



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 11:09 PM JST

PDB ID : 7C0T
Title : Crystal structure of a dinucleotide-binding protein (N81A) of ABC transporter endogenously bound to uridylyl-3'-5'-phospho-guanosine
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.
Deposited on : 2020-05-01
Resolution : 1.77 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

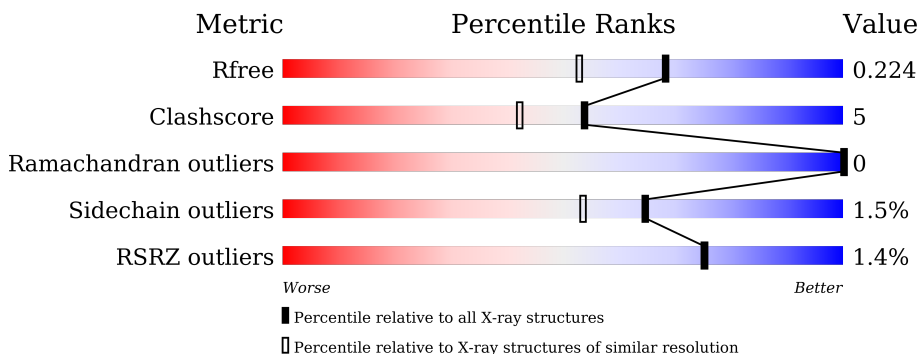
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	406	 2% 89% 8% ..
1	B	406	 % 90% 7% .

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
10	PDO	B	503	-	-	X	-
5	PEG	A	506	-	-	X	-
6	GOL	A	507	-	-	X	-
7	PGE	A	508	-	-	X	-
7	PGE	A	509	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7170 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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3083	1998	517	563	5	0	5	0
1	B	396	3089	2002	519	564	4	0	7	0

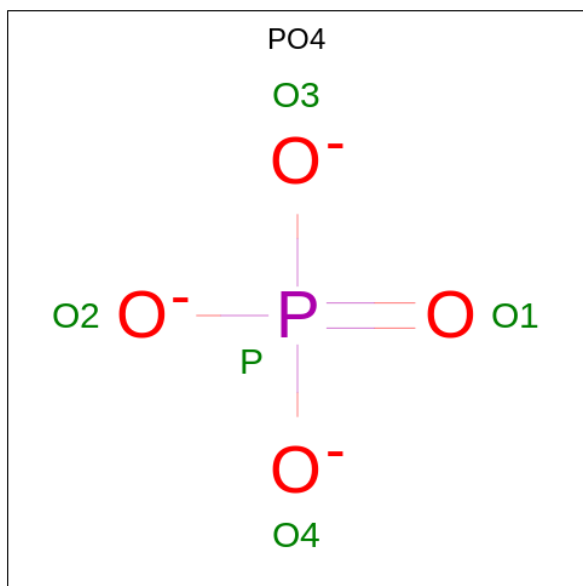
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q5SLB4
A	0	MET	-	expression tag	UNP Q5SLB4
A	81	ALA	ASN	engineered mutation	UNP Q5SLB4
A	399	HIS	-	expression tag	UNP Q5SLB4
A	400	HIS	-	expression tag	UNP Q5SLB4
A	401	HIS	-	expression tag	UNP Q5SLB4
A	402	HIS	-	expression tag	UNP Q5SLB4
A	403	HIS	-	expression tag	UNP Q5SLB4
A	404	HIS	-	expression tag	UNP Q5SLB4
B	-1	MET	-	initiating methionine	UNP Q5SLB4
B	0	MET	-	expression tag	UNP Q5SLB4
B	81	ALA	ASN	engineered mutation	UNP Q5SLB4
B	399	HIS	-	expression tag	UNP Q5SLB4
B	400	HIS	-	expression tag	UNP Q5SLB4
B	401	HIS	-	expression tag	UNP Q5SLB4
B	402	HIS	-	expression tag	UNP Q5SLB4
B	403	HIS	-	expression tag	UNP Q5SLB4
B	404	HIS	-	expression tag	UNP Q5SLB4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

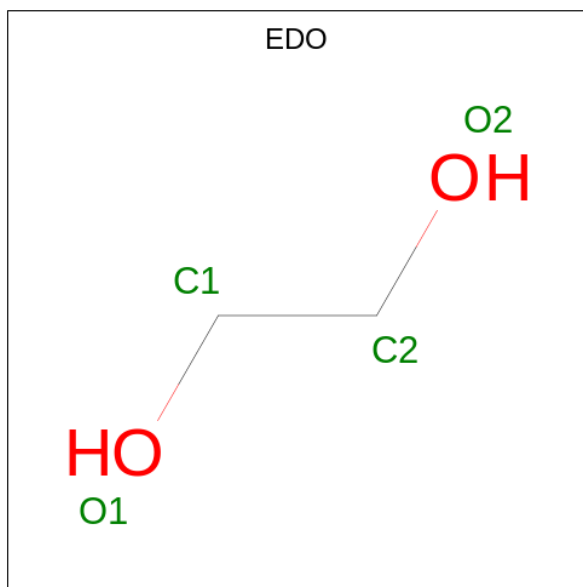
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



