



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 05:34 PM EST

PDB ID : 4S3Q  
Title : Amylomaltase MalQ from Escherichia coli in complex with maltose  
Authors : Weiss, S.C.; Schiefner, A.  
Deposited on : unknown  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

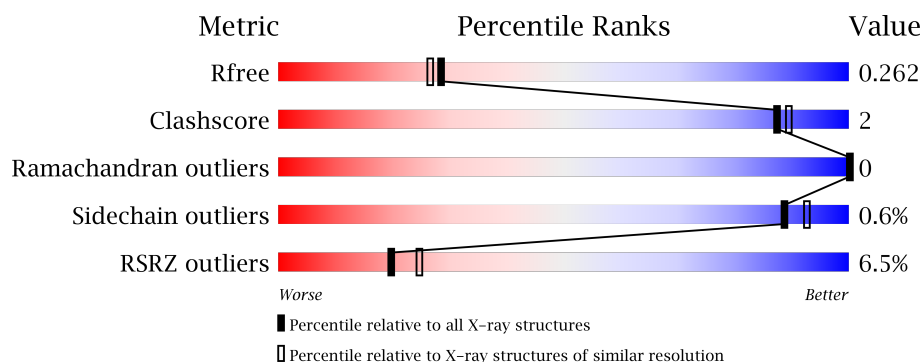
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	696	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	B	696	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	C	696	<div> <div>7%</div> <div>92%</div> <div>5%</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
2	EDO	A	701	-	-	-	X
2	EDO	C	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16868 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	0
			5440	3458	945	1005	32			
1	B	686	Total	C	N	O	S	0	0	0
			5480	3482	957	1009	32			
1	C	681	Total	C	N	O	S	0	0	0
			5430	3452	942	1004	32			

There are 24 discrepancies between the modelled and reference sequences:

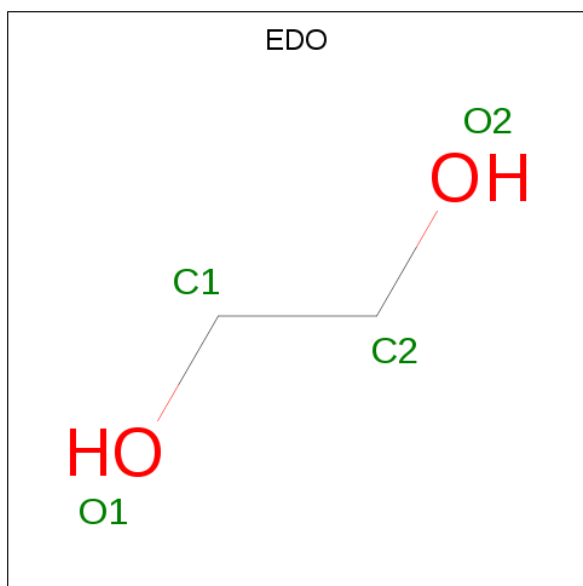
Chain	Residue	Modelled	Actual	Comment	Reference
A	689	SER	-	EXPRESSION TAG	UNP P15977
A	690	ALA	-	EXPRESSION TAG	UNP P15977
A	691	HIS	-	EXPRESSION TAG	UNP P15977
A	692	HIS	-	EXPRESSION TAG	UNP P15977
A	693	HIS	-	EXPRESSION TAG	UNP P15977
A	694	HIS	-	EXPRESSION TAG	UNP P15977
A	695	HIS	-	EXPRESSION TAG	UNP P15977
A	696	HIS	-	EXPRESSION TAG	UNP P15977
B	689	SER	-	EXPRESSION TAG	UNP P15977
B	690	ALA	-	EXPRESSION TAG	UNP P15977
B	691	HIS	-	EXPRESSION TAG	UNP P15977
B	692	HIS	-	EXPRESSION TAG	UNP P15977
B	693	HIS	-	EXPRESSION TAG	UNP P15977
B	694	HIS	-	EXPRESSION TAG	UNP P15977
B	695	HIS	-	EXPRESSION TAG	UNP P15977
B	696	HIS	-	EXPRESSION TAG	UNP P15977
C	689	SER	-	EXPRESSION TAG	UNP P15977
C	690	ALA	-	EXPRESSION TAG	UNP P15977
C	691	HIS	-	EXPRESSION TAG	UNP P15977
C	692	HIS	-	EXPRESSION TAG	UNP P15977
C	693	HIS	-	EXPRESSION TAG	UNP P15977
C	694	HIS	-	EXPRESSION TAG	UNP P15977
C	695	HIS	-	EXPRESSION TAG	UNP P15977

