



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:27 PM JST

PDB ID : 7C16  
Title : Crystal structure of a dinucleotide-binding protein (Y224A/Y246A) of ABC transporter endogenously bound to uridylyl-3'-5'-phospho-guanosine (Form I)  
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.  
Deposited on : 2020-05-02  
Resolution : 1.90 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](mailto: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>.

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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

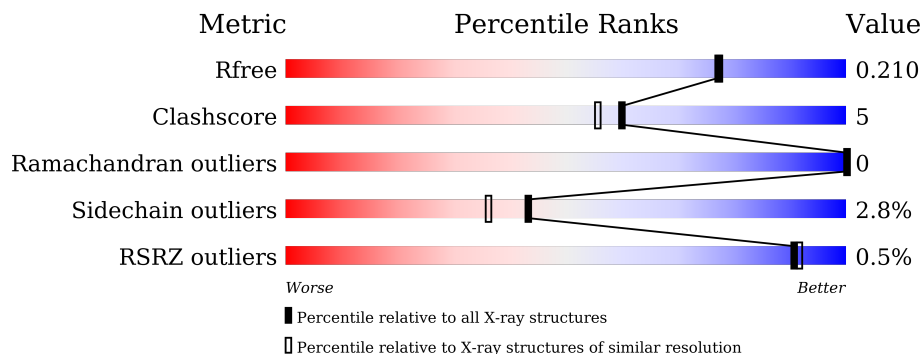
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	 88% 9% .
1	B	406	 83% 13% ..

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
3	CO2	B	502	-	-	X	-
7	PEG	A	509	-	-	X	-

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 6774 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	396	Total	C	N	O	S	0	1	0
			3042	1965	513	560	4			
1	B	395	Total	C	N	O	S	0	1	0
			3031	1958	512	558	3			

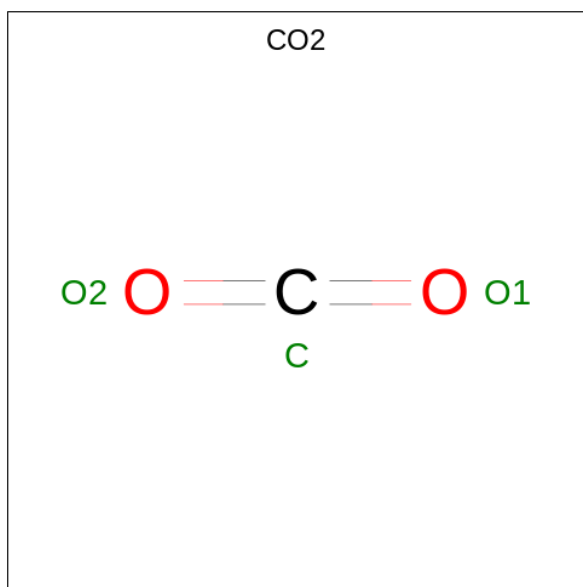
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q5SLB4
A	0	MET	-	expression tag	UNP Q5SLB4
A	224	ALA	TYR	engineered mutation	UNP Q5SLB4
A	246	ALA	TYR	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	224	ALA	TYR	engineered mutation	UNP Q5SLB4
B	246	ALA	TYR	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).

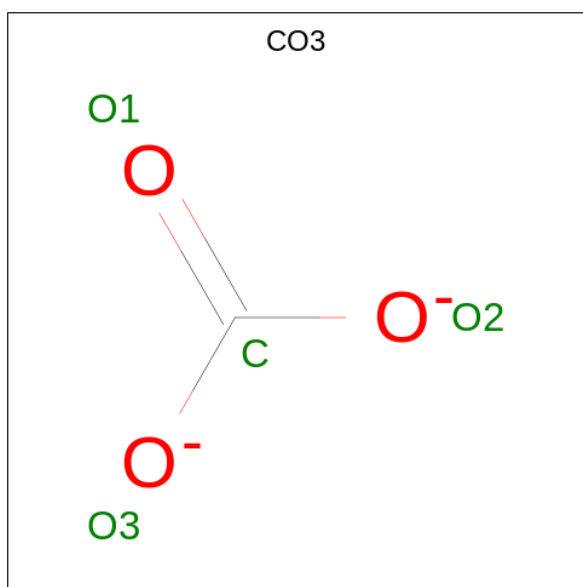
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO<sub>2</sub>).



