



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2021 – 12:32 PM JST

PDB ID : 7C0K
Title : Crystal structure of a dinucleotide-binding protein of ABC transporter endogenously bound to uridylyl-3'-5'-phospho-guanosine (Form II)
Authors : Kanaujia, S.P.; Chandravanshi, M.
Deposited on : 2020-05-01
Resolution : 1.80 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

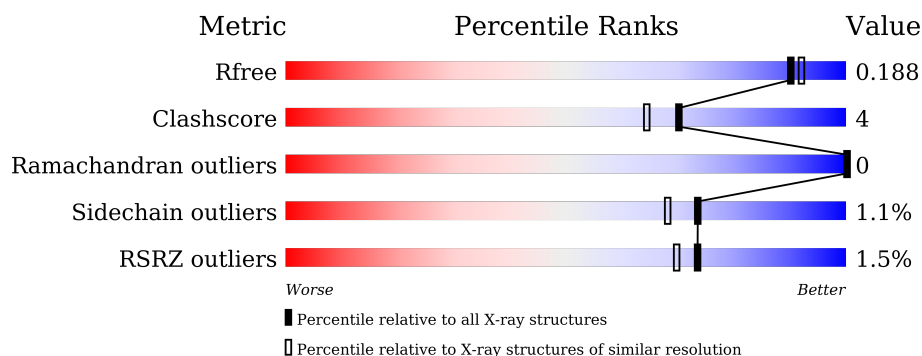
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 1% 91% 5% . . </div> </div>
1	B	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 2% 91% 7% . </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	B	517	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7081 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	396	Total	C	N	O	S	0	5	0
			3082	1998	520	560	4			
1	B	397	Total	C	N	O	S	0	4	0
			3086	1997	521	563	5			

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

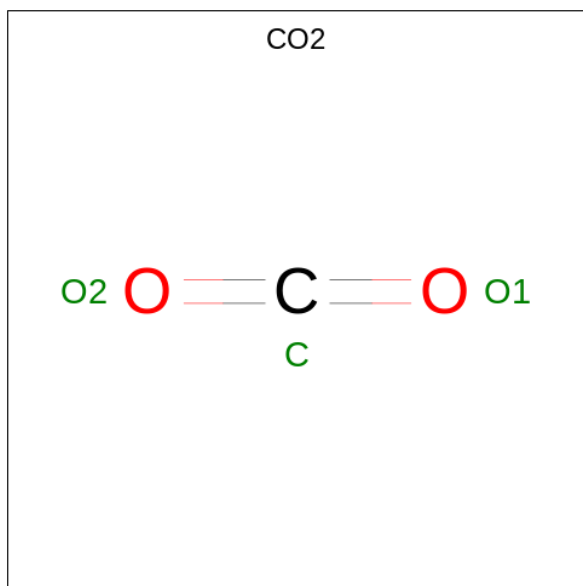
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	5	Total	Cl	0	0
			5	5		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

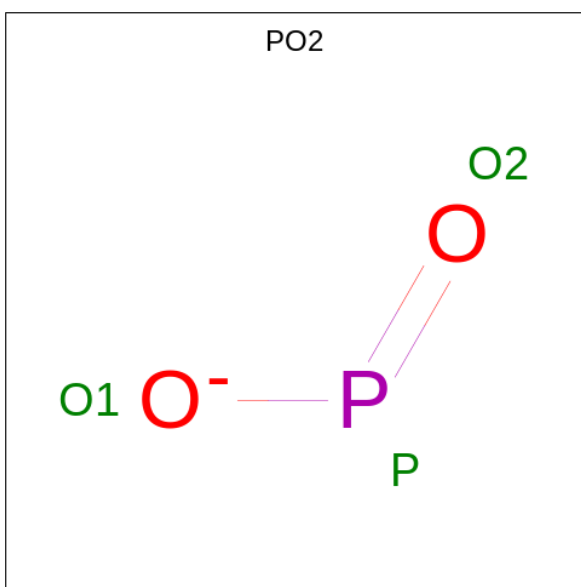
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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



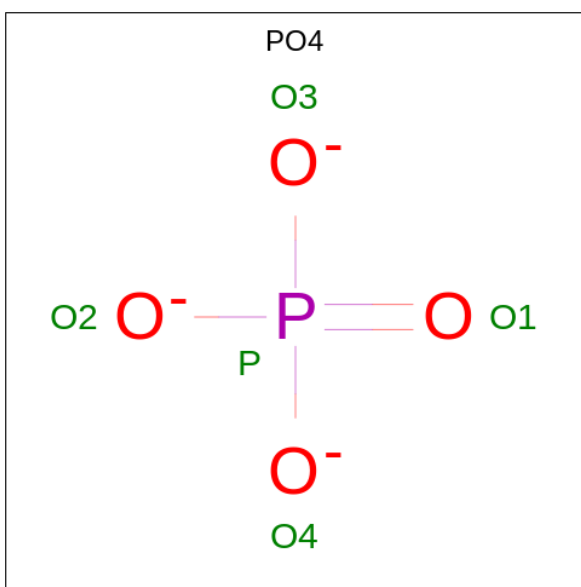
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is HYPOPHOSPHITE (three-letter code: PO2) (formula: O₂P).



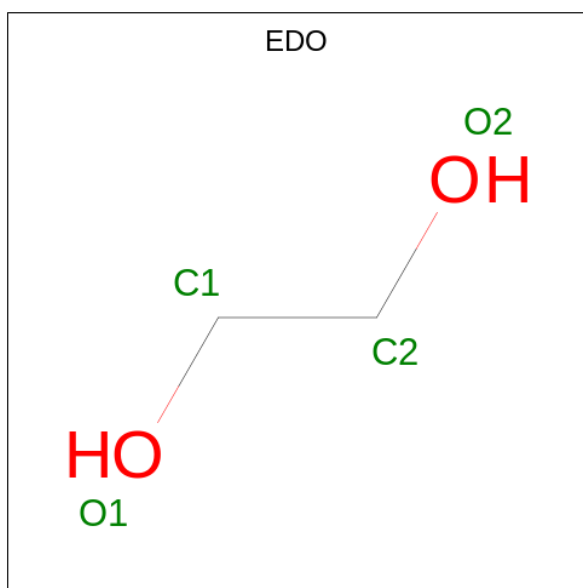
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			3	2	1		
5	A	1	Total	O	P	0	0
			3	2	1		
5	A	1	Total	O	P	0	0
			3	2	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



