



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 12:32 PM JST

PDB ID : 7C0F
Title : Crystal structure of a dinucleotide-binding protein of ABC transporter endogenously bound to uridylyl-3'-5'-phospho-guanosine (Form I)
Authors : Kanaujia, S.P.; Chandravanshi, M.
Deposited on : 2020-05-01
Resolution : 2.15 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 : 2.23.1
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) : 2.23.1

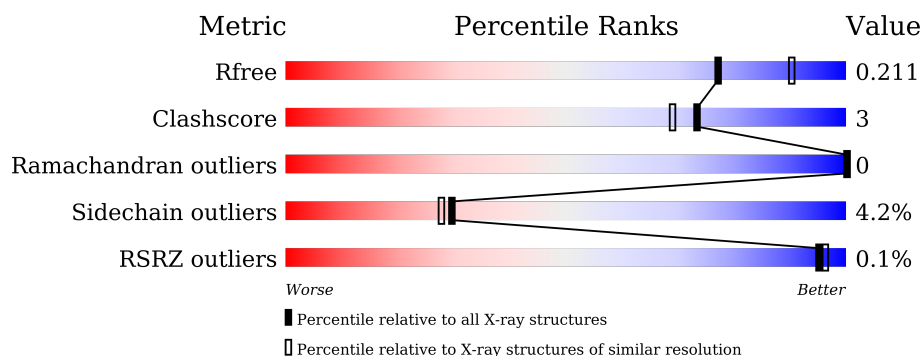
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	
1	B	406	

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
4	CO2	A	507	-	-	X	-
6	GOL	B	508	-	-	X	-
8	PDO	A	517	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 6784 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
1	A	395	Total	C	N	O	S	0	3	0
			3064	1983	519	559	3			
1	B	395	Total	C	N	O	S	0	1	0
			3050	1973	515	559	3			

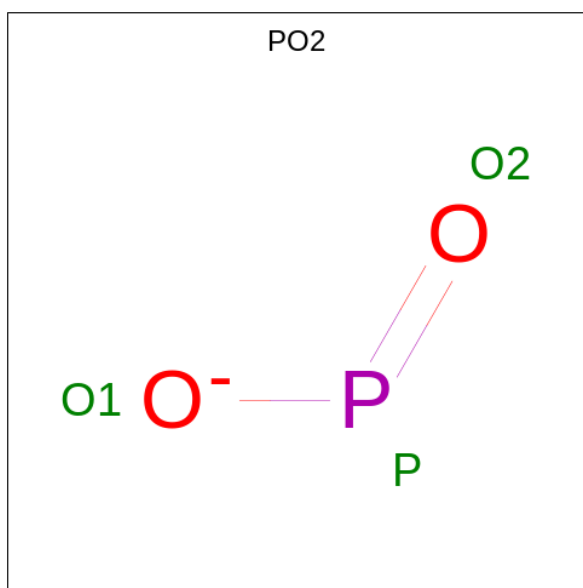
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q5SLB4
A	0	MET	-	expression tag	UNP Q5SLB4
A	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	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).

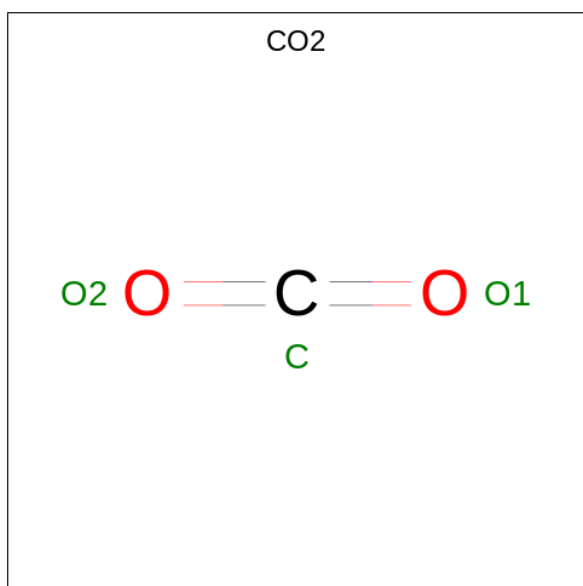
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is HYPOPHOSPHITE (three-letter code: PO2) (formula: O_2P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			3	2	1		
3	B	1	Total	O	P	0	0
			3	2	1		

- Molecule 4 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).



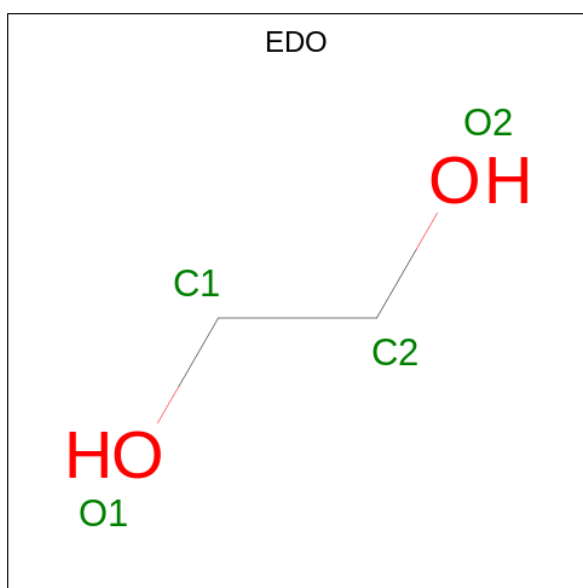
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