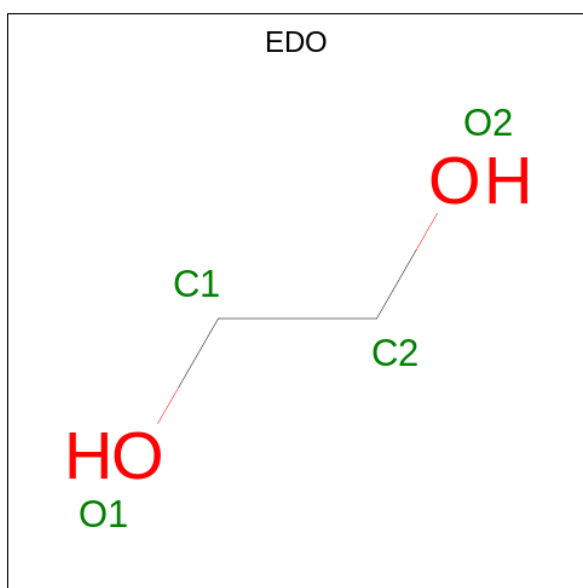
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



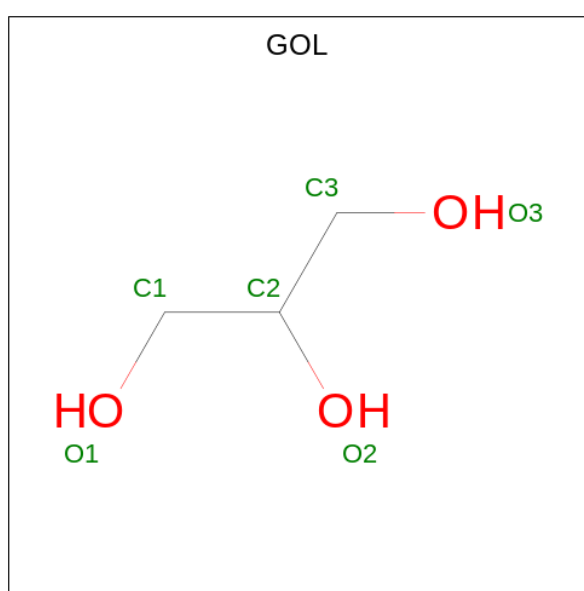
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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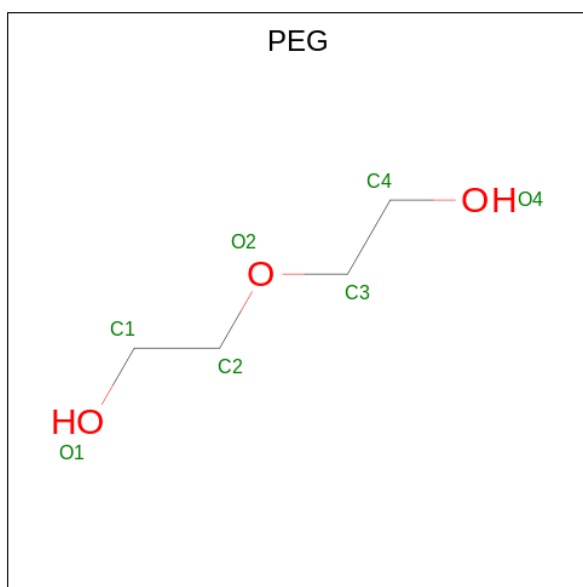
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



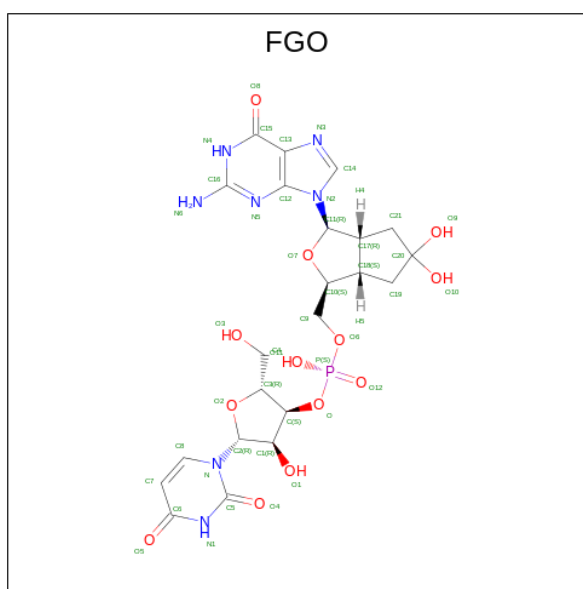
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- 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: C<sub>22</sub>H<sub>28</sub>N<sub>7</sub>O<sub>13</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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

