



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 07:07 PM EDT

PDB ID : 6D66  
Title : Crystal structure of the human dual specificity 1 catalytic domain (C258S) as a maltose binding protein fusion in complex with the designed AR protein mbp3\_16  
Authors : Gumpena, R.; Waugh, D.S.; Lountos, G.T.  
Deposited on : 2018-04-20  
Resolution : 2.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

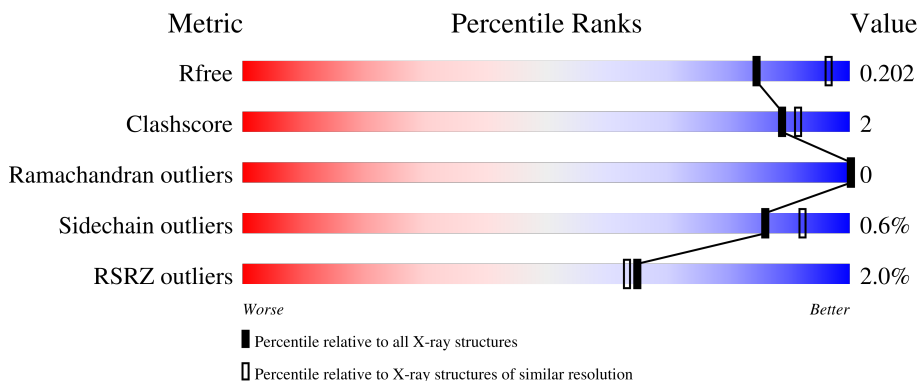
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	
2	B	136	

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
5	GLY	A	1412	-	X	-	-
9	DAL	B	204	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5428 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 Maltose-binding periplasmic protein, Dual specificity protein phosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	4032	2594	674	753	11	0	8	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0AEX9
A	83	ALA	ASP	engineered mutation	UNP P0AEX9
A	84	ALA	LYS	engineered mutation	UNP P0AEX9
A	173	ALA	GLU	engineered mutation	UNP P0AEX9
A	174	ALA	ASN	engineered mutation	UNP P0AEX9
A	240	ALA	LYS	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	367	THR	-	linker	UNP P0AEX9
A	368	ASN	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	458	SER	CYS	engineered mutation	UNP P28562
A	515	HIS	-	expression tag	UNP P28562
A	516	HIS	-	expression tag	UNP P28562
A	517	HIS	-	expression tag	UNP P28562
A	518	HIS	-	expression tag	UNP P28562
A	519	HIS	-	expression tag	UNP P28562
A	520	HIS	-	expression tag	UNP P28562

- Molecule 2 is a protein called Designed AR protein mbp3\_16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	125	951	607	157	185	2	0	1	0

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



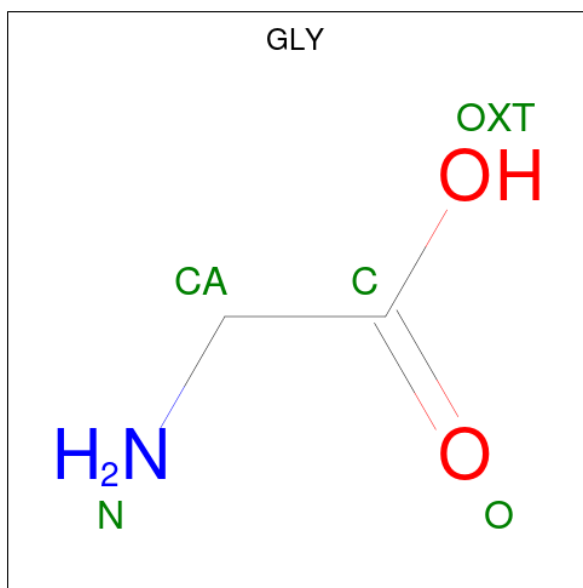
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
3	A	1	7	4	3	0	0
3	B	1	7	4	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



