



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:22 PM UTC

PDB ID : 8KCM / pdb_00008kcm
Title : MmCPDII-DNA complex containing low-dosage, light induced repaired DNA.
Authors : Maestre-Reyna, M.; Wang, P.-H.; Nango, E.; Hosokawa, Y.; Saft, M.; Furrer, A.; Yang, C.-H.; Ngura Putu, E.P.G.; Wu, W.-J.; Emmerich, H.-J.; Engilberge, S.; Caramello, N.; Wranik, M.; Glover, H.L.; Franz-Badur, S.; Wu, H.-Y.; Lee, C.-C.; Huang, W.-C.; Huang, K.-F.; Chang, Y.-K.; Liao, J.-H.; Weng, J.-H.; Gad, W.; Chang, C.-W.; Pang, A.H.; Gashi, D.; Beale, E.; Ozerov, D.; Milne, C.; Cirelli, C.; Bacellar, C.; Sugahara, M.; Owada, S.; Joti, Y.; Yamashita, A.; Tanaka, R.; Tanaka, T.; Luo, F.J.; Tono, K.; Kiontke, S.; Spadaccini, R.; Royant, A.; Yamamoto, J.; Iwata, S.; Standfuss, J.; Essen, L.-O.; Bessho, Y.; Tsai, M.-D.
Deposited on : 2023-08-08
Resolution : 2.50 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:

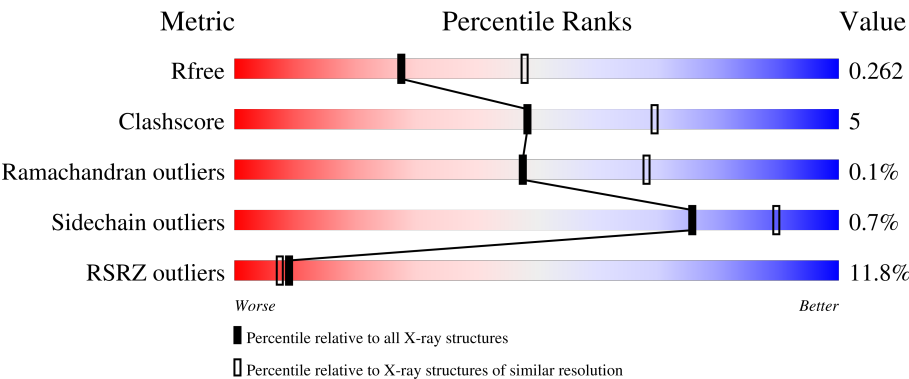
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	482	

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Buster-report

Percentile statistics

CCP4

Density-Fitness

Ideal geometry (proteins)

Ideal geometry (DNA, RNA)

Validation Pipeline (wwPDB-VP)

:

wwPDB partial adaption of 1.1.7 (2018)

: 20250101.v01 (using entries in the PDB archive January 1st 2025)

: 9.0.010 (Gargrove)

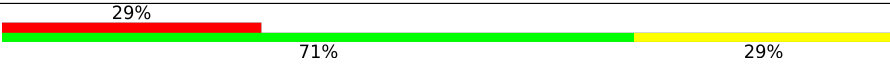
: 1.0.12

: Engh & Huber (2001)

: Parkinson et al. (1996)

: 2.49

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Mol	Chain	Length	Quality of chain
1	B	482	
2	C	14	
2	E	14	
3	D	14	
3	F	14	

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
6	GOL	A	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8706 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 Deoxyribodipyrimidine photo-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	3	0
			3557	2301	590	652	14			
1	B	428	Total	C	N	O	S	0	3	0
			3406	2197	570	625	14			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A0F8I5V2
A	-16	GLY	-	expression tag	UNP A0A0F8I5V2
A	-15	SER	-	expression tag	UNP A0A0F8I5V2
A	-14	SER	-	expression tag	UNP A0A0F8I5V2
A	-13	HIS	-	expression tag	UNP A0A0F8I5V2
A	-12	HIS	-	expression tag	UNP A0A0F8I5V2
A	-11	HIS	-	expression tag	UNP A0A0F8I5V2
A	-10	HIS	-	expression tag	UNP A0A0F8I5V2
A	-9	HIS	-	expression tag	UNP A0A0F8I5V2
A	-8	HIS	-	expression tag	UNP A0A0F8I5V2
A	-7	SER	-	expression tag	UNP A0A0F8I5V2
A	-6	SER	-	expression tag	UNP A0A0F8I5V2
A	-5	GLY	-	expression tag	UNP A0A0F8I5V2
A	-4	LEU	-	expression tag	UNP A0A0F8I5V2
A	-3	VAL	-	expression tag	UNP A0A0F8I5V2
A	-2	PRO	-	expression tag	UNP A0A0F8I5V2
A	-1	ARG	-	expression tag	UNP A0A0F8I5V2
A	0	GLY	-	expression tag	UNP A0A0F8I5V2
A	1	SER	-	expression tag	UNP A0A0F8I5V2
A	2	HIS	-	expression tag	UNP A0A0F8I5V2
A	377	THR	MET	engineered mutation	UNP A0A0F8I5V2
B	-17	MET	-	initiating methionine	UNP A0A0F8I5V2
B	-16	GLY	-	expression tag	UNP A0A0F8I5V2
B	-15	SER	-	expression tag	UNP A0A0F8I5V2
B	-14	SER	-	expression tag	UNP A0A0F8I5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP A0A0F8I5V2
B	-12	HIS	-	expression tag	UNP A0A0F8I5V2
B	-11	HIS	-	expression tag	UNP A0A0F8I5V2
B	-10	HIS	-	expression tag	UNP A0A0F8I5V2
B	-9	HIS	-	expression tag	UNP A0A0F8I5V2
B	-8	HIS	-	expression tag	UNP A0A0F8I5V2
B	-7	SER	-	expression tag	UNP A0A0F8I5V2
B	-6	SER	-	expression tag	UNP A0A0F8I5V2
B	-5	GLY	-	expression tag	UNP A0A0F8I5V2
B	-4	LEU	-	expression tag	UNP A0A0F8I5V2
B	-3	VAL	-	expression tag	UNP A0A0F8I5V2
B	-2	PRO	-	expression tag	UNP A0A0F8I5V2
B	-1	ARG	-	expression tag	UNP A0A0F8I5V2
B	0	GLY	-	expression tag	UNP A0A0F8I5V2
B	1	SER	-	expression tag	UNP A0A0F8I5V2
B	2	HIS	-	expression tag	UNP A0A0F8I5V2
B	377	THR	MET	engineered mutation	UNP A0A0F8I5V2