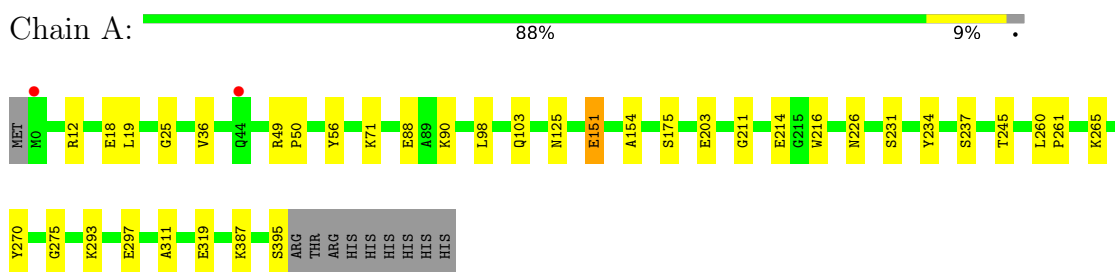
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	266	Total	O	0	0
			266	266		
9	B	269	Total	O	0	0
			269	269		

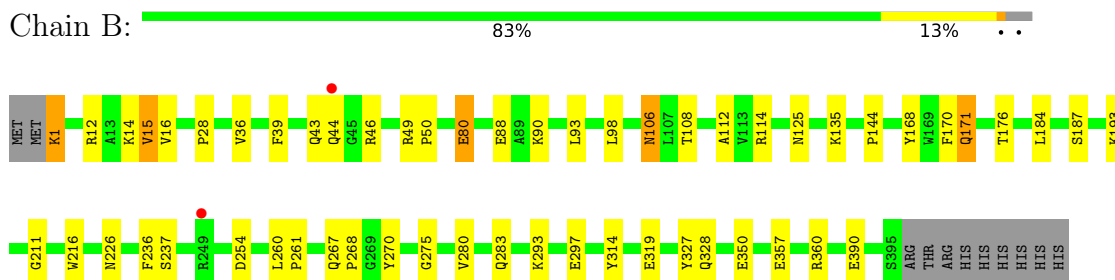
### 3 Residue-property plots [i](#)

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



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



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.52Å 121.69Å 65.40Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	58.52 – 1.90 58.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.52-1.90) 99.6 (58.52-1.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.163 , 0.204 0.170 , 0.210	Depositor DCC
$R_{free}$ test set	3511 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.339 for h,-k,-l	Xtriage
Reported twinning fraction	0.681 for H, K, L 0.319 for -h,-k,l	Depositor
Outliers	0 of 71926 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6774	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, CO2, CO3, FGO, PEG, EDO, GOL

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	1.08	7/3113 (0.2%)	1.14	4/4223 (0.1%)
1	B	1.09	8/3102 (0.3%)	1.15	8/4209 (0.2%)
All	All	1.08	15/6215 (0.2%)	1.14	12/8432 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	GLU	CD-OE2	9.17	1.35	1.25
1	A	25	GLY	C-O	7.83	1.36	1.23
1	B	357	GLU	CD-OE1	-7.33	1.17	1.25
1	B	350	GLU	CD-OE2	-6.77	1.18	1.25
1	A	175	SER	C-O	6.24	1.35	1.23
1	A	151	GLU	CD-OE1	-5.43	1.19	1.25
1	B	237	SER	C-O	5.37	1.33	1.23
1	A	18	GLU	CD-OE2	-5.35	1.19	1.25
1	A	203	GLU	CD-OE1	-5.35	1.19	1.25
1	B	270	TYR	C-O	5.29	1.33	1.23
1	B	80	GLU	CD-OE2	5.22	1.31	1.25
1	B	184	LEU	C-O	-5.05	1.13	1.23
1	B	80	GLU	CD-OE1	5.04	1.31	1.25
1	B	187	SER	CA-CB	-5.02	1.45	1.52
1	A	237	SER	CA-CB	-5.02	1.45	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	114	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	270	TYR	CB-CG-CD1	6.02	124.61	121.00
1	B	168	TYR	CB-CG-CD2	5.83	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	PHE	CB-CA-C	-5.49	99.42	110.40
1	B	327	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	56	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	B	168	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	171	GLN	CA-CB-CG	-5.08	102.23	113.40
1	A	49	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	B	360	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	56	TYR	CB-CG-CD1	5.02	124.02	121.00

