



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:44 AM GMT

PDB ID : 2BHU  
Title : CRYSTAL STRUCTURE OF DEINOCOCCUS RADIODURANS MALTOO  
LIGOSYLTREHALOSETREHALOHYDROLASE  
Authors : Timmins, J.; Leiros, H.-K.S.; Leonard, G.; Leiros, I.; Mcsweeney, S.  
Deposited on : 2005-01-18  
Resolution : 1.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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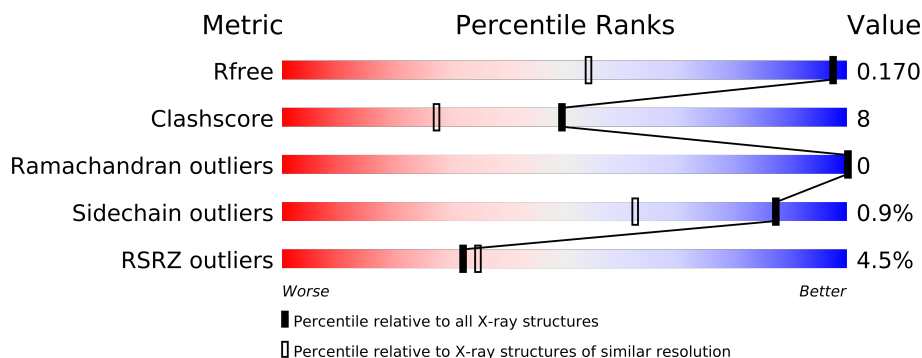
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.10 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))
$R_{free}$	66092	1400 (1.20-1.00)
Clashscore	79885	1559 (1.20-1.00)
Ramachandran outliers	78287	1474 (1.20-1.00)
Sidechain outliers	78261	1472 (1.20-1.00)
RSRZ outliers	66119	1400 (1.20-1.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	602	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TRS	A	1603[A]	-	X
2	TRS	A	1603[B]	-	X
3	PGE	A	1604[A]	-	X
3	PGE	A	1604[B]	-	X
4	MG	A	1606	-	X

## 2 Entry composition

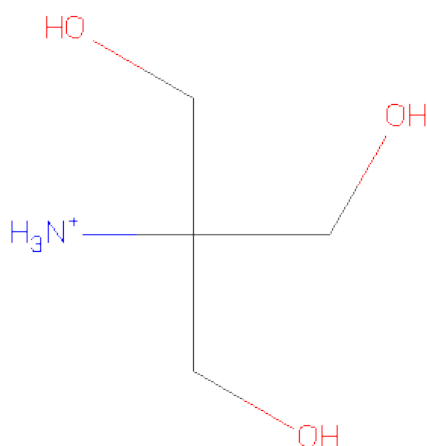
There are 5 unique types of molecules in this entry. The entry contains 6172 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MALTOOLIGOSYLTREHALOSETREHALOHYDROLASE.

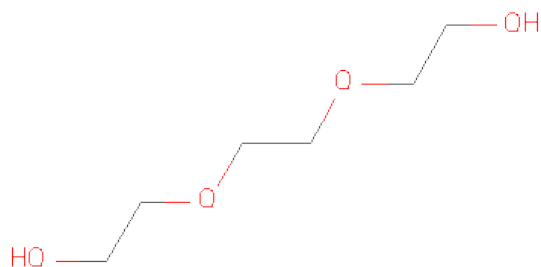
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	580	5005	3162	895	937	11	52	43	0

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	16	8	2	6	0	1

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			20	12	8		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

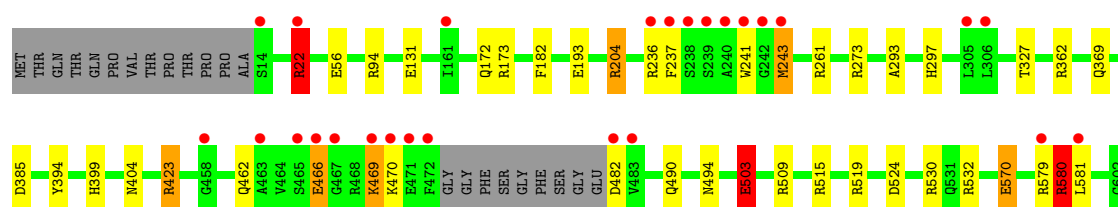
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1130	Total	O	0	0
			1130	1130		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MALTOOLIGOSYLTREHALOSETREHALOXYDROLASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.58Å 66.62Å 152.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 1.10 44.41 – 1.10	Depositor EDS
% Data completeness (in resolution range)	88.2 (44.41-1.10) 88.2 (44.41-1.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.128 , 0.159 0.143 , 0.170	Depositor DCC
$R_{free}$ test set	10891 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	7.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 216501 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, PGE, MG

