



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:12 AM UTC

PDB ID : 7ZC0 / pdb_00007zc0
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

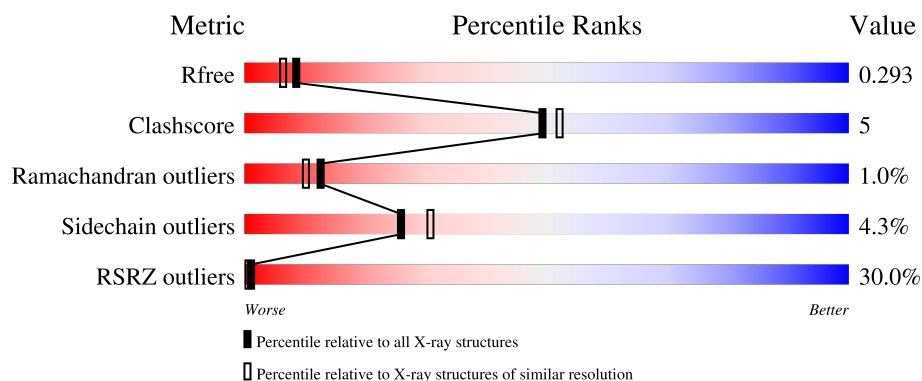
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	AAA	726	29% 82% 16% ..

2 Entry composition [i](#)

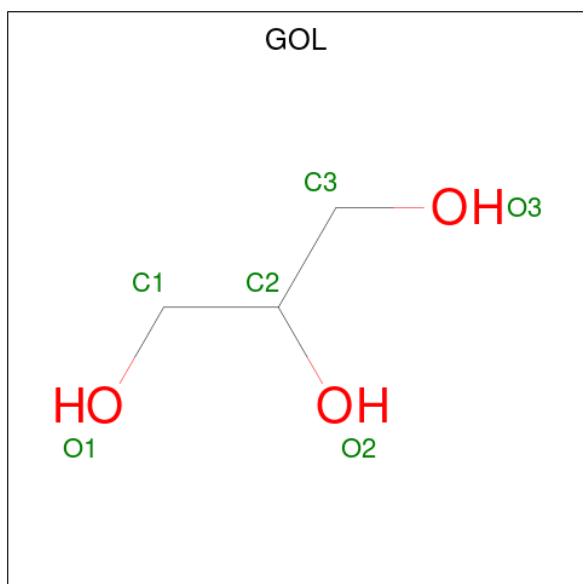
There are 4 unique types of molecules in this entry. The entry contains 5949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	AAA	710	5667	3597	957	1098	15	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

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

3 Residue-property plots

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	262.56Å 262.56Å 72.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.28 – 2.25 131.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (131.28-2.25) 99.3 (131.28-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.252 , 0.292 0.253 , 0.293	Depositor DCC
R_{free} test set	2978 reflections (4.98%)	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)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

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.

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	0.58	1/5808 (0.0%)	1.11	0/7880

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	372	HIS	CE1-NE2	5.64	1.38	1.32

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	60	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	60	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 5.

All (60) 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: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:224:MET:HE1	1:AAA:285:MET:HE2	1.80	0.63
1:AAA:608:TYR:CE2	1:AAA:609:MET:HE2	2.34	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:93:GLU:H	1:AAA:93:GLU:CD	2.16	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:608:TYR:CD2	1:AAA:609:MET:HE2	2.47	0.50
1:AAA:533:ILE:HD11	1:AAA:550:LEU:HD12	1.93	0.50
1:AAA:447:SER:O	1:AAA:466:MET:HE2	2.11	0.50
1:AAA:65:LYS:HG3	1:AAA:609:MET:HE1	1.95	0.49
1:AAA:248:LEU:HD21	1:AAA:285:MET:HE3	1.94	0.49
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:653:ILE:C	1:AAA:653:ILE:HD12	2.40	0.47
1:AAA:564:LYS:HA	1:AAA:567:MET:HE3	1.97	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:299:MET:HE1	1:AAA:321:TRP:HB3	1.99	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:684:MET:HE2	1:AAA:693:PHE:HE2	1.82	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:675:LYS:O	1:AAA:676:THR:C	2.62	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
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:615:TYR:C	1:AAA:618:PRO:HD2	2.46	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:353:GLN:CD	1:AAA:377:PHE:HB3	2.45	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%)	12 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	313	GLY
1	AAA	275	ALA

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Mol	Chain	Res	Type
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 ⓘ

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	AAA	602/614 (98%)	576 (96%)	26 (4%)	26	31