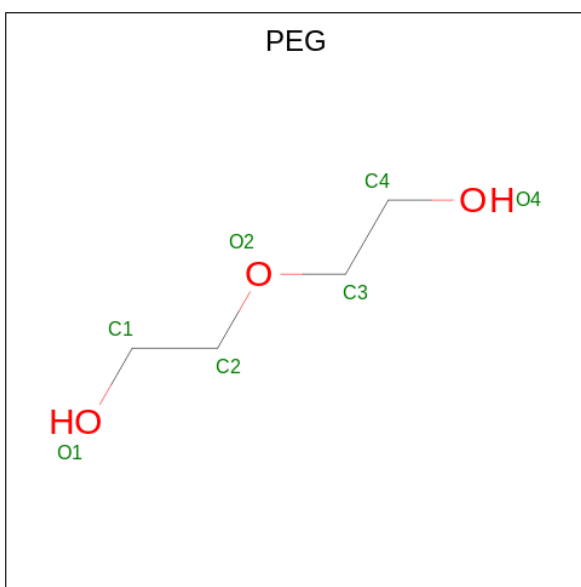
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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



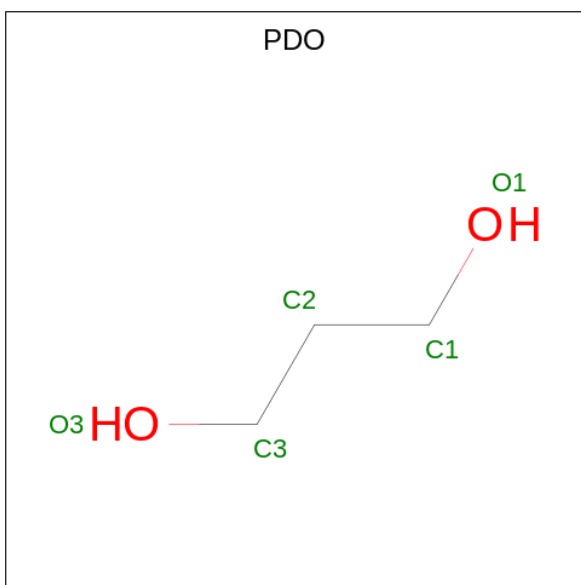
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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



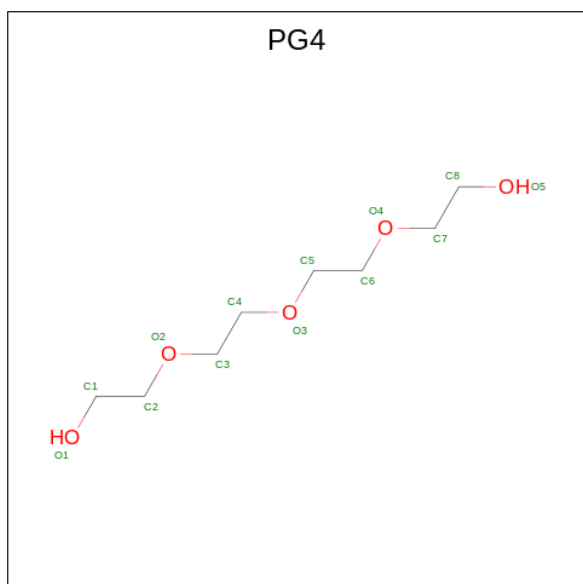
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



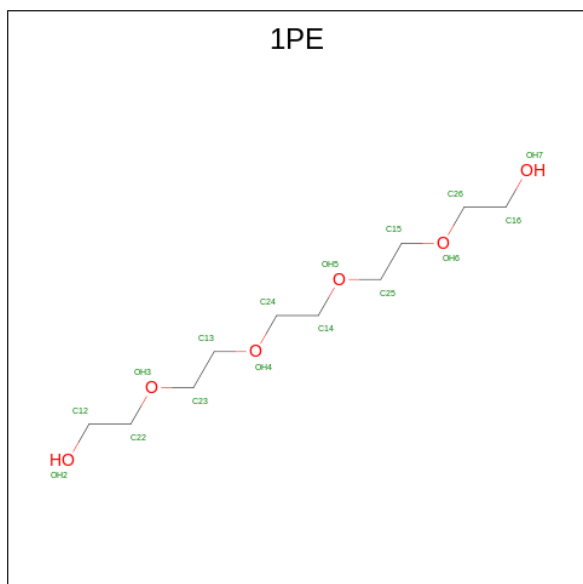
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			5	3	2		

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



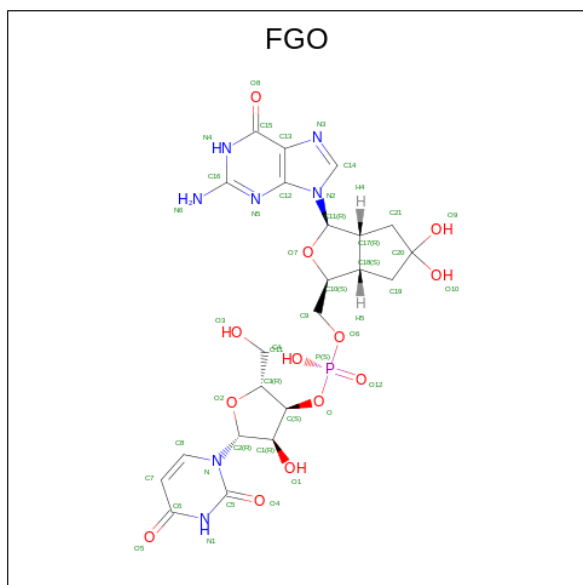
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			13	8	5		
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



