



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:34 PM BST

PDB ID : 6EQ0  
Title : Structure of the periplasmic binding protein (PBP) MelB (atu4661) in complex with galactose from agrobacterium tumefaciens C58  
Authors : Vigouroux, A.; Morera, S.  
Deposited on : 2017-10-12  
Resolution : 2.45 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 : 2.13.1  
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) : 2.13.1

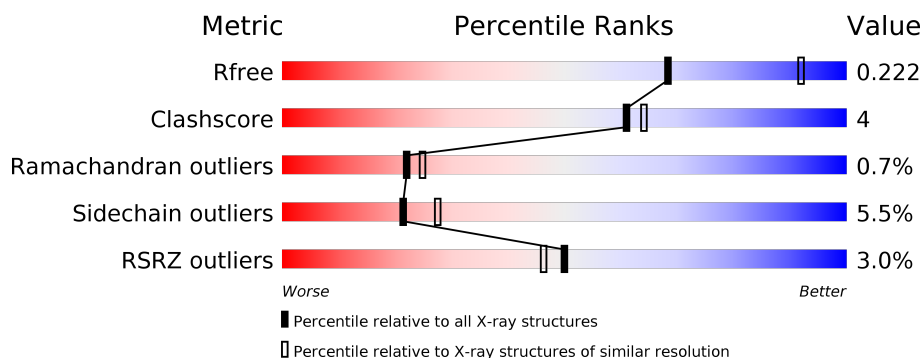
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	683	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	683	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </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
3	PEG	A	703	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10998 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.

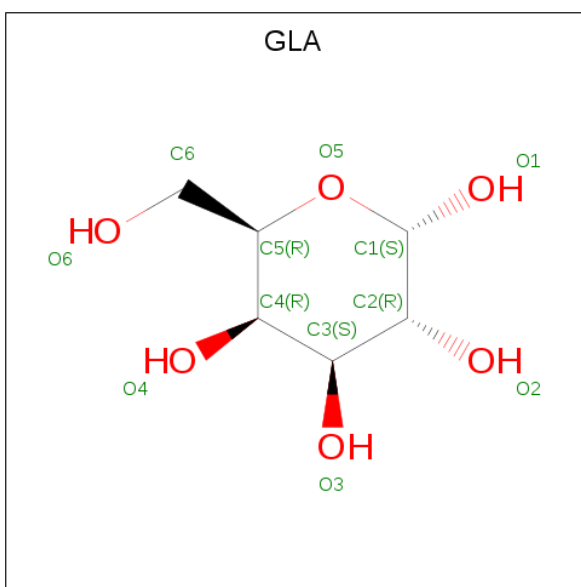
- Molecule 1 is a protein called Periplasmic alpha-galactoside-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	0	0
			5295	3380	899	1000	16			
1	B	671	Total	C	N	O	S	0	0	0
			5295	3380	899	1000	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	HIS	-	expression tag	UNP A0A083ZM57
A	679	HIS	-	expression tag	UNP A0A083ZM57
A	680	HIS	-	expression tag	UNP A0A083ZM57
A	681	HIS	-	expression tag	UNP A0A083ZM57
A	682	HIS	-	expression tag	UNP A0A083ZM57
A	683	HIS	-	expression tag	UNP A0A083ZM57
B	678	HIS	-	expression tag	UNP A0A083ZM57
B	679	HIS	-	expression tag	UNP A0A083ZM57
B	680	HIS	-	expression tag	UNP A0A083ZM57
B	681	HIS	-	expression tag	UNP A0A083ZM57
B	682	HIS	-	expression tag	UNP A0A083ZM57
B	683	HIS	-	expression tag	UNP A0A083ZM57

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- 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		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	7	Total Cl 7 7	0	0
5	A	9	Total Cl 9 9	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total Ca 5 5	0	0
6	A	12	Total Ca 12 12	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	143	Total O 143 143	0	0
7	B	110	Total O 110 110	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.84Å 73.92Å 171.10Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	46.51 – 2.45 46.51 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.51-2.45) 87.5 (46.51-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.194 , 0.241 0.200 , 0.222	Depositor DCC
$R_{free}$ test set	2480 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.145 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: GLA, CA, PEG, EDO, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	1/5448 (0.0%)	0.72	1/7413 (0.0%)
1	B	0.50	0/5448	0.72	3/7413 (0.0%)
All	All	0.52	1/10896 (0.0%)	0.72	4/14826 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	MET	SD-CE	-6.42	1.41	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	677	ASN	C-N-CA	7.47	140.38	121.70
1	B	22	ALA	C-N-CA	5.62	135.76	121.70
1	A	57	GLY	C-N-CA	5.23	134.77	121.70
1	B	57	GLY	C-N-CA	5.03	134.29	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5295	0	5113	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5295	0	5114	43	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	14	0	20	6	0
4	A	44	0	66	2	0
4	B	40	0	60	0	0
5	A	9	0	0	2	0
5	B	7	0	0	0	0
6	A	12	0	0	0	0
6	B	5	0	0	0	0
7	A	143	0	0	1	0
7	B	110	0	0	1	0
All	All	10998	0	10397	93	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 4.

