



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:54 PM GMT

PDB ID : 3VGB  
Title : Crystal structure of glycosyltrehalose trehalohydrolase (GTHase) from *Sulfolobus solfataricus* KM1  
Authors : Okazaki, N.; Tamada, T.; Feese, M.D.; Kato, M.; Miura, Y.; Komeda, T.; Kobayashi, K.; Kondo, K.; Kuroki, R.  
Deposited on : 2011-08-09  
Resolution : 2.65 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 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

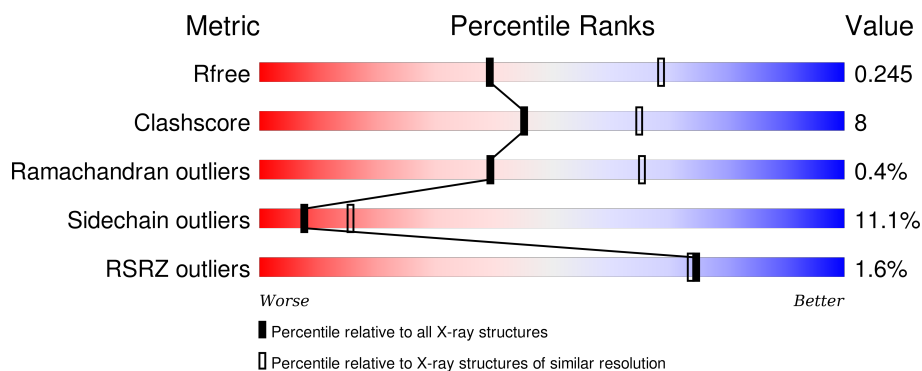
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

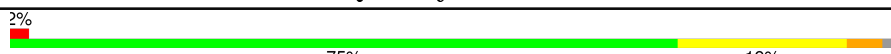
The reported resolution of this entry is 2.65 Å.

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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	558	

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	GOL	A	1101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1102	-	-	-	X
3	GOL	A	1103	-	-	-	X

## 2 Entry composition [i](#)

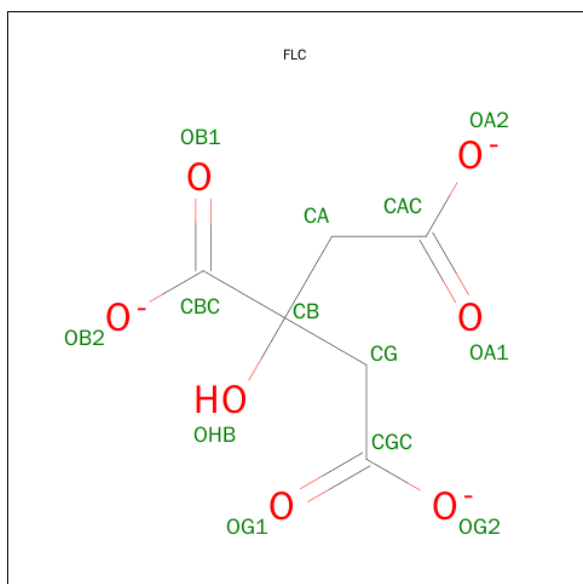
There are 4 unique types of molecules in this entry. The entry contains 4720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malto-oligosyltrehalose trehalohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4512	2907	741	855	9	0	0	0

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 2% 75% 10%
- THR PHE ALA TYR LYS ILE ASP G8 I19 E10 W16 Q20 K24 L25 Y33 I45 T46 I47 I48 V52 R53 V59 L60 D61 D62 E65 P69 A70 S71 R72 Y73 Q74 I84 E87 S88 K89 N92 I93 E94 K98 K99 E100 I104 Y105 V161 I122 I123 K124 L125 L128 I133 I138 I141 A142 Q143 V155 Y156 L157 V160 Q161 N162 V174 K179 I184 I185 L186 V193 G194 P195 N198 L203 K210 Y211 K212 W215 G216 L217 E225 S226 V229 V237 K242 E243 D252 V261 I265 L266 E267 E268 V272 V273 R278 L279 V280 R290 V291 V292 K295 E296 K297 C298 D308 R311 H312 E321 R322 Q323 L332 D333 V336 Y339 K340 R354 H357 V361 V370 V371 Y372 R387 V392 E395 S396 A402 Y409 W412 I413 F414 Y415 Y423 F427 R435 L436 L437 Q438 R444 K445 K446 E447 Q450 D453 P454 Q455 D456 E457 S458 L480 R483 R484 L487 R489 R494 V497 E501 L504 R509 E510 Y511 S518 K525 L531 L532 N535 Y536 S537 E544

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.27Å 78.27Å 282.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.78 – 2.65 67.78 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (67.78-2.65) 97.4 (67.78-2.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.202 , 0.243 0.206 , 0.245	Depositor DCC
$R_{free}$ test set	1486 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.0	EDS
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 29341 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, FLC

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	0.39	0/4628	0.55	0/6253

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	4512	0	4369	70	0
2	A	13	0	5	0	0
3	A	18	0	24	3	0
4	A	177	0	0	7	0
All	All	4720	0	4398	70	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 8.