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

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Mol	Chain	Res	Type
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 oligosaccharides 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	AAA	802	-	5,5,5	0.19	0	5,5,5	0.64	0
2	GOL	AAA	801	-	5,5,5	0.06	0	5,5,5	0.26	0
2	GOL	AAA	803	-	5,5,5	0.12	0	5,5,5	0.33	0
2	GOL	AAA	804	-	5,5,5	0.12	0	5,5,5	0.46	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	802	-	-	1/4/4/4	-
2	GOL	AAA	801	-	-	4/4/4/4	-
2	GOL	AAA	803	-	-	2/4/4/4	-
2	GOL	AAA	804	-	-	1/4/4/4	-

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 ⓘ

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, 95th 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%)	1.41	213 (30%) 1 1	20, 51, 107, 145	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	26	VAL	9.5
1	AAA	28	PHE	8.8
1	AAA	27	LEU	8.0
1	AAA	307	VAL	6.8
1	AAA	282	TRP	6.8
1	AAA	277	THR	6.4
1	AAA	303	GLY	6.1
1	AAA	735	LYS	6.0
1	AAA	281	TYR	5.9
1	AAA	276	ALA	5.4
1	AAA	288	HIS	5.1
1	AAA	271	ALA	5.1
1	AAA	269	TRP	5.1
1	AAA	272	ALA	5.0
1	AAA	256	LYS	5.0
1	AAA	247	TRP	4.8
1	AAA	311	ILE	4.8
1	AAA	29	GLN	4.8
1	AAA	253	ALA	4.7
1	AAA	722	ALA	4.7
1	AAA	484	SER	4.6
1	AAA	278	SER	4.6
1	AAA	720	ALA	4.6
1	AAA	734	THR	4.6
1	AAA	310	ILE	4.5
1	AAA	246	SER	4.4
1	AAA	238	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	237	PRO	4.4
1	AAA	30	GLY	4.4
1	AAA	694	LYS	4.3
1	AAA	275	ALA	4.2
1	AAA	289	TYR	4.2
1	AAA	244	LEU	4.2
1	AAA	257	ILE	4.2
1	AAA	236	GLY	4.0
1	AAA	500	GLY	4.0
1	AAA	273	LYS	4.0
1	AAA	693	PHE	4.0
1	AAA	314	ASP	4.0
1	AAA	501	SER	4.0
1	AAA	320	LYS	4.0
1	AAA	304	PHE	3.9
1	AAA	727	TYR	3.9
1	AAA	719	THR	3.9
1	AAA	717	LYS	3.9
1	AAA	675	LYS	3.8
1	AAA	721	ASN	3.8
1	AAA	280	GLN	3.8
1	AAA	305	ALA	3.8
1	AAA	692	VAL	3.8
1	AAA	301	GLN	3.7
1	AAA	504	ALA	3.7
1	AAA	315	ASN	3.7
1	AAA	667	ALA	3.7
1	AAA	645	PRO	3.7
1	AAA	701	SER	3.7
1	AAA	711	VAL	3.7
1	AAA	296	LEU	3.6
1	AAA	298	PHE	3.6
1	AAA	264	LEU	3.6
1	AAA	266	VAL	3.6
1	AAA	316	ALA	3.6
1	AAA	242	ASN	3.5
1	AAA	274	ASP	3.5
1	AAA	642	ASN	3.5
1	AAA	115	ALA	3.5
1	AAA	602	TYR	3.5
1	AAA	287	ILE	3.5
1	AAA	731	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	234	PHE	3.5
1	AAA	312	ASN	3.5
1	AAA	285	MET	3.5
1	AAA	254	ALA	3.4
1	AAA	332	TYR	3.4
1	AAA	639	TYR	3.4
1	AAA	482	THR	3.4
1	AAA	567	MET	3.4
1	AAA	676	THR	3.4
1	AAA	235	PHE	3.4
1	AAA	31	PRO	3.4
1	AAA	290	ALA	3.4
1	AAA	718	GLY	3.4
1	AAA	652	LEU	3.3
1	AAA	284	PRO	3.3
1	AAA	705	VAL	3.3
1	AAA	270	TYR	3.3
1	AAA	245	PRO	3.2
1	AAA	308	ASP	3.2
1	AAA	486	LYS	3.2
1	AAA	326	ILE	3.2
1	AAA	306	THR	3.2
1	AAA	232	TYR	3.2
1	AAA	111	ASN	3.2