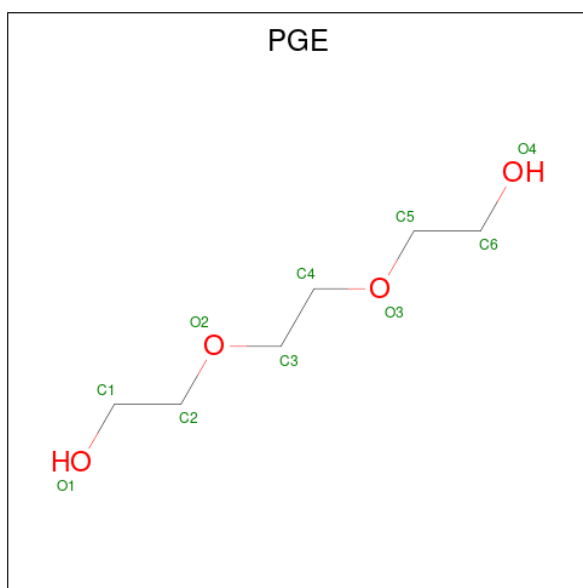
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



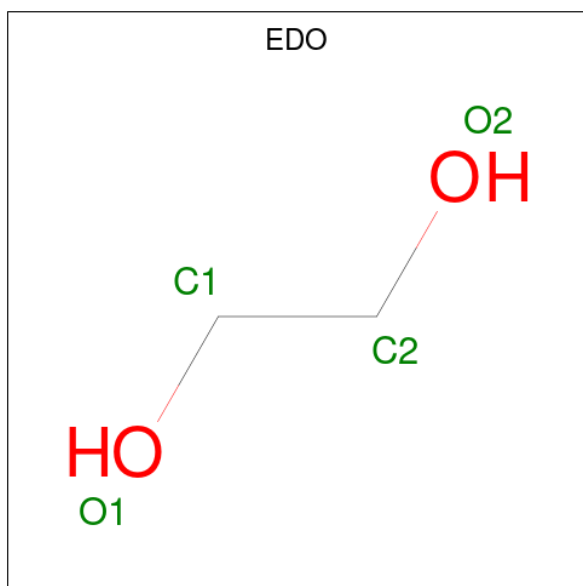
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	2	1	2		
5	A	1	Total	C	N	O	0	0
			5	2	1	2		
5	A	1	Total	C	N	O	0	0
			5	2	1	2		

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



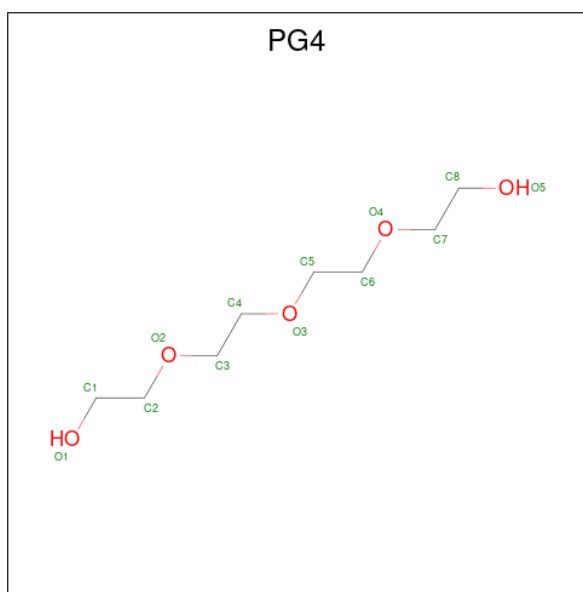
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