- Molecule 2 is a DNA chain called Repaired DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			244	115	44	73	12			
2	E	11	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

- Molecule 3 is a DNA chain called complementary oligonucleotide to the repaired DNA.

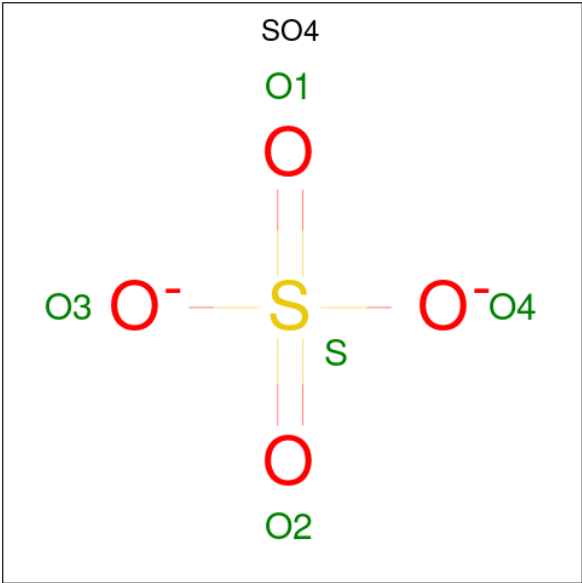
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			286	136	56	81	13			
3	F	13	Total	C	N	O	P	0	0	0
			266	126	54	74	12			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	263	Total	O	0	1
			264	264		
7	B	233	Total	O	0	0
			233	233		
7	C	21	Total	O	0	0
			21	21		

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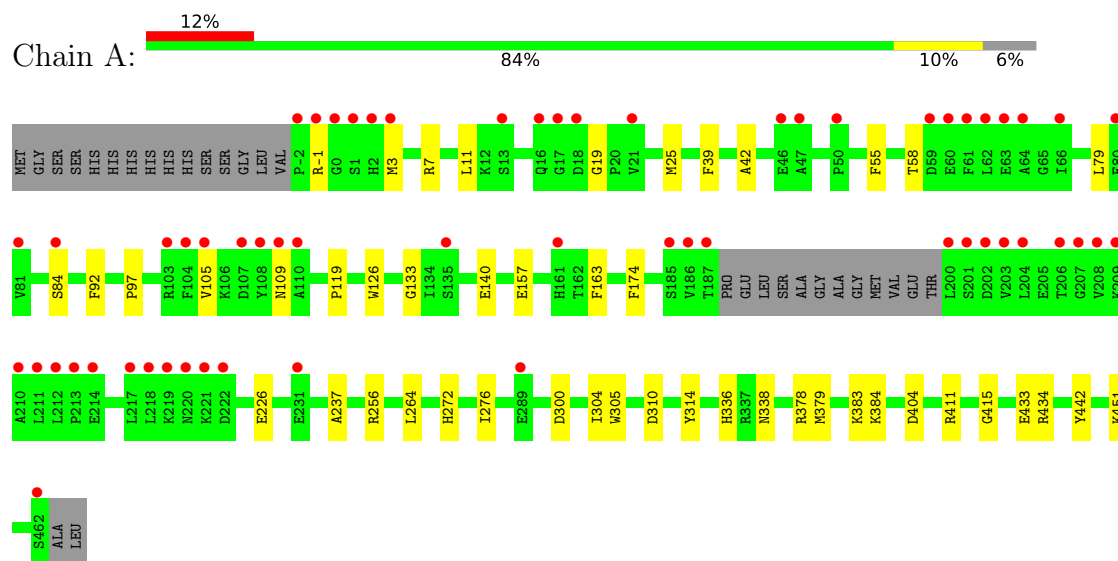
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	13	Total 13	O 13	0	0
7	E	15	Total 15	O 15	0	0
7	F	11	Total 11	O 11	0	0