All (93) 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:633:PRO:HA	3:A:703:PEG:H11	1.32	1.05
1:A:164:TRP:HA	1:A:272:MET:HE1	1.69	0.73
1:A:633:PRO:HA	3:A:703:PEG:C1	2.16	0.72
1:A:579:ILE:HG21	1:A:599:TYR:HB2	1.73	0.70
1:A:617:GLY:H	3:A:703:PEG:H42	1.54	0.70
1:B:46:PRO:HD2	1:B:49:ILE:HD12	1.77	0.67
1:A:46:PRO:HD2	1:A:49:ILE:HD12	1.78	0.65
1:A:164:TRP:HA	1:A:272:MET:CE	2.27	0.63
1:B:425:ILE:H	1:B:600:GLN:HE22	1.47	0.60
1:B:677:ASN:HB3	1:B:678:HIS:C	2.22	0.59
1:A:110:TRP:O	1:A:113:ILE:HG22	2.02	0.59
1:B:438:VAL:HG21	1:B:605:GLN:HB2	1.85	0.58
1:B:110:TRP:O	1:B:113:ILE:HG22	2.03	0.58
1:A:438:VAL:HG21	1:A:605:GLN:HB2	1.86	0.57
1:A:617:GLY:O	3:A:703:PEG:H21	2.05	0.57
1:B:240:SER:O	1:B:244:LYS:HB2	2.06	0.56
1:B:242:ILE:HG13	1:B:270:PRO:HG2	1.87	0.56
1:A:240:SER:O	1:A:244:LYS:HB2	2.06	0.55
1:A:77:ASN:ND2	1:A:648:ARG:HH12	2.04	0.55
1:B:93:VAL:HG12	1:B:111:GLY:HA3	1.87	0.55
1:A:360:PRO:O	3:A:703:PEG:H41	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HD11	1:B:137:PRO:HA	1.89	0.55
1:A:242:ILE:HG13	1:A:270:PRO:HG2	1.88	0.54
1:B:51:GLU:HA	1:B:55:LYS:HD2	1.90	0.54
1:A:127:LEU:HD11	1:A:137:PRO:HA	1.88	0.54
1:A:93:VAL:HG12	1:A:111:GLY:HA3	1.88	0.54
1:A:571:PRO:HA	1:A:574:LYS:HD2	1.90	0.54
1:B:77:ASN:ND2	1:B:648:ARG:HH12	2.06	0.53
1:A:500:GLN:HA	1:A:503:LYS:HD2	1.91	0.53
1:B:382:ARG:HA	1:B:472:LEU:HD11	1.92	0.52
1:A:677:ASN:CG	1:A:678:HIS:HA	2.29	0.52
1:B:571:PRO:HA	1:B:574:LYS:HD2	1.92	0.52
1:A:480:THR:HB	1:A:511:HIS:ND1	2.25	0.51
1:A:382:ARG:HA	1:A:472:LEU:HD11	1.92	0.51
1:B:500:GLN:HA	1:B:503:LYS:HD2	1.91	0.51
1:A:633:PRO:CA	3:A:703:PEG:H11	2.22	0.50
1:A:272:MET:HB2	5:A:718:CL:CL	2.49	0.50
1:B:297:VAL:HG12	1:B:303:GLN:HA	1.93	0.50
1:B:290:ARG:HD2	1:B:308:ASN:HD22	1.77	0.49
1:A:239:PRO:HB3	1:A:270:PRO:HB2	1.95	0.49
1:B:239:PRO:HB3	1:B:270:PRO:HB2	1.94	0.48
1:A:582:LYS:HG3	1:B:571:PRO:HG2	1.95	0.48
1:A:297:VAL:HG12	1:A:303:GLN:HA	1.95	0.48
1:A:369:MET:O	1:A:558:ASN:HB2	2.14	0.48
1:A:646:ARG:HA	1:A:649:LEU:HG	1.95	0.47
1:A:117:LEU:HD22	1:A:271:VAL:HG11	1.96	0.47
1:A:290:ARG:HD2	1:A:308:ASN:HD22	1.80	0.47
1:B:417:PHE:O	1:B:616:PRO:HD3	2.15	0.47
1:A:494:ALA:O	1:A:498:VAL:HG23	2.14	0.47
1:B:646:ARG:HA	1:B:649:LEU:HG	1.95	0.47
1:A:437:THR:HG23	1:A:604:THR:HG21	1.96	0.47
1:A:417:PHE:O	1:A:616:PRO:HD3	2.14	0.47
1:A:331:PHE:CE2	1:A:619:LEU:HD11	2.49	0.47
1:B:494:ALA:O	1:B:498:VAL:HG23	2.15	0.47