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

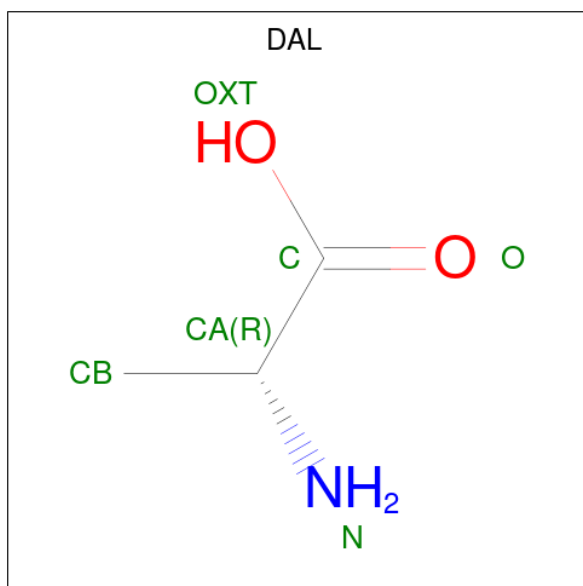
- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).





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

- Molecule 9 is D-ALANINE (three-letter code: DAL) (formula:  $C_3H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			6	3	1	2		

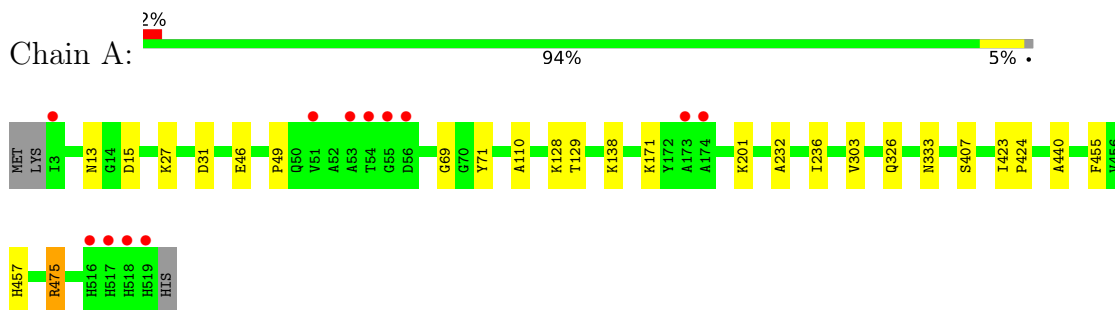
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	233	Total	O	0	0
			233	233		
10	B	74	Total	O	0	0
			74	74		

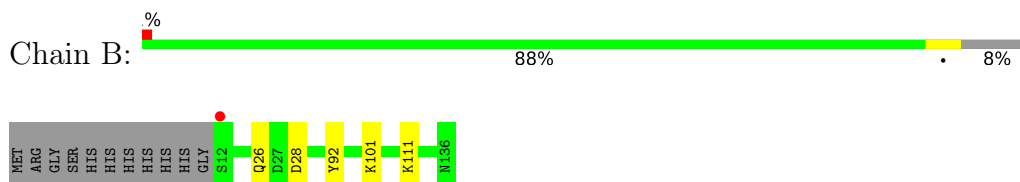
### 3 Residue-property plots [i](#)

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: Maltose-binding periplasmic protein,Dual specificity protein phosphatase 1



- Molecule 2: Designed AR protein mbp3\_16



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.97Å 79.97Å 265.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.44 – 2.23 36.44 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.44-2.23) 99.3 (36.44-2.23)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.22Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.159 , 0.202 0.159 , 0.202	Depositor DCC
$R_{free}$ test set	2135 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtrriage
Anisotropy	0.101	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: DAL, PEG, PO4, EDO, PG4, PGE

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	0.38	0/4158	0.51	0/5649
2	B	0.39	0/971	0.56	0/1317
All	All	0.38	0/5129	0.52	0/6966

There are no bond length outliers.

There are no bond angle outliers.