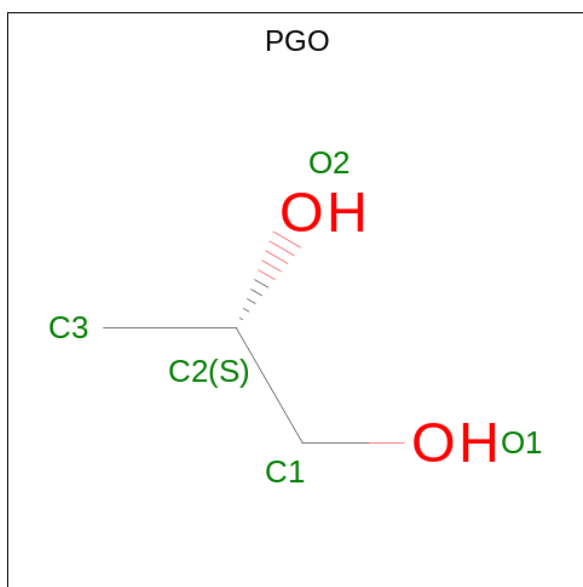
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 11 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).



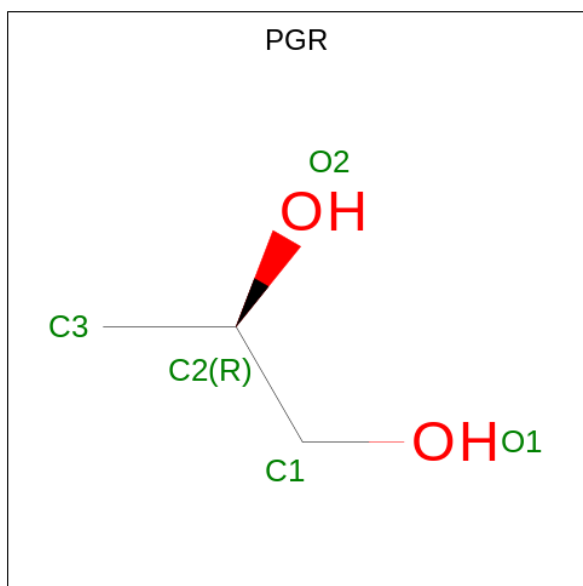
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			43	22	7	13	1		
11	B	1	Total	C	N	O	P	0	0
			43	22	7	13	1		

- Molecule 12 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



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

- Molecule 13 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: $C_3H_8O_2$).



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

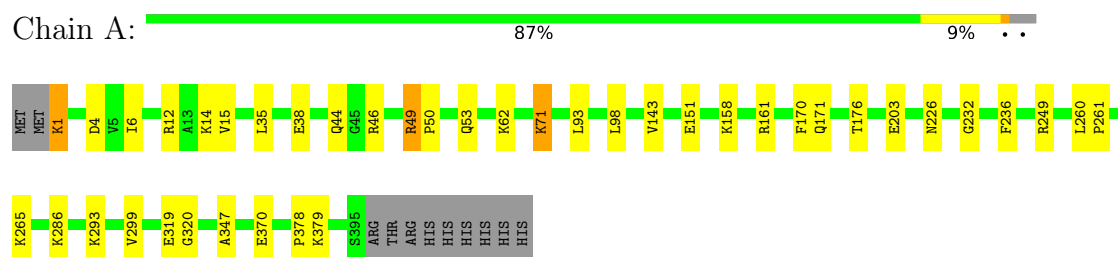
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	210	Total 210	O 210	0	0
14	B	205	Total 205	O 205	0	0

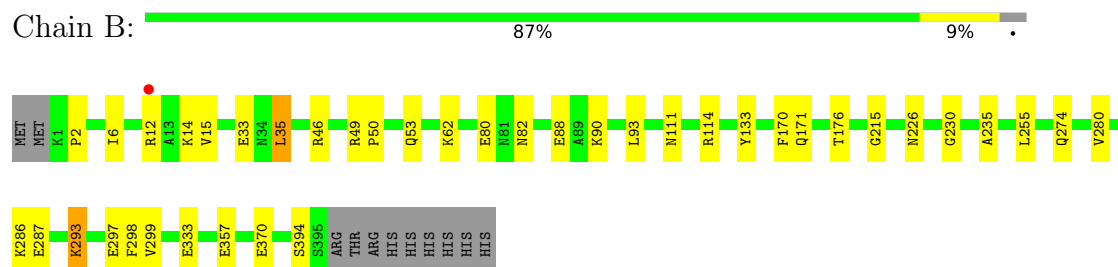
3 Residue-property plots

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: Sugar ABC transporter, periplasmic sugar-binding protein



- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.16Å 120.88Å 66.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.06 – 2.15 66.06 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.9 (66.06-2.15) 97.9 (66.06-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.158 , 0.204 0.165 , 0.211	Depositor DCC
R_{free} test set	2429 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.860 for H, K, L 0.140 for -h,-k,l	Depositor
Outliers	0 of 48537 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6784	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: 1PE, FGO, EDO, PDO, PG4, PO2, CO2, PGO, PGR, CL, GOL, PEG

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	0.90	2/3143 (0.1%)	0.98	2/4262 (0.0%)
1	B	0.94	6/3123 (0.2%)	0.98	1/4237 (0.0%)
All	All	0.92	8/6266 (0.1%)	0.98	3/8499 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	GLU	CD-OE2	6.86	1.33	1.25
1	B	357	GLU	CD-OE2	-6.81	1.18	1.25
1	A	370	GLU	CD-OE1	6.68	1.33	1.25
1	B	287	GLU	CD-OE1	6.10	1.32	1.25
1	B	80	GLU	CD-OE2	5.98	1.32	1.25
1	A	347	ALA	C-O	5.48	1.33	1.23
1	B	333	GLU	CD-OE2	5.38	1.31	1.25
1	B	215	GLY	C-O	5.00	1.31	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	CG-CD-NE	-5.98	99.24	111.80
1	B	49	ARG	CG-CD-NE	-5.94	99.32	111.80
1	A	236	PHE	CB-CA-C	-5.40	99.59	110.40

