

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7ZC0
Title	:	4,6-alpha-glucanotransferase GtfC from Geobacillus 12AMOR1
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Deposited on	:	2022-03-25
Resolution	:	2.25 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.25 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.



Motria	Whole archive	Similar resolution
wiethc	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 >=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 <=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				
			26%				
1	AAA	726	83%	14%	••		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5949 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 4,6-alpha-Glucanotransferase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	AAA	710	Total 5667	C 3597	N 957	O 1098	$\begin{array}{c} \mathrm{S} \\ 15 \end{array}$	0	0	0

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	AAA	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	AAA	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
2	AAA	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	257	Total O 257 257	0	0



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: 4,6-alpha-Glucanotransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants	262.56Å 262.56Å 72.23Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	131.28 - 2.25	Depositor
Resolution (A)	131.28 - 2.25	EDS
% Data completeness	99.3 (131.28-2.25)	Depositor
(in resolution range)	99.3 (131.28-2.25)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.16 (at 2.25 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.252 , 0.292	Depositor
n, n_{free}	0.253 , 0.293	DCC
R_{free} test set	2978 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5949	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: GOL, CA

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	AAA	0.38	0/5808	0.72	0/7880	

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 (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	AAA	5667	0	5463	49	0
2	AAA	24	0	32	3	0
3	AAA	1	0	0	0	0
4	AAA	257	0	0	4	0
All	All	5949	0	5495	49	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 (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:AAA:569:ARG:HG2	1:AAA:570:VAL:N	2.06	0.70
1:AAA:651:ASP:O	1:AAA:671:GLY:HA2	1.93	0.68
1:AAA:578:ASN:N	4:AAA:903:HOH:O	2.30	0.65
1:AAA:218:GLN:O	1:AAA:222:ARG:HD3	1.97	0.63
1:AAA:104:GLY:HA2	1:AAA:114:ARG:O	2.03	0.58
1:AAA:46:GLN:HE22	1:AAA:515:ASN:HB2	1.71	0.56
1:AAA:50:LEU:HD12	1:AAA:520:LYS:HB2	1.89	0.54
1:AAA:579:VAL:HG21	1:AAA:615:TYR:CE2	2.43	0.53
1:AAA:264:LEU:HD23	1:AAA:285:MET:HE1	1.92	0.52
1:AAA:199:TYR:O	1:AAA:396:HIS:HE1	1.94	0.50
1:AAA:42:ARG:NH2	1:AAA:440:ASN:OD1	2.43	0.50
1:AAA:533:ILE:HD11	1:AAA:550:LEU:HD12	1.93	0.50
1:AAA:357:VAL:O	2:AAA:801:GOL:H32	2.12	0.49
1:AAA:100:ARG:HG3	4:AAA:1014:HOH:O	2.13	0.49
1:AAA:617:GLU:HB2	1:AAA:618:PRO:HD3	1.96	0.48
1:AAA:487:LEU:HD22	1:AAA:672:THR:HG23	1.96	0.48
1:AAA:606:ALA:CB	1:AAA:611:LYS:HD2	2.43	0.48
1:AAA:93:GLU:H	1:AAA:93:GLU:CD	2.16	0.47
1:AAA:693:PHE:CD1	1:AAA:712:LEU:HD21	2.50	0.47
1:AAA:569:ARG:HG2	1:AAA:570:VAL:H	1.78	0.47
1:AAA:100:ARG:NH2	1:AAA:394:GLN:OE1	2.39	0.46
1:AAA:71:GLU:HB3	1:AAA:624:LYS:HE3	1.98	0.46
1:AAA:295:TYR:OH	1:AAA:322:THR:HG22	2.16	0.46
1:AAA:295:TYR:OH	1:AAA:322:THR:CG2	2.63	0.45
1:AAA:679:THR:HG22	1:AAA:715:ARG:CD	2.46	0.45
1:AAA:356:PHE:HB3	2:AAA:801:GOL:H11	1.98	0.44
1:AAA:357:VAL:O	2:AAA:801:GOL:C3	2.66	0.44
1:AAA:558:LYS:HD2	4:AAA:932:HOH:O	2.18	0.44
1:AAA:318:ILE:O	1:AAA:322:THR:HG23	2.17	0.44
1:AAA:578:ASN:HB3	1:AAA:581:SER:HB2	2.01	0.43
1:AAA:652:LEU:HD12	1:AAA:670:ILE:O	2.19	0.43
1:AAA:444:TYR:HB3	1:AAA:464:LEU:HB2	2.01	0.43
1:AAA:44:ILE:O	1:AAA:595:THR:HA	2.19	0.43
1:AAA:81:PRO:HB2	1:AAA:94:GLY:O	2.19	0.42
1:AAA:60:LYS:HE2	1:AAA:123:GLU:OE2	2.19	0.42
1:AAA:494:SER:HB3	1:AAA:496:VAL:O	2.19	0.42
1:AAA:513:VAL:HG13	1:AAA:582:GLN:OE1	2.19	0.42
1:AAA:653:ILE:C	1:AAA:653:ILE:HD12	2.40	0.42
1:AAA:323:ASN:HA	1:AAA:326:ILE:HD12	2.01	0.42
1:AAA:539:TYR:CG	1:AAA:544:PRO:HA	2.53	0.42
1:AAA:63:ALA:HB1	1:AAA:130:LYS:HD3	2.01	0.42
1:AAA:679:THR:HG22	1:AAA:715:ARG:HD2	2.01	0.42