1:A:652:ALA:HA	4:A:713:EDO:H12	1.96	0.46
1:A:336:GLN:HE22	1:A:488:ALA:H	1.63	0.46
1:B:331:PHE:CE2	1:B:619:LEU:HD11	2.50	0.46
1:B:369:MET:O	1:B:558:ASN:HB2	2.15	0.46
1:B:117:LEU:HD22	1:B:271:VAL:HG11	1.98	0.46
4:A:704:EDO:H11	4:A:712:EDO:H22	1.98	0.45
1:B:437:THR:HG23	1:B:604:THR:HG21	1.97	0.45
1:B:336:GLN:HE22	1:B:488:ALA:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TRP:CE3	1:A:272:MET:HE2	2.52	0.45
1:B:478:GLU:HB3	7:B:816:HOH:O	2.17	0.45
1:A:90:ARG:HB3	7:A:884:HOH:O	2.17	0.45
1:A:38:LYS:HE3	1:A:40:LEU:HD21	1.98	0.45
1:A:164:TRP:CD2	1:A:272:MET:HE2	2.53	0.44
1:A:554:ARG:HH11	1:A:554:ARG:HB2	1.83	0.44
1:A:481:LEU:HD11	1:A:531:VAL:HG23	2.00	0.43
1:B:376:TRP:CE2	1:B:560:ARG:HB2	2.53	0.43
1:B:24:GLY:HA3	1:B:25:LYS:HA	1.85	0.43
1:B:481:LEU:HD11	1:B:531:VAL:HG23	2.00	0.43
1:A:376:TRP:CE2	1:A:560:ARG:HB2	2.53	0.43
1:A:97:PRO:HD2	5:A:717:CL:CL	2.56	0.43
1:B:562:PRO:HG2	1:B:565:LYS:HD3	2.01	0.43
1:B:467:PHE:CE2	1:B:472:LEU:HD12	2.55	0.42
1:B:571:PRO:O	1:B:575:GLU:HG2	2.20	0.42
1:B:600:GLN:HA	1:B:600:GLN:HE21	1.84	0.42
1:A:426:SER:HA	1:A:614:GLU:OE1	2.19	0.42
1:B:289:ARG:HA	1:B:289:ARG:HD2	1.91	0.42
1:A:562:PRO:HG2	1:A:565:LYS:HD3	2.02	0.41
1:B:433:ASP:HB3	1:B:436:SER:HB2	2.02	0.41
1:A:75:THR:HG23	1:A:299:GLU:HB2	2.03	0.41
1:B:88:THR:HA	1:B:309:GLU:O	2.21	0.41
1:A:38:LYS:O	1:A:70:PRO:HD2	2.21	0.41
1:A:397:GLN:HG2	1:A:440:TYR:CE2	2.56	0.41
1:B:247:HIS:HD2	1:B:258:PHE:CZ	2.38	0.41
1:B:563:GLU:HA	1:B:564:GLY:HA2	1.68	0.41
1:A:477:VAL:HG21	1:A:506:LEU:HD23	2.04	0.40
1:B:426:SER:HA	1:B:614:GLU:OE1	2.20	0.40
1:B:75:THR:HG23	1:B:299:GLU:HB2	2.03	0.40
1:B:118:SER:HB3	1:B:236:CYS:HB3	2.04	0.40
1:B:97:PRO:HG3	1:B:286:ILE:HD11	2.02	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	669/683 (98%)	625 (93%)	39 (6%)	5 (1%)	22	25
1	B	669/683 (98%)	624 (93%)	40 (6%)	5 (1%)	22	25
All	All	1338/1366 (98%)	1249 (93%)	79 (6%)	10 (1%)	22	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	131	ASP
1	B	58	LYS
1	B	87	ASP
1	A	87	ASP
1	B	23	GLU
1	B	224	LYS
1	A	224	LYS
1	A	645	ILE
1	B	645	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/568 (98%)	529 (95%)	29 (5%)	23	30
1	B	558/568 (98%)	526 (94%)	32 (6%)	20	26
All	All	1116/1136 (98%)	1055 (94%)	61 (6%)	21	27

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	44	SER
1	A	82	VAL