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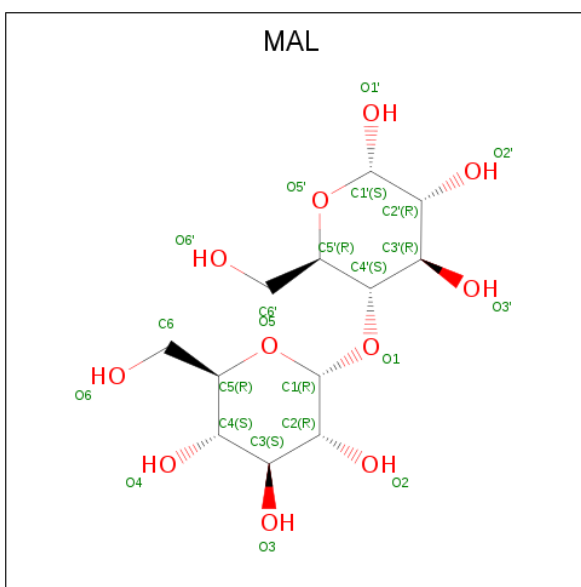
Chain	Residue	Modelled	Actual	Comment	Reference
C	696	HIS	-	EXPRESSION TAG	UNP P15977

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



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

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

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

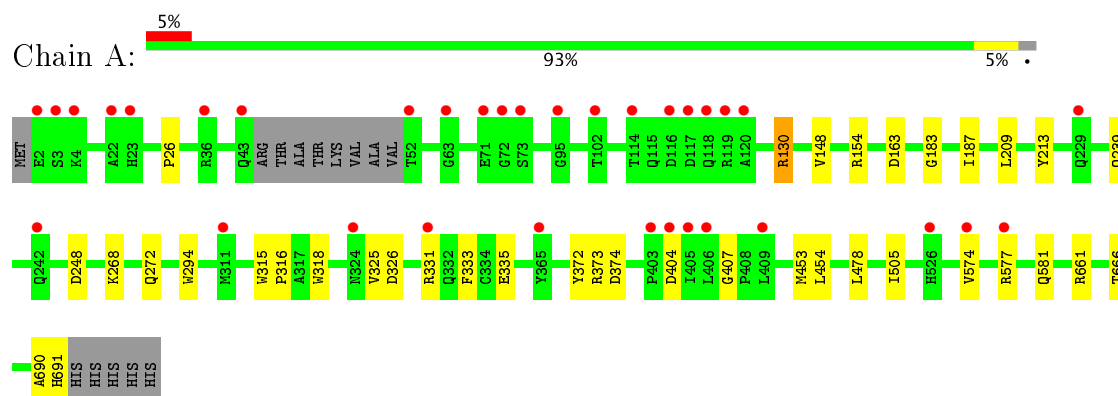
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	156	Total	O	0	0
			156	156		
5	C	137	Total	O	0	0
			137	137		

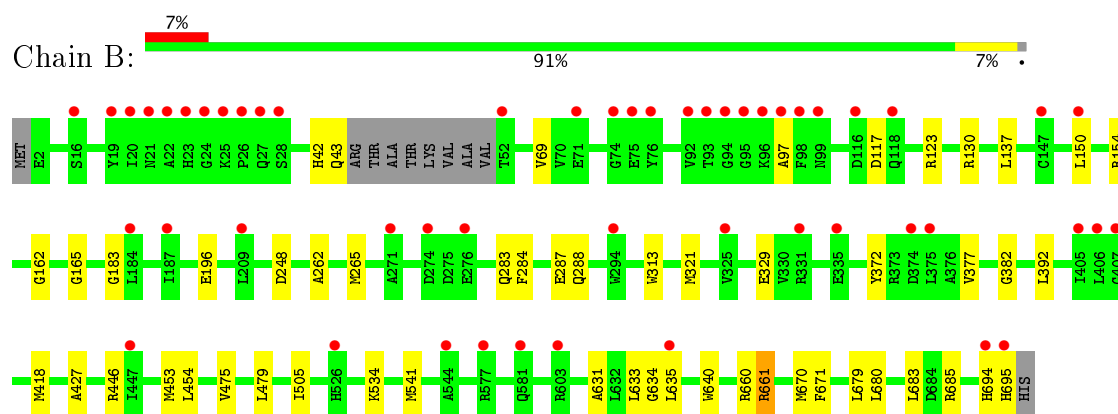
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