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	3042	0	3076	18	0
1	B	3031	0	3066	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	12	0	0	4	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
5	A	12	0	18	3	0
5	B	12	0	18	2	0
6	A	12	0	16	1	0
6	B	12	0	16	1	0
7	A	7	0	10	5	0
8	A	43	0	0	3	0
8	B	43	0	0	3	0
9	A	266	0	0	8	0
9	B	269	0	0	8	0
All	All	6774	0	6220	57	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 (57) 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:98:LEU:O	1:A:293:LYS:HD2	1.67	0.93
1:A:245:THR:HG21	1:A:311:ALA:O	1.73	0.88
3:B:502:CO2:O2	8:B:512:FGO:C19	2.23	0.86
1:B:98:LEU:O	1:B:293:LYS:HD2	1.80	0.82
1:A:88:GLU:OE2	9:A:602:HOH:O	2.00	0.79
1:A:395:SER:O	9:A:601:HOH:O	2.00	0.79
3:B:502:CO2:C	8:B:512:FGO:C19	2.64	0.76
1:A:214:GLU:OE1	4:A:503:CO3:O2	2.09	0.69
1:B:106:ASN:OD1	1:B:108:THR:HB	1.93	0.69
1:A:103:GLN:HG2	9:A:795:HOH:O	1.94	0.66
1:B:88:GLU:OE2	9:B:601:HOH:O	2.14	0.66
1:B:16:VAL:HG11	1:B:49:ARG:NH2	2.11	0.64
1:B:1:LYS:HE2	9:B:617:HOH:O	2.00	0.61
1:A:151:GLU:HG2	7:A:509:PEG:H21	1.82	0.61
5:A:505:EDO:C2	8:A:510:FGO:C19	2.79	0.60
1:B:16:VAL:HG11	1:B:49:ARG:HH22	1.68	0.59
1:A:36:VAL:HG21	1:A:50:PRO:HG3	1.86	0.58
1:B:170:PHE:HB2	1:B:176:THR:HG21	1.86	0.58
1:A:103:GLN:CG	9:A:795:HOH:O	2.52	0.57
5:B:507:EDO:H12	9:B:769:HOH:O	2.06	0.54
5:B:507:EDO:H21	9:B:769:HOH:O	2.08	0.54
5:A:505:EDO:H22	8:A:510:FGO:C19	2.38	0.53
1:A:211:GLY:HA2	1:A:216:TRP:CE2	2.46	0.51
1:B:267:GLN:HG2	1:B:268:PRO:O	2.11	0.50
5:A:505:EDO:C1	8:A:510:FGO:C19	2.91	0.48
1:B:36:VAL:HG21	1:B:50:PRO:HG3	1.96	0.48
7:A:509:PEG:H32	9:A:664:HOH:O	2.15	0.47
1:B:106:ASN:OD1	1:B:108:THR:CB	2.62	0.47
1:A:234:TYR:HB3	6:A:507:GOL:H31	1.98	0.46
7:A:509:PEG:C3	9:A:664:HOH:O	2.63	0.46
1:B:293:LYS:NZ	1:B:297:GLU:OE1	2.49	0.45
1:B:125:ASN:O	1:B:275:GLY:HA3	2.17	0.44
1:B:93:LEU:HD12	1:B:280:VAL:HG12	1.99	0.44
1:B:49:ARG:HH21	1:B:49:ARG:HB3	1.82	0.44
1:B:135:LYS:HB2	1:B:254:ASP:HB3	1.99	0.44
1:B:15:VAL:HG13	1:B:46:ARG:HG2	1.99	0.44
1:A:125:ASN:O	1:A:275:GLY:HA3	2.18	0.44
1:A:154:ALA:CB	7:A:509:PEG:H11	2.48	0.44
3:B:502:CO2:O1	9:B:602:HOH:O	2.21	0.44
1:B:39:PHE:O	1:B:43:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLU:HG2	1:B:112:ALA:HB1	2.00	0.43
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.94	0.42
1:A:151:GLU:CG	7:A:509:PEG:H21	2.47	0.42
1:B:193:LYS:NZ	1:B:390:GLU:OE2	2.41	0.42
1:B:211:GLY:HA2	1:B:216:TRP:CE2	2.54	0.42
1:A:231:SER:O	1:A:231:SER:OG	2.27	0.42
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.87	0.42
1:B:49:ARG:NH2	1:B:49:ARG:CB	2.83	0.41
1:B:171:GLN:NE2	9:B:623:HOH:O	2.54	0.41
1:B:125:ASN:HB2	1:B:314:TYR:CZ	2.56	0.41
1:B:328:GLN:HG2	6:B:511:GOL:H32	2.02	0.41
1:A:265:LYS:HE3	9:A:849:HOH:O	2.21	0.41
1:B:49:ARG:HH21	1:B:49:ARG:CB	2.34	0.40
3:B:502:CO2:C	8:B:512:FGO:C18	2.99	0.40
1:B:283:GLN:HG3	9:B:628:HOH:O	2.21	0.40
1:A:103:GLN:OE1	9:A:604:HOH:O	2.22	0.40
1:B:144:PRO:HG3	9:B:823:HOH:O	2.21	0.40