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:690:ASN:HA	1:AAA:706:ALA:O	2.20	0.42
1:AAA:248:LEU:HD23	1:AAA:270:TYR:CD2	2.55	0.41
1:AAA:684:MET:HG3	1:AAA:693:PHE:CZ	2.55	0.41
1:AAA:371:ILE:HD11	1:AAA:423:LEU:CD1	2.50	0.41
1:AAA:268:GLY:O	1:AAA:285:MET:HG2	2.20	0.40
1:AAA:157:TYR:HB2	1:AAA:357:VAL:O	2.21	0.40
1:AAA:734:THR:HA	4:AAA:981:HOH:O	2.21	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	AAA	708/726~(98%)	651 (92%)	50 (7%)	7 (1%)	15 13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	313	GLY
1	AAA	275	ALA
1	AAA	274	ASP
1	AAA	676	THR
1	AAA	708	ASN
1	AAA	30	GLY
1	AAA	294	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	602/614~(98%)	576~(96%)	26~(4%)	29 33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	27	LEU
1	AAA	114	ARG
1	AAA	184	LEU
1	AAA	227	ASP
1	AAA	239	ASP
1	AAA	255	ASN
1	AAA	270	TYR
1	AAA	300	SER
1	AAA	306	THR
1	AAA	309	ASP
1	AAA	359	GLU
1	AAA	375	TYR
1	AAA	399	ASN
1	AAA	453	GLU
1	AAA	482	THR
1	AAA	501	SER
1	AAA	503	SER
1	AAA	520	LYS
1	AAA	530	LEU
1	AAA	557	LYS
1	AAA	565	ASP
1	AAA	678	THR
1	AAA	679	THR
1	AAA	702	GLU
1	AAA	703	LYS
1	AAA	705	VAL

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)

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).