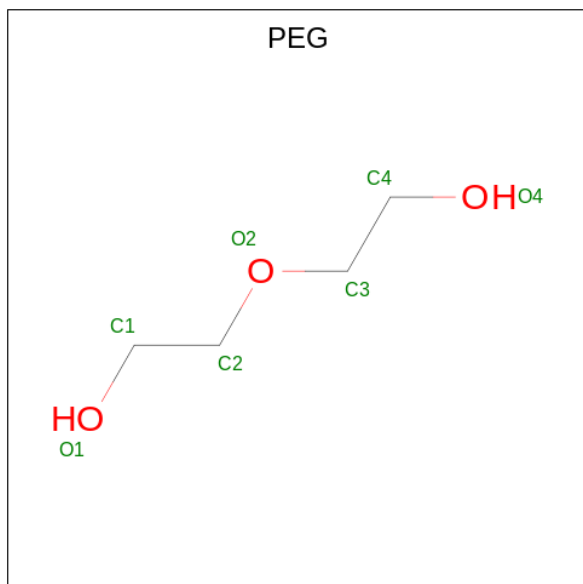
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

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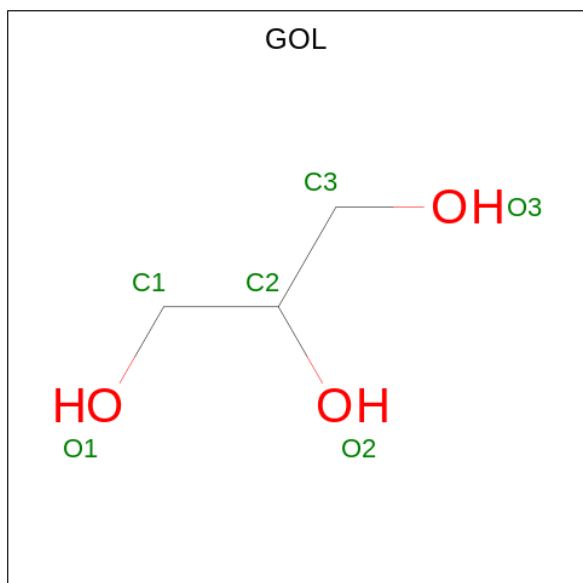
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



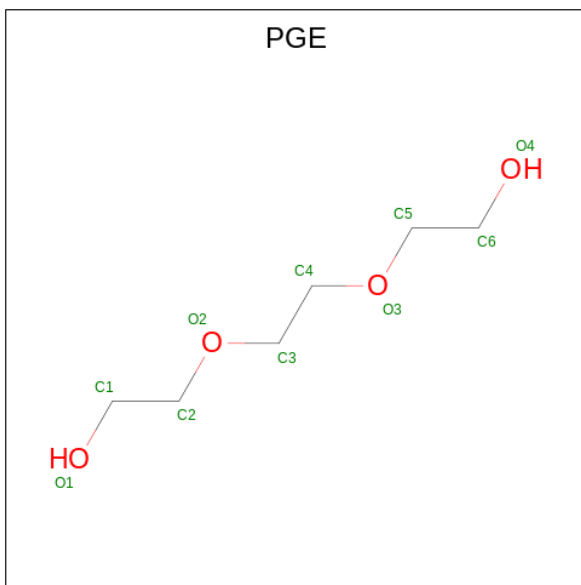
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



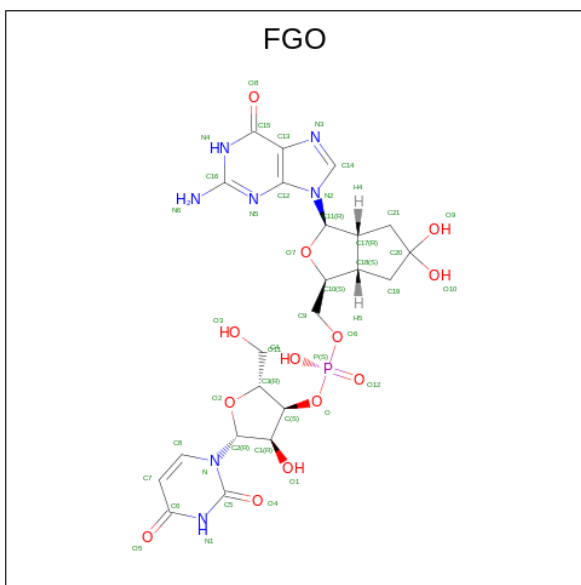
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