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	395/406 (97%)	390 (99%)	5 (1%)	0	100	100
1	B	394/406 (97%)	384 (98%)	10 (2%)	0	100	100
All	All	789/812 (97%)	774 (98%)	15 (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	308/317 (97%)	301 (98%)	7 (2%)	50	45
1	B	307/317 (97%)	297 (97%)	10 (3%)	38	29
All	All	615/634 (97%)	598 (97%)	17 (3%)	43	36

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	19	LEU
1	A	71	LYS
1	A	90	LYS
1	A	226	ASN
1	A	319	GLU
1	A	387	LYS
1	B	1	LYS
1	B	12	ARG
1	B	14	LYS
1	B	15	VAL
1	B	28	PRO
1	B	44	GLN
1	B	90	LYS
1	B	106	ASN
1	B	226	ASN
1	B	319	GLU

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

Mol	Chain	Res	Type
1	A	103	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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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
3	CO2	B	502	-	2,2,2	0.37	0	1,1,1	1.08	0
6	GOL	B	510	-	5,5,5	0.22	0	5,5,5	0.44	0
4	CO3	B	506	-	2,3,3	0.67	0	2,3,3	0.19	0
5	EDO	A	505	-	3,3,3	0.21	0	2,2,2	0.38	0
5	EDO	B	509	-	3,3,3	0.10	0	2,2,2	0.52	0
6	GOL	B	511	-	5,5,5	0.09	0	5,5,5	0.29	0
5	EDO	B	507	-	3,3,3	0.43	0	2,2,2	0.10	0
3	CO2	A	502	-	2,2,2	0.08	0	1,1,1	1.07	0
6	GOL	A	508	-	5,5,5	0.20	0	5,5,5	0.26	0
3	CO2	B	504	-	2,2,2	0.32	0	1,1,1	0.76	0
5	EDO	A	506	-	3,3,3	0.35	0	2,2,2	0.47	0
7	PEG	A	509	-	6,6,6	0.36	0	5,5,5	0.38	0
3	CO2	B	503	-	2,2,2	0.20	0	1,1,1	0.86	0
8	FGO	B	512	-	44,48,48	1.48	8 (18%)	50,75,75	2.05	14 (28%)
8	FGO	A	510	-	44,48,48	1.51	9 (20%)	50,75,75	1.76	10 (20%)
4	CO3	A	503	-	2,3,3	0.87	0	2,3,3	0.47	0
3	CO2	B	505	-	2,2,2	0.12	0	1,1,1	0.99	0
6	GOL	A	507	-	5,5,5	0.08	0	5,5,5	0.38	0
5	EDO	B	508	-	3,3,3	0.18	0	2,2,2	0.34	0
5	EDO	A	504	-	3,3,3	0.28	0	2,2,2	0.10	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	508	-	-	0/4/4/4	-
6	GOL	B	510	-	-	4/4/4/4	-
5	EDO	B	508	-	-	1/1/1/1	-
5	EDO	A	505	-	-	1/1/1/1	-
5	EDO	B	509	-	-	0/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
7	PEG	A	509	-	-	4/4/4/4	-
6	GOL	B	511	-	-	2/4/4/4	-
8	FGO	B	512	-	-	2/17/63/63	0/6/6/6
6	GOL	A	507	-	-	1/4/4/4	-
8	FGO	A	510	-	-	0/17/63/63	0/6/6/6
5	EDO	B	507	-	-	1/1/1/1	-
5	EDO	A	504	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	512	FGO	C15-N4	-4.02	1.31	1.37
8	A	510	FGO	C5-N	3.83	1.44	1.38
8	B	512	FGO	C21-C17	-3.44	1.48	1.53
8	B	512	FGO	C6-N1	-3.32	1.32	1.38
8	A	510	FGO	C6-N1	-2.95	1.33	1.38
8	B	512	FGO	C8-C7	2.85	1.41	1.35
8	A	510	FGO	C19-C18	-2.82	1.49	1.53
8	A	510	FGO	C8-C7	2.73	1.41	1.35
8	A	510	FGO	C17-C11	-2.72	1.48	1.52
8	A	510	FGO	C15-N4	-2.68	1.33	1.37
8	A	510	FGO	C16-N5	2.64	1.39	1.33
8	A	510	FGO	C21-C17	-2.64	1.49	1.53
8	B	512	FGO	C5-N	2.27	1.42	1.38
8	B	512	FGO	O7-C10	-2.21	1.40	1.45
8	B	512	FGO	C16-N5	2.11	1.38	1.33
8	B	512	FGO	C18-C17	-2.09	1.49	1.55
8	A	510	FGO	C16-N6	2.03	1.39	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	512	FGO	N1-C5-N	6.42	123.41	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	512	FGO	C6-N1-C5	-5.79	118.94	126.58
8	A	510	FGO	C6-N1-C5	-5.06	119.91	126.58
8	B	512	FGO	C13-C15-N4	4.82	122.47	113.95
8	A	510	FGO	N1-C5-N	4.78	121.24	114.89
8	A	510	FGO	C7-C6-N1	4.01	120.85	114.84
8	B	512	FGO	C7-C6-N1	3.66	120.32	114.84
8	B	512	FGO	O4-C5-N1	-3.61	114.78	121.50
8	A	510	FGO	C13-C15-N4	3.33	119.83	113.95
8	A	510	FGO	O4-C5-N1	-3.22	115.51	121.50
8	A	510	FGO	P-O-C	2.82	129.67	119.41
8	B	512	FGO	C21-C17-C11	-2.73	109.18	113.62
8	B	512	FGO	P-O-C	2.68	129.16	119.41
8	B	512	FGO	C1-C-C3	-2.63	98.56	103.22
8	B	512	FGO	O5-C6-N1	-2.60	115.49	119.31
8	B	512	FGO	C16-N4-C15	-2.58	120.34	125.10
8	A	510	FGO	C7-C8-N	-2.58	117.49	121.81
8	A	510	FGO	O8-C15-N4	-2.50	117.70	120.65
8	B	512	FGO	O8-C15-C13	-2.48	119.53	124.37
8	B	512	FGO	C7-C8-N	-2.32	117.92	121.81
8	B	512	FGO	O8-C15-N4	-2.24	118.01	120.65
8	A	510	FGO	O2-C2-N	2.15	113.29	108.36
8	B	512	FGO	C14-N3-C13	2.10	106.99	102.99
8	A	510	FGO	O3-C4-C3	-2.01	104.39	111.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	510	GOL	O1-C1-C2-C3
6	B	510	GOL	C1-C2-C3-O3
8	B	512	FGO	C-C3-C4-O3
8	B	512	FGO	O2-C3-C4-O3
7	A	509	PEG	O1-C1-C2-O2
6	B	511	GOL	O1-C1-C2-C3
5	A	505	EDO	O1-C1-C2-O2
5	A	506	EDO	O1-C1-C2-O2
5	B	507	EDO	O1-C1-C2-O2
6	B	510	GOL	O2-C2-C3-O3
5	A	504	EDO	O1-C1-C2-O2
7	A	509	PEG	C4-C3-O2-C2
6	B	511	GOL	O1-C1-C2-O2
7	A	509	PEG	O2-C3-C4-O4