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	3064	0	3106	19	0
1	B	3050	0	3080	17	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	9	0	0	2	0
4	B	9	0	0	0	0
5	A	16	0	24	1	0
5	B	4	0	6	0	0
6	A	12	0	16	1	0
6	B	24	0	32	6	0
7	A	21	0	30	1	0
7	B	7	0	10	0	0
8	A	5	0	8	4	0
9	A	13	0	18	0	0
9	B	13	0	18	0	0
10	A	16	0	22	0	0
11	A	43	0	0	0	0
11	B	43	0	0	0	0
12	B	5	0	8	1	0
13	B	5	0	8	0	0
14	A	210	0	0	6	0
14	B	205	0	0	8	0
All	All	6784	0	6386	42	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 3.

All (42) 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:171:GLN:NE2	14:A:601:HOH:O	2.02	0.90
1:B:35:LEU:HD23	1:B:298:PHE:CE2	2.13	0.83
4:A:507:CO2:O1	8:A:517:PDO:H21	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLU:OE2	14:B:601:HOH:O	2.09	0.69
1:A:203:GLU:OE1	14:A:602:HOH:O	2.10	0.69
6:B:508:GOL:C1	14:B:644:HOH:O	2.41	0.69
1:A:379:LYS:HE2	14:A:671:HOH:O	1.96	0.65
1:B:274:GLN:HE22	6:B:508:GOL:H32	1.62	0.63
6:B:507:GOL:H2	14:B:698:HOH:O	1.98	0.63
1:A:320:GLY:HA3	8:A:517:PDO:H32	1.81	0.62
1:B:171:GLN:OE1	14:B:602:HOH:O	2.16	0.61
1:B:274:GLN:HE22	6:B:508:GOL:C3	2.15	0.60
1:B:93:LEU:HD12	1:B:280:VAL:HG12	1.83	0.59
1:B:35:LEU:HD23	1:B:298:PHE:HE2	1.64	0.59
4:A:507:CO2:O1	8:A:517:PDO:C2	2.55	0.55
6:B:508:GOL:H11	14:B:644:HOH:O	2.04	0.54
7:A:516:PEG:H42	14:B:652:HOH:O	2.07	0.54
1:A:53:GLN:OE1	1:A:62:LYS:HD3	2.09	0.52
1:A:1:LYS:HB3	1:A:4:ASP:OD2	2.10	0.52
1:A:49:ARG:NH2	14:A:607:HOH:O	2.33	0.50
1:B:2:PRO:HB2	1:B:33:GLU:HB3	1.94	0.49
1:A:35:LEU:HG	14:A:613:HOH:O	2.11	0.49
1:B:53:GLN:OE1	1:B:62:LYS:HD3	2.14	0.48
1:B:82:ASN:ND2	14:B:605:HOH:O	2.36	0.48
1:B:230:GLY:H	12:B:512:PGO:H31	1.78	0.48
1:A:320:GLY:HA3	8:A:517:PDO:C3	2.44	0.47
1:A:6:ILE:HG21	1:A:50:PRO:HD2	1.96	0.46
1:A:93:LEU:HD23	1:A:98:LEU:HG	1.99	0.45
1:A:71:LYS:O	1:A:71:LYS:HG3	2.17	0.45
1:B:111:ASN:ND2	14:B:621:HOH:O	2.49	0.44
1:B:255:LEU:O	6:B:507:GOL:H11	2.18	0.44
1:B:6:ILE:HG21	1:B:50:PRO:HD2	2.00	0.44
1:B:133:TYR:HA	1:B:235:ALA:O	2.18	0.43
1:A:232:GLY:O	6:A:512:GOL:H31	2.20	0.42
1:A:143:VAL:HG22	1:A:158:LYS:HE3	2.01	0.42
1:A:170:PHE:HB2	1:A:176:THR:HG21	2.02	0.42
1:A:319:GLU:HG2	5:A:508:EDO:H21	2.03	0.41
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.94	0.41
1:A:38:GLU:OE1	14:A:603:HOH:O	2.22	0.40
1:A:151:GLU:OE2	1:A:265:LYS:NZ	2.55	0.40
1:B:170:PHE:HB2	1:B:176:THR:HG21	2.04	0.40
1:B:293:LYS:HE2	1:B:297:GLU:OE1	2.21	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	396/406 (98%)	389 (98%)	7 (2%)	0	100	100
1	B	394/406 (97%)	388 (98%)	6 (2%)	0	100	100
All	All	790/812 (97%)	777 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/319 (98%)	297 (96%)	14 (4%)	27	24
1	B	309/319 (97%)	297 (96%)	12 (4%)	32	30
All	All	620/638 (97%)	594 (96%)	26 (4%)	30	28