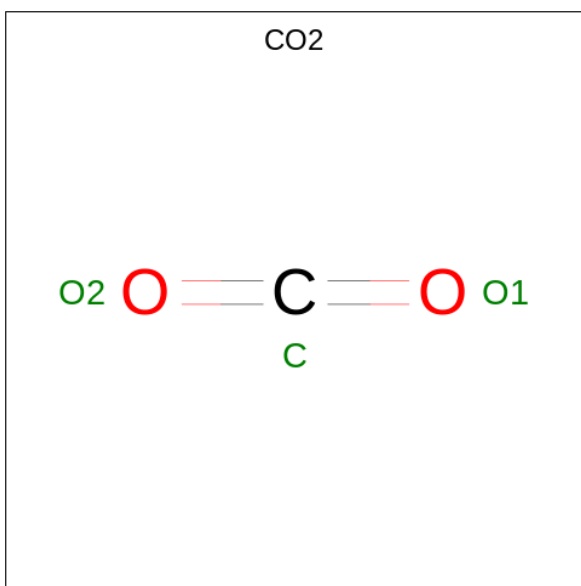
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is [(1S,3R,3aR,6aS)-3-(2-azanyl-6-oxidanylidene-1H-purin-9-yl)-5,5-bis(oxidanyl)-1,3,3a,4,6,6a-hexahydrocyclopenta[c]furan-1-yl)methyl [(2R,3S,4R,5R)-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-2-(hydroxymethyl)-4-oxidanyl-oxolan-3-yl] hydrogen phosphate (three-letter code: FGO) (formula: C₂₂H₂₈N₇O₁₃P) (labeled as "Ligand of Interest" by depositor).



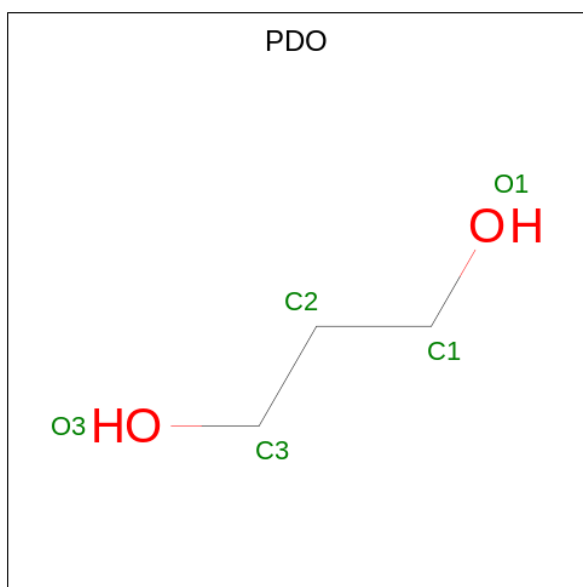
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
8	A	1	43	22	7	13	1	0	0
8	B	1	43	22	7	13	1	0	0

- Molecule 9 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
9	B	1	3	1 2	0	0

- Molecule 10 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			5	3	2		

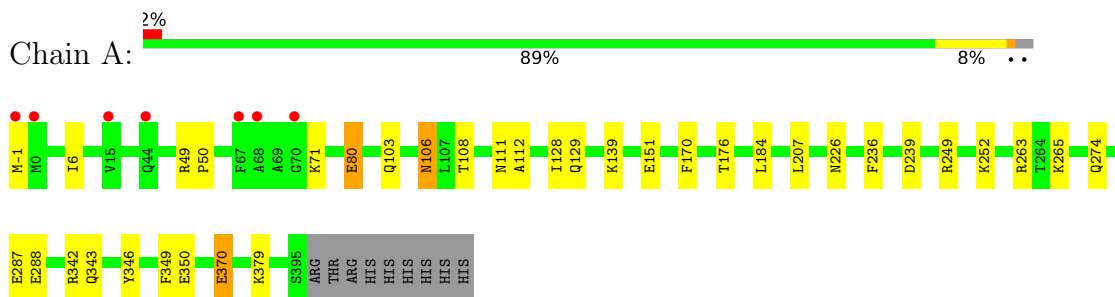
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	409	Total	O	0	0
			409	409		
11	B	436	Total	O	0	0
			436	436		

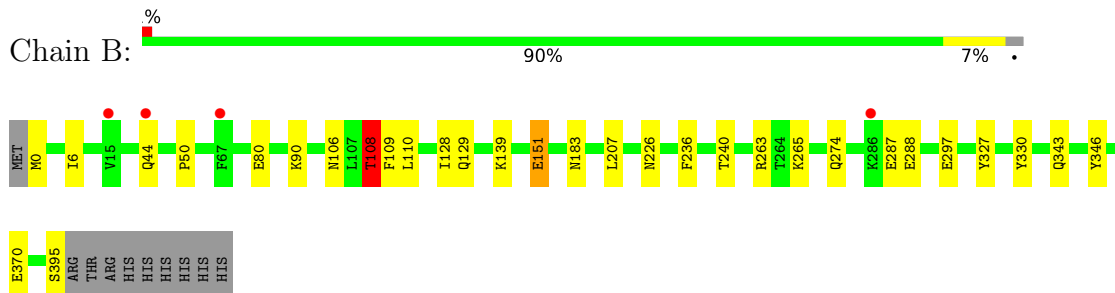
3 Residue-property plots [i](#)