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	17.97	33/5142 (0.6%)	5.15	51/6994 (0.7%)

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	6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22[A]	ARG	CZ-NH2	642.51	9.68	1.33
1	A	22[B]	ARG	CZ-NH2	642.51	9.68	1.33
1	A	22[A]	ARG	CZ-NH1	575.45	8.81	1.33
1	A	22[B]	ARG	CZ-NH1	575.45	8.81	1.33
1	A	503[A]	GLU	CD-OE2	232.20	3.81	1.25
1	A	503[B]	GLU	CD-OE2	232.20	3.81	1.25
1	A	503[A]	GLU	CD-OE1	138.59	2.78	1.25
1	A	503[B]	GLU	CD-OE1	138.59	2.78	1.25
1	A	466	GLU	CD-OE2	109.17	2.45	1.25
1	A	580	ARG	CZ-NH2	45.79	1.92	1.33
1	A	503[A]	GLU	CG-CD	40.58	2.12	1.51
1	A	503[B]	GLU	CG-CD	40.58	2.12	1.51
1	A	482	ASP	CB-CG	28.85	2.12	1.51
1	A	243[A]	MET	CG-SD	27.26	2.52	1.81
1	A	243[B]	MET	CG-SD	27.26	2.52	1.81
1	A	243[A]	MET	SD-CE	20.13	2.90	1.77
1	A	243[B]	MET	SD-CE	20.13	2.90	1.77
1	A	519[A]	ARG	NE-CZ	18.09	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519[B]	ARG	NE-CZ	18.09	1.56	1.33
1	A	193[A]	GLU	CD-OE2	14.10	1.41	1.25
1	A	193[B]	GLU	CD-OE2	14.10	1.41	1.25
1	A	22[A]	ARG	CB-CG	9.73	1.78	1.52
1	A	22[B]	ARG	CB-CG	9.73	1.78	1.52
1	A	469	LYS	CD-CE	9.67	1.75	1.51
1	A	579	ARG	CD-NE	-7.91	1.33	1.46
1	A	462	GLN	CD-NE2	7.52	1.51	1.32
1	A	22[A]	ARG	CA-CB	-6.96	1.38	1.53
1	A	22[B]	ARG	CA-CB	-6.96	1.38	1.53
1	A	193[A]	GLU	CD-OE1	6.90	1.33	1.25
1	A	193[B]	GLU	CD-OE1	6.90	1.33	1.25
1	A	466	GLU	CG-CD	-6.33	1.42	1.51
1	A	470	LYS	CG-CD	-6.30	1.31	1.52
1	A	580	ARG	CZ-NH1	-6.13	1.25	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22[A]	ARG	NE-CZ-NH1	-187.50	26.55	120.30
1	A	22[B]	ARG	NE-CZ-NH1	-187.50	26.55	120.30
1	A	22[A]	ARG	NE-CZ-NH2	-178.16	31.22	120.30
1	A	22[B]	ARG	NE-CZ-NH2	-178.16	31.22	120.30
1	A	22[A]	ARG	NH1-CZ-NH2	-96.56	13.18	119.40
1	A	22[B]	ARG	NH1-CZ-NH2	-96.56	13.18	119.40
1	A	503[A]	GLU	OE1-CD-OE2	-73.93	34.59	123.30
1	A	503[B]	GLU	OE1-CD-OE2	-73.93	34.59	123.30
1	A	580	ARG	NE-CZ-NH1	56.44	148.52	120.30
1	A	503[A]	GLU	CG-CD-OE2	-42.34	33.61	118.30
1	A	503[B]	GLU	CG-CD-OE2	-42.34	33.61	118.30
1	A	519[A]	ARG	NE-CZ-NH1	-31.91	104.35	120.30
1	A	519[B]	ARG	NE-CZ-NH1	-31.91	104.35	120.30
1	A	503[A]	GLU	CG-CD-OE1	-31.21	55.87	118.30
1	A	503[B]	GLU	CG-CD-OE1	-31.21	55.87	118.30
1	A	519[A]	ARG	NE-CZ-NH2	30.27	135.44	120.30
1	A	519[B]	ARG	NE-CZ-NH2	30.27	135.44	120.30
1	A	580	ARG	NH1-CZ-NH2	-26.41	90.35	119.40
1	A	469	LYS	CD-CE-NZ	-19.60	66.62	111.70
1	A	243[A]	MET	CG-SD-CE	-19.20	69.48	100.20
1	A	243[B]	MET	CG-SD-CE	-19.20	69.48	100.20
1	A	580	ARG	NE-CZ-NH2	-17.71	111.44	120.30
1	A	519[A]	ARG	CD-NE-CZ	15.71	145.60	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519[B]	ARG	CD-NE-CZ	15.71	145.60	123.60
1	A	482	ASP	CA-CB-CG	-12.80	85.25	113.40
1	A	243[A]	MET	CB-CG-SD	-10.60	80.61	112.40
1	A	243[B]	MET	CB-CG-SD	-10.60	80.61	112.40
1	A	22[A]	ARG	CB-CG-CD	-9.52	86.86	111.60
1	A	22[B]	ARG	CB-CG-CD	-9.52	86.86	111.60
1	A	570	GLU	OE1-CD-OE2	-9.22	112.24	123.30
1	A	22[A]	ARG	CB-CA-C	6.87	124.15	110.40
1	A	22[B]	ARG	CB-CA-C	6.87	124.15	110.40
1	A	579	ARG	CG-CD-NE	6.81	126.10	111.80
1	A	193[A]	GLU	CG-CD-OE1	-6.66	104.97	118.30