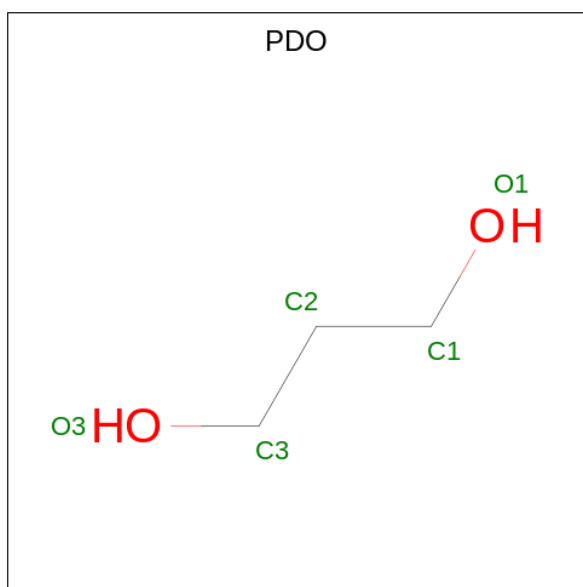
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



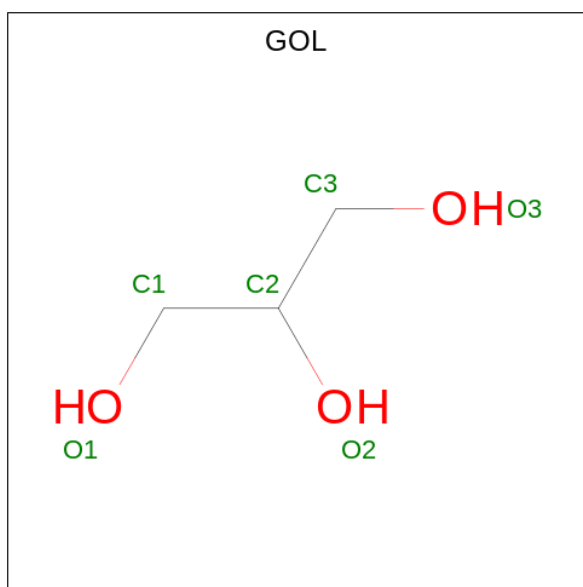
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total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

- 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		
8	A	1	Total	C	O	0	0
			5	3	2		
8	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



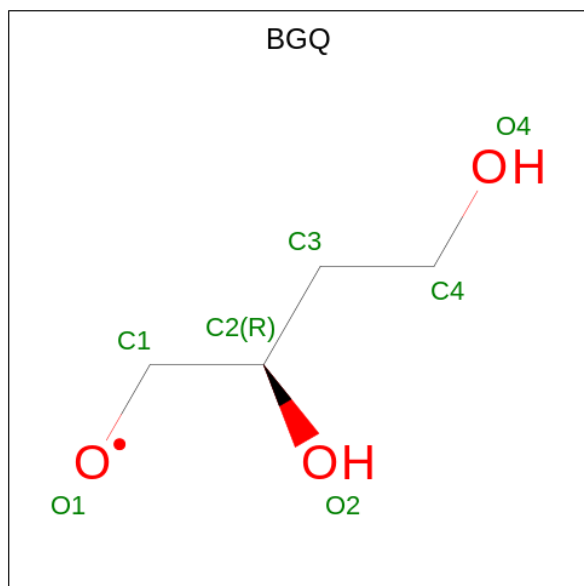
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

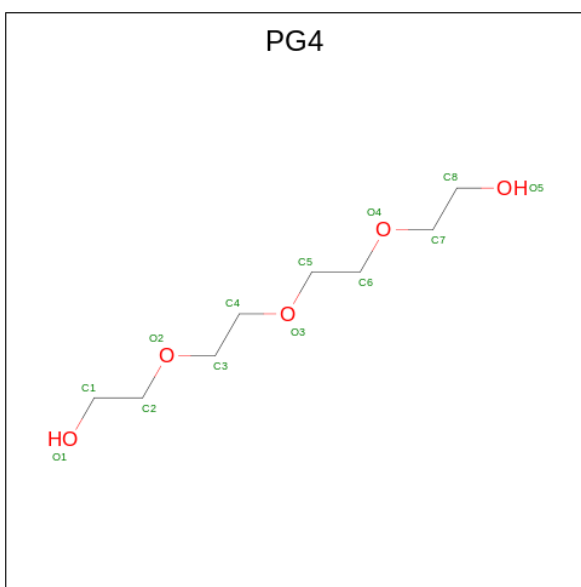
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total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

- Molecule 10 is 2-HYDROXY BUTANE-1,4-DIOL (three-letter code: BGQ) (formula: C₄H₉O₃).



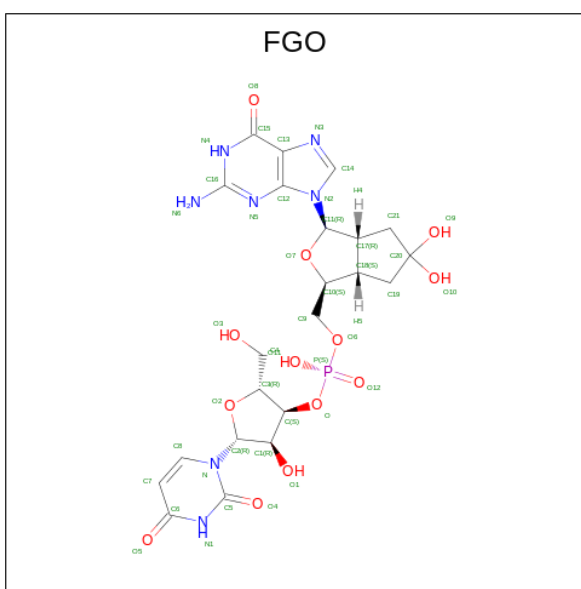
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 12 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).



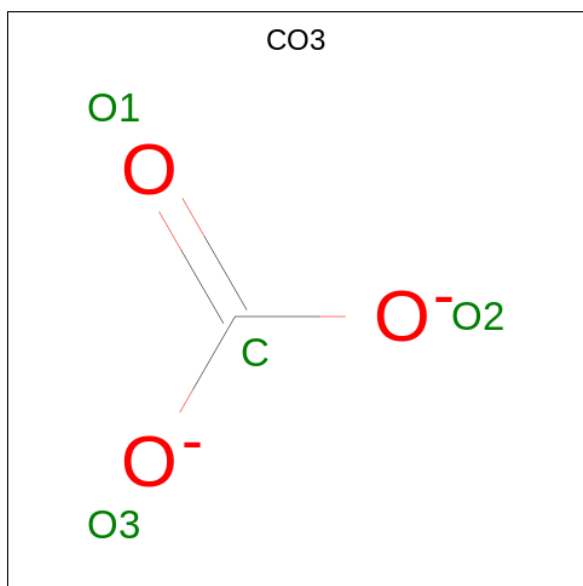
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			43	22	7	13	1		

Continued on next page...