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: Sugar ABC transporter, periplasmic sugar-binding protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.61Å 58.34Å 123.48Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	60.67 – 1.77 60.67 – 1.77	Depositor EDS
% Data completeness (in resolution range)	95.2 (60.67-1.77) 95.2 (60.67-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.181 , 0.219 0.189 , 0.224	Depositor DCC
R_{free} test set	4376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: EDO, PO4, GOL, FGO, CL, PEG, PDO, PGE, CO2

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	1.01	6/3168 (0.2%)	1.01	3/4295 (0.1%)
1	B	1.01	9/3180 (0.3%)	1.03	9/4311 (0.2%)
All	All	1.01	15/6348 (0.2%)	1.02	12/8606 (0.1%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80[A]	GLU	CD-OE2	11.82	1.38	1.25
1	B	80[B]	GLU	CD-OE2	11.82	1.38	1.25
1	A	80	GLU	CD-OE2	8.18	1.34	1.25
1	A	287	GLU	CD-OE1	7.94	1.34	1.25
1	A	139	LYS	C-O	7.32	1.37	1.23
1	B	287	GLU	CD-OE1	7.06	1.33	1.25
1	B	288	GLU	CD-OE2	6.99	1.33	1.25
1	B	288	GLU	CD-OE1	6.47	1.32	1.25
1	A	288	GLU	CD-OE1	6.36	1.32	1.25
1	B	297[A]	GLU	CD-OE2	5.60	1.31	1.25
1	B	297[B]	GLU	CD-OE2	5.60	1.31	1.25
1	A	288	GLU	CD-OE2	5.52	1.31	1.25
1	A	370	GLU	CD-OE1	5.46	1.31	1.25
1	B	151	GLU	CD-OE1	-5.11	1.20	1.25
1	B	139	LYS	C-O	5.02	1.32	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	A	346	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	B	80[A]	GLU	CB-CA-C	6.53	123.45	110.40
1	B	80[B]	GLU	CB-CA-C	6.53	123.45	110.40
1	B	327	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	236	PHE	CB-CA-C	-5.78	98.83	110.40
1	B	236	PHE	CB-CA-C	-5.68	99.05	110.40
1	B	109	PHE	CB-CG-CD1	5.66	124.76	120.80
1	B	346	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	49	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	236	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	B	108	THR	N-CA-CB	-5.17	100.48	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	LYS	Mainchain