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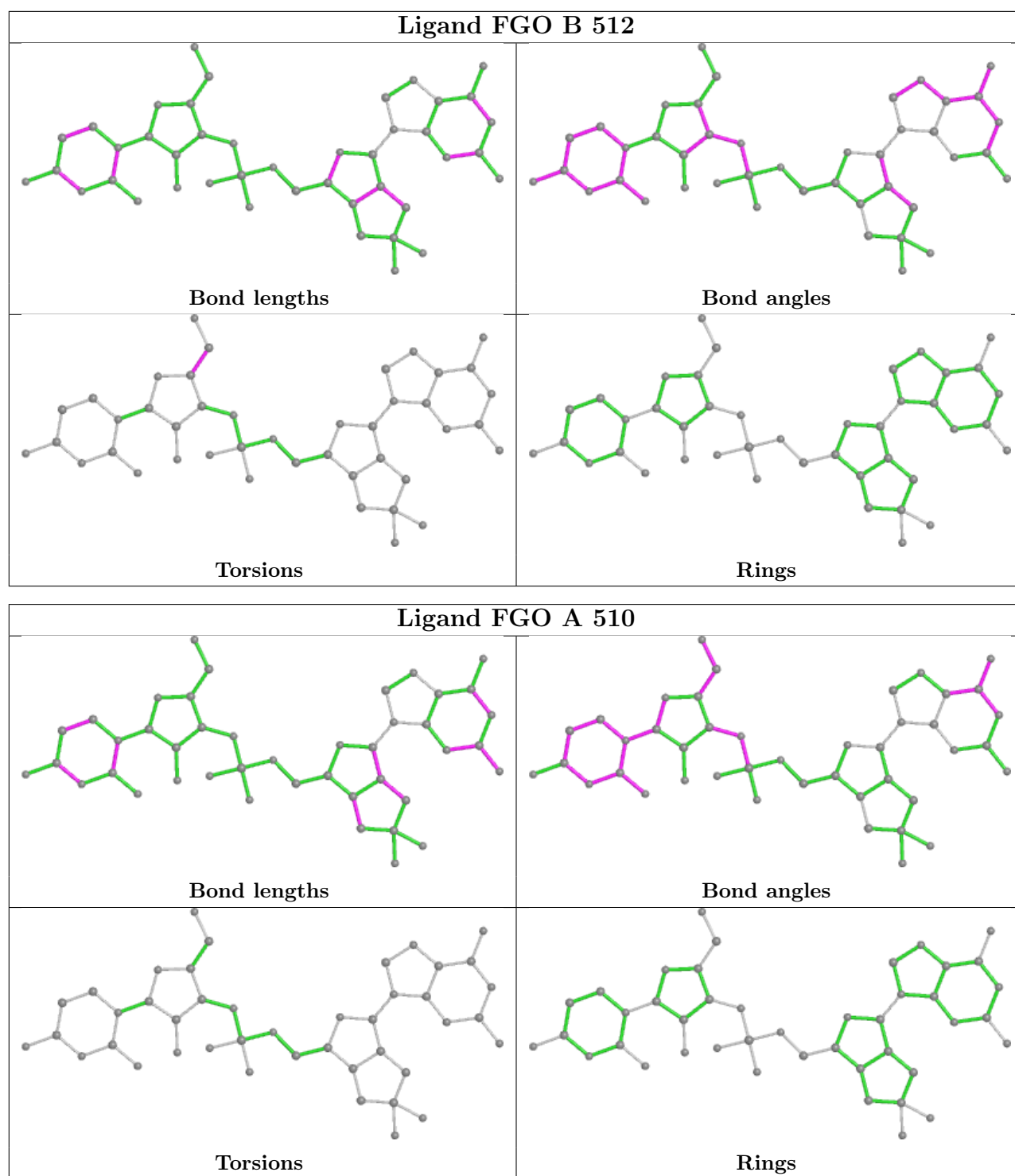
Mol	Chain	Res	Type	Atoms
7	A	509	PEG	C1-C2-O2-C3
5	B	508	EDO	O1-C1-C2-O2
6	A	507	GOL	C1-C2-C3-O3
6	B	510	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	CO2	4	0
5	A	505	EDO	3	0
6	B	511	GOL	1	0
5	B	507	EDO	2	0
7	A	509	PEG	5	0
8	B	512	FGO	3	0
8	A	510	FGO	3	0
4	A	503	CO3	1	0
6	A	507	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	396/406 (97%)	-0.24	2 (0%) 91 92	8, 16, 33, 53	0
1	B	395/406 (97%)	-0.26	2 (0%) 91 92	8, 16, 30, 50	0
All	All	791/812 (97%)	-0.25	4 (0%) 91 92	8, 16, 33, 53	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	GLN	2.7
1	A	44	GLN	2.5
1	A	0	MET	2.4
1	B	249	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	EDO	A	504	4/4	0.82	0.14	30,33,34,37	0

