,5,5	0.72	0
7	PEG	B	304	-	6,6,6	0.55	0	5,5,5	0.91	0
6	1PE	A	803	-	15,15,15	1.11	0	14,14,14	1.15	0
4	MCN	A	801	5	42,48,48	3.16	13 (30%)	55,74,74	2.31	15 (27%)
8	FAD	B	301	-	58,58,58	1.47	11 (18%)	85,89,89	1.93	19 (22%)
10	ACY	B	305	-	3,3,3	1.14	0	3,3,3	1.20	0
7	PEG	B	302	-	6,6,6	0.68	0	5,5,5	0.56	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
7	PEG	A	804	-	-	3/4/4/4	-
9	PG4	B	303	-	-	7/10/10/10	-
11	FES	C	201	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FES	C	202	3	-	-	0/1/1/1
7	PEG	C	203	-	-	1/4/4/4	-
7	PEG	B	304	-	-	3/4/4/4	-
6	1PE	A	803	-	-	7/13/13/13	-
4	MCN	A	801	5	-	3/22/54/54	0/5/5/5
8	FAD	B	301	-	-	0/34/50/50	0/6/6/6
7	PEG	B	302	-	-	4/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	MCN	C6'-N5'	10.23	1.46	1.32
4	A	801	MCN	PA-O3A	8.94	1.69	1.59
4	A	801	MCN	C7'-N8'	8.69	1.50	1.30
4	A	801	MCN	C6'-C7	7.93	1.56	1.43
4	A	801	MCN	C2'-N3'	4.90	1.43	1.35
8	B	301	FAD	C5B-C4B	3.88	1.63	1.51
8	B	301	FAD	O4B-C1B	3.82	1.50	1.42
4	A	801	MCN	O5'-C5'	-3.50	1.31	1.44