1	AAA	223	VAL	3.2
1	AAA	295	TYR	3.1
1	AAA	309	ASP	3.1
1	AAA	114	ARG	3.1
1	AAA	240	PRO	3.1
1	AAA	614	LEU	3.1
1	AAA	716	VAL	3.0
1	AAA	714	ILE	3.0
1	AAA	72	TRP	3.0
1	AAA	265	PRO	3.0
1	AAA	248	LEU	3.0
1	AAA	263	TYR	3.0
1	AAA	313	GLY	3.0
1	AAA	638	GLY	3.0
1	AAA	286	LEU	2.9
1	AAA	640	THR	2.9
1	AAA	224	MET	2.9
1	AAA	648	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	321	TRP	2.9
1	AAA	318	ILE	2.9
1	AAA	708	ASN	2.9
1	AAA	712	LEU	2.9
1	AAA	243	TYR	2.8
1	AAA	325	TYR	2.8
1	AAA	699	PHE	2.8
1	AAA	323	ASN	2.8
1	AAA	723	LEU	2.8
1	AAA	319	ALA	2.8
1	AAA	239	ASP	2.8
1	AAA	615	TYR	2.8
1	AAA	251	ALA	2.8
1	AAA	436	ASN	2.8
1	AAA	260	VAL	2.8
1	AAA	704	LEU	2.7
1	AAA	636	ILE	2.7
1	AAA	483	PRO	2.7
1	AAA	291	LYS	2.7
1	AAA	259	THR	2.7
1	AAA	249	GLU	2.7
1	AAA	680	ILE	2.7
1	AAA	650	GLN	2.6
1	AAA	227	ASP	2.6
1	AAA	698	GLY	2.6
1	AAA	283	LYS	2.6
1	AAA	324	ALA	2.6
1	AAA	250	GLU	2.6
1	AAA	193	GLY	2.6
1	AAA	673	ASN	2.6
1	AAA	322	THR	2.6
1	AAA	570	VAL	2.6
1	AAA	647	THR	2.6
1	AAA	682	VAL	2.6
1	AAA	568	LYS	2.6
1	AAA	317	GLU	2.6
1	AAA	706	ALA	2.6
1	AAA	279	ASP	2.5
1	AAA	677	ASP	2.5
1	AAA	481	GLY	2.5
1	AAA	300	SER	2.5
1	AAA	328	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	610	SER	2.5
1	AAA	438	LEU	2.5
1	AAA	225	THR	2.5
1	AAA	686	THR	2.5
1	AAA	668	VAL	2.5
1	AAA	702	GLU	2.5
1	AAA	713	THR	2.5
1	AAA	299	MET	2.5
1	AAA	630	ALA	2.5
1	AAA	297	SER	2.4
1	AAA	302	HIS	2.4
1	AAA	643	THR	2.4
1	AAA	679	THR	2.4
1	AAA	255	ASN	2.4
1	AAA	611	LYS	2.4
1	AAA	505	HIS	2.4
1	AAA	89	ALA	2.3
1	AAA	228	ASN	2.3
1	AAA	733	PRO	2.3
1	AAA	88	MET	2.3
1	AAA	241	ARG	2.3
1	AAA	485	GLN	2.3
1	AAA	724	VAL	2.3
1	AAA	122	ASP	2.3
1	AAA	651	ASP	2.3
1	AAA	36	GLY	2.3
1	AAA	294	GLY	2.3
1	AAA	663	TYR	2.3
1	AAA	197	ALA	2.3
1	AAA	233	ARG	2.3
1	AAA	603	GLN	2.3
1	AAA	68	LEU	2.2
1	AAA	726	GLY	2.2
1	AAA	644	SER	2.2
1	AAA	581	SER	2.2
1	AAA	608	TYR	2.2
1	AAA	732	VAL	2.2
1	AAA	261	ASP	2.2
1	AAA	541	THR	2.2
1	AAA	606	ALA	2.2
1	AAA	689	ALA	2.2
1	AAA	715	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	728	LEU	2.2
1	AAA	258	ASN	2.2
1	AAA	293	LYS	2.2
1	AAA	502	GLY	2.2
1	AAA	629	TYR	2.1
1	AAA	700	HIS	2.1
1	AAA	685	GLY	2.1
1	AAA	262	THR	2.1
1	AAA	327	GLN	2.1
1	AAA	110	PRO	2.1
1	AAA	231	PRO	2.1
1	AAA	674	PRO	2.1
1	AAA	119	GLY	2.1
1	AAA	267	ASP	2.0
1	AAA	292	ASP	2.0
1	AAA	268	GLY	2.0
1	AAA	557	LYS	2.0
1	AAA	628	ALA	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	GOL	AAA	804	6/6	0.82	0.18	52,56,57,57	0
2	GOL	AAA	802	6/6	0.84	0.16	36,39,42,48	0
2	GOL	AAA	803	6/6	0.90	0.14	31,36,38,40	0
2	GOL	AAA	801	6/6	0.95	0.09	38,40,41,42	0
3	CA	AAA	805	1/1	0.98	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.