Continued from previous page...

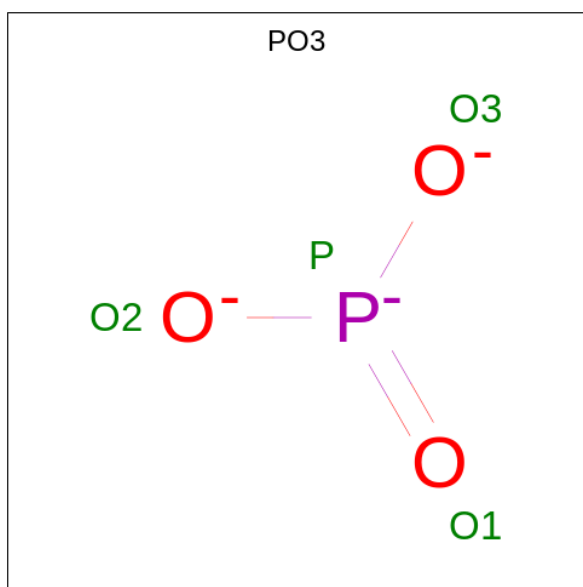
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	P	0	0
			43	22	7	13	1		

- Molecule 13 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

- Molecule 14 is PHOSPHITE ION (three-letter code: PO3) (formula: O₃P).



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

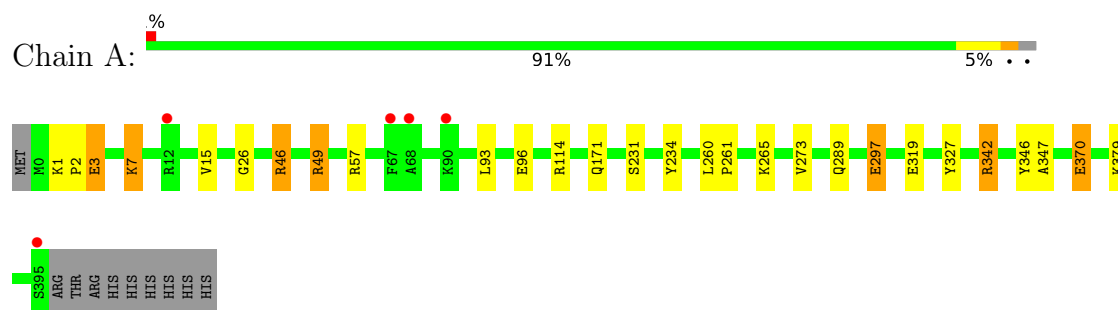
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	310	Total	O	0	0
			310	310		
15	B	327	Total	O	0	0
			327	327		

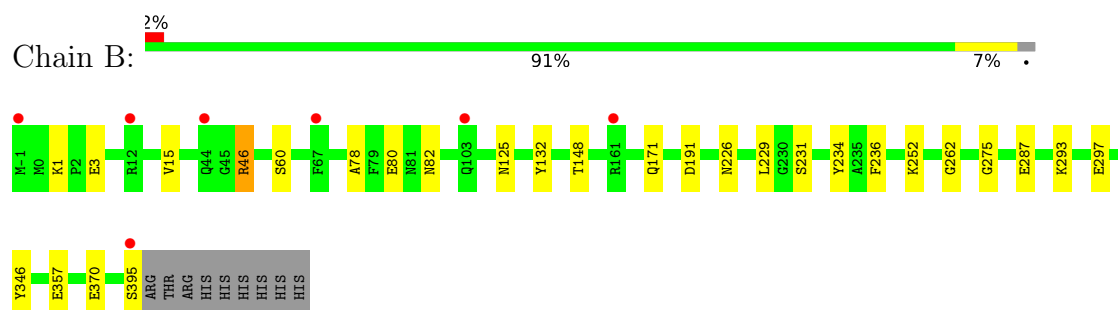
3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.17Å 57.52Å 121.14Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	46.57 – 1.80 46.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.57-1.80) 99.9 (46.57-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.146 , 0.176 0.159 , 0.188	Depositor DCC
R_{free} test set	4082 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7081	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: GOL, CO3, PO4, FGO, CO2, CL, PDO, PO2, EDO, PO3, PG4, BGQ, NA

