



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:51 am GMT

PDB ID : 3FAX
Title : The crystal structure of GBS pullulanase SAP in complex with maltotetraose
Authors : Gourlay, L.J.
Deposited on : 2008-11-18
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

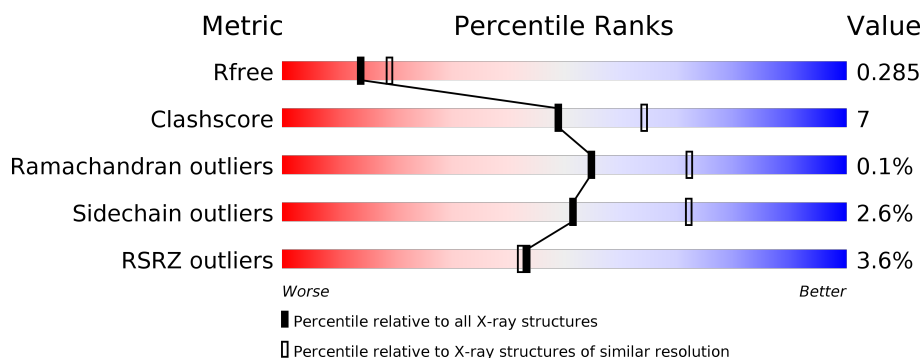
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 ≥ 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	877	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6190 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 Reticulocyte binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	1	0
			6088	3854	1034	1187	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	GLU	-	EXPRESSION TAG	UNP Q3DB05
A	1217	HIS	-	EXPRESSION TAG	UNP Q3DB05
A	1218	HIS	-	EXPRESSION TAG	UNP Q3DB05
A	1219	HIS	-	EXPRESSION TAG	UNP Q3DB05
A	1220	HIS	-	EXPRESSION TAG	UNP Q3DB05
A	1221	HIS	-	EXPRESSION TAG	UNP Q3DB05
A	1222	HIS	-	EXPRESSION TAG	UNP Q3DB05

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

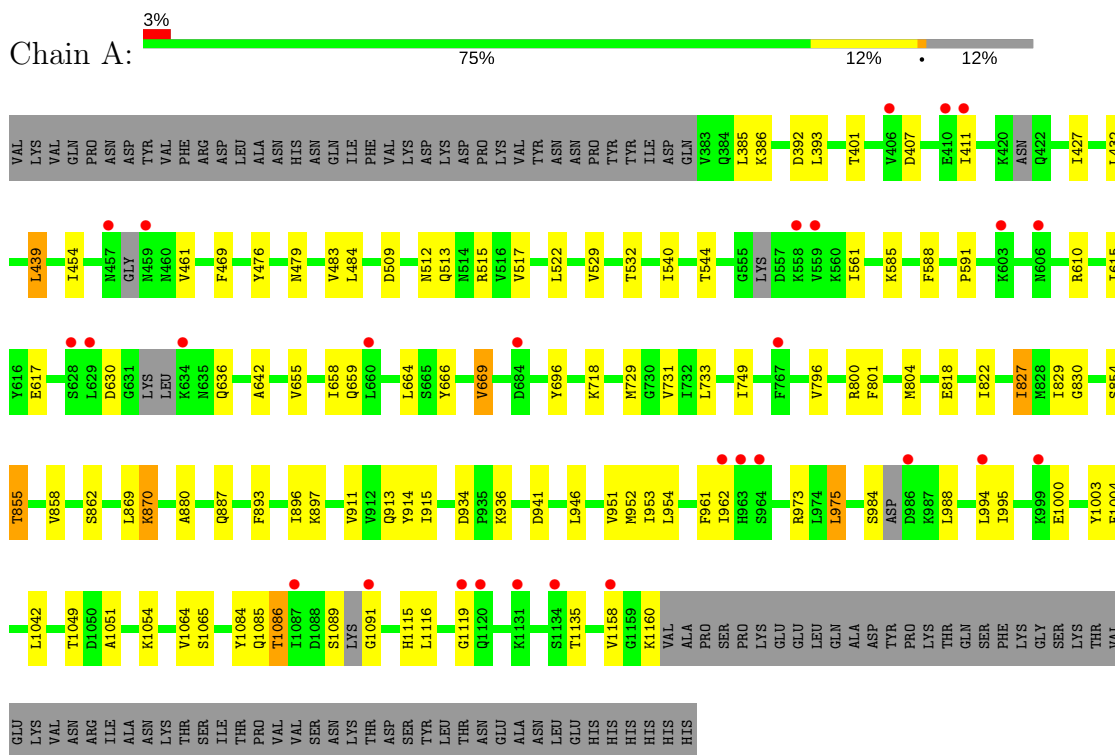
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total 63	O 63	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Reticulocyte binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.21Å 102.86Å 171.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 39.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.40) 99.5 (39.61-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.221 , 0.283 0.231 , 0.285	Depositor DCC
R_{free} test set	1726 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6190	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, GLC, CL