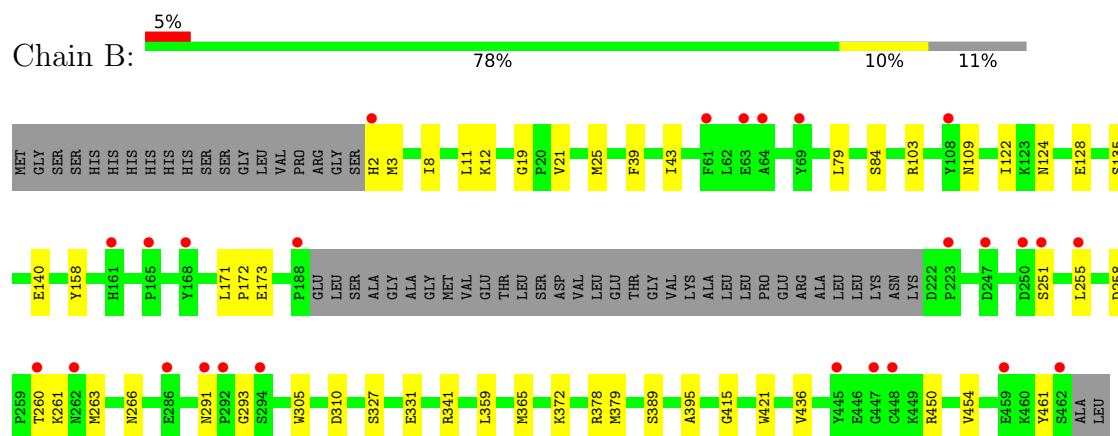
3 Residue-property plots [i](#)

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: Deoxyribodipyrimidine photo-lyase



• Molecule 1: Deoxyribodipyrimidine photo-lyase

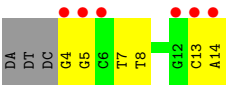


• Molecule 2: Repaired DNA

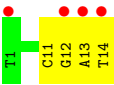




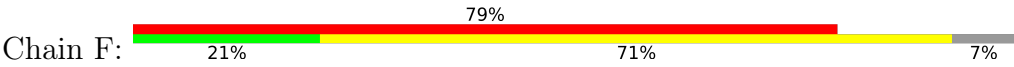
● Molecule 2: Repaired DNA



● Molecule 3: complementary oligonucleotide to the repaired DNA



● Molecule 3: complementary oligonucleotide to the repaired DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.83Å 115.04Å 167.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.50 49.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.29-2.50) 99.9 (49.29-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.218 , 0.259 0.221 , 0.262	Depositor DCC
R_{free} test set	2425 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	3.2	Xtriage
Anisotropy	3.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GOL, SO4, 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	0.19	1/3665 (0.0%)	0.36	0/4973
1	B	0.17	0/3513	0.34	0/4769
2	C	0.52	0/272	0.68	0/417
2	E	0.58	0/251	0.73	0/385
3	D	0.37	0/321	0.54	0/494
3	F	0.36	0/299	0.63	0/460
All	All	0.24	1/8321 (0.0%)	0.41	0/11498

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
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLY	C-O	-5.83	1.20	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	103	ARG	Sidechain
1	B	378	ARG	Sidechain

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	3557	0	3353	32	0
1	B	3406	0	3214	35	0
2	C	244	0	135	7	0
2	E	225	0	124	7	0
3	D	286	0	158	2	0
3	F	266	0	146	7	0
4	A	53	0	31	2	0
4	B	53	0	31	1	0
5	A	5	0	0	0	0
6	A	30	0	40	6	0
6	B	24	0	32	1	0
7	A	264	0	0	6	0
7	B	233	0	0	5	0
7	C	21	0	0	1	0
7	D	13	0	0	0	0
7	E	15	0	0	0	0
7	F	11	0	0	1	0
All	All	8706	0	7264	82	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 5.