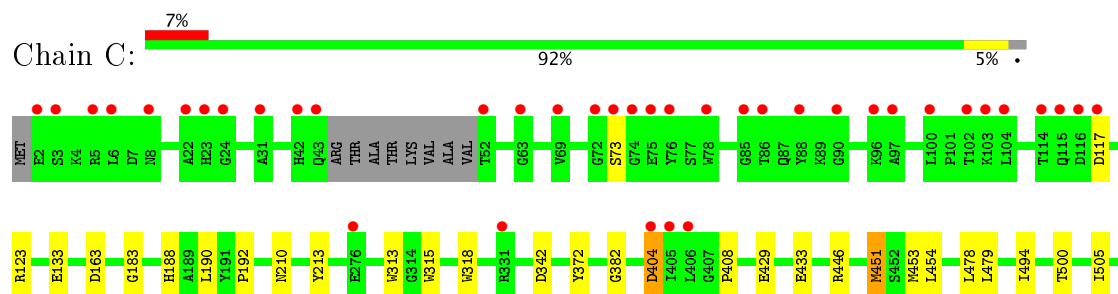
#### • Molecule 1: 4-alpha-glucanotransferase



#### • Molecule 1: 4-alpha-glucanotransferase



#### • Molecule 1: 4-alpha-glucanotransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.13Å 77.02Å 128.40Å 76.11° 75.48° 66.31°	Depositor
Resolution (Å)	34.23 – 2.10 34.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.23-2.10) 88.9 (34.23-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.221 , 0.258 0.225 , 0.262	Depositor DCC
$R_{free}$ test set	6970 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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: IOD, MAL, EDO

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	0.50	0/5586	0.67	5/7592 (0.1%)
1	B	0.48	0/5630	0.66	2/7652 (0.0%)
1	C	0.48	0/5575	0.66	3/7577 (0.0%)
All	All	0.49	0/16791	0.66	10/22821 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	661	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	661	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	661	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	451	MET	CG-SD-CE	-5.46	91.46	100.20
1	A	130	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	661	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	374	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	661	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	130	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	373	ARG	NE-CZ-NH2	-5.00	117.80	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	5440	0	5292	25	0
1	B	5480	0	5320	32	0
1	C	5430	0	5285	22	0
2	A	8	0	12	0	0
2	B	8	0	12	1	0
2	C	4	0	6	3	0
3	A	23	0	22	0	0
4	A	3	0	0	1	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
5	A	174	0	0	3	0
5	B	156	0	0	1	0
5	C	137	0	0	2	0
All	All	16868	0	15949	77	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 2.