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Mol	Chain	Res	Type
1	A	114	ASP
1	A	131	ASP
1	A	150	ASP
1	A	154	LEU
1	A	156	MET
1	A	189	SER
1	A	213	THR
1	A	229	THR
1	A	279	SER
1	A	299	GLU
1	A	303	GLN
1	A	313	LYS
1	A	351	ASN
1	A	378	ASN
1	A	384	GLN
1	A	388	GLU
1	A	429	THR
1	A	460	ASP
1	A	479	ILE
1	A	492	SER
1	A	500	GLN
1	A	507	ARG
1	A	514	ASP
1	A	532	ARG
1	A	554	ARG
1	A	594	ASP
1	B	19	GLN
1	B	25	LYS
1	B	44	SER
1	B	82	VAL
1	B	133	LYS
1	B	150	ASP
1	B	154	LEU
1	B	156	MET
1	B	189	SER
1	B	213	THR
1	B	229	THR
1	B	279	SER
1	B	288	LEU
1	B	299	GLU
1	B	300	LYS
1	B	303	GLN

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Mol	Chain	Res	Type
1	B	313	LYS
1	B	346	ARG
1	B	351	ASN
1	B	378	ASN
1	B	388	GLU
1	B	429	THR
1	B	454	ILE
1	B	492	SER
1	B	500	GLN
1	B	514	ASP
1	B	532	ARG
1	B	554	ARG
1	B	594	ASP
1	B	600	GLN
1	B	676	ILE
1	B	677	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	303	GLN
1	A	308	ASN
1	A	323	GLN
1	A	336	GLN
1	A	339	ASN
1	A	544	ASN
1	A	622	ASN
1	B	77	ASN
1	B	308	ASN
1	B	323	GLN
1	B	336	GLN
1	B	339	ASN
1	B	466	ASN
1	B	543	GLN
1	B	544	ASN
1	B	600	GLN
1	B	622	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 58 ligands modelled in this entry, 33 are monoatomic - leaving 25 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	$\# Z  > 2$
4	EDO	B	707	-	3,3,3	0.62	0	2,2,2	0.30	0
4	EDO	A	707	-	3,3,3	0.71	0	2,2,2	0.15	0
4	EDO	B	702	-	3,3,3	0.63	0	2,2,2	0.24	0
4	EDO	B	706	-	3,3,3	0.79	0	2,2,2	0.26	0
4	EDO	B	710	-	3,3,3	0.56	0	2,2,2	0.42	0
4	EDO	A	705	-	3,3,3	0.58	0	2,2,2	0.42	0
4	EDO	B	709	-	3,3,3	0.63	0	2,2,2	0.31	0
4	EDO	A	709	-	3,3,3	0.77	0	2,2,2	0.29	0
4	EDO	A	713	-	3,3,3	0.52	0	2,2,2	0.23	0
4	EDO	B	704	-	3,3,3	0.63	0	2,2,2	0.24	0
4	EDO	A	704	-	3,3,3	0.63	0	2,2,2	0.18	0
4	EDO	B	705	-	3,3,3	0.58	0	2,2,2	0.31	0
4	EDO	A	708	-	3,3,3	0.65	0	2,2,2	0.18	0
4	EDO	A	711	-	3,3,3	0.73	0	2,2,2	0.22	0
4	EDO	A	712	-	3,3,3	0.59	0	2,2,2	0.32	0
4	EDO	B	708	-	3,3,3	0.63	0	2,2,2	0.26	0
2	GLA	A	701	6	12,12,12	0.85	0	17,17,17	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	710	-	3,3,3	0.72	0	2,2,2	0.10	0
3	PEG	A	702	-	6,6,6	0.13	0	5,5,5	0.12	0
3	PEG	A	703	-	6,6,6	0.36	0	5,5,5	0.42	0
4	EDO	A	714	-	3,3,3	0.58	0	2,2,2	0.33	0
4	EDO	B	711	-	3,3,3	0.75	0	2,2,2	0.23	0
4	EDO	A	706	-	3,3,3	0.73	0	2,2,2	0.30	0
4	EDO	B	703	-	3,3,3	0.70	0	2,2,2	0.15	0
2	GLA	B	701	6	12,12,12	0.26	0	17,17,17	0.55	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