8	B	301	FAD	C4X-N5	3.45	1.38	1.30
8	B	301	FAD	C8M-C8	2.53	1.55	1.51
4	A	801	MCN	C4-N3	2.46	1.39	1.34
8	B	301	FAD	C8A-N9A	-2.35	1.33	1.37
8	B	301	FAD	C10-N1	2.33	1.37	1.33
4	A	801	MCN	C4'-N3'	2.30	1.41	1.36
8	B	301	FAD	C4A-N3A	2.27	1.38	1.34
8	B	301	FAD	C5'-C4'	2.23	1.54	1.51
4	A	801	MCN	PB-O3A	2.18	1.61	1.59
4	A	801	MCN	O4D-C4D	2.15	1.49	1.45
8	B	301	FAD	C8A-N7A	2.13	1.35	1.31
4	A	801	MCN	C6-C5	2.12	1.40	1.35
8	B	301	FAD	C7M-C7	2.09	1.54	1.51
4	A	801	MCN	C3'-C4D	-2.09	1.47	1.53
4	A	801	MCN	C4A-N5'	2.05	1.41	1.37
8	B	301	FAD	C5X-N5	2.04	1.43	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	MCN	O9'-C7-C6'	-9.07	106.79	120.97
8	B	301	FAD	O4B-C1B-N9A	-7.90	92.92	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	301	FAD	N3A-C2A-N1A	-5.99	119.51	128.58
4	A	801	MCN	C5'-C4D-C3'	-5.84	94.21	115.21
8	B	301	FAD	C5A-C4A-N3A	-5.25	119.48	126.72
4	A	801	MCN	O9'-C7-N8'	-4.62	109.03	115.12
8	B	301	FAD	N3A-C4A-N9A	4.24	134.38	127.17
4	A	801	MCN	O2-C2-N3	-4.14	115.80	122.33
8	B	301	FAD	C4X-C10-N10	4.12	122.39	116.48