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	6/3167 (0.2%)	1.09	11/4296 (0.3%)
1	B	1.00	7/3168 (0.2%)	1.07	7/4295 (0.2%)
All	All	1.00	13/6335 (0.2%)	1.08	18/8591 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	GLU	CD-OE2	14.43	1.41	1.25
1	B	297	GLU	CD-OE2	8.10	1.34	1.25
1	B	370	GLU	CD-OE2	8.02	1.34	1.25
1	B	80	GLU	CD-OE2	7.70	1.34	1.25
1	B	370	GLU	CD-OE1	7.64	1.34	1.25
1	A	370	GLU	CD-OE2	6.46	1.32	1.25
1	A	370	GLU	CD-OE1	6.36	1.32	1.25
1	B	287	GLU	CD-OE1	6.06	1.32	1.25
1	A	3	GLU	CD-OE1	5.82	1.32	1.25
1	B	229	LEU	C-O	5.79	1.34	1.23
1	A	96	GLU	CD-OE2	5.71	1.31	1.25
1	B	252	LYS	C-O	5.58	1.33	1.23
1	A	319	GLU	CD-OE2	5.03	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	114[A]	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	114[B]	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	346	TYR	CB-CG-CD1	7.39	125.43	121.00
1	A	327	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	B	236	PHE	CB-CA-C	-6.66	97.08	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	A	46	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	342	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	346	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	346	TYR	CB-CG-CD1	5.91	124.55	121.00
1	B	297	GLU	OE1-CD-OE2	5.70	130.15	123.30
1	B	132	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	114[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	114[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	49	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	15	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	B	46	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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	3082	0	3137	21	0
1	B	3086	0	3130	11	0
2	A	1	0	0	0	0
2	B	5	0	0	1	0
3	A	1	0	0	0	0
4	A	12	0	0	0	0
4	B	6	0	0	0	0
5	A	9	0	0	0	0
6	A	5	0	0	0	0
7	A	16	0	24	5	0
7	B	28	0	41	10	0
8	A	10	0	16	0	0
8	B	5	0	8	0	0
9	A	36	0	48	3	0
9	B	24	0	32	3	0
10	A	7	0	9	2	0
11	A	13	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	43	0	0	0	0
12	B	43	0	0	0	0
13	B	8	0	0	0	0
14	B	4	0	0	0	0
15	A	310	0	0	14	0
15	B	327	0	0	14	1
All	All	7081	0	6463	46	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (46) 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)
9:A:517:GOL:H2	15:A:672:HOH:O	1.32	1.24
1:A:379:LYS:HD3	15:A:741:HOH:O	1.56	1.02
7:B:516:EDO:H11	15:B:733:HOH:O	1.72	0.87
7:A:511:EDO:H21	15:A:782:HOH:O	1.75	0.85
1:B:171:GLN:OE1	15:B:601:HOH:O	1.95	0.83
1:A:297:GLU:HB2	7:A:513:EDO:H11	1.62	0.82
7:B:517:EDO:H22	15:B:709:HOH:O	1.80	0.81
1:A:342:ARG:HH22	7:A:511:EDO:H22	1.45	0.79
7:B:516:EDO:H21	15:B:795:HOH:O	1.87	0.73
2:B:502:CL:CL	15:B:867:HOH:O	2.48	0.69
1:A:370:GLU:HG2	15:A:784:HOH:O	1.98	0.63
9:B:521:GOL:H12	15:B:827:HOH:O	1.99	0.63
1:B:234:TYR:HB3	9:B:522:GOL:H12	1.82	0.61
1:A:46:ARG:HD2	15:A:720:HOH:O	2.04	0.58
7:B:516:EDO:C2	15:B:795:HOH:O	2.49	0.58
1:A:234:TYR:HB3	9:A:520:GOL:H12	1.86	0.57
1:B:60:SER:HB2	7:B:517:EDO:H12	1.87	0.57
7:B:514:EDO:H21	15:B:627:HOH:O	2.05	0.56
9:B:521:GOL:C1	15:B:827:HOH:O	2.56	0.54
1:A:26:GLY:H	10:A:523:BGQ:C3	2.20	0.54
1:A:26:GLY:H	10:A:523:BGQ:H31C	1.73	0.53
1:A:297:GLU:OE1	7:A:513:EDO:O2	2.27	0.53
1:A:57[A]:ARG:HG3	15:A:844:HOH:O	2.11	0.50
1:A:3:GLU:HB2	15:A:744:HOH:O	2.13	0.49
7:B:514:EDO:H22	15:B:702:HOH:O	2.11	0.49
1:A:7:LYS:HE2	15:A:868:HOH:O	2.14	0.48
1:A:93[B]:LEU:HD11	1:A:289:GLN:CD	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:519:GOL:O2	15:A:602:HOH:O	2.20	0.48
1:A:231:SER:HB3	15:A:617:HOH:O	2.13	0.48
1:A:171:GLN:OE1	15:A:601:HOH:O	2.20	0.47
1:B:82:ASN:ND2	7:B:517:EDO:O2	2.25	0.47
1:B:46:ARG:HD2	15:B:796:HOH:O	2.15	0.45
1:A:1:LYS:HB3	1:A:2:PRO:HD2	1.99	0.45
1:B:60:SER:OG	1:B:357[B]:GLU:OE1	2.12	0.44
1:B:78:ALA:HA	7:B:517:EDO:H22	2.00	0.44
7:A:511:EDO:C2	15:A:782:HOH:O	2.49	0.43
1:A:93[B]:LEU:HD11	1:A:289:GLN:NE2	2.34	0.43
7:B:514:EDO:C2	15:B:627:HOH:O	2.65	0.43
1:B:125:ASN:O	1:B:275:GLY:HA3	2.20	0.42
1:A:273:VAL:CG2	1:A:347:ALA:HB1	2.50	0.41
1:A:49:ARG:NH2	15:A:614:HOH:O	2.50	0.41
1:B:148:THR:HA	1:B:262:GLY:O	2.21	0.41
1:B:293:LYS:HD3	15:B:772:HOH:O	2.21	0.40
1:B:231:SER:HB3	15:B:695:HOH:O	2.21	0.40
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.96	0.40
1:A:265:LYS:CE	15:A:616:HOH:O	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:606:HOH:O	15:B:891:HOH:O[2_656]	2.16	0.04