All (70) 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:133:ILE:HD11	1:A:413:ILE:HD12	1.48	0.95
1:A:354:ARG:HG3	1:A:354:ARG:HH11	1.49	0.76
1:A:264:HIS:HD2	1:A:266:LEU:H	1.36	0.73
1:A:105:TYR:HB2	1:A:133:ILE:HG12	1.71	0.71
1:A:321:GLU:HB3	1:A:323:GLN:NE2	2.06	0.71
1:A:104:ILE:HB	1:A:412:MET:HG3	1.73	0.71
1:A:311:HIS:HD2	1:A:312:HIS:ND1	1.89	0.70
1:A:92:ASN:O	1:A:278:ARG:NH2	2.24	0.69
1:A:143:GLN:HE22	1:A:162:ASN:H	1.42	0.67
1:A:387:ARG:HD2	1:A:423:ASN:O	1.95	0.67
1:A:395:GLU:OE1	1:A:535:ASN:ND2	2.30	0.64
1:A:535:ASN:HB3	1:A:537:SER:H	1.63	0.62
1:A:174:VAL:HB	1:A:184:VAL:HG11	1.82	0.61
1:A:387:ARG:NH2	1:A:415:MET:O	2.34	0.61
1:A:252:ASP:OD1	3:A:1103:GOL:H31	2.00	0.61
1:A:392:VAL:HB	1:A:396:SER:HB2	1.83	0.61
1:A:141:ILE:HD12	1:A:160:VAL:HG13	1.85	0.58
1:A:72:ARG:HG2	4:A:2089:HOH:O	2.05	0.57
1:A:124:LYS:HE2	3:A:1101:GOL:H32	1.87	0.56
1:A:427:PHE:HB3	1:A:450:GLN:HE22	1.72	0.55
1:A:444:ARG:NH1	1:A:450:GLN:HE21	2.05	0.55
1:A:264:HIS:CD2	1:A:266:LEU:H	2.21	0.55
1:A:453:ASP:HB3	1:A:456:ASP:HB2	1.88	0.55
1:A:437:ILE:HG23	1:A:455:GLN:HG3	1.90	0.54
1:A:226:SER:HA	1:A:229:VAL:HG13	1.88	0.54
1:A:354:ARG:HH11	1:A:354:ARG:CG	2.20	0.54
1:A:357:HIS:HE1	4:A:2026:HOH:O	1.91	0.53
1:A:427:PHE:HB2	1:A:444:ARG:NH2	2.25	0.51
1:A:53:ARG:HB3	1:A:84:ILE:O	2.11	0.51
1:A:480:LEU:HD13	1:A:532:LEU:HD23	1.93	0.51
1:A:321:GLU:HB3	1:A:323:GLN:HE21	1.76	0.50
1:A:100:GLU:HG2	4:A:2004:HOH:O	2.12	0.50
1:A:531:LEU:HD21	1:A:557:LYS:HG3	1.94	0.50
1:A:155:VAL:CG2	1:A:198:ASN:HB2	2.42	0.49
1:A:415:MET:O	1:A:415:MET:HG3	2.13	0.49
1:A:16:TRP:HZ2	1:A:225:GLU:HG2	1.79	0.48
1:A:494:ARG:HH12	1:A:509:ARG:HD3	1.79	0.48
1:A:71:SER:CB	1:A:74:GLN:HE22	2.26	0.47
1:A:308:ASP:OD1	1:A:372:TYR:OH	2.27	0.47
1:A:24:LYS:HB2	1:A:59:VAL:HG13	1.95	0.47
1:A:333:ASP:HA	1:A:336:VAL:HG13	1.95	0.47
1:A:157:LEU:HD11	4:A:2071:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ARG:HD2	1:A:444:ARG:HA	1.62	0.46
1:A:332:LEU:HD21	1:A:504:LEU:HD23	1.98	0.46
1:A:52:VAL:HA	1:A:53:ARG:HA	1.66	0.46
1:A:487:LEU:HG	1:A:511:TYR:HB3	1.96	0.46
1:A:141:ILE:HG12	1:A:186:LEU:HD11	1.98	0.45
1:A:409:TYR:O	1:A:484:ARG:NH2	2.49	0.45
1:A:402:ALA:HA	1:A:480:LEU:HD21	1.99	0.44
1:A:273:VAL:HG21	1:A:280:VAL:HG22	1.99	0.44
1:A:493:ARG:HD2	4:A:2012:HOH:O	2.17	0.44
1:A:268:GLU:O	1:A:272:VAL:HG23	2.18	0.44
1:A:10:GLU:HB2	1:A:48:ASN:HA	1.99	0.44
1:A:124:LYS:CE	3:A:1101:GOL:H32	2.48	0.43
1:A:89:LYS:HG3	1:A:243:GLU:OE1	2.19	0.43
1:A:194:GLY:HA2	1:A:195:PRO:HD3	1.86	0.43
1:A:295:LYS:HE3	4:A:2157:HOH:O	2.19	0.43
1:A:133:ILE:CD1	1:A:413:ILE:HD12	2.35	0.42
1:A:20:GLN:OE1	1:A:60:LEU:HB3	2.18	0.42
1:A:354:ARG:NH1	1:A:354:ARG:CG	2.82	0.42
1:A:89:LYS:HG2	1:A:242:LYS:HB3	2.00	0.42
1:A:544:GLU:HG2	1:A:544:GLU:H	1.37	0.42
1:A:297:LYS:O	1:A:298:CYS:HB2	2.20	0.41
1:A:122:ILE:HA	1:A:125:LEU:HD22	2.02	0.41
1:A:210:LYS:HD3	4:A:2137:HOH:O	2.21	0.41
1:A:155:VAL:HG21	1:A:198:ASN:HB2	2.03	0.40
1:A:10:GLU:CB	1:A:48:ASN:HA	2.51	0.40
1:A:69:PRO:HG2	1:A:203:LEU:HD11	2.04	0.40
1:A:435:LYS:HD2	1:A:435:LYS:HA	1.90	0.40
1:A:138:ILE:HD13	1:A:184:VAL:HG23	2.04	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	548/558 (98%)	524 (96%)	22 (4%)	2 (0%)	39 65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	LYS
1	A	62	ASP

