



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 10:59 AM BST

PDB ID : 7C64  
Title : Crystal structure of beta-glycosides-binding protein of ABC transporter in an open state (Form II)  
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.  
Deposited on : 2020-05-21  
Resolution : 1.63 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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

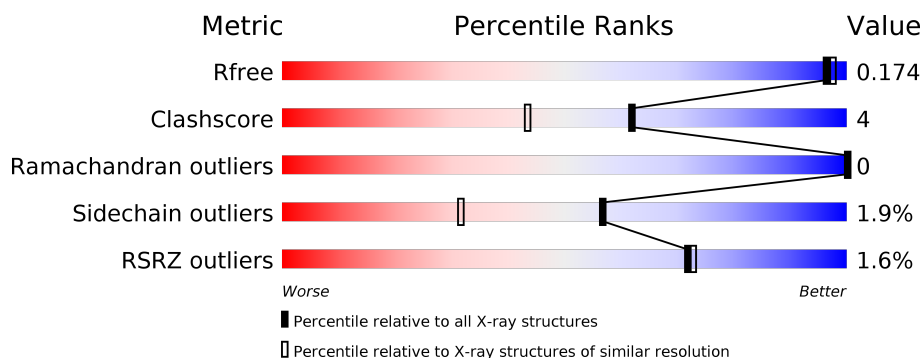
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 on 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	423	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div>
1	B	423	<div> <div style="width: 87%;"></div> <div style="width: 9%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></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
8	MRY	A	511	-	X	-	-
8	MRY	B	512	-	X	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7498 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	415	Total	C	N	O	S	0	6	0
			3201	2060	549	581	11			
1	B	415	Total	C	N	O	S	0	11	0
			3234	2086	555	582	11			

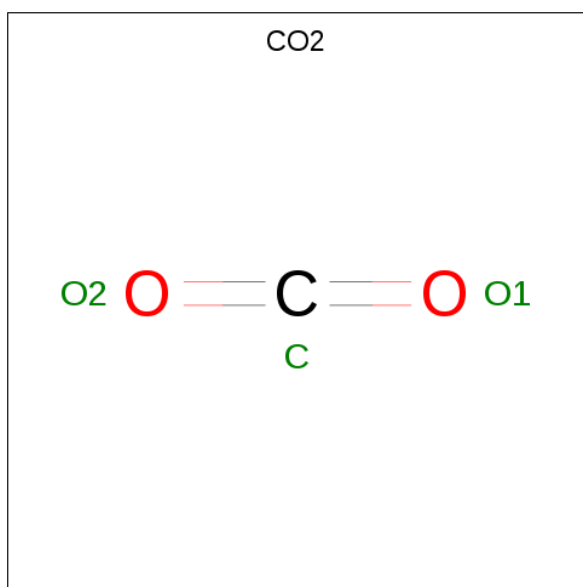
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53W80
A	417	HIS	-	expression tag	UNP Q53W80
A	418	HIS	-	expression tag	UNP Q53W80
A	419	HIS	-	expression tag	UNP Q53W80
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
A	422	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80
B	421	HIS	-	expression tag	UNP Q53W80
B	422	HIS	-	expression tag	UNP Q53W80

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Cl	0	0
			5	5		
2	A	3	Total	Cl	0	0
			3	3		

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



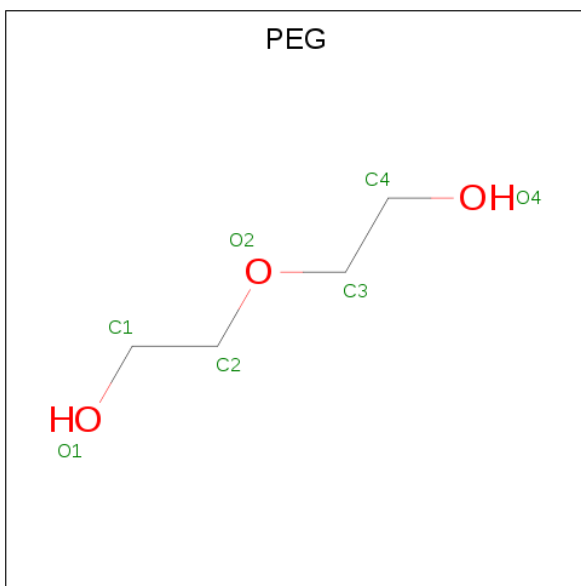
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