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	399/406 (98%)	393 (98%)	6 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	399/406 (98%)	393 (98%)	6 (2%)	0	100	100
All	All	798/812 (98%)	786 (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	314/319 (98%)	312 (99%)	2 (1%)	86	84
1	B	314/319 (98%)	309 (98%)	5 (2%)	62	54
All	All	628/638 (98%)	621 (99%)	7 (1%)	73	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	15	VAL
1	B	1	LYS
1	B	3	GLU
1	B	191	ASP
1	B	226	ASN
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	267	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 48 ligands modelled in this entry, 7 are monoatomic - leaving 41 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	EDO	B	512	-	3,3,3	0.15	0	2,2,2	0.11	0
7	EDO	B	517	-	3,3,3	0.56	0	2,2,2	0.56	0
5	PO2	A	509	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	A	514	-	3,3,3	0.53	0	2,2,2	0.24	0
5	PO2	A	507	-	0,2,2	0.00	-	0,1,1	0.00	-
8	PDO	A	516	-	4,4,4	0.17	0	3,3,3	0.14	0
11	PG4	A	524	-	12,12,12	0.25	0	11,11,11	0.30	0
7	EDO	B	514	-	3,3,3	0.34	0	2,2,2	0.43	0
9	GOL	A	520	-	5,5,5	0.17	0	5,5,5	0.38	0
9	GOL	B	520	-	5,5,5	0.05	0	5,5,5	0.23	0
9	GOL	A	522	-	5,5,5	0.17	0	5,5,5	0.60	0
4	CO2	A	506	-	2,2,2	0.04	0	1,1,1	0.98	0
7	EDO	A	511	-	3,3,3	0.22	0	2,2,2	0.50	0
7	EDO	A	513	-	3,3,3	0.58	0	2,2,2	0.96	0
13	CO3	B	508	-	0,3,3	0.00	-	0,3,3	0.00	-
12	FGO	B	523	-	40,48,48	1.90	10 (25%)	39,75,75	2.07	8 (20%)
9	GOL	B	521	-	5,5,5	0.05	0	5,5,5	0.20	0
7	EDO	B	515	-	3,3,3	0.21	0	2,2,2	0.35	0
14	PO3	B	510	-	0,3,3	0.00	-	0,3,3	0.00	-
7	EDO	B	516	-	3,3,3	0.49	0	2,2,2	1.44	0
9	GOL	A	519	-	5,5,5	0.11	0	5,5,5	0.31	0
4	CO2	A	505	-	2,2,2	0.20	0	1,1,1	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	A	521	-	5,5,5	0.16	0	5,5,5	0.69	0
4	CO2	A	503	-	2,2,2	0.24	0	1,1,1	0.71	0
9	GOL	A	517	-	5,5,5	0.23	0	5,5,5	0.35	0
4	CO2	A	504	-	2,2,2	0.18	0	1,1,1	0.95	0
9	GOL	A	518	-	5,5,5	0.10	0	5,5,5	0.38	0
12	FGO	A	525	-	40,48,48	1.92	10 (25%)	39,75,75	1.44	5 (12%)
4	CO2	B	507	-	2,2,2	0.19	0	1,1,1	0.72	0
7	EDO	B	511	-	3,3,3	0.62	0	2,2,2	0.25	0
8	PDO	A	515	-	4,4,4	0.31	0	3,3,3	0.25	0
6	PO4	A	510	-	4,4,4	0.65	0	6,6,6	0.48	0
9	GOL	B	522	-	5,5,5	0.16	0	5,5,5	0.64	0
7	EDO	B	513	-	3,3,3	0.12	0	2,2,2	0.09	0
13	CO3	B	509	-	0,3,3	0.00	-	0,3,3	0.00	-
10	BGQ	A	523	-	6,6,6	0.46	0	4,6,6	0.73	0
5	PO2	A	508	-	0,2,2	0.00	-	0,1,1	0.00	-
8	PDO	B	518	-	4,4,4	0.21	0	3,3,3	0.48	0
4	CO2	B	506	-	2,2,2	0.37	0	1,1,1	0.67	0
9	GOL	B	519	-	5,5,5	0.06	0	5,5,5	0.22	0
7	EDO	A	512	-	3,3,3	0.15	0	2,2,2	0.22	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	EDO	B	512	-	-	1/1/1/1	-
7	EDO	B	517	-	-	0/1/1/1	-
7	EDO	A	514	-	-	1/1/1/1	-
8	PDO	A	516	-	-	1/2/2/2	-
11	PG4	A	524	-	-	1/10/10/10	-
7	EDO	B	514	-	-	1/1/1/1	-
9	GOL	A	520	-	-	2/4/4/4	-
9	GOL	B	520	-	-	4/4/4/4	-
9	GOL	A	522	-	-	2/4/4/4	-
7	EDO	A	511	-	-	0/1/1/1	-
7	EDO	A	513	-	-	1/1/1/1	-
12	FGO	B	523	-	-	1/15/63/63	0/6/6/6
9	GOL	B	521	-	-	4/4/4/4	-
7	EDO	B	515	-	-	0/1/1/1	-
7	EDO	B	516	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	A	519	-	-	4/4/4/4	-
9	GOL	A	521	-	-	2/4/4/4	-
9	GOL	A	517	-	-	3/4/4/4	-
9	GOL	A	518	-	-	4/4/4/4	-
12	FGO	A	525	-	-	0/15/63/63	0/6/6/6
7	EDO	B	511	-	-	1/1/1/1	-
8	PDO	A	515	-	-	1/2/2/2	-
9	GOL	B	522	-	-	4/4/4/4	-
7	EDO	B	513	-	-	1/1/1/1	-
10	BGQ	A	523	-	-	3/5/5/5	-
8	PDO	B	518	-	-	1/2/2/2	-
9	GOL	B	519	-	-	3/4/4/4	-
7	EDO	A	512	-	-	1/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	525	FGO	C8-N	5.70	1.42	1.35
12	A	525	FGO	C19-C18	-5.65	1.44	1.53
12	B	523	FGO	C21-C17	-5.37	1.45	1.53
12	B	523	FGO	C8-N	4.71	1.41	1.35
12	B	523	FGO	C19-C18	-3.90	1.47	1.53
12	A	525	FGO	C21-C17	-3.68	1.47	1.53
12	B	523	FGO	O5-C6	3.32	1.32	1.24
12	B	523	FGO	C15-C13	3.17	1.46	1.41
12	A	525	FGO	O5-C6	3.10	1.32	1.24
12	A	525	FGO	C15-C13	3.02	1.46	1.41
12	A	525	FGO	O2-C2	2.45	1.44	1.41
12	B	523	FGO	C5-N1	-2.39	1.33	1.38
12	B	523	FGO	C18-C17	-2.37	1.49	1.55
12	A	525	FGO	C18-C17	-2.25	1.49	1.55
12	B	523	FGO	C21-C20	-2.23	1.48	1.52
12	B	523	FGO	O2-C2	2.22	1.44	1.41
12	B	523	FGO	C8-C7	2.20	1.42	1.38
12	A	525	FGO	C1-C2	-2.15	1.50	1.53
12	A	525	FGO	C6-N1	2.11	1.36	1.33
12	A	525	FGO	C5-N1	-2.01	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	523	FGO	C11-N2-C12	-5.58	116.84	126.64
12	B	523	FGO	C15-C13-C12	-4.56	116.44	120.80
12	B	523	FGO	C13-C15-N4	-4.54	117.22	123.43
12	A	525	FGO	C11-N2-C12	-4.23	119.21	126.64
12	B	523	FGO	C15-N4-C16	4.05	122.37	115.93
12	B	523	FGO	O2-C2-C1	-4.05	101.00	106.93
12	A	525	FGO	C21-C17-C11	-3.67	107.66	113.62
12	A	525	FGO	C13-C15-N4	-3.62	118.47	123.43
12	B	523	FGO	C21-C17-C11	-3.38	108.14	113.62
12	B	523	FGO	C16-N5-C12	-2.70	112.27	115.36
12	B	523	FGO	N6-C16-N4	-2.67	113.09	117.25
12	A	525	FGO	C15-C13-C12	-2.52	118.40	120.80
12	A	525	FGO	C15-N4-C16	2.10	119.26	115.93