All (82) 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:383:LYS:HB3	6:A:503:GOL:H12	1.55	0.89
1:B:140:GLU:OE2	7:B:601:HOH:O	2.02	0.77
1:B:124:ASN:HB2	6:B:503:GOL:H11	1.66	0.76
1:B:25:MET:HE1	1:B:79:LEU:HD21	1.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:O	7:B:602:HOH:O	2.07	0.72
2:C:14:DA:N7	7:C:101:HOH:O	2.21	0.71
3:F:7:DA:N3	7:F:101:HOH:O	2.27	0.68
1:B:12:LYS:NZ	1:B:135:SER:HA	2.08	0.68
1:A:272:HIS:NE2	7:A:605:HOH:O	2.27	0.67
1:A:25:MET:HE1	1:A:79:LEU:HD21	1.78	0.66
1:B:3:MET:HE2	1:B:39:PHE:HB2	1.78	0.66
1:A:300:ASP:OD1	7:A:601:HOH:O	2.14	0.65
1:A:442:TYR:CD1	6:A:503:GOL:H2	2.33	0.64
1:B:327:SER:O	1:B:331:GLU:HG3	1.98	0.63
1:A:442:TYR:HD1	6:A:503:GOL:H2	1.63	0.63
1:B:291:ASN:OD1	1:B:293:GLY:N	2.32	0.63
1:B:255:LEU:HD12	1:B:263:MET:HG3	1.80	0.61
1:B:124:ASN:O	1:B:128:GLU:HG3	2.01	0.60
1:B:8:ILE:HD13	1:B:39:PHE:CE1	2.37	0.60
1:A:58:THR:HG22	1:A:97:PRO:HD3	1.84	0.59
1:B:258:ASP:OD1	1:B:260:THR:OG1	2.20	0.59
1:A:3:MET:HE1	1:A:39:PHE:HA	1.83	0.58
1:A:434:ARG:NH1	7:A:610:HOH:O	2.36	0.58
1:B:2:HIS:N	7:B:613:HOH:O	2.38	0.56
1:A:11:LEU:HD11	1:A:140:GLU:HB2	1.86	0.56
1:B:12:LYS:HZ1	1:B:135:SER:HA	1.69	0.56
1:B:379:MET:SD	2:E:8:DT:C6	2.99	0.55
3:F:1:DT:H2'	3:F:2:DG:C8	2.42	0.55
3:F:5:DC:H2''	3:F:6:DG:C8	2.41	0.55
1:A:379:MET:SD	2:C:8:DT:C6	3.01	0.54
2:E:4:DG:H4'	2:E:5:DG:OP1	2.08	0.53
1:B:359:LEU:HD13	1:B:454:VAL:HG13	1.91	0.53
1:A:55:PHE:HB3	1:A:92:PHE:HD1	1.74	0.52
2:E:13:DC:H2''	2:E:14:DA:C8	2.44	0.52
1:A:336:HIS:NE2	1:A:433:GLU:OE2	2.43	0.51
1:B:389[A]:SER:OG	1:B:395:ALA:HB2	2.10	0.51
1:A:314:TYR:O	6:A:507:GOL:H11	2.12	0.50
3:F:11:DC:H2''	3:F:12:DG:C8	2.47	0.50
1:B:8:ILE:HD13	1:B:39:PHE:CD1	2.47	0.50
1:A:157:GLU:HG3	1:A:163:PHE:CD1	2.46	0.49
1:A:119:PRO:O	6:A:506:GOL:H11	2.12	0.49
1:B:305:TRP:CE3	2:E:7:DT:H72	2.47	0.49
1:B:251:SER:OG	1:B:263:MET:SD	2.70	0.48
1:A:451:LYS:NZ	2:C:10:DG:OP2	2.43	0.48
1:B:11:LEU:HD11	1:B:140:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASN:OD1	1:B:291:ASN:C	2.56	0.48
1:B:171:LEU:N	1:B:172:PRO:HD2	2.29	0.47
3:F:4:DG:H2''	3:F:5:DC:H5''	1.95	0.47
1:A:256:ARG:NH2	7:A:621:HOH:O	2.47	0.47
1:B:450[B]:ARG:NH2	7:B:625:HOH:O	2.48	0.47
1:B:19:GLY:HA3	1:B:109:ASN:O	2.14	0.46
1:A:226:GLU:OE2	7:A:602:HOH:O	2.20	0.46
3:D:11:DC:H2''	3:D:12:DG:C8	2.51	0.45
2:E:7:DT:C4	2:E:8:DT:C4	3.05	0.45
1:B:415:GLY:HA2	4:B:501:FAD:N5	2.33	0.44
1:A:300:ASP:HA	1:A:304:ILE:HD12	1.99	0.44
1:A:237:ALA:HB1	1:A:276:ILE:HB	2.00	0.44
1:A:7:ARG:NH2	1:A:174:PHE:O	2.46	0.44
2:C:3:DC:H2''	2:C:4:DG:C8	2.53	0.43
1:A:19:GLY:HA3	1:A:109:ASN:O	2.19	0.43
1:B:421:TRP:CE2	2:E:8:DT:H71	2.54	0.43
1:A:442:TYR:HA	6:A:503:GOL:H11	2.01	0.43
1:B:122:ILE:HD12	1:B:122:ILE:HA	1.89	0.42
1:A:3:MET:HE2	1:A:42:ALA:CB	2.50	0.42
1:B:21:VAL:HG21	1:B:43:ILE:HG22	2.02	0.42
2:C:4:DG:H2''	2:C:5:DG:O5'	2.20	0.42
1:A:305:TRP:CE3	2:C:7:DT:H72	2.55	0.42
1:A:415:GLY:HA2	4:A:501:FAD:N5	2.35	0.42
3:D:13:DA:H2''	3:D:14:DT:H5'	2.01	0.42
1:B:341:ARG:CZ	1:B:436:VAL:HG13	2.50	0.42
1:A:58:THR:HG21	1:A:126:TRP:CZ2	2.54	0.42
1:A:264:LEU:HB3	4:A:501:FAD:O2P	2.20	0.41
1:A:384:LYS:HA	1:A:384:LYS:HD3	1.87	0.41
1:B:305:TRP:CD2	2:E:7:DT:H72	2.56	0.41
3:F:7:DA:H2''	3:F:8:DA:C8	2.56	0.41
1:B:365:MET:HB3	1:B:461:TYR:HB3	2.03	0.41
1:A:404:ASP:HB3	1:A:411:ARG:HG3	2.03	0.41
1:B:158:TYR:CZ	3:F:10:DC:H4'	2.56	0.40
1:B:266:ASN:HA	1:B:372:LYS:HE3	2.02	0.40
1:B:173:GLU:OE1	7:B:603:HOH:O	2.22	0.40
2:C:7:DT:C4	2:C:8:DT:C4	3.09	0.40
1:A:338:ASN:ND2	7:A:606:HOH:O	2.29	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	452/482 (94%)	441 (98%)	10 (2%)	1 (0%)	43	63
1	B	427/482 (89%)	420 (98%)	7 (2%)	0	100	100
All	All	879/964 (91%)	861 (98%)	17 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG

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	354/416 (85%)	351 (99%)	3 (1%)	73	88
1	B	346/416 (83%)	344 (99%)	2 (1%)	78	91
All	All	700/832 (84%)	695 (99%)	5 (1%)	76	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	105	VAL
1	A	310	ASP
1	B	84	SER
1	B	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	124	ASN
1	B	48	ASN
1	B	124	ASN

5.3.3 RNA [i](#)

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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	B	502	-	5,5,5	0.87	0	5,5,5	1.14	0
6	GOL	A	506	-	5,5,5	1.01	0	5,5,5	0.92	0
6	GOL	A	504	-	5,5,5	1.03	0	5,5,5	0.86	0
5	SO4	A	502	-	4,4,4	0.56	0	6,6,6	0.13	0
6	GOL	A	503	-	5,5,5	0.93	0	5,5,5	1.09	0
6	GOL	A	507	-	5,5,5	0.90	0	5,5,5	1.06	0
6	GOL	B	503	-	5,5,5	0.86	0	5,5,5	1.24	1 (20%)
4	FAD	B	501	-	58,58,58	0.33	0	85,89,89	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	504	-	5,5,5	0.89	0	5,5,5	0.99	0
6	GOL	A	505	-	5,5,5	0.87	0	5,5,5	1.09	0
4	FAD	A	501	-	58,58,58	0.45	0	85,89,89	0.37	0
6	GOL	B	505	-	5,5,5	0.09	0	5,5,5	0.40	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
6	GOL	B	502	-	-	4/4/4/4	-
6	GOL	A	506	-	-	1/4/4/4	-
6	GOL	A	504	-	-	0/4/4/4	-
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	A	503	-	-	2/4/4/4	-
6	GOL	B	503	-	-	4/4/4/4	-
4	FAD	B	501	-	-	3/34/50/50	0/6/6/6
6	GOL	B	504	-	-	0/4/4/4	-
6	GOL	A	505	-	-	1/4/4/4	-
4	FAD	A	501	-	-	3/34/50/50	0/6/6/6
6	GOL	B	505	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	GOL	C3-C2-C1	-2.24	103.57	111.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	B	502	GOL	O1-C1-C2-O2
6	B	502	GOL	O1-C1-C2-C3
6	B	502	GOL	O2-C2-C3-O3
6	B	503	GOL	O1-C1-C2-O2

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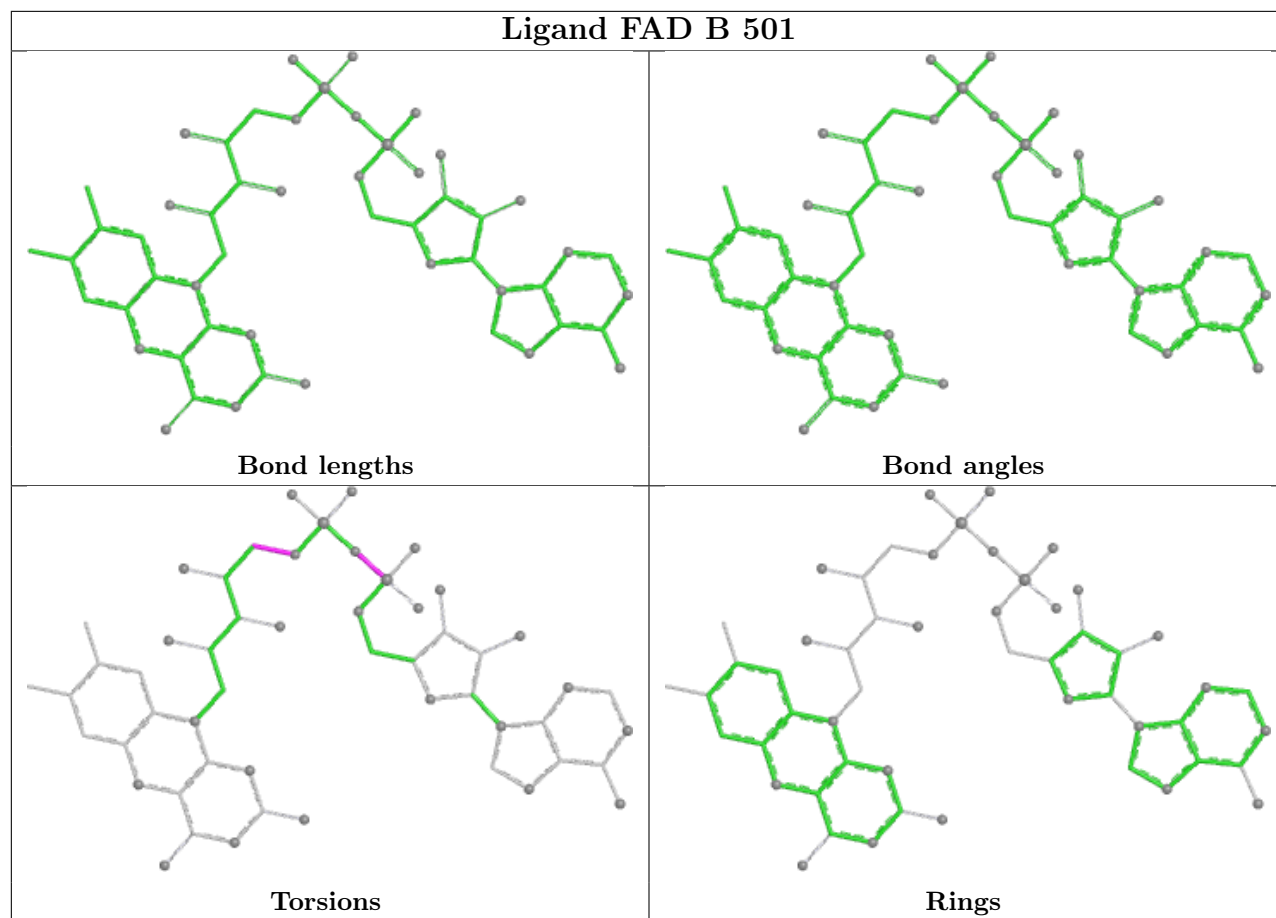
Mol	Chain	Res	Type	Atoms
6	B	503	GOL	O1-C1-C2-C3
6	B	503	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
6	B	502	GOL	C1-C2-C3-O3
6	B	503	GOL	O2-C2-C3-O3
6	A	506	GOL	O1-C1-C2-C3
6	A	505	GOL	O1-C1-C2-O2
6	B	505	GOL	C1-C2-C3-O3
4	A	501	FAD	P-O3P-PA-O1A
6	A	503	GOL	O2-C2-C3-O3
6	B	505	GOL	O2-C2-C3-O3
4	A	501	FAD	C4'-C5'-O5'-P
4	B	501	FAD	C4'-C5'-O5'-P
4	B	501	FAD	P-O3P-PA-O1A
4	B	501	FAD	P-O3P-PA-O2A
4	A	501	FAD	P-O3P-PA-O2A