5.2 Too-close contacts [i](#)

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	3083	0	3134	35	0
1	B	3089	0	3144	22	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	8	0	12	0	0
5	A	7	0	10	5	0
6	A	6	0	8	6	0
6	B	6	0	8	0	0
7	A	20	0	28	22	0
8	A	43	0	0	0	0
8	B	43	0	0	0	0
9	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	5	0	7	6	0
11	A	409	0	0	8	0
11	B	436	0	0	8	0
All	All	7170	0	6351	67	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 (67) 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:80:GLU:HB2	7:A:509:PGE:H1	1.29	1.10
1:B:263[B]:ARG:HH21	1:B:263[B]:ARG:HG3	1.06	1.05
1:A:106:ASN:OD1	1:A:108:THR:HB	1.58	1.04
7:A:509:PGE:H12	11:A:675:HOH:O	1.57	1.03
10:B:503:PDO:H31	11:B:717:HOH:O	1.69	0.92
1:A:249:ARG:NH1	11:A:601:HOH:O	2.04	0.88
1:A:111:ASN:HB3	11:A:794:HOH:O	1.74	0.85
1:A:239:ASP:HA	5:A:506:PEG:H12	1.60	0.84
1:A:263:ARG:HG3	6:A:507:GOL:H12	1.58	0.83
1:B:263[B]:ARG:HG3	1:B:263[B]:ARG:NH2	1.85	0.81
1:B:274:GLN:HE22	10:B:503:PDO:H12	1.46	0.80
1:A:80:GLU:CB	7:A:509:PGE:H1	2.12	0.78
1:A:350:GLU:O	7:A:509:PGE:C2	2.32	0.78
1:B:207:LEU:HD12	11:B:853:HOH:O	1.82	0.78
1:A:263:ARG:CG	6:A:507:GOL:H12	2.15	0.76
1:A:350:GLU:O	7:A:509:PGE:H22	1.86	0.75
1:A:349:PHE:HB3	7:A:509:PGE:H22	1.69	0.74
5:A:506:PEG:H42	11:A:751:HOH:O	1.89	0.73
1:A:263:ARG:HD2	6:A:507:GOL:H31	1.73	0.70
1:B:274:GLN:HE22	10:B:503:PDO:C1	2.04	0.69
1:A:239:ASP:HA	5:A:506:PEG:C1	2.22	0.69
1:B:263[B]:ARG:HH21	1:B:263[B]:ARG:CG	1.94	0.66
1:B:274:GLN:NE2	10:B:503:PDO:H12	2.10	0.66
1:A:370:GLU:HG2	11:A:864:HOH:O	1.95	0.66
7:A:508:PGE:H32	7:A:508:PGE:H62	1.76	0.66
1:B:44:GLN:HB2	11:B:910:HOH:O	1.97	0.63
1:B:108:THR:HG21	11:B:700:HOH:O	1.98	0.63
1:A:207:LEU:HD12	11:A:872:HOH:O	1.98	0.63
1:B:370:GLU:HG2	11:B:638:HOH:O	1.98	0.62
1:B:106:ASN:OD1	1:B:108:THR:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:O	7:A:509:PGE:H2	2.01	0.59
7:A:508:PGE:H52	7:A:509:PGE:O4	2.03	0.59
1:B:151:GLU:OE2	1:B:265:LYS:NZ	2.35	0.58
7:A:508:PGE:O1	7:A:508:PGE:H3	2.03	0.58
7:A:508:PGE:H42	11:A:606:HOH:O	2.04	0.57
1:A:151:GLU:OE2	1:A:265:LYS:NZ	2.39	0.55
7:A:508:PGE:H52	7:A:509:PGE:C6	2.38	0.54
7:A:508:PGE:H32	7:A:508:PGE:C6	2.38	0.53
1:A:112:ALA:HB2	7:A:509:PGE:H6	1.90	0.53
1:B:263[A]:ARG:NH1	11:B:607:HOH:O	2.42	0.53
7:A:508:PGE:C5	7:A:509:PGE:O4	2.59	0.51
1:B:330:TYR:CD2	11:B:661:HOH:O	2.55	0.50
1:A:263:ARG:HD2	6:A:507:GOL:C3	2.41	0.50
1:A:112:ALA:HA	7:A:509:PGE:H4	1.94	0.50
1:A:184:LEU:HA	6:A:507:GOL:H32	1.93	0.49
1:A:263:ARG:HG3	6:A:507:GOL:C1	2.37	0.48
1:B:263[B]:ARG:HD2	1:B:263[B]:ARG:HA	1.46	0.48
1:A:112:ALA:HA	7:A:509:PGE:C4	2.45	0.47
1:B:183:ASN:O	1:B:263[B]:ARG:HD3	2.15	0.47
1:B:90:LYS:N	1:B:90:LYS:HD3	2.31	0.46
1:A:274:GLN:HE22	5:A:506:PEG:C2	2.29	0.46
1:B:240:THR:HB	10:B:503:PDO:H12	1.98	0.46
1:A:112:ALA:CB	7:A:509:PGE:H4	2.47	0.45
1:A:6:ILE:HG21	1:A:50:PRO:HD2	2.00	0.44
1:A:170:PHE:HB2	1:A:176:THR:HG21	2.00	0.44
1:A:129:GLN:HE21	5:A:506:PEG:C1	2.30	0.43
1:A:349:PHE:CE1	7:A:509:PGE:H62	2.53	0.43
1:B:129:GLN:HE21	10:B:503:PDO:H22	1.84	0.43
1:B:128:ILE:HG12	1:B:343:GLN:HG3	1.99	0.43
1:A:342[A]:ARG:HH11	1:A:342[A]:ARG:HG3	1.82	0.43
1:A:379:LYS:HD2	11:A:1003:HOH:O	2.17	0.42
1:B:0:MET:HB2	11:B:912:HOH:O	2.20	0.42
1:A:128:ILE:HG12	1:A:343:GLN:HG3	2.01	0.42
1:A:112:ALA:N	7:A:509:PGE:H6	2.35	0.41
1:A:112:ALA:HB2	7:A:509:PGE:C6	2.50	0.41
1:A:349:PHE:HD1	7:A:508:PGE:H6	1.86	0.41
1:B:6:ILE:HG21	1:B:50:PRO:HD2	2.03	0.41

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	400/406 (98%)	393 (98%)	7 (2%)	0	100	100
1	B	401/406 (99%)	396 (99%)	5 (1%)	0	100	100
All	All	801/812 (99%)	789 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	314/318 (99%)	309 (98%)	5 (2%)	62	51
1	B	315/318 (99%)	311 (99%)	4 (1%)	69	59
All	All	629/636 (99%)	620 (99%)	9 (1%)	65	56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	71	LYS
1	A	103	GLN
1	A	106	ASN
1	A	226	ASN
1	B	108	THR
1	B	110	LEU
1	B	226	ASN