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	515	PDO	O1-C1-C2-C3
9	A	518	GOL	O1-C1-C2-C3
9	A	518	GOL	C1-C2-C3-O3
9	A	519	GOL	O1-C1-C2-C3
9	A	519	GOL	C1-C2-C3-O3
9	A	522	GOL	O1-C1-C2-C3
9	B	519	GOL	C1-C2-C3-O3
9	B	520	GOL	O1-C1-C2-C3
9	B	520	GOL	C1-C2-C3-O3
9	B	521	GOL	C1-C2-C3-O3
9	B	521	GOL	O2-C2-C3-O3
9	B	522	GOL	O1-C1-C2-C3
10	A	523	BGQ	C1-C2-C3-C4
10	A	523	BGQ	O2-C2-C3-C4
12	B	523	FGO	C1-C2-N-C8
11	A	524	PG4	O4-C7-C8-O5
9	A	519	GOL	O1-C1-C2-O2
9	B	520	GOL	O1-C1-C2-O2
9	B	520	GOL	O2-C2-C3-O3
9	B	522	GOL	O1-C1-C2-O2
9	A	517	GOL	O1-C1-C2-C3
9	A	517	GOL	C1-C2-C3-O3
9	A	521	GOL	C1-C2-C3-O3
9	B	521	GOL	O1-C1-C2-C3
9	B	522	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	518	GOL	O1-C1-C2-O2
9	A	518	GOL	O2-C2-C3-O3
9	A	519	GOL	O2-C2-C3-O3
9	A	522	GOL	O1-C1-C2-O2
9	B	519	GOL	O2-C2-C3-O3
7	A	513	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2
7	B	511	EDO	O1-C1-C2-O2
9	B	522	GOL	O2-C2-C3-O3
7	B	512	EDO	O1-C1-C2-O2
8	B	518	PDO	O1-C1-C2-C3
9	A	521	GOL	O2-C2-C3-O3
7	B	513	EDO	O1-C1-C2-O2
9	A	520	GOL	O1-C1-C2-C3
7	B	514	EDO	O1-C1-C2-O2
9	A	520	GOL	O1-C1-C2-O2
7	A	512	EDO	O1-C1-C2-O2
9	B	519	GOL	O1-C1-C2-C3
9	A	517	GOL	O1-C1-C2-O2
10	A	523	BGQ	C2-C3-C4-O4
8	A	516	PDO	C1-C2-C3-O3
9	B	521	GOL	O1-C1-C2-O2

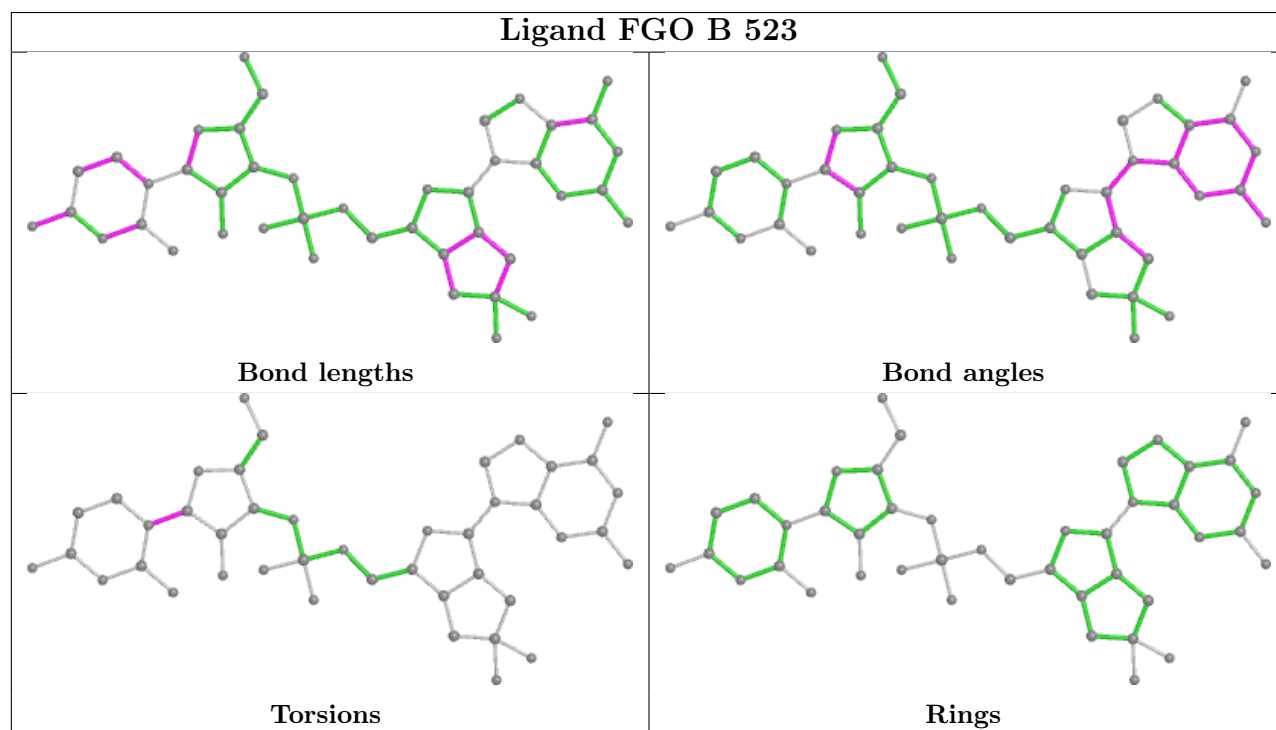
There are no ring outliers.