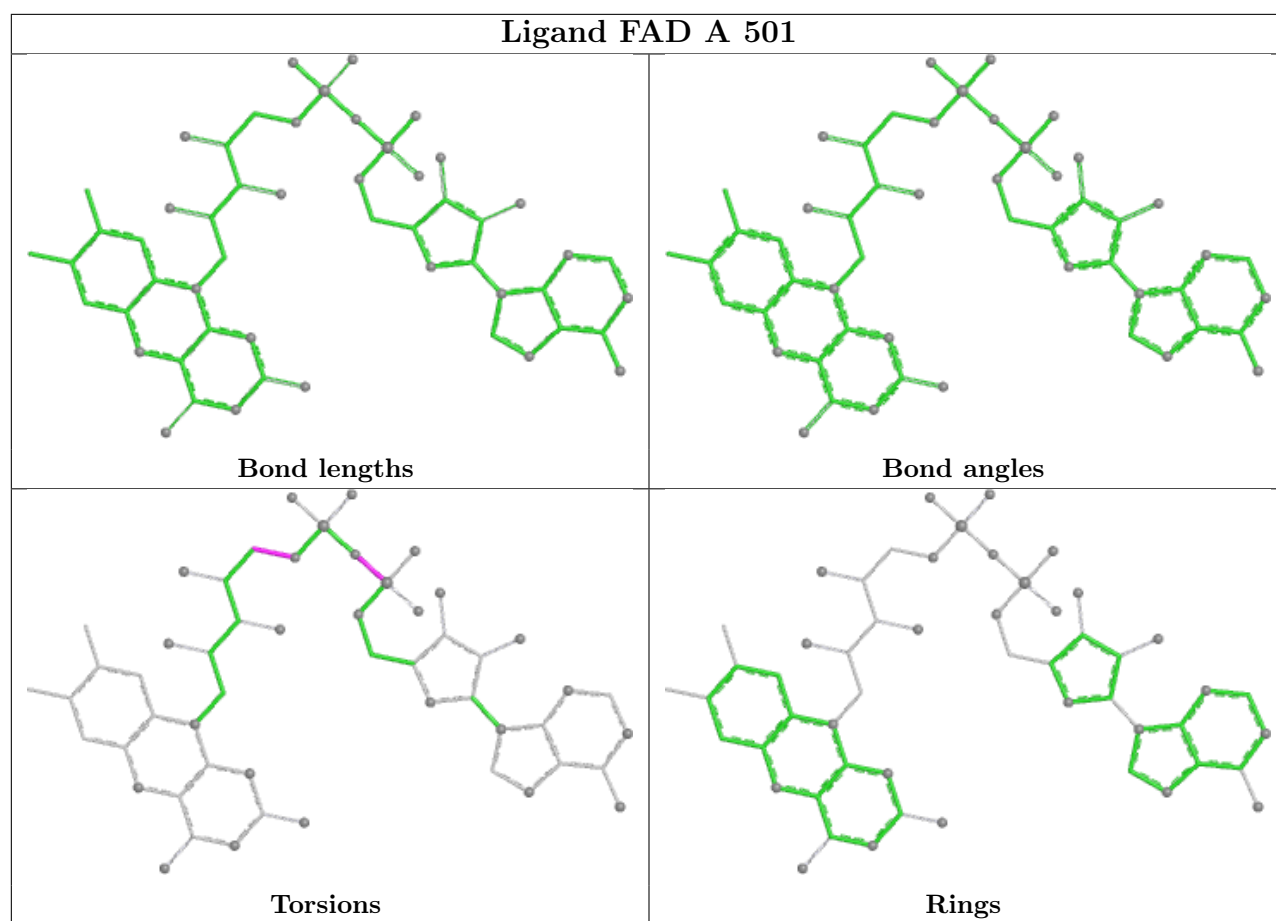
There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	506	GOL	1	0
6	A	503	GOL	4	0
6	A	507	GOL	1	0
6	B	503	GOL	1	0
4	B	501	FAD	1	0
4	A	501	FAD	2	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 ⓘ