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Mol	Chain	Res	Type
1	B	395	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	274	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
6	GOL	A	507	-	5,5,5	0.20	0	5,5,5	0.54	0
3	PO4	A	503	-	4,4,4	1.10	0	6,6,6	0.56	0
8	FGO	A	510	-	44,48,48	1.77	7 (15%)	50,75,75	1.67	12 (24%)
9	CO2	B	501	-	2,2,2	0.35	0	1,1,1	1.26	0
3	PO4	B	502	-	4,4,4	0.98	0	6,6,6	0.44	0
4	EDO	A	504	-	3,3,3	0.04	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PDO	B	503	-	4,4,4	0.78	0	3,3,3	0.58	0
6	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.66	0
5	PEG	A	506	-	6,6,6	0.52	0	5,5,5	0.36	0
7	PGE	A	508	-	9,9,9	0.36	0	8,8,8	0.63	0
8	FGO	B	505	-	44,48,48	1.78	7 (15%)	50,75,75	1.63	12 (24%)
4	EDO	A	505	-	3,3,3	0.18	0	2,2,2	0.08	0
7	PGE	A	509	-	9,9,9	0.20	0	8,8,8	0.36	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	A	507	-	-	2/4/4/4	-
8	FGO	A	510	-	-	0/17/63/63	0/6/6/6
4	EDO	A	504	-	-	0/1/1/1	-
10	PDO	B	503	-	-	0/2/2/2	-
6	GOL	B	504	-	-	0/4/4/4	-
5	PEG	A	506	-	-	4/4/4/4	-
7	PGE	A	508	-	-	5/7/7/7	-
8	FGO	B	505	-	-	0/17/63/63	0/6/6/6
4	EDO	A	505	-	-	1/1/1/1	-
7	PGE	A	509	-	-	3/7/7/7	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	505	FGO	C19-C18	-5.95	1.44	1.53
8	A	510	FGO	C19-C18	-5.74	1.44	1.53
8	A	510	FGO	C21-C17	-4.48	1.46	1.53
8	B	505	FGO	O5-C6	4.41	1.33	1.24
8	A	510	FGO	O5-C6	4.36	1.33	1.24
8	B	505	FGO	C21-C17	-4.16	1.47	1.53
8	B	505	FGO	C8-C7	3.97	1.44	1.35
8	A	510	FGO	C8-C7	3.72	1.43	1.35
8	A	510	FGO	C5-N1	-3.67	1.31	1.38
8	B	505	FGO	C15-N4	-2.83	1.33	1.37
8	A	510	FGO	O8-C15	2.40	1.28	1.23
8	B	505	FGO	C5-N1	-2.34	1.33	1.38
8	A	510	FGO	C15-N4	-2.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	505	FGO	O2-C3	-2.02	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	505	FGO	N1-C5-N	4.15	120.40	114.89
8	A	510	FGO	C7-C6-N1	4.13	121.01	114.84
8	B	505	FGO	C7-C6-N1	3.97	120.78	114.84
8	A	510	FGO	N1-C5-N	3.96	120.14	114.89
8	B	505	FGO	O5-C6-N1	-3.30	114.47	119.31
8	A	510	FGO	O5-C6-N1	-3.25	114.53	119.31
8	A	510	FGO	C6-N1-C5	-2.93	122.72	126.58
8	A	510	FGO	C14-N3-C13	2.89	108.50	102.99
8	A	510	FGO	O4-C5-N	-2.89	118.95	122.79
8	A	510	FGO	O8-C15-N4	2.86	124.03	120.65
8	B	505	FGO	O9-C20-C19	-2.84	101.18	110.56
8	A	510	FGO	O2-C2-C1	-2.74	100.66	106.64
8	B	505	FGO	O9-C20-C21	2.69	119.47	110.56
8	A	510	FGO	N6-C16-N5	-2.67	114.54	119.74
8	A	510	FGO	C3-O2-C2	2.61	115.22	109.47
8	B	505	FGO	C8-C7-C6	-2.60	115.97	119.52
8	B	505	FGO	O4-C5-N	-2.58	119.36	122.79
8	B	505	FGO	N6-C16-N5	-2.57	114.74	119.74
8	B	505	FGO	C6-N1-C5	-2.43	123.37	126.58
8	B	505	FGO	C14-N3-C13	2.28	107.33	102.99
8	B	505	FGO	C2-N-C8	2.21	125.65	120.84
8	A	510	FGO	C8-C7-C6	-2.12	116.62	119.52
8	B	505	FGO	O7-C10-C18	-2.11	101.07	104.89
8	A	510	FGO	N4-C16-N5	2.11	127.25	123.32

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	507	GOL	C1-C2-C3-O3
7	A	508	PGE	C1-C2-O2-C3
7	A	509	PGE	O2-C3-C4-O3
5	A	506	PEG	O1-C1-C2-O2
5	A	506	PEG	O2-C3-C4-O4
4	A	505	EDO	O1-C1-C2-O2
7	A	508	PGE	O3-C5-C6-O4
7	A	509	PGE	O3-C5-C6-O4