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	4032	0	3963	16	0
2	B	951	0	927	4	0
3	A	14	0	20	0	0
3	B	7	0	10	1	0
4	A	5	0	0	0	0
5	A	15	0	6	0	0
6	A	30	0	42	1	0
7	A	36	0	54	0	0
7	B	12	0	18	2	0
8	A	13	0	18	0	0
9	B	6	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	233	0	0	2	0
10	B	74	0	0	0	0
All	All	5428	0	5064	19	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 (19) 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)
2:B:28:ASP:HB2	7:B:205:EDO:H21	1.73	0.70
1:A:171:LYS:NZ	10:A:1504:HOH:O	2.33	0.62
1:A:13:ASN:ND2	1:A:15:ASP:OD1	2.37	0.57
1:A:475:ARG:HH11	1:A:475:ARG:HG3	1.75	0.50
1:A:69:GLY:HA3	1:A:333:ASN:O	2.13	0.49
1:A:407:SER:O	1:A:424:PRO:HA	2.15	0.46
2:B:101:LYS:HZ3	3:B:203:PEG:H32	1.81	0.46
1:A:27:LYS:NZ	1:A:31:ASP:OD1	2.41	0.45
1:A:455:PHE:CE2	1:A:457:HIS:HB3	2.51	0.45
1:A:128[B]:LYS:HG3	1:A:129:THR:HG23	1.99	0.45
1:A:110:ALA:HA	1:A:303:VAL:HA	1.99	0.44
1:A:232:ALA:O	1:A:236:ILE:HG13	2.18	0.43
1:A:49:PRO:HG3	1:A:71:TYR:CE1	2.53	0.43
1:A:138:LYS:NZ	2:B:92:TYR:OH	2.52	0.42
1:A:423:ILE:HD11	1:A:440:ALA:HB2	2.02	0.42
1:A:171:LYS:HD3	10:A:1566:HOH:O	2.19	0.42
1:A:326:GLN:NE2	6:A:1404:PGE:H3	2.36	0.41
1:A:46:GLU:O	1:A:49:PRO:HD2	2.21	0.41
2:B:26:GLN:C	7:B:205:EDO:H22	2.42	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	523/520 (101%)	511 (98%)	12 (2%)	0	100	100
2	B	124/136 (91%)	123 (99%)	1 (1%)	0	100	100
All	All	647/656 (99%)	634 (98%)	13 (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	413/414 (100%)	411 (100%)	2 (0%)	88	94
2	B	95/105 (90%)	94 (99%)	1 (1%)	73	84
All	All	508/519 (98%)	505 (99%)	3 (1%)	86	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LYS
1	A	475	ARG
2	B	111	LYS

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

### 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](#)

24 ligands are modelled in this entry.