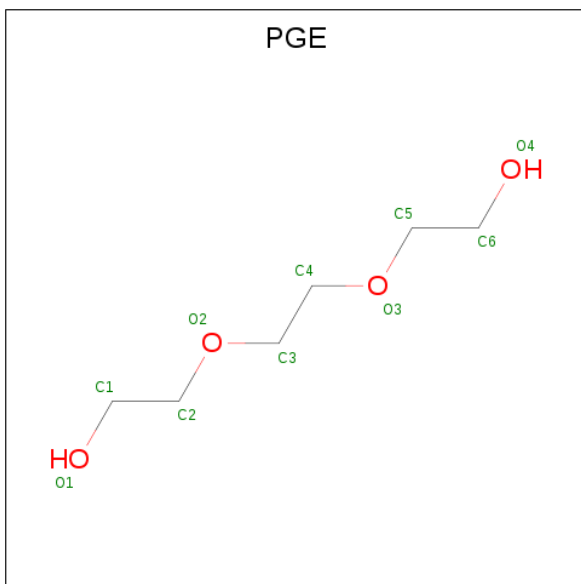
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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



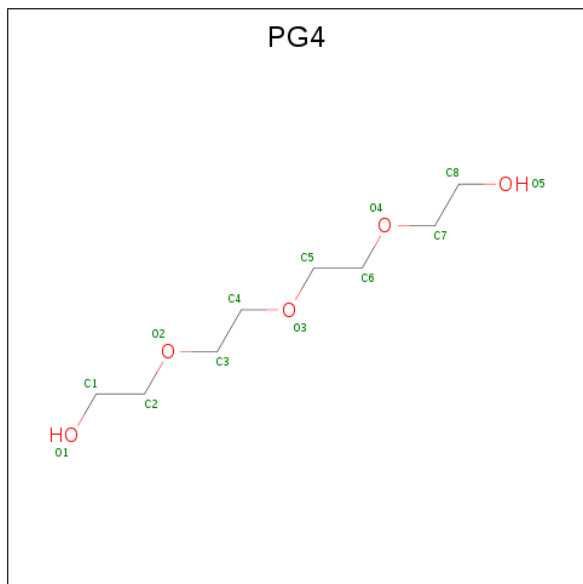
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



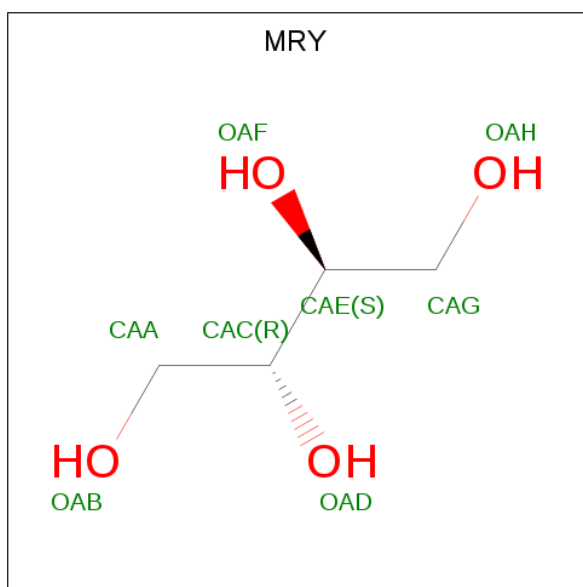
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



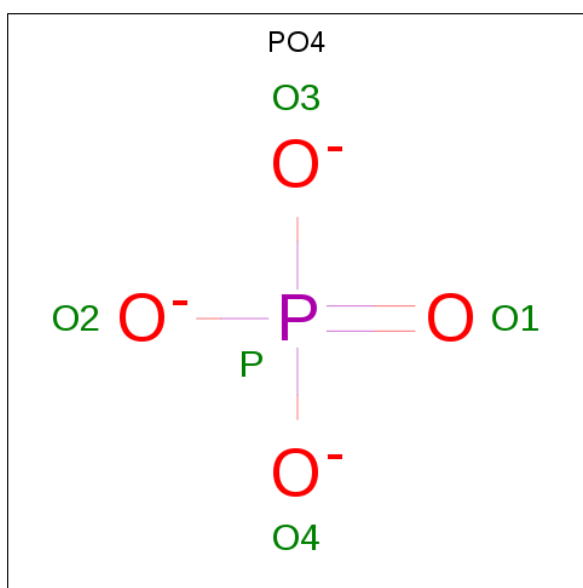
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is MESO-ERYTHRITOL (three-letter code: MRY) (formula:  $C_4H_{10}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	4	4		
8	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