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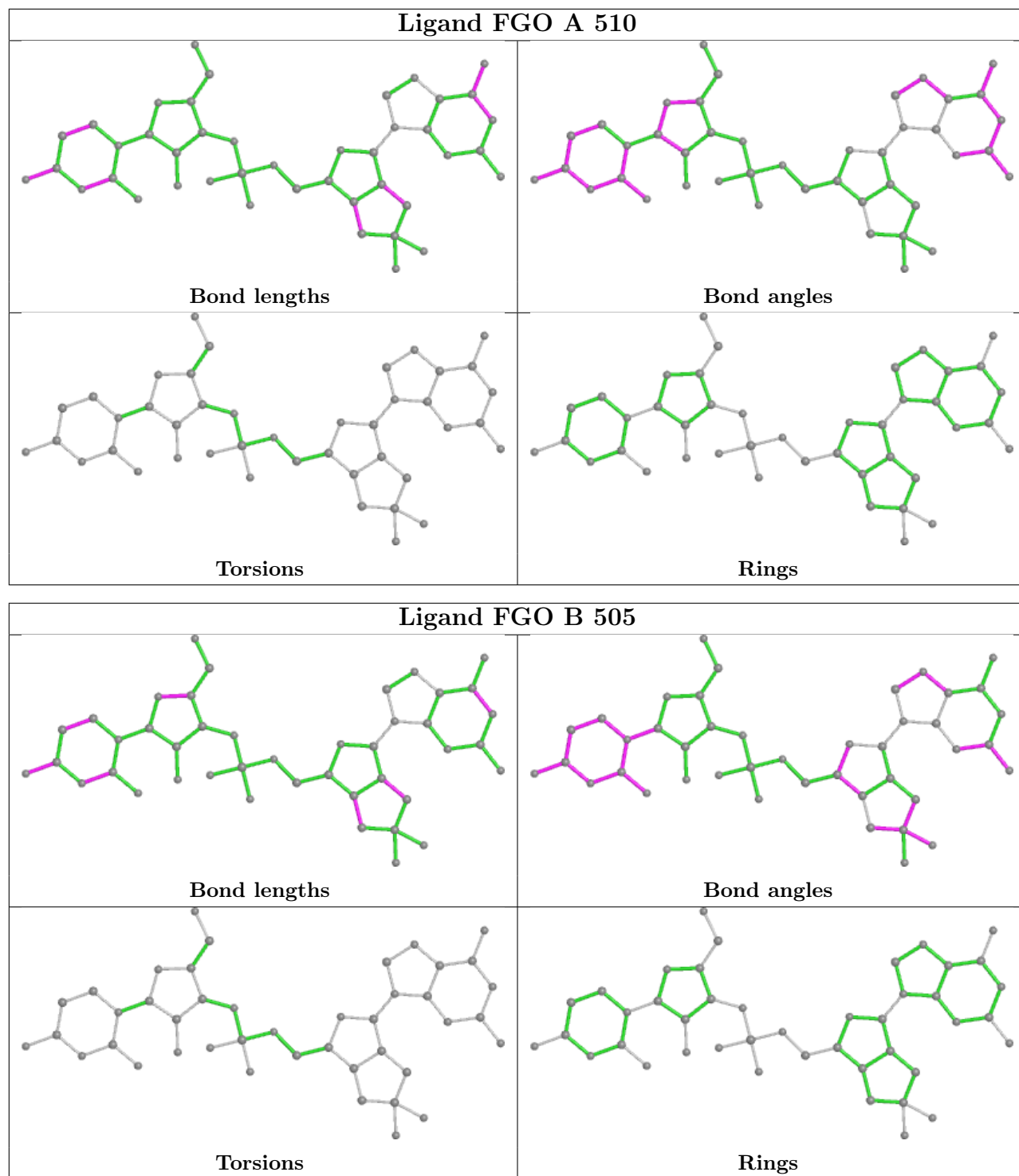
Mol	Chain	Res	Type	Atoms
5	A	506	PEG	C4-C3-O2-C2
7	A	508	PGE	C4-C3-O2-C2
5	A	506	PEG	C1-C2-O2-C3
7	A	508	PGE	O2-C3-C4-O3
7	A	509	PGE	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
7	A	508	PGE	C6-C5-O3-C4

There are no ring outliers.

5 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	GOL	6	0
10	B	503	PDO	6	0
5	A	506	PEG	5	0
7	A	508	PGE	8	0
7	A	509	PGE	17	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

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	397/406 (97%)	0.03	7 (1%) 68 68	6, 16, 35, 64	0
1	B	396/406 (97%)	-0.00	4 (1%) 82 82	7, 16, 32, 59	0
All	All	793/812 (97%)	0.01	11 (1%) 75 75	6, 16, 34, 64	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLN	7.0
1	B	44	GLN	5.0
1	A	68	ALA	3.5
1	A	67	PHE	3.2
1	A	-1	MET	2.8
1	B	67	PHE	2.7
1	A	70	GLY	2.6
1	A	15	VAL	2.2
1	B	286	LYS	2.2
1	A	0	MET	2.0
1	B	15	VAL	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 monosaccharides in this entry.