4	EDO	B	707	-	-	0/1/1/1	-
4	EDO	A	707	-	-	0/1/1/1	-
4	EDO	B	702	-	-	0/1/1/1	-
4	EDO	B	706	-	-	0/1/1/1	-
4	EDO	B	710	-	-	0/1/1/1	-
4	EDO	A	705	-	-	1/1/1/1	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	A	709	-	-	1/1/1/1	-
4	EDO	A	713	-	-	0/1/1/1	-
4	EDO	B	704	-	-	0/1/1/1	-
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	B	705	-	-	0/1/1/1	-
4	EDO	A	708	-	-	0/1/1/1	-
4	EDO	A	711	-	-	0/1/1/1	-
4	EDO	A	712	-	-	0/1/1/1	-
4	EDO	B	708	-	-	0/1/1/1	-
2	GLA	A	701	6	-	0/2/22/22	0/1/1/1
4	EDO	A	710	-	-	0/1/1/1	-
3	PEG	A	702	-	-	2/4/4/4	-
3	PEG	A	703	-	-	2/4/4/4	-
4	EDO	A	714	-	-	0/1/1/1	-
4	EDO	B	711	-	-	1/1/1/1	-
4	EDO	A	706	-	-	0/1/1/1	-
4	EDO	B	703	-	-	1/1/1/1	-
2	GLA	B	701	6	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GLA	C1-O5-C5	2.73	118.82	113.66
2	A	701	GLA	C3-C4-C5	-2.28	106.17	110.24
2	A	701	GLA	O5-C5-C6	2.26	112.06	106.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	711	EDO	O1-C1-C2-O2
4	A	709	EDO	O1-C1-C2-O2
3	A	703	PEG	C4-C3-O2-C2
3	A	702	PEG	C1-C2-O2-C3
3	A	702	PEG	C4-C3-O2-C2
3	A	703	PEG	C1-C2-O2-C3
4	A	705	EDO	O1-C1-C2-O2
4	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	713	EDO	1	0
4	A	704	EDO	1	0
4	A	712	EDO	1	0
3	A	703	PEG	6	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	671/683 (98%)	-0.07	17 (2%) 57 53	24, 58, 98, 164	0
1	B	671/683 (98%)	0.13	23 (3%) 45 41	34, 67, 107, 139	0
All	All	1342/1366 (98%)	0.03	40 (2%) 50 46	24, 63, 104, 164	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	8.6
1	A	22	ALA	7.9
1	B	59	LEU	5.0
1	A	21	PRO	4.6
1	A	456	LEU	4.3
1	A	471	THR	3.9
1	B	56	ALA	3.9
1	B	252	LYS	3.5
1	A	467	PHE	3.4
1	A	567	LEU	3.3
1	B	188	VAL	3.2
1	B	67	PRO	3.2
1	A	563	GLU	3.1
1	A	444	LEU	3.1
1	A	474	GLY	2.9
1	A	469	LYS	2.8
1	B	50	THR	2.8
1	B	64	GLU	2.7
1	B	211	ASP	2.7
1	B	132	ALA	2.7
1	B	242	ILE	2.6
1	A	468	PRO	2.6
1	A	572	PHE	2.6
1	B	568	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	215	GLU	2.6
1	A	16	GLU	2.5
1	B	61	PRO	2.5
1	A	604	THR	2.4
1	B	75	THR	2.4
1	A	19	GLN	2.4
1	B	459	THR	2.3
1	A	588	ASP	2.3
1	B	214	VAL	2.2
1	B	57	GLY	2.1
1	B	293	TYR	2.1
1	B	378	ASN	2.1
1	B	68	GLU	2.0
1	B	103	ILE	2.0
1	A	475	ARG	2.0
1	B	668	GLY	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
4	EDO	A	706	4/4	0.72	0.27	49,49,54,55	0
4	EDO	B	702	4/4	0.73	0.21	79,79,79,79	0