1	A	193[B]	GLU	CG-CD-OE1	-6.66	104.97	118.30
1	A	94	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	530	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	182	PHE	CB-CG-CD1	6.07	125.05	120.80
1	A	362	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	394	TYR	CB-CG-CD1	5.68	124.41	121.00
1	A	362	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	423	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	469	LYS	CB-CG-CD	5.49	125.86	111.60
1	A	532	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	515	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	193[A]	GLU	CG-CD-OE2	5.37	129.03	118.30
1	A	193[B]	GLU	CG-CD-OE2	5.37	129.03	118.30
1	A	261	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	423	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	524	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	394	TYR	CB-CG-CD2	-5.17	117.89	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22[A]	ARG	Sidechain
1	A	466	GLU	Sidechain
1	A	503[A]	GLU	Sidechain
1	A	509[A]	ARG	Sidechain
1	A	570	GLU	Sidechain
1	A	580	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5005	0	14	37	3
2	A	16	0	0	0	0
3	A	20	0	0	1	0
4	A	1	0	0	0	0
5	A	1130	0	0	15	2
All	All	6172	0	14	37	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (37) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22[A]:ARG:CG	1:A:22[A]:ARG:CB	1.78	1.58
1:A:503[B]:GLU:CG	1:A:503[B]:GLU:CD	1.95	1.34
1:A:243[B]:MET:CG	1:A:243[B]:MET:SD	2.23	1.25
1:A:503[A]:GLU:CG	1:A:503[A]:GLU:CD	2.12	1.17
1:A:404[B]:ASN:OD1	5:A:2834:HOH:O	1.62	1.13
1:A:22[A]:ARG:CD	1:A:22[A]:ARG:CB	2.27	1.12
1:A:172:GLN:OE1	5:A:2453:HOH:O	1.81	0.98
1:A:243[A]:MET:CG	1:A:243[A]:MET:SD	2.52	0.98
1:A:423:ARG:CD	5:A:2863:HOH:O	2.16	0.94
1:A:581[A]:LEU:CD1	5:A:3112:HOH:O	2.17	0.91
1:A:204[A]:ARG:CG	5:A:2519:HOH:O	2.21	0.88
1:A:503[B]:GLU:CB	1:A:503[B]:GLU:CD	2.46	0.83
1:A:327[B]:THR:CG2	5:A:2710:HOH:O	2.26	0.83
1:A:243[A]:MET:SD	1:A:243[A]:MET:CB	2.70	0.80
1:A:580:ARG:CZ	5:A:3089:HOH:O	2.30	0.79
1:A:22[A]:ARG:NH2	1:A:22[A]:ARG:NH1	2.29	0.79
1:A:503[B]:GLU:CG	1:A:503[B]:GLU:OE1	2.36	0.74
1:A:503[B]:GLU:CG	1:A:503[B]:GLU:OE2	2.35	0.74
1:A:503[A]:GLU:CG	1:A:503[A]:GLU:OE2	2.35	0.74
1:A:503[A]:GLU:CG	1:A:503[A]:GLU:OE1	2.37	0.73
1:A:369[B]:GLN:NE2	3:A:1604[B]:PGE:C4	2.56	0.69
1:A:56[B]:GLU:OE2	5:A:2171:HOH:O	2.10	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22[A]:ARG:CG	1:A:22[A]:ARG:CA	2.64	0.67
1:A:469:LYS:CE	1:A:469:LYS:CG	2.75	0.64
1:A:56[A]:GLU:OE2	5:A:2169:HOH:O	2.16	0.61
1:A:204[A]:ARG:NH1	5:A:2535:HOH:O	2.32	0.61
1:A:131:GLU:OE2	1:A:399:HIS:CD2	2.54	0.61
1:A:503[A]:GLU:OE1	1:A:503[A]:GLU:OE2	2.19	0.59
1:A:503[B]:GLU:OE1	1:A:503[B]:GLU:OE2	2.20	0.58
1:A:404[A]:ASN:ND2	5:A:2837:HOH:O	2.40	0.55
1:A:490:GLN:NE2	1:A:494[A]:ASN:OD1	2.42	0.52
1:A:243[B]:MET:CB	1:A:243[B]:MET:SD	2.99	0.47
1:A:56[B]:GLU:CG	5:A:2171:HOH:O	2.62	0.47
1:A:241:TRP:CZ2	5:A:2297:HOH:O	2.70	0.44
1:A:404[B]:ASN:ND2	5:A:2837:HOH:O	2.52	0.41
1:A:237:PHE:C	5:A:2595:HOH:O	2.59	0.41
1:A:293:ALA:O	1:A:297[A]:HIS:CD2	2.74	0.40