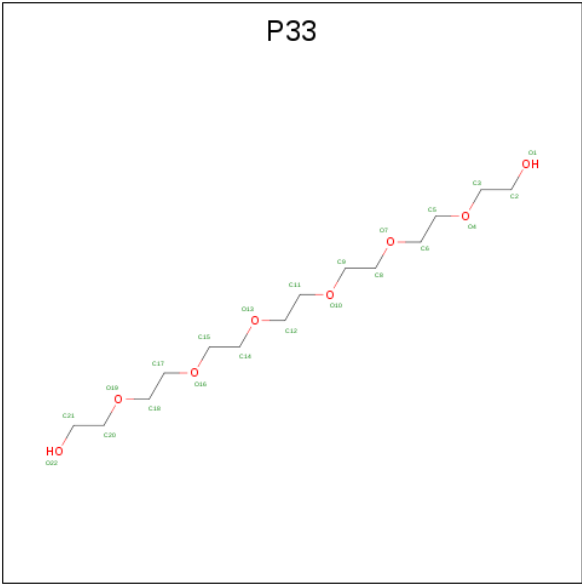


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is 3,6,9,12,15,18-HEXAOXAIICOSANE-1,20-DIOL (three-letter code: P33)



(formula: C<sub>14</sub>H<sub>30</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			22	14	8		

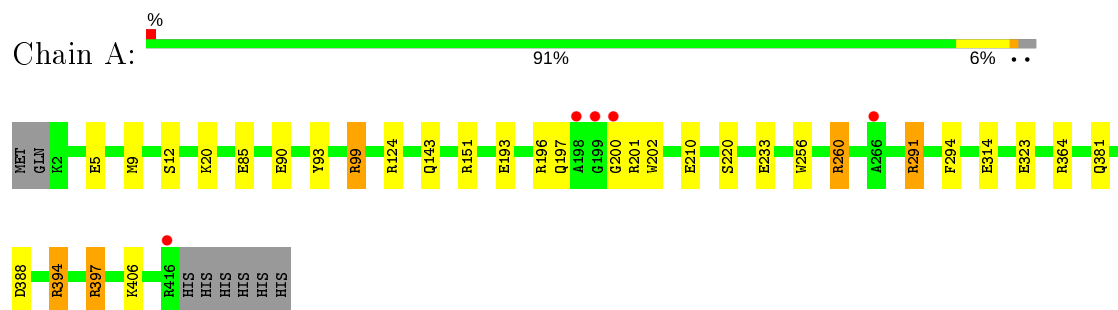
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	482	Total	O	0	0
			482	482		
11	B	452	Total	O	0	0
			452	452		