4	EDO	A	709	4/4	0.74	0.19	54,55,59,59	0
5	CL	A	718	1/1	0.74	0.17	76,76,76,76	0
4	EDO	B	707	4/4	0.76	0.13	76,78,79,81	0
6	CA	A	726	1/1	0.78	0.16	85,85,85,85	0
6	CA	A	731	1/1	0.78	0.12	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	703	4/4	0.78	0.23	70,71,72,72	0
4	EDO	A	710	4/4	0.81	0.30	62,62,64,64	0
4	EDO	B	705	4/4	0.82	0.15	91,92,94,95	0
4	EDO	B	708	4/4	0.82	0.17	76,77,77,78	0
4	EDO	B	704	4/4	0.82	0.17	66,67,70,73	0
6	CA	A	725	1/1	0.83	0.08	82,82,82,82	0
4	EDO	B	706	4/4	0.83	0.14	42,45,46,47	0
4	EDO	A	708	4/4	0.84	0.14	71,72,74,76	0
6	CA	B	722	1/1	0.85	0.12	79,79,79,79	0
6	CA	A	735	1/1	0.86	0.16	171,171,171,171	0
5	CL	B	714	1/1	0.87	0.12	73,73,73,73	0
5	CL	B	712	1/1	0.88	0.12	82,82,82,82	0
4	EDO	A	707	4/4	0.88	0.22	41,44,47,48	0
4	EDO	A	713	4/4	0.88	0.28	42,42,43,43	0
4	EDO	A	711	4/4	0.89	0.12	62,63,63,64	0
3	PEG	A	702	7/7	0.89	0.16	61,63,64,66	0
6	CA	B	723	1/1	0.90	0.07	91,91,91,91	0
3	PEG	A	703	7/7	0.90	0.32	39,42,46,48	0
6	CA	A	729	1/1	0.90	0.15	81,81,81,81	0
6	CA	A	733	1/1	0.91	0.04	94,94,94,94	0
4	EDO	B	709	4/4	0.91	0.18	53,55,55,55	0
4	EDO	A	704	4/4	0.91	0.09	64,65,65,65	0
4	EDO	B	711	4/4	0.91	0.09	62,63,63,63	0
5	CL	A	720	1/1	0.91	0.09	60,60,60,60	0
6	CA	A	734	1/1	0.92	0.08	68,68,68,68	0
4	EDO	A	705	4/4	0.92	0.14	56,59,64,66	0
5	CL	B	717	1/1	0.92	0.07	77,77,77,77	0
4	EDO	A	714	4/4	0.93	0.12	51,51,53,53	0
4	EDO	A	712	4/4	0.93	0.17	54,54,54,55	0
4	EDO	B	710	4/4	0.93	0.20	60,61,61,62	0
5	CL	A	715	1/1	0.93	0.07	49,49,49,49	0
5	CL	A	719	1/1	0.93	0.07	68,68,68,68	0
2	GLA	B	701	12/12	0.94	0.13	35,41,45,45	0
6	CA	B	721	1/1	0.94	0.06	74,74,74,74	0
2	GLA	A	701	12/12	0.94	0.13	33,39,46,54	0
5	CL	B	713	1/1	0.94	0.17	97,97,97,97	0
6	CA	A	727	1/1	0.95	0.06	79,79,79,79	0
6	CA	A	732	1/1	0.95	0.17	81,81,81,81	0
6	CA	B	719	1/1	0.95	0.07	54,54,54,54	0
5	CL	B	718	1/1	0.95	0.15	92,92,92,92	0
5	CL	A	716	1/1	0.95	0.07	51,51,51,51	0
5	CL	B	716	1/1	0.96	0.17	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	A	723	1/1	0.96	0.06	65,65,65,65	0
6	CA	B	720	1/1	0.96	0.07	89,89,89,89	0
5	CL	B	715	1/1	0.96	0.05	79,79,79,79	0
6	CA	A	728	1/1	0.97	0.13	91,91,91,91	0
6	CA	A	730	1/1	0.97	0.23	81,81,81,81	0
5	CL	A	721	1/1	0.98	0.10	64,64,64,64	0
5	CL	A	717	1/1	0.98	0.07	60,60,60,60	0
5	CL	A	722	1/1	0.98	0.06	65,65,65,65	0
6	CA	A	724	1/1	0.98	0.15	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.