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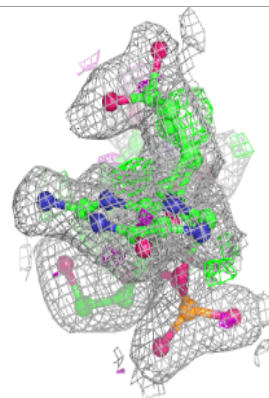
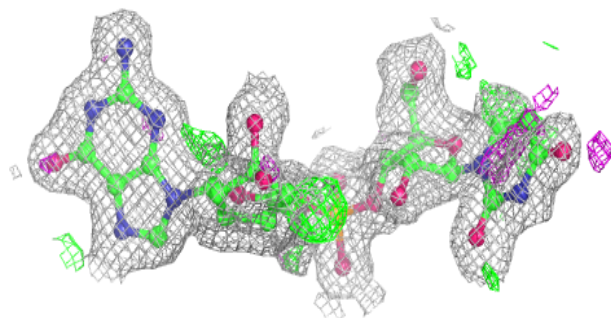
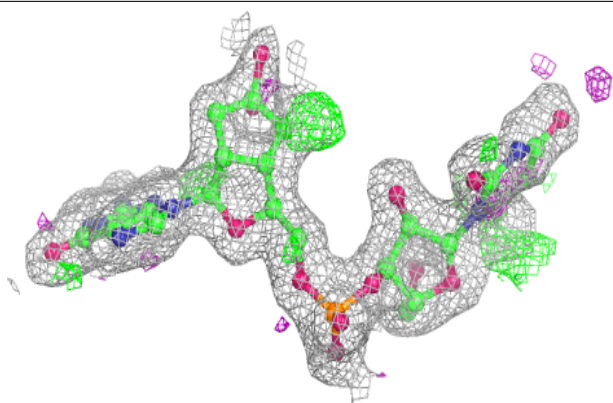
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CO2	B	502	3/3	0.84	0.11	32,32,35,37	0
7	PEG	A	509	7/7	0.84	0.16	23,31,39,39	0
3	CO2	B	504	3/3	0.86	0.18	31,31,32,35	0
6	GOL	B	511	6/6	0.87	0.25	33,33,36,36	0
3	CO2	B	503	3/3	0.88	0.12	40,40,44,44	0
4	CO3	A	503	4/4	0.89	0.12	38,38,39,41	0
5	EDO	A	506	4/4	0.90	0.13	27,29,34,36	0
5	EDO	B	509	4/4	0.90	0.16	22,27,28,36	0
2	CL	B	501	1/1	0.91	0.09	50,50,50,50	0
4	CO3	B	506	4/4	0.93	0.13	36,41,42,44	0
5	EDO	A	505	4/4	0.94	0.13	28,29,30,30	0
6	GOL	A	507	6/6	0.94	0.12	28,31,31,32	0
6	GOL	B	510	6/6	0.94	0.14	17,21,22,30	0
2	CL	A	501	1/1	0.94	0.10	55,55,55,55	0
5	EDO	B	507	4/4	0.94	0.09	23,24,24,25	0
8	FGO	A	510	43/43	0.94	0.13	10,18,35,42	0
5	EDO	B	508	4/4	0.95	0.16	16,20,22,26	0
6	GOL	A	508	6/6	0.95	0.13	19,20,25,33	0
8	FGO	B	512	43/43	0.95	0.12	11,16,34,39	0
3	CO2	B	505	3/3	0.96	0.09	30,30,32,33	0
3	CO2	A	502	3/3	0.96	0.08	28,28,31,35	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.