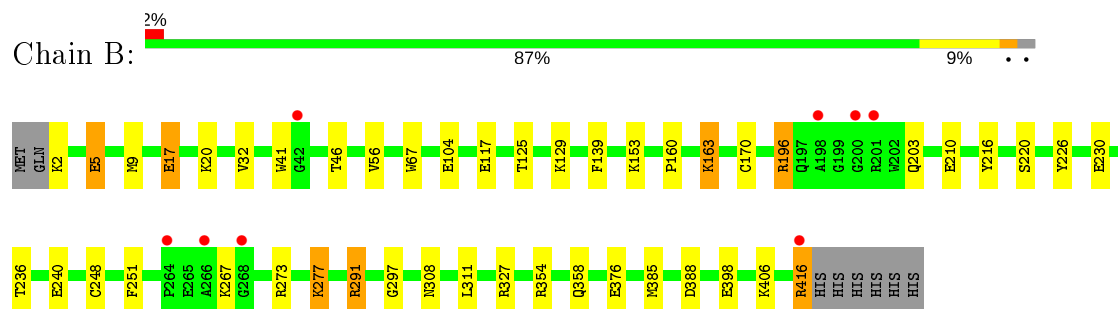
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	57.46 Å 100.71 Å 66.26 Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	50.36 – 1.63 50.35 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.36-1.63) 99.9 (50.35-1.63)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.54 (at 1.63 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.133 , 0.166 0.142 , 0.174	Depositor DCC
$R_{free}$ test set	4480 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO2, MRY, CL, PO4, EDO, PG4, PGE, P33, 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	1.07	13/3307 (0.4%)	1.26	18/4501 (0.4%)
1	B	1.06	8/3355 (0.2%)	1.15	5/4560 (0.1%)
All	All	1.07	21/6662 (0.3%)	1.21	23/9061 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLU	CD-OE1	13.48	1.40	1.25
1	B	210	GLU	CD-OE1	10.87	1.37	1.25
1	B	5	GLU	CD-OE2	9.86	1.36	1.25
1	B	17	GLU	CD-OE1	9.27	1.35	1.25
1	B	41	TRP	C-O	-8.00	1.08	1.23
1	A	314	GLU	CD-OE2	7.47	1.33	1.25
1	B	220	SER	CB-OG	-7.41	1.32	1.42
1	A	201	ARG	C-O	7.23	1.37	1.23
1	A	210	GLU	CD-OE2	6.93	1.33	1.25
1	B	376	GLU	CD-OE2	6.61	1.32	1.25
1	A	193	GLU	CD-OE2	6.38	1.32	1.25
1	A	260	ARG	CD-NE	-6.35	1.35	1.46
1	A	200	GLY	C-O	6.28	1.33	1.23
1	A	220	SER	CB-OG	-6.16	1.34	1.42
1	A	85[A]	GLU	CD-OE2	-6.13	1.19	1.25
1	A	85[B]	GLU	CD-OE2	-6.13	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	GLU	CD-OE1	5.87	1.32	1.25
1	A	5	GLU	CD-OE2	5.70	1.31	1.25
1	A	90	GLU	CD-OE2	-5.68	1.19	1.25
1	A	12	SER	CA-CB	-5.34	1.45	1.52
1	B	240	GLU	CD-OE1	5.05	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ARG	NE-CZ-NH1	-28.96	105.82	120.30
1	A	260	ARG	NE-CZ-NH2	17.85	129.22	120.30
1	A	260	ARG	CG-CD-NE	-9.08	92.74	111.80
1	B	327	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	A	124	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	260	ARG	CD-NE-CZ	7.54	134.16	123.60
1	A	260	ARG	CB-CG-CD	-7.41	92.33	111.60
1	B	216	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	A	294	PHE	CB-CG-CD2	-6.72	116.10	120.80
1	B	291	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	364	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	291	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	93	TYR	CB-CG-CD2	6.09	124.65	121.00
1	A	143	GLN	CB-CG-CD	5.80	126.69	111.60
1	A	202	TRP	N-CA-CB	5.74	120.94	110.60
1	A	394	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	388	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	397	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	388	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	151	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	139	PHE	CA-C-O	-5.08	109.44	120.10
1	A	151	ARG	CG-CD-NE	-5.07	101.16	111.80
1	A	260	ARG	NH1-CZ-NH2	5.02	124.92	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLN	Mainchain

## 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	3201	0	3178	9	0
1	B	3234	0	3241	39	0
2	A	3	0	0	0	0
2	B	5	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	8	0	12	1	0
5	A	14	0	20	2	0
5	B	7	0	10	0	0
6	A	10	0	14	5	0
6	B	20	0	28	1	0
7	A	13	0	18	2	0
8	A	8	0	9	3	0
8	B	8	0	9	3	0
9	B	5	0	0	0	0
10	B	22	0	30	6	0
11	A	482	0	0	7	3
11	B	452	0	0	18	3
All	All	7498	0	6569	57	3