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	12	ARG
1	A	14	LYS
1	A	15	VAL
1	A	44	GLN
1	A	46	ARG
1	A	71	LYS
1	A	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	ASN
1	A	249	ARG
1	A	286	LYS
1	A	293	LYS
1	A	299	VAL
1	A	378	PRO
1	B	12	ARG
1	B	14	LYS
1	B	15	VAL
1	B	35	LEU
1	B	46	ARG
1	B	90	LYS
1	B	114	ARG
1	B	226	ASN
1	B	286	LYS
1	B	293	LYS
1	B	299	VAL
1	B	394	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	B	226	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	B	511	-	6,6,6	0.17	0	5,5,5	0.07	0
6	GOL	B	509	-	5,5,5	0.18	0	5,5,5	0.28	0
4	CO2	B	503	-	2,2,2	0.02	0	1,1,1	0.86	0
9	PG4	B	514	-	12,12,12	0.18	0	11,11,11	0.25	0
11	FGO	A	520	-	40,48,48	1.29	6 (15%)	39,75,75	2.10	8 (20%)
4	CO2	B	505	-	2,2,2	0.11	0	1,1,1	0.86	0
13	PGR	B	513	-	3,4,4	0.33	0	1,4,4	0.08	0
5	EDO	A	508	-	3,3,3	0.28	0	2,2,2	0.29	0
5	EDO	A	510	-	3,3,3	0.24	0	2,2,2	0.18	0
9	PG4	A	518	-	12,12,12	0.27	0	11,11,11	0.18	0
8	PDO	A	517	-	4,4,4	0.29	0	3,3,3	0.79	0
4	CO2	A	505	-	2,2,2	0.19	0	1,1,1	0.78	0
6	GOL	A	513	-	5,5,5	0.12	0	5,5,5	0.44	0
4	CO2	B	504	-	2,2,2	0.31	0	1,1,1	0.93	0
7	PEG	A	514	-	6,6,6	0.18	0	5,5,5	0.10	0
6	GOL	A	512	-	5,5,5	0.13	0	5,5,5	0.50	0
5	EDO	A	509	-	3,3,3	0.08	0	2,2,2	0.29	0
10	1PE	A	519	-	15,15,15	0.44	0	14,14,14	0.84	0
4	CO2	A	506	-	2,2,2	0.02	0	1,1,1	0.81	0
5	EDO	A	511	-	3,3,3	0.39	0	2,2,2	0.07	0
6	GOL	B	510	-	5,5,5	0.09	0	5,5,5	0.37	0
6	GOL	B	507	-	5,5,5	0.12	0	5,5,5	0.38	0
6	GOL	B	508	-	5,5,5	0.20	0	5,5,5	0.53	0
5	EDO	B	506	-	3,3,3	0.07	0	2,2,2	0.36	0
7	PEG	A	516	-	6,6,6	0.09	0	5,5,5	0.11	0
3	PO2	A	504	-	0,2,2	0.00	-	0,1,1	0.00	-
11	FGO	B	515	-	40,48,48	1.68	9 (22%)	39,75,75	1.82	9 (23%)
12	PGO	B	512	-	3,4,4	0.57	0	1,4,4	0.20	0
3	PO2	B	502	-	0,2,2	0.00	-	0,1,1	0.00	-
7	PEG	A	515	-	6,6,6	0.19	0	5,5,5	0.32	0
4	CO2	A	507	-	2,2,2	0.36	0	1,1,1	0.99	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	B	511	-	-	2/4/4/4	-
6	GOL	B	509	-	-	1/4/4/4	-
9	PG4	B	514	-	-	4/10/10/10	-
11	FGO	A	520	-	-	1/15/63/63	0/6/6/6
13	PGR	B	513	-	-	0/2/2/2	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
9	PG4	A	518	-	-	4/10/10/10	-
8	PDO	A	517	-	-	1/2/2/2	-
6	GOL	A	513	-	-	4/4/4/4	-
7	PEG	A	514	-	-	2/4/4/4	-
6	GOL	A	512	-	-	4/4/4/4	-
5	EDO	A	509	-	-	1/1/1/1	-
10	1PE	A	519	-	-	1/13/13/13	-
5	EDO	A	511	-	-	0/1/1/1	-
6	GOL	B	510	-	-	0/4/4/4	-
6	GOL	B	507	-	-	4/4/4/4	-
6	GOL	B	508	-	-	4/4/4/4	-
5	EDO	B	506	-	-	1/1/1/1	-
7	PEG	A	516	-	-	3/4/4/4	-
11	FGO	B	515	-	-	2/15/63/63	0/6/6/6
12	PGO	B	512	-	-	2/2/2/2	-
7	PEG	A	515	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	515	FGO	C15-C13	5.25	1.50	1.41
11	B	515	FGO	C21-C17	-4.32	1.46	1.53
11	A	520	FGO	O7-C11	3.30	1.45	1.41
11	A	520	FGO	C15-C13	3.11	1.46	1.41
11	A	520	FGO	C21-C17	-3.01	1.48	1.53
11	B	515	FGO	C19-C20	-2.52	1.47	1.52
11	A	520	FGO	C5-N1	-2.37	1.33	1.38
11	B	515	FGO	C16-N4	2.31	1.39	1.35
11	B	515	FGO	C5-N1	-2.22	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	515	FGO	C21-C20	-2.18	1.48	1.52
11	B	515	FGO	C19-C18	-2.16	1.50	1.53
11	A	520	FGO	C17-C11	-2.14	1.49	1.52
11	B	515	FGO	C18-C10	-2.10	1.49	1.53
11	B	515	FGO	C15-N4	2.09	1.36	1.33
11	A	520	FGO	C19-C18	-2.03	1.50	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	520	FGO	C15-C13-C12	-6.78	114.33	120.80
11	A	520	FGO	C11-N2-C12	-5.67	116.68	126.64
11	B	515	FGO	C15-C13-C12	-4.21	116.78	120.80
11	B	515	FGO	C12-C13-N3	-4.01	105.22	109.40
11	A	520	FGO	C16-N5-C12	3.80	119.69	115.36
11	B	515	FGO	C16-N5-C12	3.76	119.65	115.36
11	A	520	FGO	C12-C13-N3	-3.63	105.61	109.40
11	B	515	FGO	C13-C15-N4	-3.50	118.64	123.43
11	B	515	FGO	C11-N2-C12	-3.37	120.72	126.64
11	A	520	FGO	N5-C16-N4	-3.33	122.78	127.22
11	A	520	FGO	C15-N4-C16	3.33	121.21	115.93
11	A	520	FGO	O2-C2-C1	-3.25	102.18	106.93
11	B	515	FGO	N5-C16-N4	-3.01	123.21	127.22
11	B	515	FGO	O2-C2-C1	-3.00	102.55	106.93
11	B	515	FGO	C15-N4-C16	2.89	120.52	115.93
11	B	515	FGO	O-C-C3	-2.71	100.28	110.08
11	A	520	FGO	C13-C15-N4	-2.56	119.93	123.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	512	GOL	C1-C2-C3-O3
6	A	513	GOL	O1-C1-C2-C3
6	B	507	GOL	C1-C2-C3-O3
6	B	507	GOL	O2-C2-C3-O3
6	B	508	GOL	C1-C2-C3-O3
8	A	517	PDO	C1-C2-C3-O3
11	A	520	FGO	C1-C2-N-C8
11	B	515	FGO	O2-C2-N-C8
11	B	515	FGO	C1-C2-N-C8
12	B	512	PGO	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