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
9	DAL	B	204	-	5,5,5	1.02	1 (20%)	6,6,6	1.58	1 (16%)
3	PEG	A	1417	-	6,6,6	0.46	0	5,5,5	0.26	0
7	EDO	A	1409	-	3,3,3	0.48	0	2,2,2	0.44	0
7	EDO	A	1410	-	3,3,3	0.55	0	2,2,2	0.20	0
5	GLY	A	1413	-	4,4,4	1.05	0	3,4,4	1.83	2 (66%)
7	EDO	B	201	-	3,3,3	0.52	0	2,2,2	0.26	0
7	EDO	B	202	-	3,3,3	0.47	0	2,2,2	0.33	0
3	PEG	B	203	-	6,6,6	0.47	0	5,5,5	0.36	0
6	PGE	A	1415	-	9,9,9	0.32	0	8,8,8	0.36	0
5	GLY	A	1412	-	4,4,4	1.10	1 (25%)	3,4,4	1.79	2 (66%)
7	EDO	A	1418	-	3,3,3	0.53	0	2,2,2	0.14	0
4	PO4	A	1402	-	4,4,4	0.86	0	6,6,6	0.51	0
6	PGE	A	1411	-	9,9,9	0.44	0	8,8,8	0.38	0
8	PG4	A	1408	-	12,12,12	0.50	0	11,11,11	0.25	0
7	EDO	A	1407	-	3,3,3	0.50	0	2,2,2	0.24	0
7	EDO	A	1406	-	3,3,3	0.49	0	2,2,2	0.42	0
6	PGE	A	1404	-	9,9,9	0.32	0	8,8,8	0.31	0
7	EDO	A	1405	-	3,3,3	0.47	0	2,2,2	0.39	0
7	EDO	B	205	-	3,3,3	0.43	0	2,2,2	0.41	0
5	GLY	A	1403	-	4,4,4	1.04	0	3,4,4	1.58	1 (33%)
7	EDO	A	1414	-	3,3,3	0.47	0	2,2,2	0.45	0
7	EDO	A	1419	-	3,3,3	0.50	0	2,2,2	0.32	0
3	PEG	A	1401	-	6,6,6	0.48	0	5,5,5	0.38	0
7	EDO	A	1416	-	3,3,3	0.50	0	2,2,2	0.20	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
9	DAL	B	204	-	-	4/4/4/4	-
3	PEG	A	1417	-	-	2/4/4/4	-
7	EDO	A	1409	-	-	1/1/1/1	-
7	EDO	A	1410	-	-	0/1/1/1	-
5	GLY	A	1413	-	-	0/2/2/2	-
7	EDO	B	201	-	-	0/1/1/1	-
7	EDO	B	202	-	-	1/1/1/1	-
3	PEG	B	203	-	-	3/4/4/4	-
6	PGE	A	1415	-	-	3/7/7/7	-
5	GLY	A	1412	-	-	2/2/2/2	-
7	EDO	A	1418	-	-	1/1/1/1	-
6	PGE	A	1411	-	-	3/7/7/7	-
8	PG4	A	1408	-	-	7/10/10/10	-
7	EDO	A	1407	-	-	0/1/1/1	-
7	EDO	A	1406	-	-	0/1/1/1	-
6	PGE	A	1404	-	-	5/7/7/7	-
7	EDO	A	1405	-	-	0/1/1/1	-
7	EDO	B	205	-	-	0/1/1/1	-
5	GLY	A	1403	-	-	0/2/2/2	-
7	EDO	A	1414	-	-	0/1/1/1	-
7	EDO	A	1419	-	-	1/1/1/1	-
3	PEG	A	1401	-	-	2/4/4/4	-
7	EDO	A	1416	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	204	DAL	OXT-C	-2.11	1.23	1.30
5	A	1412	GLY	OXT-C	-2.08	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	204	DAL	OXT-C-O	-3.17	116.89	124.09
5	A	1413	GLY	OXT-C-O	-2.33	117.48	123.30
5	A	1412	GLY	OXT-C-O	-2.25	117.70	123.30
5	A	1413	GLY	OXT-C-CA	2.11	121.83	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1412	GLY	OXT-C-CA	2.08	121.74	113.45
5	A	1403	GLY	OXT-C-CA	2.01	121.44	113.45