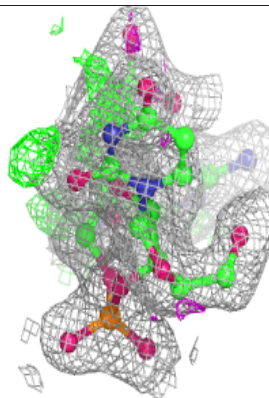
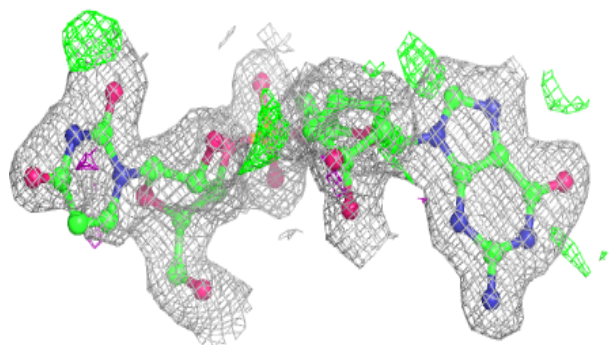
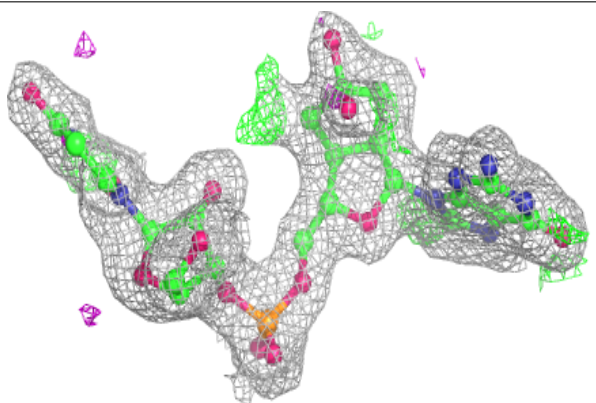


**Electron density around FGO A 510:**

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

**Electron density around FGO B 512:**

$2mF_o-DF_c$  (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.