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	0/6211	0.54	0/8401

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	6088	0	5998	82	0
2	A	34	0	30	0	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	63	0	0	1	0
All	All	6190	0	6028	82	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 7.

All (82) 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:1160:LYS:O	1:A:1160:LYS:HD3	1.43	1.19
1:A:1064:VAL:HG22	1:A:1086:THR:HG23	1.48	0.95
1:A:411:ILE:HG21	1:A:439:LEU:HD21	1.46	0.94
1:A:801:PHE:HB2	1:A:804:MET:HE3	1.50	0.93
1:A:1160:LYS:O	1:A:1160:LYS:CD	2.24	0.86
1:A:1085:GLN:HE21	1:A:1116:LEU:HD21	1.47	0.80
1:A:818:GLU:O	1:A:822:ILE:HD12	1.82	0.79
1:A:484:LEU:HD23	1:A:544:THR:HG22	1.64	0.79
1:A:896:ILE:HD13	1:A:1084:TYR:CE2	2.22	0.74
1:A:522:LEU:HD22	1:A:532:THR:HB	1.70	0.72
1:A:1119:GLY:HA3	1:A:1158:VAL:HG22	1.72	0.71
1:A:513:GLN:HE21	1:A:585:LYS:HZ3	1.40	0.70
1:A:655:VAL:HG23	1:A:729:MET:HE3	1.74	0.70
1:A:995:ILE:HD13	1:A:1004:PHE:CD2	2.27	0.69
1:A:386:LYS:HE3	1:A:401:THR:HG22	1.76	0.68
1:A:1085:GLN:HE22	1:A:1115:HIS:CE1	2.11	0.67
1:A:484:LEU:CD2	1:A:544:THR:HG22	2.24	0.67
1:A:869:LEU:HD13	1:A:952:MET:HE3	1.77	0.67
1:A:513:GLN:HE21	1:A:585:LYS:NZ	1.92	0.66
1:A:804:MET:CE	1:A:858:VAL:HG11	2.27	0.64
1:A:411:ILE:CG2	1:A:439:LEU:HD21	2.23	0.63
1:A:1051:ALA:O	1:A:1086:THR:HG21	2.01	0.60
1:A:484:LEU:HD11	1:A:588:PHE:HB3	1.83	0.60
1:A:994:LEU:HD12	1:A:1003:TYR:CZ	2.36	0.60
1:A:951:VAL:HG22	1:A:1042:LEU:HD21	1.85	0.59
1:A:973:ARG:HG3	1:A:975:LEU:HD13	1.85	0.59
1:A:385:LEU:HD21	1:A:461:VAL:HG12	1.84	0.58
1:A:666:TYR:HE1	1:A:669:VAL:HG11	1.69	0.58
1:A:870:LYS:HD2	1:A:915:ILE:HB	1.86	0.57
1:A:561:ILE:HD13	1:A:749:ILE:HG12	1.88	0.56
1:A:659:GLN:HE22	1:A:829:ILE:HD11	1.72	0.56
1:A:1054:LYS:HZ3	1:A:1086:THR:HG22	1.71	0.55
1:A:636:GLN:O	1:A:642:ALA:HB2	2.07	0.55
1:A:1054:LYS:NZ	1:A:1086:THR:HG22	2.22	0.54
1:A:1089:SER:O	1:A:1091:GLY:N	2.41	0.54
1:A:954:LEU:HD21	1:A:962:ILE:HD11	1.90	0.54
1:A:610:ARG:HB3	1:A:827:ILE:HD12	1.90	0.53
1:A:658:ILE:HG13	1:A:729:MET:HE2	1.91	0.53