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	453/482 (93%)	0.70	59 (13%) 7 6	3, 14, 49, 64	3 (0%)
1	B	428/482 (88%)	0.71	26 (6%) 27 23	6, 20, 38, 51	3 (0%)
2	C	12/14 (85%)	1.32	4 (33%) 1 1	10, 30, 55, 66	0
2	E	11/14 (78%)	2.52	6 (54%) 0 0	28, 40, 68, 72	0
3	D	14/14 (100%)	1.90	4 (28%) 1 1	23, 42, 63, 66	0
3	F	13/14 (92%)	3.18	11 (84%) 0 0	45, 57, 73, 79	0
All	All	931/1020 (91%)	0.79	110 (11%) 9 7	3, 18, 49, 79	6 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	VAL	6.8
1	A	201	SER	5.9
1	A	220	ASN	5.7
3	D	13	DA	5.2
1	A	217	LEU	5.2
1	A	1	SER	4.9
3	F	13	DA	4.9
2	E	13	DC	4.8
1	B	462	SER	4.8
1	A	-2	PRO	4.6
1	A	208	VAL	4.5
1	A	2	HIS	4.3
1	A	222	ASP	4.3
3	F	5	DC	4.3
1	A	214	GLU	4.2
1	A	210	ALA	4.2
1	A	207	GLY	4.1
1	A	218	LEU	4.0
1	A	187	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	GLU	3.9
1	B	161	HIS	3.9
1	A	47	ALA	3.9
3	F	3	DC	3.9
3	F	11	DC	3.9
3	F	4	DG	3.8
1	B	459	GLU	3.8
3	D	14	DT	3.8
1	A	213	PRO	3.7
3	F	12	DG	3.7
2	C	3	DC	3.7
2	E	12	DG	3.7
1	B	108	TYR	3.7
1	A	206	THR	3.6
1	A	18	ASP	3.6
1	A	211	LEU	3.6
1	A	62	LEU	3.6
1	B	291	ASN	3.5
1	A	16	GLN	3.5
1	B	2	HIS	3.5
1	A	203	VAL	3.4
1	B	445	TYR	3.4
2	E	5	DG	3.4
1	A	219	LYS	3.4
2	E	6	DC	3.3
1	A	21	VAL	3.3
1	A	60	GLU	3.3
1	A	61	PHE	3.3
3	F	1	DT	3.3
1	A	0	GLY	3.3
2	E	4	DG	3.2
1	A	212	LEU	3.2
1	A	462	SER	3.2
1	A	200	LEU	3.2
1	A	64	ALA	3.1
1	B	165	PRO	3.1
3	D	1	DT	3.1
1	A	-1	ARG	3.1
1	A	59	ASP	3.1
1	A	185	SER	3.1
2	E	14	DA	3.1
1	B	447	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	221	LYS	3.0
3	F	2	DG	3.0
1	A	107	ASP	3.0
1	A	209	LYS	3.0
1	A	81	VAL	2.9
2	C	14	DA	2.9
1	A	105	VAL	2.9
3	D	12	DG	2.9
2	C	13	DC	2.8
1	A	63	GLU	2.7
1	B	255	LEU	2.7
1	B	64	ALA	2.7
1	B	251	SER	2.6
1	A	109	ASN	2.6
1	B	448	CYS	2.6
1	B	260	THR	2.5
1	B	292	PRO	2.5
1	A	202	ASP	2.5
1	A	13	SER	2.4
1	A	3	MET	2.4
1	B	286	GLU	2.4
1	A	135	SER	2.3
3	F	10	DC	2.3
1	A	108	TYR	2.3
1	B	262	ASN	2.3
1	A	204	LEU	2.3
1	A	46	GLU	2.3
1	B	168	TYR	2.3
3	F	6	DG	2.3
1	A	231	GLU	2.2
1	A	104	PHE	2.2
1	A	50	PRO	2.2
1	A	66[A]	ILE	2.2
3	F	8	DA	2.2
1	A	80	GLU	2.2
1	A	289	GLU	2.2
1	B	223	PRO	2.2
1	B	69	TYR	2.1
1	A	17	GLY	2.1
1	A	110	ALA	2.1
1	B	294	SER	2.1
2	C	4	DG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	161	HIS	2.1
1	B	247	ASP	2.1
1	A	84	SER	2.1
1	B	61	PHE	2.0
1	B	250	ASP	2.0
1	B	188	PRO	2.0
1	A	103	ARG	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](#)