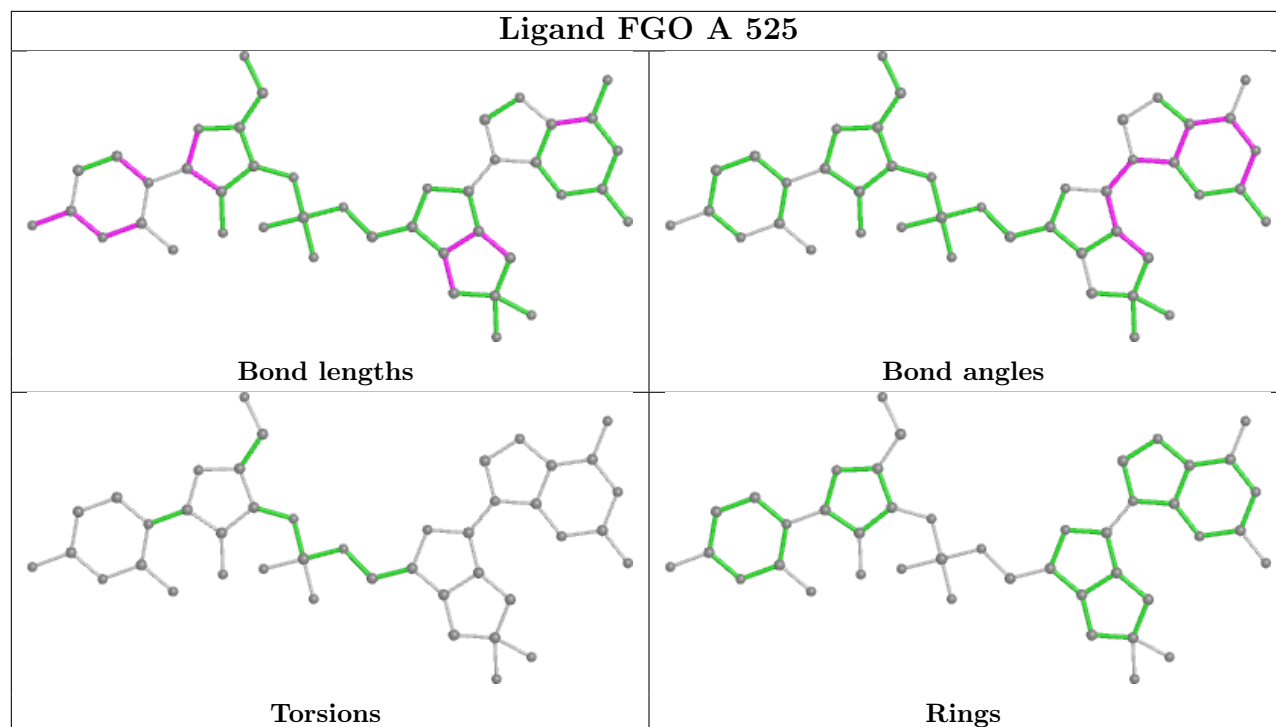
11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	517	EDO	4	0
7	B	514	EDO	3	0
9	A	520	GOL	1	0
7	A	511	EDO	3	0
7	A	513	EDO	2	0
9	B	521	GOL	2	0
7	B	516	EDO	3	0
9	A	519	GOL	1	0
9	A	517	GOL	1	0
9	B	522	GOL	1	0
10	A	523	BGQ	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	396/406 (97%)	-0.14	5 (1%) 77 74	9, 18, 41, 66	0
1	B	397/406 (97%)	-0.17	7 (1%) 68 64	9, 17, 34, 60	0
All	All	793/812 (97%)	-0.15	12 (1%) 73 70	9, 17, 36, 66	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ARG	4.4
1	A	67	PHE	4.2
1	B	12	ARG	4.1
1	A	68	ALA	4.1
1	B	67	PHE	3.1
1	B	395	SER	2.8
1	B	44	GLN	2.8
1	A	395	SER	2.3
1	A	90	LYS	2.2
1	B	103	GLN	2.2
1	B	-1	MET	2.1
1	B	161	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

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.

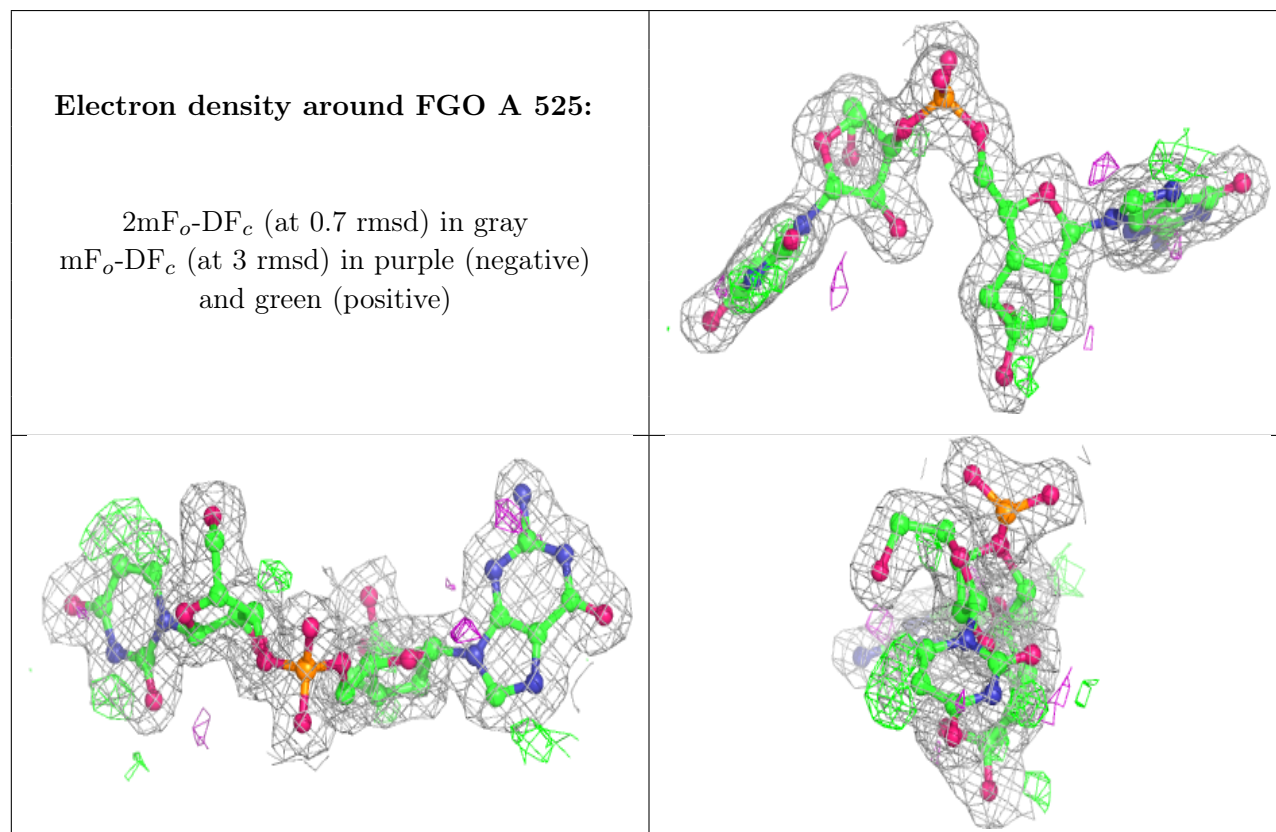
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	B	512	4/4	0.67	0.19	50,50,51,54	0
10	BGQ	A	523	7/7	0.75	0.18	47,49,55,56	0
4	CO2	A	504	3/3	0.76	0.12	45,45,48,51	0
7	EDO	B	514	4/4	0.77	0.18	37,39,42,47	0
7	EDO	A	512	4/4	0.77	0.18	42,47,48,50	0
4	CO2	A	505	3/3	0.80	0.14	53,53,56,57	0
7	EDO	B	515	4/4	0.81	0.19	38,41,44,47	0
8	PDO	B	518	5/5	0.81	0.18	34,41,46,51	0
5	PO2	A	509	3/3	0.81	0.14	52,52,60,65	0
13	CO3	B	509	4/4	0.82	0.20	35,36,39,39	0
14	PO3	B	510	4/4	0.82	0.13	49,54,63,65	0
13	CO3	B	508	4/4	0.83	0.27	42,46,46,50	0
9	GOL	A	517	6/6	0.84	0.24	29,33,33,34	0
11	PG4	A	524	13/13	0.85	0.15	31,36,45,52	0
9	GOL	A	522	6/6	0.86	0.28	30,41,44,47	0
7	EDO	A	511	4/4	0.86	0.12	31,33,37,39	0
9	GOL	B	521	6/6	0.87	0.18	45,47,48,48	0
8	PDO	A	516	5/5	0.87	0.16	39,44,50,52	0
5	PO2	A	507	3/3	0.88	0.14	50,50,52,58	0
8	PDO	A	515	5/5	0.88	0.13	40,40,42,48	0
7	EDO	B	513	4/4	0.88	0.12	49,52,53,59	0
7	EDO	B	511	4/4	0.88	0.18	39,40,44,46	0
9	GOL	A	521	6/6	0.89	0.16	23,30,35,41	0
2	CL	B	504	1/1	0.90	0.09	65,65,65,65	0
9	GOL	A	519	6/6	0.90	0.16	39,42,43,46	0
9	GOL	B	519	6/6	0.90	0.20	30,49,52,59	0
2	CL	A	501	1/1	0.91	0.07	37,37,37,37	0
9	GOL	B	520	6/6	0.91	0.18	22,40,46,54	0
7	EDO	B	516	4/4	0.91	0.14	25,26,27,29	0
4	CO2	A	506	3/3	0.91	0.16	42,42,43,52	0
6	PO4	A	510	5/5	0.92	0.16	49,50,56,58	0
9	GOL	A	518	6/6	0.93	0.18	18,28,39,48	0
7	EDO	A	514	4/4	0.93	0.14	24,29,33,40	0
4	CO2	B	507	3/3	0.94	0.11	28,28,32,40	0
9	GOL	A	520	6/6	0.94	0.12	19,22,24,28	0
2	CL	B	503	1/1	0.95	0.09	31,31,31,31	0
2	CL	B	502	1/1	0.95	0.07	48,48,48,48	0