6.4 Ligands

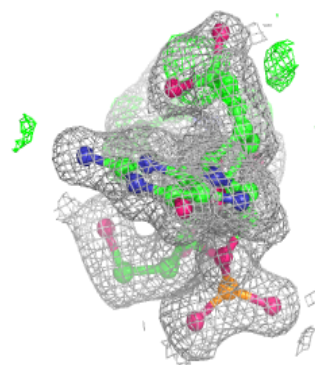
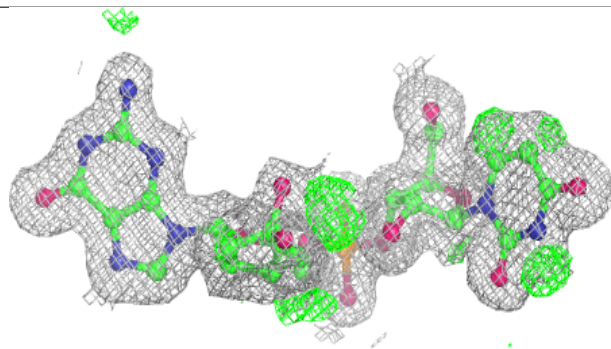
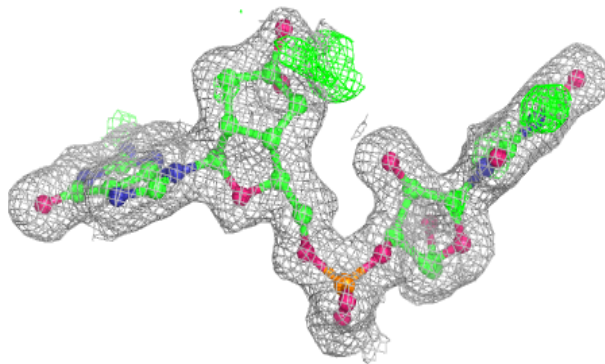
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	502	1/1	0.73	0.08	57,57,57,57	0
3	PO4	B	502	5/5	0.74	0.24	42,45,49,56	0
6	GOL	A	507	6/6	0.75	0.22	33,38,39,41	0
9	CO2	B	501	3/3	0.77	0.13	29,29,33,35	0
3	PO4	A	503	5/5	0.84	0.18	36,45,45,48	0
4	EDO	A	504	4/4	0.86	0.09	31,36,37,37	0
7	PGE	A	508	10/10	0.87	0.22	23,25,30,31	0
7	PGE	A	509	10/10	0.89	0.28	26,33,37,37	0
5	PEG	A	506	7/7	0.90	0.21	17,24,28,31	0
6	GOL	B	504	6/6	0.91	0.15	16,21,26,28	0
4	EDO	A	505	4/4	0.92	0.10	34,38,41,41	0
10	PDO	B	503	5/5	0.93	0.17	17,20,23,26	0
8	FGO	B	505	43/43	0.95	0.10	8,13,18,31	0
8	FGO	A	510	43/43	0.96	0.10	9,12,18,31	0
2	CL	A	501	1/1	0.98	0.07	33,33,33,33	0

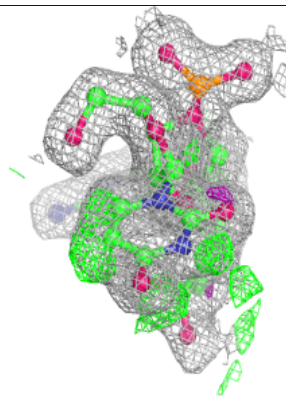
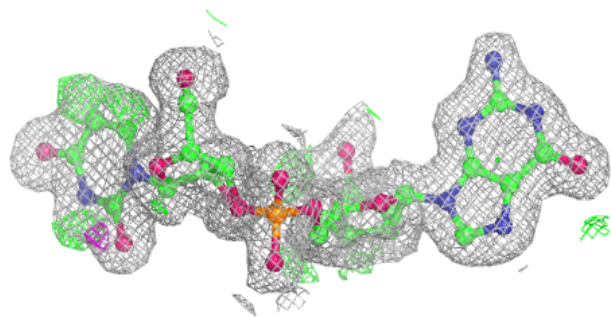
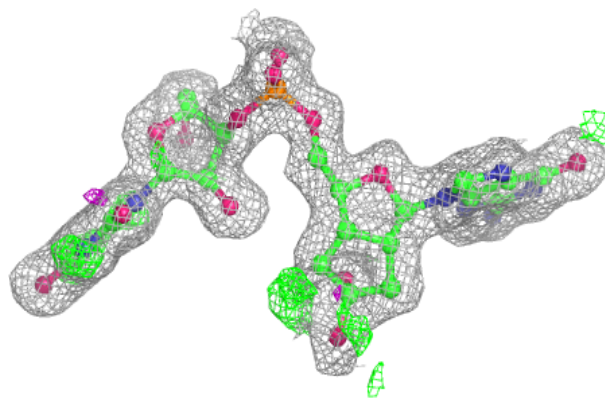
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FGO B 505:

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

**Electron density around FGO A 510:**

$2mF_o-DF_c$ (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.