All (77) 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:283:GLN:NE2	1:B:287:GLU:OE2	2.26	0.65
1:B:137:LEU:HD22	1:B:631:ALA:HB1	1.81	0.61
1:B:262:ALA:HA	1:B:265:MET:HE2	1.83	0.61
1:C:123:ARG:NH1	1:C:429:GLU:OE2	2.30	0.60
1:A:294:TRP:CH2	1:A:325:VAL:HG22	2.35	0.60
1:A:268:LYS:O	1:A:272:GLN:NE2	2.36	0.59
1:A:574:VAL:HA	1:A:577:ARG:HD2	1.83	0.58
4:A:706:IOD:I	5:A:880:HOH:O	2.87	0.57
1:A:130:ARG:NH2	5:A:832:HOH:O	2.37	0.57
1:C:190:LEU:N	2:C:701:EDO:H12	2.19	0.57
1:C:210:ASN:HA	2:C:701:EDO:O1	2.05	0.57
1:C:192:PRO:HD3	2:C:701:EDO:H11	1.86	0.57
1:A:294:TRP:CZ3	1:A:325:VAL:CG2	2.88	0.56
1:C:429:GLU:O	1:C:433:GLU:HG2	2.06	0.56
1:B:130:ARG:NH2	5:B:939:HOH:O	2.39	0.55
1:A:690:ALA:O	1:A:691:HIS:C	2.45	0.54
1:B:42:HIS:O	1:B:43:GLN:HG2	2.08	0.54
1:B:454:LEU:HD22	1:B:505:ILE:HG13	1.90	0.53
1:A:335:GLU:HG2	1:B:534:LYS:HE3	1.91	0.53
1:A:335:GLU:CG	1:B:534:LYS:HE3	2.38	0.53
1:C:451:MET:HE2	1:C:500:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:MET:HE1	1:B:479:LEU:HD23	1.92	0.52
1:C:372:TYR:CE1	1:C:494:ILE:HD13	2.45	0.51
1:C:404:ASP:O	1:C:408:PRO:HA	2.11	0.51
1:B:313:TRP:CZ3	1:B:382:GLY:HA3	2.45	0.51
1:A:453:MET:HE3	1:A:478:LEU:HB3	1.94	0.50
1:B:640:TRP:CE2	1:B:680:LEU:HD21	2.46	0.50
1:A:26:PRO:HG2	5:C:860:HOH:O	2.12	0.49
1:A:315:TRP:HA	1:A:318:TRP:CD2	2.47	0.49
1:C:453:MET:CE	1:C:479:LEU:HD23	2.43	0.49
1:B:262:ALA:HA	1:B:265:MET:CE	2.43	0.48
1:B:165:GLY:HA2	2:B:701:EDO:C2	2.44	0.48
1:B:453:MET:CE	1:B:479:LEU:HD23	2.43	0.48
1:A:154:ARG:NH2	1:A:248:ASP:HA	2.29	0.47
1:B:69:VAL:HG22	1:B:97:ALA:HB2	1.95	0.47
1:A:326:ASP:O	1:A:331:ARG:NH1	2.47	0.47
1:A:404:ASP:OD1	1:A:407:GLY:N	2.46	0.47
1:A:294:TRP:CH2	1:A:325:VAL:CG2	2.99	0.46
1:A:574:VAL:HG22	1:A:577:ARG:NH1	2.31	0.46
1:B:372:TYR:CE1	1:B:446:ARG:HB2	2.51	0.46
1:C:315:TRP:HA	1:C:318:TRP:CD2	2.49	0.46
1:B:154:ARG:NH2	1:B:248:ASP:OD1	2.48	0.46
1:A:335:GLU:HG2	1:B:534:LYS:CE	2.46	0.46
1:B:541:MET:HE2	1:B:634:GLY:HA3	1.98	0.46
1:C:183:GLY:HA2	1:C:372:TYR:HB3	1.98	0.46