8	B	301	FAD	C2A-N3A-C4A	3.95	121.48	111.83
4	A	801	MCN	C7-N8'-C4B	3.92	122.19	117.01
4	A	801	MCN	N1'-C2'-N3'	-3.47	122.80	127.21
4	A	801	MCN	C4B-C4A-N5'	-3.44	118.51	122.35
8	B	301	FAD	N9A-C8A-N7A	-3.36	109.17	113.94
8	B	301	FAD	C4A-N9A-C8A	3.33	109.24	105.74
4	A	801	MCN	C2'-N1'-C4B	3.33	119.07	115.48
4	A	801	MCN	O2B-PB-O3A	3.23	116.02	107.27
8	B	301	FAD	C2B-C1B-N9A	3.11	121.04	113.30
4	A	801	MCN	C6'-N5'-C4A	3.03	123.39	117.06
8	B	301	FAD	C4-N3-C2	-2.75	120.76	125.64
4	A	801	MCN	O5'-PA-O1A	2.67	119.51	108.94
8	B	301	FAD	C5A-N7A-C8A	2.50	107.39	103.45
4	A	801	MCN	O4D-C4D-C5'	2.50	117.34	109.33
4	A	801	MCN	O4'-C4'-C4A	2.44	124.06	119.53
4	A	801	MCN	O2A-PA-O5'	-2.33	97.01	107.57
4	A	801	MCN	C5-C6-N1	-2.25	118.18	121.84
8	B	301	FAD	C4X-C4-N3	2.25	118.98	113.25
8	B	301	FAD	C4A-C5A-N7A	-2.20	108.07	110.58
8	B	301	FAD	C5A-C6A-N6A	-2.16	117.94	123.29
8	B	301	FAD	C4A-N9A-C1B	-2.16	121.58	126.63
8	B	301	FAD	C10-C4X-N5	-2.14	120.43	124.81
8	B	301	FAD	C4X-C10-N1	-2.10	119.43	124.59