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 (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:B:170:CYS:CB	1:B:248[B]:CYS:SG	2.61	0.89
1:B:358[B]:GLN:OE1	11:B:601:HOH:O	1.95	0.83
1:B:5:GLU:CD	11:B:610:HOH:O	2.17	0.83
1:B:170:CYS:HB2	1:B:248[B]:CYS:SG	2.19	0.82
6:A:509:PGE:HO4	7:A:510:PG4:HO1	1.09	0.81
1:B:203:GLN:NE2	11:B:602:HOH:O	2.16	0.74
1:A:406:LYS:HE3	11:A:999:HOH:O	1.89	0.73
5:A:507:PEG:O1	5:A:508:PEG:O1	2.10	0.70
1:B:160:PRO:O	1:B:163[A]:LYS:HD3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HE2	1:B:308:ASN:OD1	1.94	0.68
1:B:358[B]:GLN:CG	11:B:601:HOH:O	2.42	0.67
1:B:163[B]:LYS:HE3	1:B:163[B]:LYS:HA	1.77	0.66
1:B:125:THR:O	1:B:129[A]:LYS:HG3	1.96	0.65
1:B:398:GLU:HG3	2:B:504:CL:CL	2.34	0.64
1:B:291:ARG:NH1	11:B:608:HOH:O	2.31	0.64
1:B:117:GLU:OE1	10:B:511:P33:H22A	2.02	0.59
1:A:99:ARG:NH1	11:A:606:HOH:O	2.36	0.59
8:A:511:MRY:HAG1	11:A:1003:HOH:O	2.05	0.56
1:A:256:TRP:HB2	6:A:509:PGE:H32	1.87	0.56
1:B:358[B]:GLN:CD	11:B:601:HOH:O	2.37	0.55
6:B:510:PGE:H2	11:B:969:HOH:O	2.04	0.55
1:B:163[B]:LYS:HA	1:B:163[B]:LYS:CE	2.36	0.55
1:B:20:LYS:HE3	11:B:633:HOH:O	2.08	0.54
1:A:260:ARG:HG2	6:A:509:PGE:H12	1.92	0.51
1:B:358[B]:GLN:HG3	11:B:601:HOH:O	2.08	0.51
1:B:32:VAL:HG11	1:B:311:LEU:HD21	1.93	0.49
1:B:416:ARG:HD3	11:B:602:HOH:O	2.12	0.49
1:B:196:ARG:NH1	11:B:614:HOH:O	2.45	0.48
1:B:163[A]:LYS:NZ	1:B:163[A]:LYS:HA	2.28	0.48
8:B:512:MRY:HAA1	11:B:761:HOH:O	2.12	0.48
1:B:117:GLU:OE1	10:B:511:P33:C2	2.61	0.48
1:B:406:LYS:HE3	11:B:1008:HOH:O	2.13	0.47
1:B:273:ARG:O	1:B:277[A]:LYS:HD3	2.14	0.47
1:B:354:ARG:HH21	8:B:512:MRY:CAA	2.28	0.47
6:A:509:PGE:O4	7:A:510:PG4:O1	1.95	0.45
1:B:2:LYS:N	11:B:617:HOH:O	2.49	0.45
1:A:397:ARG:HH22	4:A:505:EDO:H21	1.81	0.45
1:B:196:ARG:CZ	11:B:695:HOH:O	2.65	0.45
1:A:20:LYS:HE3	11:A:615:HOH:O	2.18	0.44
1:A:233:GLU:OE1	1:B:17:GLU:OE2	2.36	0.44
1:B:297:GLY:H	10:B:511:P33:C2	2.31	0.44
1:B:67:TRP:HE1	10:B:511:P33:H121	1.83	0.43
8:A:511:MRY:HAG2	11:A:607:HOH:O	2.19	0.43
1:B:277[B]:LYS:HE3	1:B:277[B]:LYS:HB2	1.42	0.43
1:A:291:ARG:NH2	11:A:627:HOH:O	2.52	0.42
1:B:236:THR:HG23	11:B:717:HOH:O	2.20	0.41
1:A:381:GLN:OE1	1:B:56:VAL:HG12	2.19	0.41
5:A:508:PEG:H31	1:B:46:THR:HG21	2.02	0.41
8:A:511:MRY:CAG	11:A:607:HOH:O	2.68	0.41
1:B:297:GLY:H	10:B:511:P33:H21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:509:PGE:H3	6:A:509:PGE:H1	1.88	0.41
1:B:385:MET:HB2	1:B:385:MET:HE2	1.76	0.40
10:B:511:P33:H61	11:B:791:HOH:O	2.21	0.40
8:B:512:MRY:HAG1	11:B:977:HOH:O	2.21	0.40
1:B:153:LYS:HE2	1:B:226:TYR:CE1	2.57	0.40
1:B:163[B]:LYS:CE	1:B:163[B]:LYS:CA	2.98	0.40