1:B:183:GLY:HA2	1:B:372:TYR:HB3	1.98	0.46
1:B:196:GLU:OE1	1:B:660:ARG:NH2	2.41	0.45
1:C:372:TYR:CE1	1:C:446:ARG:HB2	2.51	0.45
1:A:154:ARG:HB2	1:A:666:THR:HA	1.99	0.45
1:B:150:LEU:O	1:B:162:GLY:HA3	2.17	0.44
1:B:123:ARG:HD2	1:B:427:ALA:HB1	2.00	0.44
1:B:633:LEU:HD21	1:B:635:LEU:HD21	2.00	0.44
1:B:321:MET:SD	1:B:329:GLU:HG2	2.58	0.44
1:C:454:LEU:HD22	1:C:505:ILE:CG1	2.48	0.44
1:C:163:ASP:HB2	1:C:213:TYR:O	2.18	0.43
1:C:188:HIS:HB2	5:C:903:HOH:O	2.17	0.43
1:B:679:LEU:O	1:B:683:LEU:HG	2.18	0.43
1:A:315:TRP:N	1:A:316:PRO:CD	2.82	0.43
1:C:453:MET:HE1	1:C:479:LEU:HD23	2.01	0.43
1:B:694:HIS:CG	1:B:695:HIS:H	2.36	0.43
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.54	0.43
1:C:313:TRP:CZ3	1:C:382:GLY:HA3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:HG	1:B:418:MET:HG3	2.01	0.42
5:A:915:HOH:O	1:B:685:ARG:HD3	2.18	0.42
1:B:284:PHE:O	1:B:288:GLN:HG2	2.19	0.42
1:A:454:LEU:HD22	1:A:505:ILE:HG13	2.02	0.42
1:A:333:PHE:CD1	1:A:333:PHE:C	2.93	0.42
1:C:527:GLU:O	1:C:528:LYS:HB2	2.20	0.41
1:A:163:ASP:HB2	1:A:213:TYR:O	2.20	0.41
1:A:187:ILE:HD12	1:A:209:LEU:HD22	2.03	0.41
1:C:623:ARG:HG2	1:C:686:ARG:HG3	2.02	0.41
1:C:565:LYS:HD3	1:C:576:LEU:CD2	2.50	0.41
1:B:454:LEU:HA	1:B:475:VAL:HB	2.02	0.41
1:B:670:MET:HE3	1:B:671:PHE:CE2	2.56	0.41
1:C:453:MET:HE3	1:C:478:LEU:HB3	2.01	0.40
1:C:133:GLU:OE2	1:C:515:TYR:OH	2.26	0.40
1:A:183:GLY:HA2	1:A:372:TYR:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/696 (97%)	660 (97%)	18 (3%)	0	100	100
1	B	682/696 (98%)	666 (98%)	16 (2%)	0	100	100
1	C	677/696 (97%)	662 (98%)	15 (2%)	0	100	100
All	All	2037/2088 (98%)	1988 (98%)	49 (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	570/582 (98%)	567 (100%)	3 (0%)	91	94
1	B	574/582 (99%)	571 (100%)	3 (0%)	91	94
1	C	569/582 (98%)	564 (99%)	5 (1%)	82	87
All	All	1713/1746 (98%)	1702 (99%)	11 (1%)	89	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	VAL
1	A	239	GLN
1	A	581	GLN
1	B	117	ASP
1	B	377	VAL
1	B	661	ARG
1	C	73	SER
1	C	117	ASP
1	C	342	ASP
1	C	404	ASP
1	C	689	SER