Mal	Turne	Chain	Dec	Tiple	В	ond leng	gths	B	Bond ang	gles
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GOL	AAA	804	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.45	0
2	GOL	AAA	802	-	$5,\!5,\!5$	0.19	0	$5,\!5,\!5$	0.63	0
2	GOL	AAA	801	-	$5,\!5,\!5$	0.06	0	$5,\!5,\!5$	0.27	0
2	GOL	AAA	803	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.34	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	GOL	AAA	804	-	-	1/4/4/4	-
2	GOL	AAA	802	-	-	1/4/4/4	-
2	GOL	AAA	801	-	-	4/4/4/4	-
2	GOL	AAA	803	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	AAA	801	GOL	O1-C1-C2-C3
2	AAA	801	GOL	C1-C2-C3-O3
2	AAA	801	GOL	O2-C2-C3-O3
2	AAA	803	GOL	C1-C2-C3-O3
2	AAA	801	GOL	O1-C1-C2-O2
2	AAA	802	GOL	O2-C2-C3-O3
2	AAA	804	GOL	O2-C2-C3-O3
2	AAA	803	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	801	GOL	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 (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^{th} 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	$OWAB(Å^2)$	Q<0.9
1	AAA	710/726~(97%)	1.75	190 (26%) 0 0	20, 51, 107, 145	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	277	THR	12.1
1	AAA	281	TYR	11.5
1	AAA	310	ILE	9.0
1	AAA	273	LYS	7.8
1	AAA	316	ALA	7.8
1	AAA	500	GLY	7.2
1	AAA	288	HIS	7.2
1	AAA	28	PHE	7.1
1	AAA	603	GLN	7.0
1	AAA	639	TYR	6.6
1	AAA	309	ASP	6.3
1	AAA	313	GLY	6.3
1	AAA	727	TYR	6.3
1	AAA	282	TRP	6.3
1	AAA	306	THR	6.3
1	AAA	289	TYR	6.2
1	AAA	300	SER	6.0
1	AAA	305	ALA	5.9
1	AAA	667	ALA	5.9
1	AAA	693	PHE	5.8
1	AAA	287	ILE	5.8
1	AAA	314	ASP	5.6
1	AAA	257	ILE	5.4
1	AAA	271	ALA	5.4
1	AAA	694	LYS	5.2
1	AAA	676	THR	5.2
1	AAA	269	TRP	5.2



$7 \mathrm{ZC0}$

Mol	Chain	Res	Type	RSRZ
1	AAA	692	VAL	5.1
1	AAA	256	LYS	4.7
1	AAA	26	VAL	4.6
1	AAA	304	PHE	4.5
1	AAA	280	GLN	4.5
1	AAA	275	ALA	4.4
1	AAA	322	THR	4.3
1	AAA	615	TYR	4.3
1	AAA	717	LYS	4.2
1	AAA	244	LEU	4.2
1	AAA	652	LEU	4.2
1	AAA	30	GLY	4.2
1	AAA	234	PHE	4.2
1	AAA	317	GLU	4.1
1	AAA	735	LYS	4.1
1	AAA	248	LEU	4.1
1	AAA	614	LEU	4.1
1	AAA	675	LYS	4.0
1	AAA	701	SER	4.0
1	AAA	731	TRP	3.9
1	AAA	307	VAL	3.9
1	AAA	513	VAL	3.9
1	AAA	315	ASN	3.9
1	AAA	274	ASP	3.8
1	AAA	713	THR	3.8
1	AAA	238	ASN	3.7
1	AAA	484	SER	3.7
1	AAA	272	ALA	3.7
1	AAA	266	VAL	3.6
1	AAA	623	LEU	3.6
1	AAA	72	TRP	3.6
1	AAA	111	ASN	3.6
1	AAA	722	ALA	3.5
1	AAA	303	GLY	3.4
1	AAA	31	PRO	3.4
1	AAA	477	THR	3.4
1	AAA	249	GLU	3.4
1	AAA	567	MET	3.4
1	AAA	321	TRP	3.4
1	AAA	571	ASP	3.3
1	AAA	611	LYS	3.3
1	AAA	88	MET	3.3



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Mol	Chain	Res	Type	RSRZ
1	AAA	237	PRO	3.3
1	AAA	114	ARG	3.3
1	AAA	704	LEU	3.2
1	AAA	75	THR	3.2
1	AAA	265	PRO	3.2
1	AAA	293	LYS	3.2
1	AAA	575	ALA	3.2
1	AAA	481	GLY	3.2
1	AAA	638	GLY	3.2
1	AAA	645	PRO	3.2
1	AAA	619	ILE	3.2
1	AAA	711	VAL	3.2
1	AAA	653	ILE	3.1
1	AAA	643	THR	3.1
1	AAA	284	PRO	3.1
1	AAA	581	SER	3.1
1	AAA	708	ASN	3.1
1	AAA	301	GLN	3.1
1	AAA	283	LYS	3.1
1	AAA	258	ASN	3.1
1	AAA	602	TYR	3.0
1	AAA	243	TYR	3.0
1	AAA	488	SER	3.0
1	AAA	312	ASN	2.9
1	AAA	270	TYR	2.9
1	AAA	646	GLU	2.9
1	AAA	278	SER	2.9
1	AAA	228	ASN	2.9
1	AAA	285	MET	2.9
1	AAA	673	ASN	2.9
1	AAA	262	THR	2.9
1	AAA	346	THR	2.9
1	AAA	705	VAL	2.9
1	AAA	245	PRO	2.8
1	AAA	716	VAL	2.8
1	AAA	296	LEU	2.8
1	AAA	604	THR	2.8
1	AAA	263	TYR	2.8
1	AAA	276	ALA	2.8
1	AAA	642	ASN	2.8
1	AAA	318	ILE	2.7
1	AAA	700	HIS	2.7