All (3) 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)
11:A:798:HOH:O	11:B:630:HOH:O[2_655]	1.84	0.36
11:A:909:HOH:O	11:B:903:HOH:O[1_556]	2.08	0.12
11:A:892:HOH:O	11:B:820:HOH:O[1_556]	2.10	0.10

## 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	419/423 (99%)	415 (99%)	4 (1%)	0	100	100
1	B	424/423 (100%)	418 (99%)	6 (1%)	0	100	100
All	All	843/846 (100%)	833 (99%)	10 (1%)	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	320/322 (99%)	316 (99%)	4 (1%)	69	47
1	B	325/322 (101%)	315 (97%)	10 (3%)	40	13
All	All	645/644 (100%)	631 (98%)	14 (2%)	57	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	99	ARG
1	A	196	ARG
1	A	394	ARG
1	B	9	MET
1	B	163[A]	LYS
1	B	163[B]	LYS
1	B	196	ARG
1	B	230	GLU
1	B	251	PHE
1	B	267	LYS
1	B	277[A]	LYS
1	B	277[B]	LYS
1	B	416	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	PGE	B	510	-	9,9,9	0.38	0	8,8,8	0.42	0
5	PEG	A	507	-	6,6,6	0.20	0	5,5,5	0.22	0
5	PEG	A	508	-	6,6,6	0.21	0	5,5,5	0.24	0
4	EDO	A	506	-	3,3,3	0.17	0	2,2,2	0.08	0
6	PGE	B	509	-	9,9,9	0.23	0	8,8,8	0.19	0
4	EDO	A	505	-	3,3,3	0.50	0	2,2,2	0.39	0
8	MRY	A	511	-	7,7,7	2.51	4 (57%)	8,8,8	3.47	6 (75%)
3	CO2	B	506	-	2,2,2	0.08	0	1,1,1	1.02	0
7	PG4	A	510	-	12,12,12	0.16	0	11,11,11	0.27	0
3	CO2	A	504	-	2,2,2	0.07	0	1,1,1	1.08	0
8	MRY	B	512	-	7,7,7	2.21	3 (42%)	8,8,8	3.80	6 (75%)
5	PEG	B	508	-	6,6,6	0.31	0	5,5,5	0.31	0
10	P33	B	511	-	21,21,21	0.66	0	20,20,20	1.51	3 (15%)
6	PGE	A	509	-	9,9,9	0.22	0	8,8,8	0.19	0
9	PO4	B	507	-	4,4,4	0.67	0	6,6,6	0.42	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	PGE	B	510	-	-	4/7/7/7	-
5	PEG	A	507	-	-	1/4/4/4	-
5	PEG	A	508	-	-	1/4/4/4	-
4	EDO	A	506	-	-	0/1/1/1	-
6	PGE	B	509	-	-	1/7/7/7	-
4	EDO	A	505	-	-	1/1/1/1	-
8	MRY	A	511	-	-	6/8/8/8	-
7	PG4	A	510	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MRY	B	512	-	-	7/8/8/8	-
5	PEG	B	508	-	-	2/4/4/4	-
10	P33	B	511	-	-	8/19/19/19	-
6	PGE	A	509	-	-	2/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	511	MRY	OAH-CAG	-4.69	1.22	1.42
8	B	512	MRY	OAH-CAG	-4.52	1.23	1.42
8	A	511	MRY	CAG-CAE	-3.38	1.43	1.52
8	B	512	MRY	CAG-CAE	-2.51	1.45	1.52
8	B	512	MRY	CAE-CAC	-2.25	1.47	1.52
8	A	511	MRY	CAE-CAC	-2.24	1.47	1.52
8	A	511	MRY	CAA-CAC	-2.07	1.46	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	512	MRY	OAD-CAC-CAE	-7.78	93.74	109.72
8	A	511	MRY	OAB-CAA-CAC	-6.65	96.57	111.07
10	B	511	P33	O4-C3-C2	4.84	131.32	110.07
8	B	512	MRY	OAB-CAA-CAC	-4.19	101.93	111.07
8	B	512	MRY	CAA-CAC-CAE	4.01	121.82	113.11
8	A	511	MRY	OAD-CAC-CAE	-3.84	101.84	109.72
8	A	511	MRY	OAH-CAG-CAE	-3.55	103.35	111.07
10	B	511	P33	O1-C2-C3	2.92	128.75	111.81
8	A	511	MRY	OAF-CAE-CAC	2.81	115.51	109.72
8	B	512	MRY	OAD-CAC-CAA	-2.66	102.91	109.14
8	A	511	MRY	OAD-CAC-CAA	-2.62	103.00	109.14
8	B	512	MRY	OAF-CAE-CAG	2.34	114.63	109.14
8	A	511	MRY	CAA-CAC-CAE	2.26	118.03	113.11
8	B	512	MRY	OAF-CAE-CAC	2.01	113.86	109.72
10	B	511	P33	O13-C14-C15	2.00	119.42	110.39