1:A:479:ASN:HD21	1:A:483:VAL:HG21	1.74	0.53
1:A:664:LEU:HD12	5:A:9:HOH:O	2.08	0.52
1:A:1160:LYS:O	1:A:1160:LYS:CG	2.57	0.52
1:A:1051:ALA:HB1	1:A:1086:THR:HB	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:THR:HG23	1:A:1135:THR:O	2.11	0.51
1:A:476:TYR:CD2	1:A:529:VAL:HG21	2.47	0.50
1:A:664:LEU:HD13	1:A:696:TYR:HA	1.92	0.50
1:A:655:VAL:HG23	1:A:729:MET:CE	2.41	0.49
1:A:610:ARG:HB3	1:A:827:ILE:CD1	2.43	0.49
1:A:615:ILE:HD13	1:A:829:ILE:HD13	1.96	0.48
1:A:854:SER:O	1:A:855:THR:HG23	2.14	0.48
1:A:880:ALA:HA	1:A:887:GLN:HE21	1.78	0.48
1:A:804:MET:HE1	1:A:858:VAL:HG11	1.96	0.47
1:A:862:SER:HB2	1:A:911:VAL:HG13	1.96	0.47
1:A:893:PHE:CZ	1:A:897:LYS:HD2	2.50	0.47
1:A:915:ILE:HG23	1:A:953:ILE:HD11	1.96	0.47
1:A:666:TYR:CE1	1:A:669:VAL:HG11	2.50	0.46
1:A:1085:GLN:HE21	1:A:1116:LEU:CD2	2.24	0.46
1:A:392:ASP:HA	1:A:469:PHE:CD1	2.51	0.46
1:A:733:LEU:CD1	1:A:796:VAL:HG21	2.46	0.45
1:A:869:LEU:HD22	1:A:952:MET:HE1	1.98	0.45
1:A:984:SER:O	1:A:988:LEU:HD13	2.17	0.44
1:A:515:ARG:HH21	1:A:517:VAL:HG22	1.83	0.44
1:A:934:ASP:OD2	1:A:936:LYS:HB2	2.18	0.44
1:A:1119:GLY:CA	1:A:1158:VAL:HG22	2.44	0.43
1:A:870:LYS:HA	1:A:880:ALA:HB3	1.99	0.43
1:A:801:PHE:CB	1:A:804:MET:HE3	2.35	0.43
1:A:869:LEU:HD22	1:A:952:MET:CE	2.49	0.42
1:A:509:ASP:HB3	1:A:512:ASN:O	2.20	0.42
1:A:615:ILE:CD1	1:A:829:ILE:HD13	2.50	0.42
1:A:733:LEU:HD12	1:A:796:VAL:HG21	2.02	0.42
1:A:995:ILE:N	1:A:995:ILE:HD12	2.34	0.41
1:A:946:LEU:HD23	1:A:946:LEU:C	2.41	0.41
1:A:385:LEU:HD21	1:A:454:ILE:HB	2.02	0.41
1:A:995:ILE:HD13	1:A:1004:PHE:CE2	2.54	0.41
1:A:427:ILE:CG2	1:A:427:ILE:O	2.68	0.41
1:A:591:PRO:O	1:A:718:LYS:NZ	2.54	0.41
1:A:432:LEU:N	1:A:432:LEU:HD12	2.36	0.41
1:A:804:MET:CE	1:A:830:GLY:HA3	2.51	0.41
1:A:517:VAL:CG1	1:A:540:ILE:HD11	2.51	0.41
1:A:951:VAL:HG22	1:A:1042:LEU:CD2	2.49	0.41
1:A:827:ILE:HA	1:A:827:ILE:HD13	1.63	0.40
1:A:617:GLU:HB2	1:A:961:PHE:CZ	2.56	0.40
1:A:427:ILE:HG23	1:A:427:ILE:O	2.22	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	758/877 (86%)	715 (94%)	42 (6%)	1 (0%)	55 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	630	ASP