### 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	487/494 (99%)	433 (89%)	54 (11%)	8 15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	20	GLN
1	A	25	LEU
1	A	45	ILE
1	A	53	ARG
1	A	65	GLU
1	A	72	ARG
1	A	74	GLN
1	A	87	GLU
1	A	93	ASN
1	A	94	GLU
1	A	98	LYS
1	A	121	VAL
1	A	125	LEU
1	A	128	LEU
1	A	155	VAL
1	A	174	VAL
1	A	179	LYS
1	A	184	VAL

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Mol	Chain	Res	Type
1	A	193	VAL
1	A	215	TRP
1	A	217	LEU
1	A	225	GLU
1	A	229	VAL
1	A	237	VAL
1	A	280	VAL
1	A	290	ARG
1	A	292	VAL
1	A	323	GLN
1	A	332	LEU
1	A	336	VAL
1	A	339	TYR
1	A	340	LYS
1	A	361	VAL
1	A	370	VAL
1	A	435	LYS
1	A	438	GLN
1	A	444	ARG
1	A	445	LYS
1	A	446	LYS
1	A	447	GLU
1	A	456	ASP
1	A	458	SER
1	A	483	MET
1	A	487	LEU
1	A	497	VAL
1	A	501	GLU
1	A	509	ARG
1	A	518	SER
1	A	525	LYS
1	A	531	LEU
1	A	544	GLU
1	A	553	PHE
1	A	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	93	ASN
1	A	143	GLN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	264	HIS
1	A	301	ASN
1	A	311	HIS
1	A	323	GLN
1	A	357	HIS
1	A	450	GLN
1	A	499	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
2	FLC	A	1001	-	3,12,12	0.57	0	3,17,17	0.59	0
3	GOL	A	1101	-	5,5,5	0.34	0	5,5,5	0.25	0
3	GOL	A	1102	-	5,5,5	0.33	0	5,5,5	0.28	0
3	GOL	A	1103	-	5,5,5	0.32	0	5,5,5	0.36	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	FLC	A	1001	-	-	0/6/16/16	0/0/0/0
3	GOL	A	1101	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1102	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1103	-	-	0/4/4/4	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	2	0
3	A	1103	GOL	1	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	550/558 (98%)	0.24	9 (1%) 74 74	24, 40, 78, 101	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	GLY	4.7
1	A	211	TYR	3.9
1	A	212	LYS	2.8
1	A	46	THR	2.7
1	A	217	LEU	2.7
1	A	9	ASN	2.5
1	A	33	TYR	2.3
1	A	446	LYS	2.1
1	A	52	VAL	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1102	6/6	0.94	0.38	6.45	65,66,66,67	0
3	GOL	A	1101	6/6	0.82	0.33	4.28	79,80,81,81	0
3	GOL	A	1103	6/6	0.90	0.29	3.47	58,58,59,59	0
2	FLC	A	1001	13/13	0.96	0.14	-1.10	49,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.