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	512	MRY	CAA-CAC-CAE-OAF

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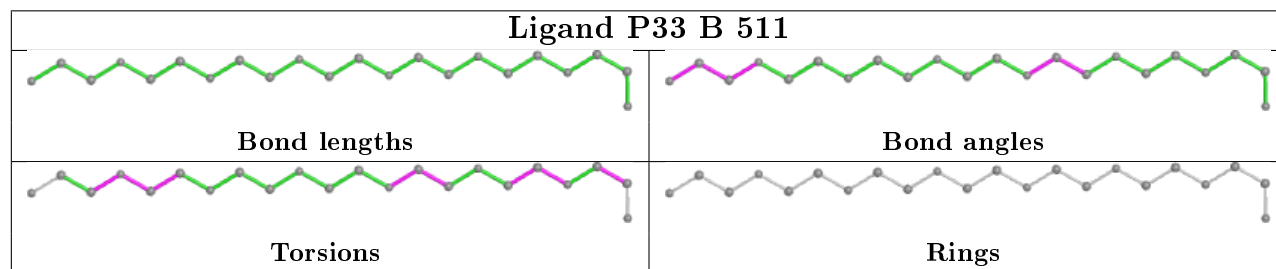
Mol	Chain	Res	Type	Atoms
8	B	512	MRY	CAA-CAC-CAE-CAG
8	B	512	MRY	OAD-CAC-CAE-OAF
8	B	512	MRY	OAD-CAC-CAE-CAG
8	B	512	MRY	CAC-CAE-CAG-OAH
8	A	511	MRY	CAA-CAC-CAE-OAF
8	A	511	MRY	CAA-CAC-CAE-CAG
8	A	511	MRY	OAD-CAC-CAE-OAF
8	A	511	MRY	OAD-CAC-CAE-CAG
8	A	511	MRY	CAC-CAE-CAG-OAH
8	A	511	MRY	OAF-CAE-CAG-OAH
10	B	511	P33	C6-C5-O4-C3
10	B	511	P33	C15-C14-O13-C12
10	B	511	P33	O13-C14-C15-O16
10	B	511	P33	O4-C5-C6-O7
5	A	508	PEG	O1-C1-C2-O2
6	B	510	PGE	C6-C5-O3-C4
10	B	511	P33	O19-C20-C21-O22
7	A	510	PG4	O4-C7-C8-O5
10	B	511	P33	O16-C17-C18-O19
6	B	510	PGE	C4-C3-O2-C2
8	B	512	MRY	OAB-CAA-CAC-OAD
8	B	512	MRY	OAF-CAE-CAG-OAH
7	A	510	PG4	C6-C5-O3-C4
10	B	511	P33	C2-C3-O4-C5
6	B	509	PGE	C4-C3-O2-C2
5	B	508	PEG	O1-C1-C2-O2
6	B	510	PGE	C3-C4-O3-C5
6	A	509	PGE	C1-C2-O2-C3
5	A	507	PEG	C1-C2-O2-C3
7	A	510	PG4	C1-C2-O2-C3
5	B	508	PEG	C4-C3-O2-C2
7	A	510	PG4	O3-C5-C6-O4
10	B	511	P33	C17-C18-O19-C20
6	A	509	PGE	O2-C3-C4-O3
4	A	505	EDO	O1-C1-C2-O2
7	A	510	PG4	O1-C1-C2-O2
6	B	510	PGE	O2-C3-C4-O3