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	664/762 (87%)	647 (97%)	17 (3%)	51 72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LEU
1	A	407	ASP
1	A	439	LEU
1	A	669	VAL
1	A	731	VAL
1	A	800	ARG
1	A	827	ILE
1	A	855	THR
1	A	870	LYS
1	A	913	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	914	TYR
1	A	941	ASP
1	A	975	LEU
1	A	1000	GLU
1	A	1049	THR
1	A	1065	SER
1	A	1086	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	A	479	ASN
1	A	513	GLN
1	A	514	ASN
1	A	526	ASN
1	A	659	GLN
1	A	694	GLN
1	A	752	ASN
1	A	875	ASN
1	A	887	GLN
1	A	890	GLN
1	A	895	ASN
1	A	913	GLN
1	A	1016	ASN
1	A	1085	GLN
1	A	1115	HIS

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](#)

3 carbohydrates 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	BGC	A	1	2	12,12,12	0.50	0	17,17,17	1.06	1 (5%)
2	GLC	A	2	2	11,11,12	0.61	0	13,15,17	0.84	0
2	GLC	A	3	2	11,11,12	0.60	0	13,15,17	1.08	1 (7%)

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	BGC	A	1	2	-	0/2/22/22	0/1/1/1
2	GLC	A	2	2	-	0/2/19/22	0/1/1/1
2	GLC	A	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	BGC	C1-C2-C3	-2.07	106.91	110.65
2	A	3	GLC	C1-C2-C3	2.83	113.24	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	A	771/877 (87%)	0.03	28 (3%)	43 42	20, 35, 49, 72	22 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ILE	4.5
1	A	999	LYS	3.9
1	A	406	VAL	3.6
1	A	411	ILE	3.2
1	A	603	LYS	3.0
1	A	1119	GLY	3.0
1	A	629	LEU	3.0
1	A	684	ASP	2.9
1	A	634	LYS	2.9
1	A	606	ASN	2.8
1	A	457	ASN	2.8
1	A	994	LEU	2.8
1	A	986	ASP	2.7
1	A	962	ILE	2.7
1	A	559	VAL	2.7
1	A	964	SER	2.7
1	A	660	LEU	2.6
1	A	558	LYS	2.6
1	A	1131	LYS	2.5
1	A	1158	VAL	2.5
1	A	1091	GLY	2.5
1	A	459	ASN	2.4
1	A	410	GLU	2.3
1	A	628	SER	2.3
1	A	963	HIS	2.3
1	A	1120	GLN	2.1
1	A	767	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1134	SER	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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	A	3	11/12	0.88	0.14	0.11	58,59,62,63	0
2	GLC	A	2	11/12	0.96	0.12	-0.38	48,54,54,56	0
2	BGC	A	1	12/12	0.81	0.23	-	59,66,67,68	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	4	1/1	0.96	0.03	-2.44	45,45,45,45	0
3	CA	A	1224	1/1	0.98	0.04	-2.66	43,43,43,43	0
3	CA	A	1223	1/1	0.97	0.06	-2.72	30,30,30,30	0
4	CL	A	1226	1/1	0.98	0.06	-3.33	29,29,29,29	0
3	CA	A	1225	1/1	0.95	0.09	-	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.