8	B	301	FAD	O2P-P-O3P	2.06	112.84	107.27
8	B	301	FAD	C4-C4X-C10	2.03	120.42	116.93

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	MCN	C5'-O5'-PA-O1A
4	A	801	MCN	C5'-O5'-PA-O3A
9	B	303	PG4	O3-C5-C6-O4
7	B	302	PEG	O1-C1-C2-O2
6	A	803	1PE	OH4-C13-C23-OH3

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

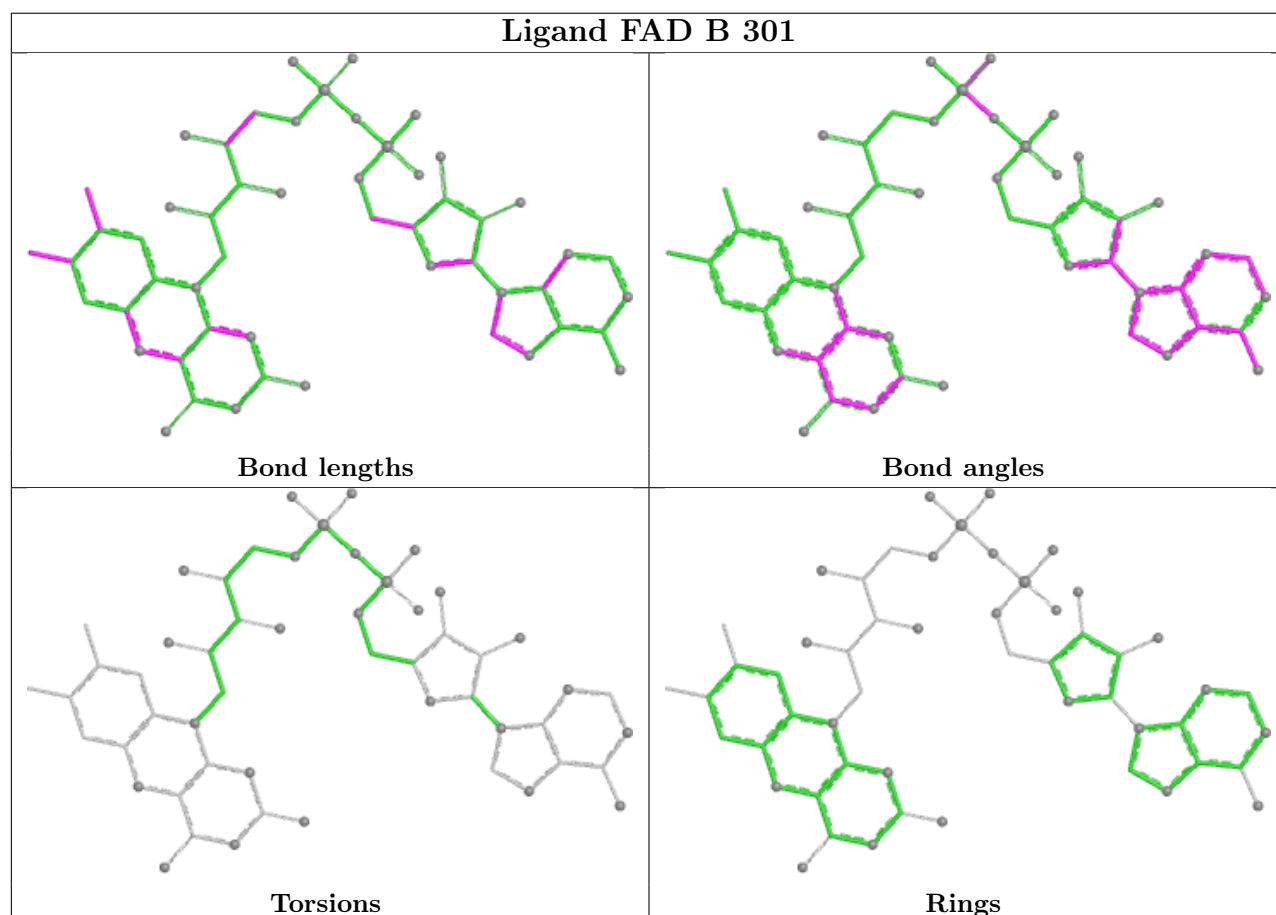
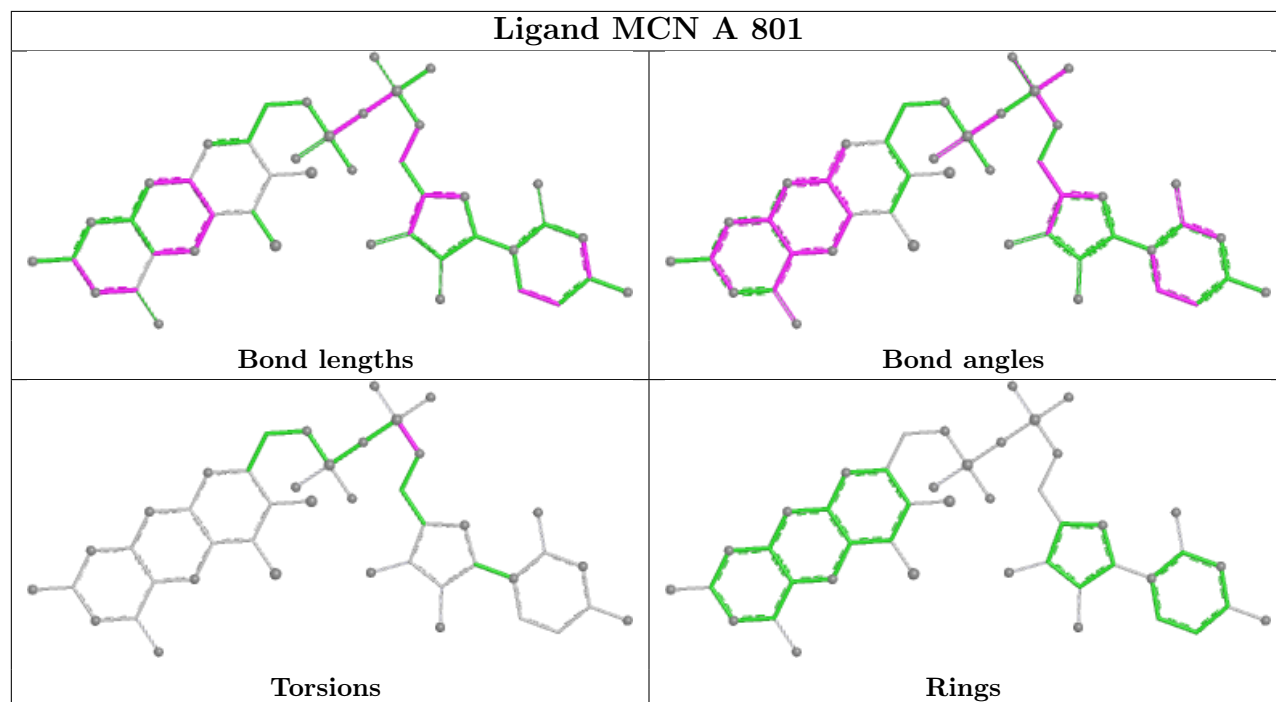
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	203	PEG	1	0
6	A	803	1PE	1	0
4	A	801	MCN	1	0
7	B	302	PEG	4	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%)	-0.33	3 (0%) 88 87	15, 28, 50, 80	0
2	B	274/278 (98%)	-0.15	1 (0%) 88 87	22, 35, 58, 88	0
3	C	161/168 (95%)	-0.46	0 100 100	17, 25, 52, 77	0
All	All	1136/1152 (98%)	-0.31	4 (0%) 88 87	15, 29, 53, 88	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	LEU	4.2
1	A	516	ASP	2.9
1	A	530	LYS	2.2
1	A	368	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

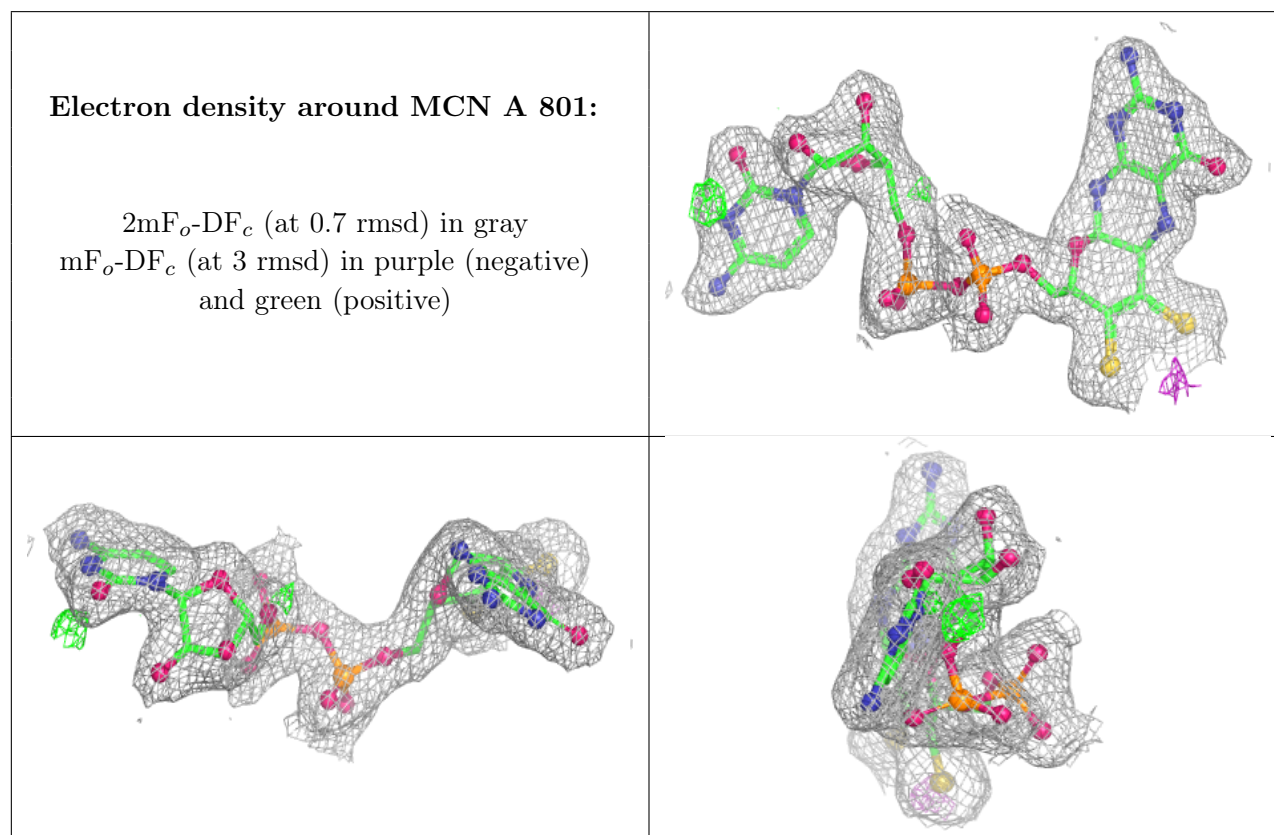
There are no oligosaccharides in this entry.