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1412	GLY	O-C-CA-N
5	A	1412	GLY	OXT-C-CA-N
6	A	1415	PGE	O2-C3-C4-O3
6	A	1404	PGE	O2-C3-C4-O3
6	A	1404	PGE	O1-C1-C2-O2
7	A	1419	EDO	O1-C1-C2-O2
3	B	203	PEG	O1-C1-C2-O2
6	A	1411	PGE	O2-C3-C4-O3
3	A	1401	PEG	O1-C1-C2-O2
8	A	1408	PG4	O1-C1-C2-O2
9	B	204	DAL	O-C-CA-CB
9	B	204	DAL	OXT-C-CA-CB
6	A	1404	PGE	O3-C5-C6-O4
8	A	1408	PG4	O2-C3-C4-O3
8	A	1408	PG4	C8-C7-O4-C6
6	A	1415	PGE	C6-C5-O3-C4
3	A	1417	PEG	C4-C3-O2-C2
6	A	1411	PGE	C4-C3-O2-C2
6	A	1415	PGE	C3-C4-O3-C5
6	A	1411	PGE	C3-C4-O3-C5
6	A	1404	PGE	C1-C2-O2-C3
3	A	1417	PEG	O1-C1-C2-O2
3	B	203	PEG	O2-C3-C4-O4
7	A	1409	EDO	O1-C1-C2-O2
7	A	1418	EDO	O1-C1-C2-O2
7	B	202	EDO	O1-C1-C2-O2
9	B	204	DAL	OXT-C-CA-N
8	A	1408	PG4	C5-C6-O4-C7
8	A	1408	PG4	C4-C3-O2-C2
8	A	1408	PG4	C3-C4-O3-C5
6	A	1404	PGE	C3-C4-O3-C5
8	A	1408	PG4	O3-C5-C6-O4
9	B	204	DAL	O-C-CA-N
3	A	1401	PEG	C1-C2-O2-C3
3	B	203	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	PEG	1	0
6	A	1404	PGE	1	0
7	B	205	EDO	2	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 [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	517/520 (99%)	-0.52	12 (2%) 60 58	18, 29, 53, 72	0
2	B	125/136 (91%)	-0.65	1 (0%) 86 85	19, 27, 41, 65	0
All	All	642/656 (97%)	-0.55	13 (2%) 65 63	18, 28, 53, 72	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	3.7
1	A	519	HIS	3.7
1	A	517	HIS	3.6
1	A	54	THR	3.4
1	A	3	ILE	2.8
2	B	12	SER	2.7
1	A	174	ALA	2.6
1	A	55	GLY	2.5
1	A	518	HIS	2.5
1	A	56	ASP	2.4
1	A	516	HIS	2.4
1	A	173	ALA	2.3
1	A	51	VAL	2.2

### 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
3	PEG	A	1401	7/7	0.80	0.18	44,49,60,63	0
6	PGE	A	1411	10/10	0.80	0.34	29,51,56,57	0
7	EDO	A	1406	4/4	0.81	0.24	47,55,56,62	0
7	EDO	A	1410	4/4	0.83	0.16	45,46,49,54	0
5	GLY	A	1403	5/5	0.84	0.11	41,53,56,58	0
7	EDO	A	1409	4/4	0.84	0.16	46,52,53,54	0
6	PGE	A	1415	10/10	0.84	0.18	44,60,65,65	0
7	EDO	B	201	4/4	0.84	0.23	42,46,58,65	0
7	EDO	B	202	4/4	0.85	0.13	47,52,54,57	0
7	EDO	A	1418	4/4	0.86	0.17	53,53,58,67	0
3	PEG	B	203	7/7	0.87	0.27	56,60,70,72	0
3	PEG	A	1417	7/7	0.87	0.21	48,54,59,64	0
7	EDO	A	1407	4/4	0.88	0.22	52,53,55,58	0
5	GLY	A	1413	5/5	0.88	0.12	47,50,58,62	0
6	PGE	A	1404	10/10	0.89	0.16	34,43,53,59	0
9	DAL	B	204	6/6	0.89	0.18	46,48,55,57	0
8	PG4	A	1408	13/13	0.91	0.21	38,53,61,66	0
7	EDO	A	1419	4/4	0.91	0.14	45,46,50,54	0
7	EDO	A	1405	4/4	0.92	0.09	52,54,55,56	0
7	EDO	A	1414	4/4	0.92	0.17	46,48,49,53	0
7	EDO	A	1416	4/4	0.93	0.27	54,59,61,63	0
5	GLY	A	1412	5/5	0.94	0.14	54,58,61,72	0
7	EDO	B	205	4/4	0.94	0.32	39,48,48,54	0
4	PO4	A	1402	5/5	1.00	0.10	19,21,22,23	0

## 6.5 Other polymers

There are no such residues in this entry.