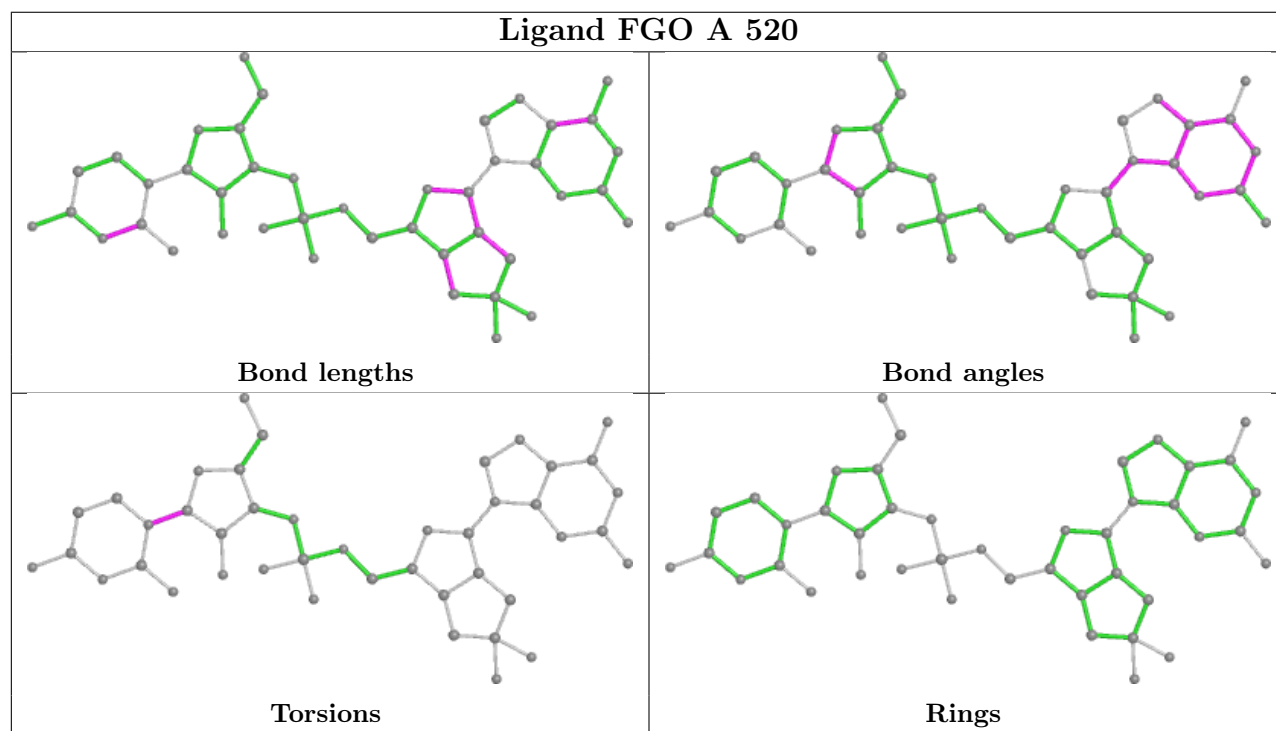
Mol	Chain	Res	Type	Atoms
12	B	512	PGO	O1-C1-C2-O2
9	A	518	PG4	O3-C5-C6-O4
6	A	513	GOL	O1-C1-C2-O2
7	B	511	PEG	O1-C1-C2-O2
7	A	516	PEG	O1-C1-C2-O2
6	A	512	GOL	O1-C1-C2-C3
6	A	513	GOL	C1-C2-C3-O3
6	B	508	GOL	O1-C1-C2-C3
6	B	509	GOL	O1-C1-C2-C3
9	B	514	PG4	O4-C7-C8-O5
6	A	512	GOL	O2-C2-C3-O3
6	B	508	GOL	O2-C2-C3-O3
7	A	514	PEG	O1-C1-C2-O2
7	A	514	PEG	O2-C3-C4-O4
5	A	509	EDO	O1-C1-C2-O2
7	A	516	PEG	O2-C3-C4-O4
9	B	514	PG4	O3-C5-C6-O4
9	B	514	PG4	O2-C3-C4-O3
5	A	508	EDO	O1-C1-C2-O2
5	A	510	EDO	O1-C1-C2-O2
10	A	519	1PE	OH2-C12-C22-OH3
7	A	516	PEG	C1-C2-O2-C3
9	A	518	PG4	C1-C2-O2-C3
9	A	518	PG4	C6-C5-O3-C4
5	B	506	EDO	O1-C1-C2-O2
7	A	515	PEG	O2-C3-C4-O4
6	B	507	GOL	O1-C1-C2-C3
6	A	513	GOL	O2-C2-C3-O3
6	B	508	GOL	O1-C1-C2-O2
9	B	514	PG4	C5-C6-O4-C7
7	A	515	PEG	O1-C1-C2-O2
9	A	518	PG4	O1-C1-C2-O2
7	A	515	PEG	C1-C2-O2-C3
6	A	512	GOL	O1-C1-C2-O2
6	B	507	GOL	O1-C1-C2-O2
7	A	515	PEG	C4-C3-O2-C2
7	B	511	PEG	O2-C3-C4-O4