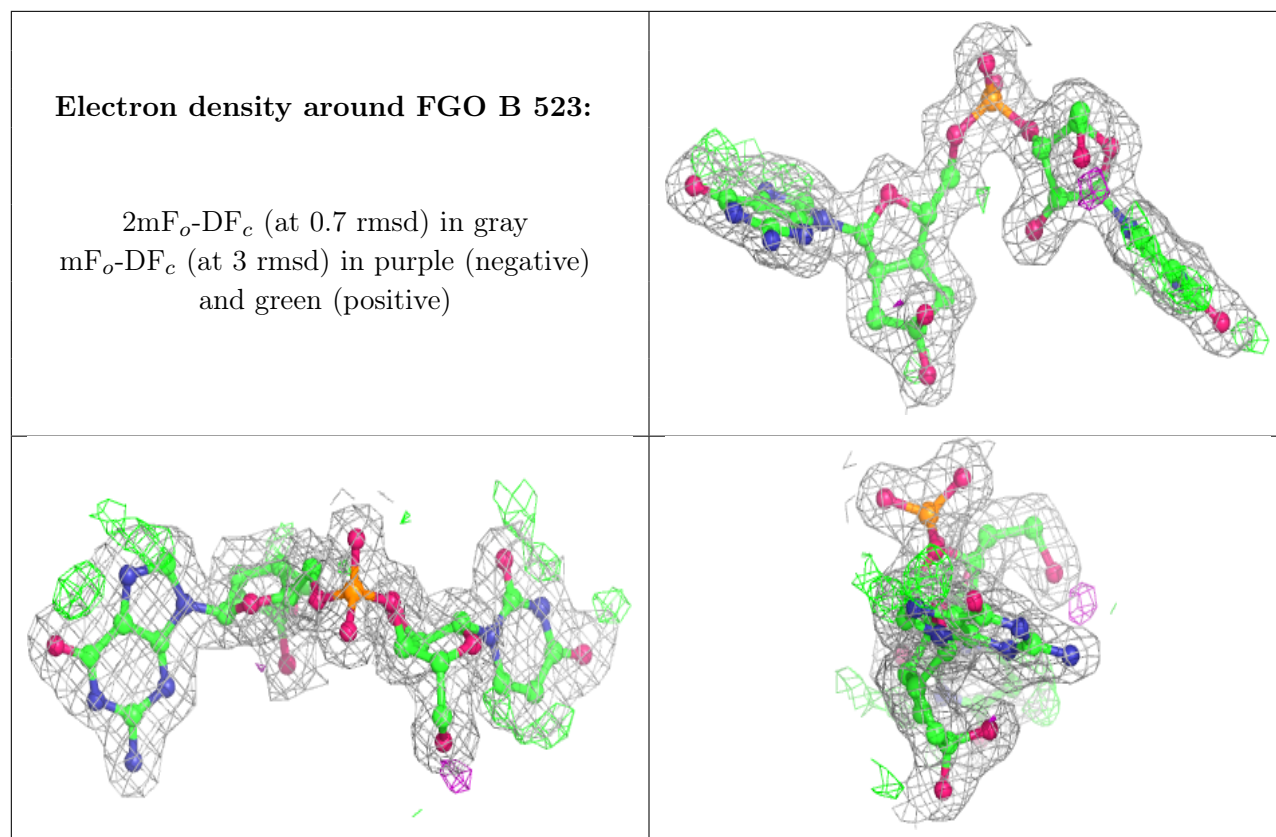
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	A	502	1/1	0.95	0.15	34,34,34,34	0
7	EDO	A	513	4/4	0.95	0.14	22,26,29,31	0
4	CO2	B	506	3/3	0.96	0.21	27,27,27,38	0
4	CO2	A	503	3/3	0.96	0.10	23,23,24,42	0
12	FGO	A	525	43/43	0.96	0.09	11,15,23,31	0
12	FGO	B	523	43/43	0.96	0.10	9,15,23,28	0
2	CL	B	505	1/1	0.96	0.05	42,42,42,42	0
5	PO2	A	508	3/3	0.96	0.09	33,33,38,44	0
9	GOL	B	522	6/6	0.96	0.16	22,26,28,29	0
7	EDO	B	517	4/4	0.97	0.20	22,25,25,28	0
2	CL	B	501	1/1	0.99	0.07	26,26,26,26	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.