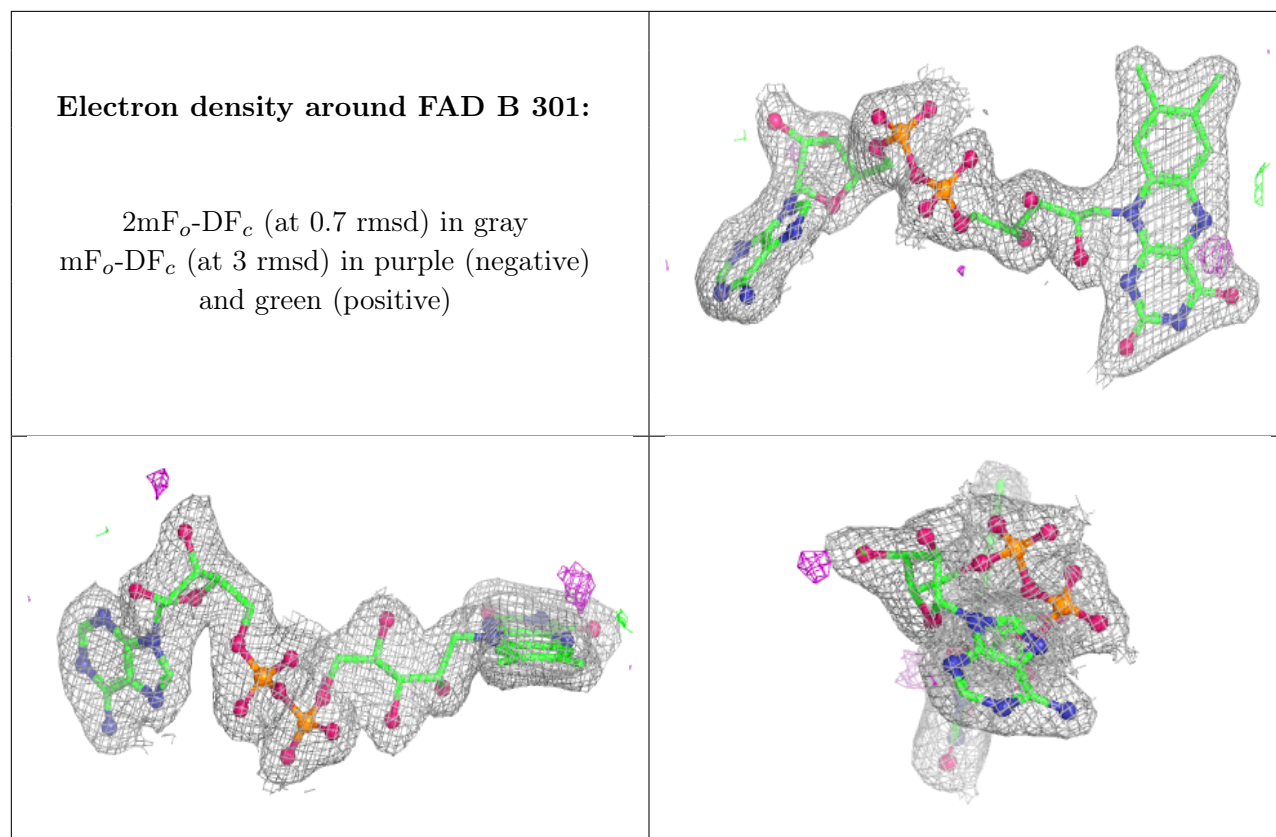
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	A	803	16/16	0.84	0.15	43,47,51,52	0
7	PEG	B	302	7/7	0.84	0.15	43,50,61,66	0
7	PEG	A	804	7/7	0.85	0.12	47,51,60,60	0
7	PEG	B	304	7/7	0.86	0.14	46,51,57,59	0
7	PEG	C	203	7/7	0.88	0.12	39,43,49,50	0
9	PG4	B	303	13/13	0.89	0.12	44,47,56,58	0
10	ACY	B	305	4/4	0.91	0.11	35,36,36,37	0
4	MCN	A	801	44/44	0.98	0.05	19,24,27,34	0
8	FAD	B	301	53/53	0.98	0.05	21,27,32,36	0
11	FES	C	202	4/4	0.99	0.03	21,21,22,23	0
11	FES	C	201	4/4	1.00	0.02	20,21,21,23	0
5	MO	A	802	1/1	1.00	0.04	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.