All (5) 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	Distance(Å)	Clash(Å)
1:A:236[A]:ARG:NH2	1:A:297[A]:HIS:ND1[4_455]	1.46	0.74
1:A:236[A]:ARG:NH2	1:A:297[A]:HIS:CG[4_455]	1.63	0.57
1:A:236[A]:ARG:NH2	1:A:297[A]:HIS:CB[4_455]	1.89	0.31
5:A:2346:HOH:O	5:A:2662:HOH:O[4_555]	1.93	0.27
5:A:2202:HOH:O	5:A:2818:HOH:O[4_455]	2.11	0.09

## 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	623/602 (104%)	617 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	513/484 (106%)	508 (99%)	5 (1%)	85 59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	A	204[A]	ARG
1	A	204[B]	ARG
1	A	273	ARG
1	A	385	ASP

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 chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	TRS	A	1603[A]	-	7,7,7	1.13	1 (14%)	9,9,9	1.51	1 (11%)
2	TRS	A	1603[B]	-	7,7,7	0.72	0	9,9,9	1.06	1 (11%)
3	PGE	A	1604[A]	-	9,9,9	1.50	3 (33%)	8,8,8	1.16	0
3	PGE	A	1604[B]	1	9,9,9	0.99	0	8,8,8	0.97	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	TRS	A	1603[A]	-	-	0/9/9/9	0/0/0/0
2	TRS	A	1603[B]	-	-	0/9/9/9	0/0/0/0
3	PGE	A	1604[A]	-	-	0/7/7/7	0/0/0/0
3	PGE	A	1604[B]	1	-	0/7/7/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1603[A]	TRS	C3-C	-2.55	1.47	1.53
3	A	1604[A]	PGE	C5-C6	2.43	1.62	1.49
3	A	1604[A]	PGE	O3-C4	2.28	1.51	1.42
3	A	1604[A]	PGE	O3-C5	2.22	1.51	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1603[A]	TRS	C3-C-N	-3.23	99.53	108.30
2	A	1603[B]	TRS	C3-C-N	2.05	113.86	108.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	580/602 (96%)	-0.14	26 (4%)	32 35	4, 8, 18, 40	34 (5%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22[A]	ARG	6.7
1	A	236[A]	ARG	6.1
1	A	241	TRP	5.0
1	A	472	PHE	4.9
1	A	240	ALA	4.4
1	A	470	LYS	4.3
1	A	239[A]	SER	4.2
1	A	469	LYS	4.1
1	A	482	ASP	3.8
1	A	463	ALA	3.4
1	A	467	GLY	3.3
1	A	243[A]	MET	3.2
1	A	465	SER	3.1
1	A	242	GLY	2.8
1	A	483	VAL	2.7
1	A	466	GLU	2.7
1	A	237	PHE	2.6
1	A	238	SER	2.5
1	A	471	GLU	2.5
1	A	305[A]	LEU	2.3
1	A	581[A]	LEU	2.3
1	A	458	GLY	2.1
1	A	579	ARG	2.1
1	A	14	SER	2.0
1	A	306[A]	LEU	2.0
1	A	161[A]	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PGE	A	1604[A]	10/10	0.26	16.33	14,19,30,32	10
3	PGE	A	1604[B]	10/10	0.26	16.15	0,0,0,0	10
2	TRS	A	1603[A]	8/8	0.11	2.66	9,11,13,15	8
2	TRS	A	1603[B]	8/8	0.11	2.66	15,17,17,18	8
4	MG	A	1606	1/1	0.12	2.49	10,10,10,10	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.