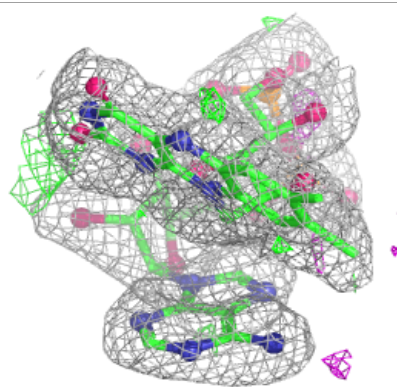
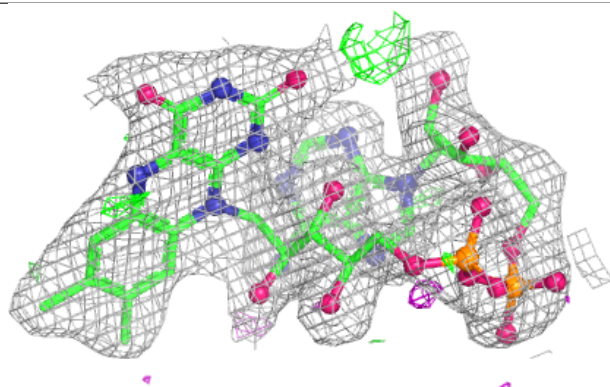
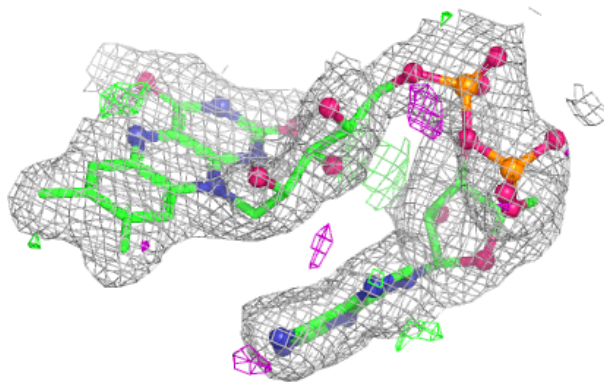
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	505	6/6	0.70	0.23	24,30,37,46	0
6	GOL	B	502	6/6	0.75	0.18	32,37,39,43	0
6	GOL	B	503	6/6	0.82	0.20	17,21,29,34	0
6	GOL	A	504	6/6	0.85	0.17	28,37,41,42	0
6	GOL	A	507	6/6	0.85	0.24	21,32,38,43	0
6	GOL	A	503	6/6	0.89	0.28	9,16,20,21	0
6	GOL	B	504	6/6	0.89	0.15	27,29,33,35	0
6	GOL	B	505	6/6	0.89	0.15	24,33,37,37	0
5	SO4	A	502	5/5	0.92	0.14	26,30,34,36	0
6	GOL	A	506	6/6	0.93	0.15	12,15,19,26	0
4	FAD	B	501	53/53	0.93	0.11	7,15,26,31	0
4	FAD	A	501	53/53	0.96	0.09	1,3,5,12	0

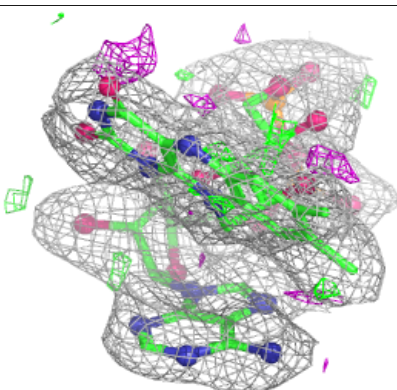
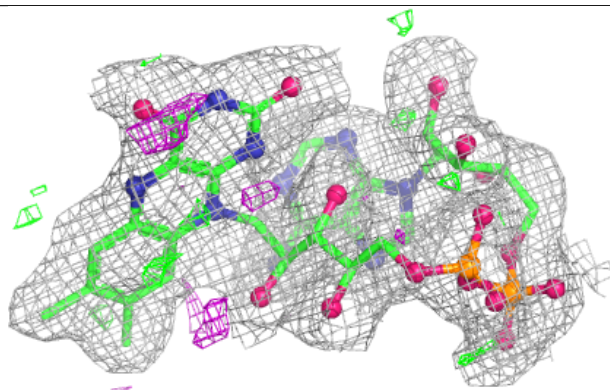
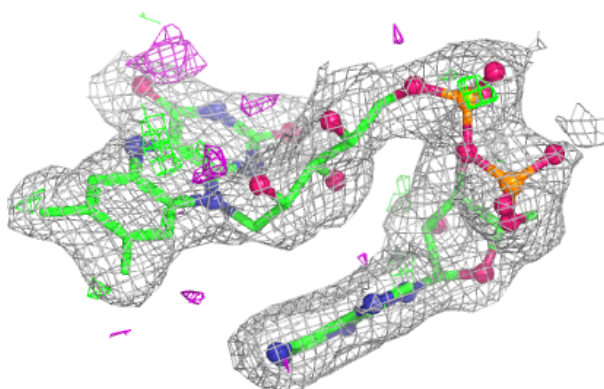
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 501:

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

**Electron density around FAD A 501:**

$2mF_o-DF_c$ (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.