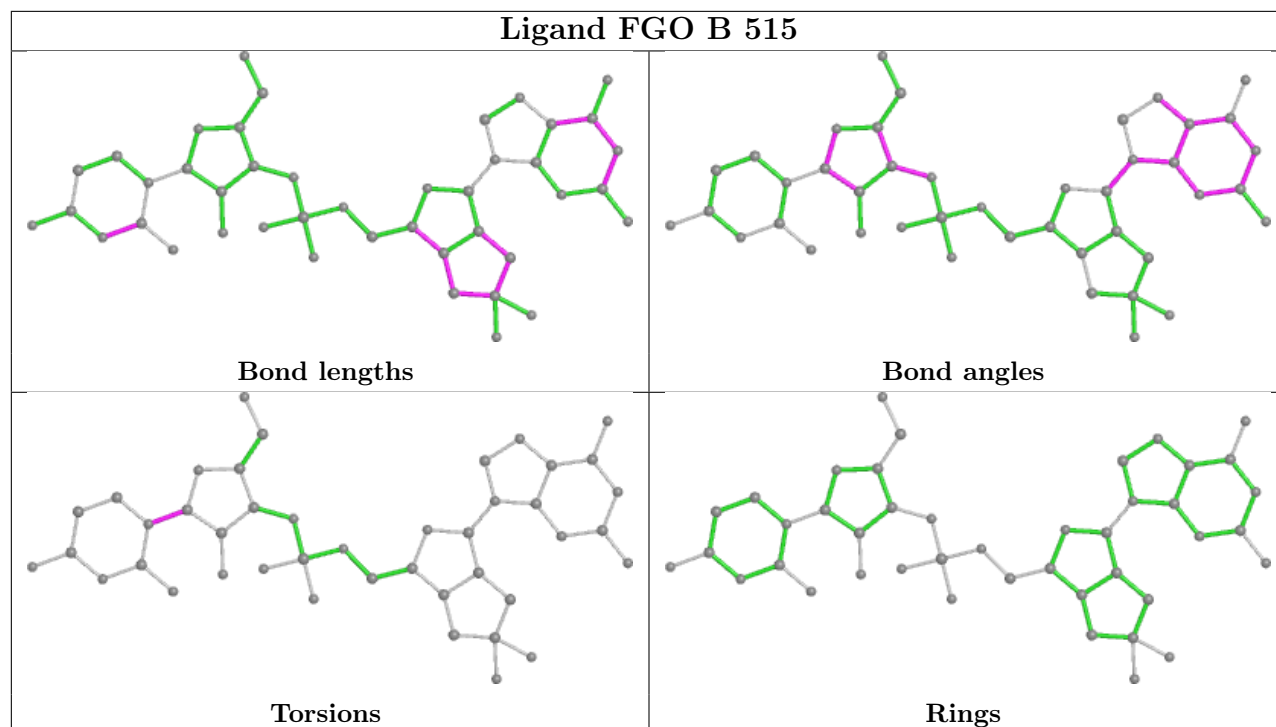
There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	EDO	1	0
8	A	517	PDO	4	0
6	A	512	GOL	1	0
6	B	507	GOL	2	0
6	B	508	GOL	4	0
7	A	516	PEG	1	0
12	B	512	PGO	1	0
4	A	507	CO2	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 [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	395/406 (97%)	-0.67	0	100	100	11, 20, 42, 64	0
1	B	395/406 (97%)	-0.69	1 (0%)	94	95	10, 20, 39, 74	0
All	All	790/812 (97%)	-0.68	1 (0%)	95	96	10, 20, 42, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	ARG	2.5

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 [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
13	PGR	B	513	5/5	0.77	0.17	41,43,44,46	0
5	EDO	A	510	4/4	0.84	0.14	35,42,44,47	0
4	CO2	A	505	3/3	0.85	0.17	44,44,48,49	0
7	PEG	A	516	7/7	0.87	0.15	42,51,62,62	0

Continued on next page...