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Mol	Chain	Res	Type	RSRZ
1	AAA	682	VAL	2.7
1	AAA	734	THR	2.7
1	AAA	723	LEU	2.7
1	AAA	227	ASP	2.6
1	AAA	719	THR	2.6
1	AAA	689	ALA	2.6
1	AAA	416	THR	2.6
1	AAA	686	THR	2.6
1	AAA	489	THR	2.5
1	AAA	618	PRO	2.5
1	AAA	320	LYS	2.5
1	AAA	685	GLY	2.5
1	AAA	674	PRO	2.5
1	AAA	151	ASN	2.5
1	AAA	299	MET	2.5
1	AAA	628	ALA	2.5
1	AAA	308	ASP	2.5
1	AAA	726	GLY	2.5
1	AAA	230	LYS	2.5
1	AAA	504	ALA	2.5
1	AAA	714	ILE	2.5
1	AAA	625	MET	2.5
1	AAA	290	ALA	2.4
1	AAA	73	GLY	2.4
1	AAA	223	VAL	2.4
1	AAA	138	VAL	2.4
1	AAA	608	TYR	2.4
1	AAA	473	THR	2.4
1	AAA	468	TRP	2.4
1	AAA	622	LEU	2.4
1	AAA	724	VAL	2.4
1	AAA	89	ALA	2.4
1	AAA	720	ALA	2.4
1	AAA	225	THR	2.4
1	AAA	721	ASN	2.4
1	AAA	596	ILE	2.3
1	AAA	569	ARG	2.3
1	AAA	45	PHE	2.3
1	AAA	286	LEU	2.3
1	AAA	712	LEU	2.3
1	AAA	469	ALA	2.3
1	AAA	33	TYR	2.3



1200

Mol	Chain	Res	Type	RSRZ
1	AAA	554	GLU	2.3
1	AAA	538	LYS	2.3
1	AAA	302	HIS	2.3
1	AAA	561	ALA	2.3
1	AAA	584	ALA	2.3
1	AAA	470	LEU	2.2
1	AAA	703	LYS	2.2
1	AAA	400	TRP	2.2
1	AAA	264	LEU	2.2
1	AAA	695	ASP	2.2
1	AAA	598	TYR	2.2
1	AAA	491	ALA	2.2
1	AAA	574	TYR	2.1
1	AAA	621	LYS	2.1
1	AAA	61	ILE	2.1
1	AAA	103	LEU	2.1
1	AAA	620	THR	2.1
1	AAA	436	ASN	2.1
1	AAA	501	SER	2.1
1	AAA	412	ILE	2.1
1	AAA	201	TYR	2.1
1	AAA	212	GLY	2.1
1	AAA	136	LEU	2.1
1	AAA	557	LYS	2.1
1	AAA	43	VAL	2.1
1	AAA	325	TYR	2.1
1	AAA	122	ASP	2.0
1	AAA	553	LYS	2.0
1	AAA	482	THR	2.0
1	AAA	651	ASP	2.0
1	AAA	232	TYR	2.0
1	AAA	663	TYR	2.0
1	AAA	46	GLN	2.0
1	AAA	525	THR	2.0
1	AAA	340	SER	2.0
1	AAA	247	TRP	2.0
1	AAA	397	TRP	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^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	GOL	AAA	804	6/6	0.55	0.33	$52,\!56,\!57,\!57$	0
2	GOL	AAA	803	6/6	0.72	0.34	31,36,38,40	0
2	GOL	AAA	802	6/6	0.75	0.26	36,39,42,48	0
2	GOL	AAA	801	6/6	0.92	0.20	38,40,41,42	0
3	CA	AAA	805	1/1	0.98	0.16	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.