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	510	PGE	1	0
5	A	507	PEG	1	0
5	A	508	PEG	2	0
4	A	505	EDO	1	0
8	A	511	MRY	3	0
7	A	510	PG4	2	0
8	B	512	MRY	3	0
10	B	511	P33	6	0
6	A	509	PGE	5	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, 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	415/423 (98%)	-0.16	5 (1%) 79 79	6, 11, 23, 44	0
1	B	415/423 (98%)	-0.16	8 (1%) 66 67	6, 11, 24, 57	0
All	All	830/846 (98%)	-0.16	13 (1%) 72 73	6, 11, 23, 57	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	GLY	3.9
1	B	266	ALA	3.7
1	B	200	GLY	3.6
1	A	198	ALA	3.4
1	B	198	ALA	3.4
1	B	268	GLY	3.0
1	B	201	ARG	2.9
1	B	42	GLY	2.3
1	A	266	ALA	2.3
1	A	199	GLY	2.1
1	B	416	ARG	2.1
1	A	416	ARG	2.0
1	B	264	PRO	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 ⓘ

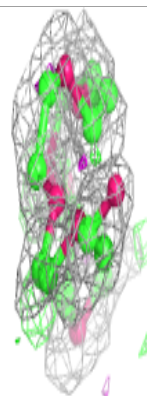
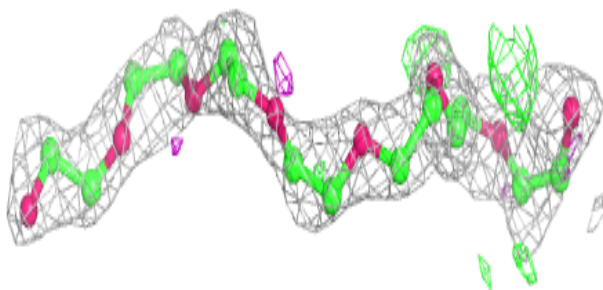
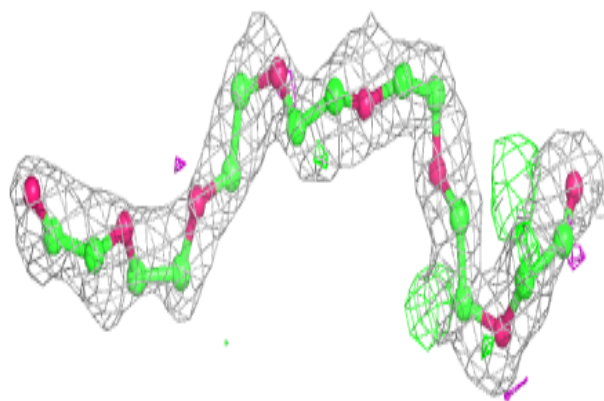
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	PEG	B	508	7/7	0.79	0.12	40,43,44,44	0
6	PGE	B	509	10/10	0.80	0.13	34,38,46,49	0
8	MRY	A	511	8/8	0.81	0.26	24,29,36,40	0
10	P33	B	511	22/22	0.82	0.15	23,38,45,45	0
6	PGE	B	510	10/10	0.82	0.13	25,31,36,42	0
8	MRY	B	512	8/8	0.83	0.20	23,32,36,36	0
3	CO2	A	504	3/3	0.83	0.10	38,38,39,44	0
4	EDO	A	505	4/4	0.84	0.14	36,37,40,43	0
4	EDO	A	506	4/4	0.84	0.17	31,31,33,33	0
5	PEG	A	507	7/7	0.85	0.13	27,32,35,38	0
7	PG4	A	510	13/13	0.86	0.12	23,29,45,48	0
5	PEG	A	508	7/7	0.86	0.11	35,41,44,48	0
3	CO2	B	506	3/3	0.87	0.10	35,35,35,44	0
6	PGE	A	509	10/10	0.89	0.17	26,31,37,45	0
2	CL	A	503	1/1	0.89	0.08	41,41,41,41	0
9	PO4	B	507	5/5	0.91	0.20	35,36,40,42	0
2	CL	B	505	1/1	0.92	0.08	33,33,33,33	0
2	CL	B	504	1/1	0.95	0.06	35,35,35,35	0
2	CL	B	503	1/1	0.98	0.04	41,41,41,41	0
2	CL	B	502	1/1	0.99	0.04	21,21,21,21	0
2	CL	A	502	1/1	0.99	0.06	20,20,20,20	0
2	CL	B	501	1/1	1.00	0.08	10,10,10,10	0
2	CL	A	501	1/1	1.00	0.07	14,14,14,14	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 P33 B 511:**

$2mF_o-DF_c$  (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.