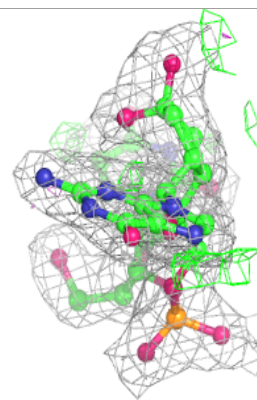
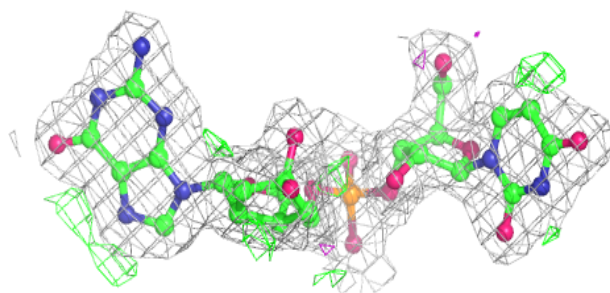
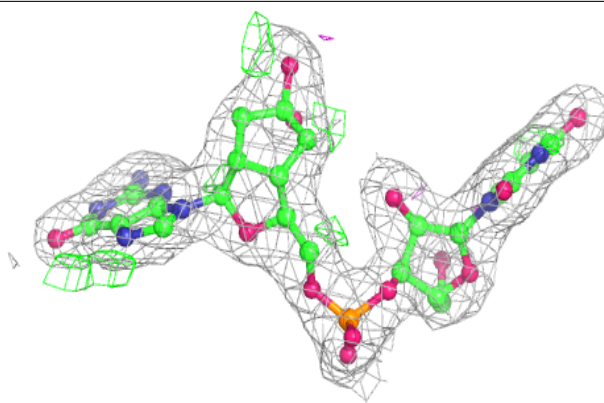
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PEG	B	511	7/7	0.89	0.13	47,52,57,58	0
7	PEG	A	515	7/7	0.90	0.14	41,44,48,49	0
2	CL	A	501	1/1	0.90	0.06	51,51,51,51	0
4	CO2	A	507	3/3	0.90	0.07	35,35,47,48	0
2	CL	A	503	1/1	0.90	0.07	55,55,55,55	0
12	PGO	B	512	5/5	0.91	0.10	24,24,27,29	0
5	EDO	A	508	4/4	0.92	0.13	39,39,42,43	0
9	PG4	A	518	13/13	0.92	0.14	37,43,54,55	0
6	GOL	B	507	6/6	0.93	0.15	36,40,41,42	0
7	PEG	A	514	7/7	0.93	0.12	37,44,54,55	0
5	EDO	A	509	4/4	0.93	0.11	43,44,47,52	0
3	PO2	A	504	3/3	0.93	0.10	39,39,48,56	0
9	PG4	B	514	13/13	0.94	0.11	32,36,52,57	0
4	CO2	B	505	3/3	0.94	0.08	48,48,50,51	0
5	EDO	B	506	4/4	0.94	0.11	38,39,41,46	0
8	PDO	A	517	5/5	0.95	0.11	21,26,29,32	0
2	CL	A	502	1/1	0.95	0.04	50,50,50,50	0
6	GOL	A	513	6/6	0.95	0.10	26,37,43,44	0
10	1PE	A	519	16/16	0.95	0.11	26,29,36,42	0
4	CO2	B	504	3/3	0.95	0.08	32,32,39,40	0
6	GOL	B	508	6/6	0.95	0.12	30,30,37,38	0
2	CL	B	501	1/1	0.96	0.06	42,42,42,42	0
4	CO2	A	506	3/3	0.96	0.05	43,43,43,46	0
3	PO2	B	502	3/3	0.96	0.19	46,46,47,58	0
6	GOL	B	509	6/6	0.96	0.09	18,23,27,31	0
6	GOL	B	510	6/6	0.96	0.08	21,25,27,27	0
11	FGO	A	520	43/43	0.97	0.09	14,19,25,30	0
11	FGO	B	515	43/43	0.97	0.09	12,17,24,27	0
6	GOL	A	512	6/6	0.97	0.09	25,30,32,33	0
5	EDO	A	511	4/4	0.97	0.14	22,26,27,28	0
4	CO2	B	503	3/3	0.98	0.07	35,35,36,41	0

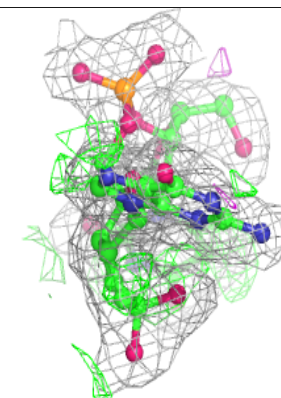
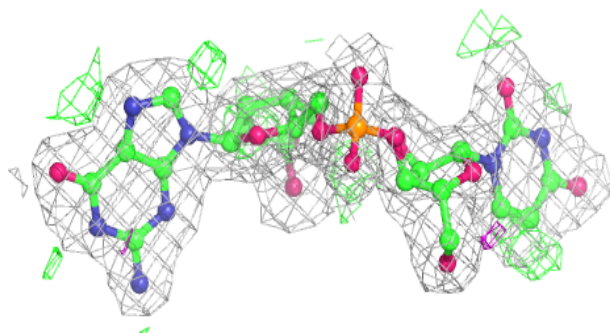
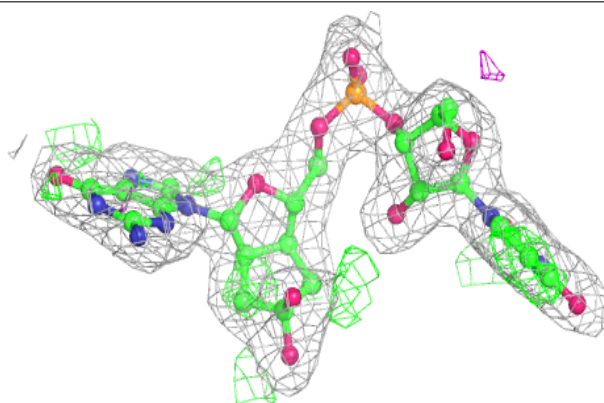
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FGO A 520:

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

**Electron density around FGO B 515:**

$2mF_o-DF_c$ (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.