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

Mol	Chain	Res	Type
1	C	239	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z  > 2$
2	EDO	A	701	-	3,3,3	0.58	0	2,2,2	0.17	0
2	EDO	A	702	-	3,3,3	0.49	0	2,2,2	0.26	0
3	MAL	A	703	-	24,24,24	0.60	0	35,35,35	0.89	0
2	EDO	B	701	-	3,3,3	0.30	0	2,2,2	0.29	0
2	EDO	B	702	-	3,3,3	0.44	0	2,2,2	0.47	0
2	EDO	C	701	-	3,3,3	0.46	0	2,2,2	0.37	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
2	EDO	A	701	-	-	0/1/1/1	0/0/0/0
2	EDO	A	702	-	-	0/1/1/1	0/0/0/0
3	MAL	A	703	-	-	0/8/48/48	0/2/2/2
2	EDO	B	701	-	-	0/1/1/1	0/0/0/0
2	EDO	B	702	-	-	0/1/1/1	0/0/0/0
2	EDO	C	701	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	EDO	1	0
2	C	701	EDO	3	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	682/696 (97%)	0.32	34 (4%)	30 36	24, 36, 62, 81	0
1	B	686/696 (98%)	0.45	52 (7%)	15 19	27, 37, 58, 87	0
1	C	681/696 (97%)	0.37	48 (7%)	17 22	25, 37, 63, 98	0
All	All	2049/2088 (98%)	0.38	134 (6%)	20 25	24, 37, 62, 98	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	9.2
1	A	405	ILE	7.7
1	B	95	GLY	5.7
1	C	2	GLU	5.5
1	B	23	HIS	5.4
1	C	3	SER	4.9
1	C	5	ARG	4.8
1	C	23	HIS	4.6
1	B	74	GLY	4.4
1	C	74	GLY	4.3
1	A	2	GLU	4.3
1	A	117	ASP	4.2
1	B	406	LEU	4.1
1	C	22	ALA	4.0
1	B	274	ASP	4.0
1	A	72	GLY	3.9
1	A	404	ASP	3.8
1	A	574	VAL	3.8
1	C	96	LYS	3.8
1	A	102	THR	3.8
1	A	52	THR	3.8
1	C	102	THR	3.8
1	A	22	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	694	HIS	3.8
1	C	75	GLU	3.7
1	B	405	ILE	3.7
1	C	43	GLN	3.5
1	C	117	ASP	3.5
1	A	43	GLN	3.5
1	C	72	GLY	3.5
1	C	103	LYS	3.5
1	A	120	ALA	3.5
1	B	20	ILE	3.5
1	C	116	ASP	3.4
1	B	27	GLN	3.4
1	C	97	ALA	3.3
1	B	577	ARG	3.2
1	B	447	ILE	3.2
1	B	24	GLY	3.1
1	B	25	LYS	3.1
1	C	689	SER	3.1
1	B	28	SER	3.1
1	A	406	LEU	3.0
1	C	526	HIS	3.0
1	A	118	GLN	3.0
1	B	96	LYS	3.0
1	A	3	SER	3.0
1	B	695	HIS	3.0
1	B	75	GLU	2.9
1	B	118	GLN	2.9
1	C	76	TYR	2.9
1	C	73	SER	2.9
1	C	6	LEU	2.8
1	B	21	ASN	2.8
1	C	86	THR	2.8
1	A	114	THR	2.7
1	C	115	GLN	2.7
1	B	209	LEU	2.7
1	B	93	THR	2.7
1	A	116	ASP	2.6
1	C	603	ARG	2.6
1	B	325	VAL	2.6
1	B	98	PHE	2.6
1	C	31	ALA	2.6
1	B	331	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	276	GLU	2.6
1	A	119	ARG	2.6
1	A	23	HIS	2.6
1	C	585	LEU	2.6
1	A	4	LYS	2.5
1	A	324	ASN	2.5
1	A	63	GLY	2.5
1	B	635	LEU	2.5
1	C	406	LEU	2.5
1	B	116	ASP	2.5
1	B	271	ALA	2.5
1	C	78	TRP	2.4
1	B	147	CYS	2.4
1	B	99	ASN	2.4
1	C	85	GLY	2.4
1	B	97	ALA	2.4
1	B	71	GLU	2.4
1	B	187	ILE	2.4
1	A	409	LEU	2.4
1	C	42	HIS	2.4
1	C	90	GLY	2.4
1	A	71	GLU	2.3
1	C	331	ARG	2.3
1	B	26	PRO	2.3
1	C	114	THR	2.3
1	C	582	ASP	2.3
1	B	150	LEU	2.3
1	A	242	GLN	2.3
1	B	19	TYR	2.3
1	C	610	LEU	2.3
1	A	526	HIS	2.2
1	C	577	ARG	2.2
1	C	8	ASN	2.2
1	B	526	HIS	2.2
1	B	544	ALA	2.2
1	C	88	TYR	2.2
1	A	311	MET	2.2
1	A	73	SER	2.2
1	A	403	PRO	2.2
1	B	335	GLU	2.2
1	A	229	GLN	2.2
1	C	100	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	577	ARG	2.2
1	A	365	TYR	2.2
1	C	404	ASP	2.1
1	C	574	VAL	2.1
1	B	407	GLY	2.1
1	C	52	THR	2.1
1	A	331	ARG	2.1
1	B	94	GLY	2.1
1	C	276	GLU	2.1
1	B	52	THR	2.1
1	C	405	ILE	2.1
1	B	603	ARG	2.1
1	C	24	GLY	2.1
1	B	375	LEU	2.1
1	B	92	VAL	2.1
1	B	16	SER	2.0
1	B	294	TRP	2.0
1	C	104	LEU	2.0
1	C	69	VAL	2.0
1	B	374	ASP	2.0
1	B	76	TYR	2.0
1	B	184	LEU	2.0
1	C	579	LEU	2.0
1	A	36	ARG	2.0
1	A	95	GLY	2.0
1	B	581	GLN	2.0
1	C	63	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	701	4/4	0.89	0.28	6.21	39,39,39,41	0
2	EDO	C	701	4/4	0.92	0.19	2.52	29,30,30,31	0
3	MAL	A	703	23/23	0.77	0.20	1.95	45,53,61,66	0
2	EDO	B	702	4/4	0.94	0.25	1.35	35,35,35,37	0
2	EDO	A	702	4/4	0.96	0.17	-0.19	26,28,28,29	0
2	EDO	B	701	4/4	0.95	0.12	-0.24	31,33,36,40	0
4	IOD	B	704	1/1	0.96	0.10	-0.92	76,76,76,76	0
4	IOD	C	703	1/1	0.96	0.10	-1.10	83,83,83,83	0
4	IOD	B	703	1/1	0.97	0.05	-1.42	52,52,52,52	0
4	IOD	A	706	1/1	0.96	0.07	-2.95	75,75,75,75	0
4	IOD	A	704	1/1	0.97	0.06	-3.07	46,46,46,46	0
4	IOD	A	705	1/1	0.96	0.05	-3.92	69,69,69,69	0
4	IOD	C	702	1/1	0.96	0.05	-	69,69,69,69	0
4	IOD	B	705	1/1	0.94	0.06	-	69,69,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.