



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:50 pm GMT

PDB ID : 4J5T
Title : Crystal structure of Processing alpha-Glucosidase I
Authors : Barker, M.K.; Rose, D.R.
Deposited on : 2013-02-09
Resolution : 2.04 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

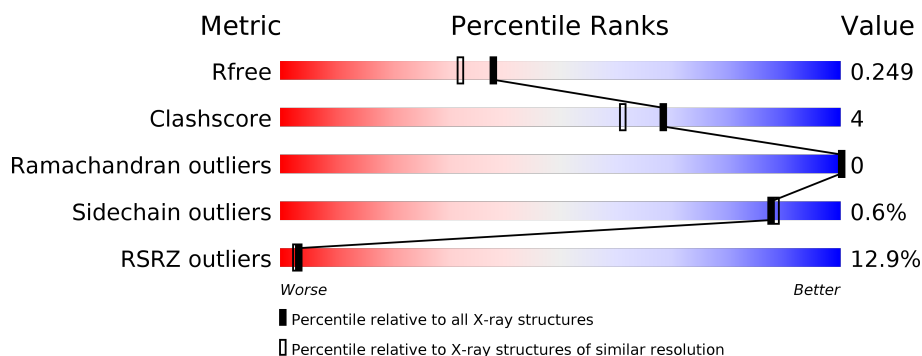
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.04 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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	811	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6838 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 Mannosyl-oligosaccharide glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	788	Total	C	N	O	S	0	7	0
			6497	4163	1074	1233	27			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP P53008
A	-1	GLU	-	EXPRESSION TAG	UNP P53008
A	0	PHE	-	EXPRESSION TAG	UNP P53008
A	1	MET	-	EXPRESSION TAG	UNP P53008
A	801	ARG	-	EXPRESSION TAG	UNP P53008
A	802	SER	-	EXPRESSION TAG	UNP P53008
A	803	HIS	-	EXPRESSION TAG	UNP P53008
A	804	HIS	-	EXPRESSION TAG	UNP P53008
A	805	HIS	-	EXPRESSION TAG	UNP P53008
A	806	HIS	-	EXPRESSION TAG	UNP P53008
A	807	HIS	-	EXPRESSION TAG	UNP P53008
A	808	HIS	-	EXPRESSION TAG	UNP P53008

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

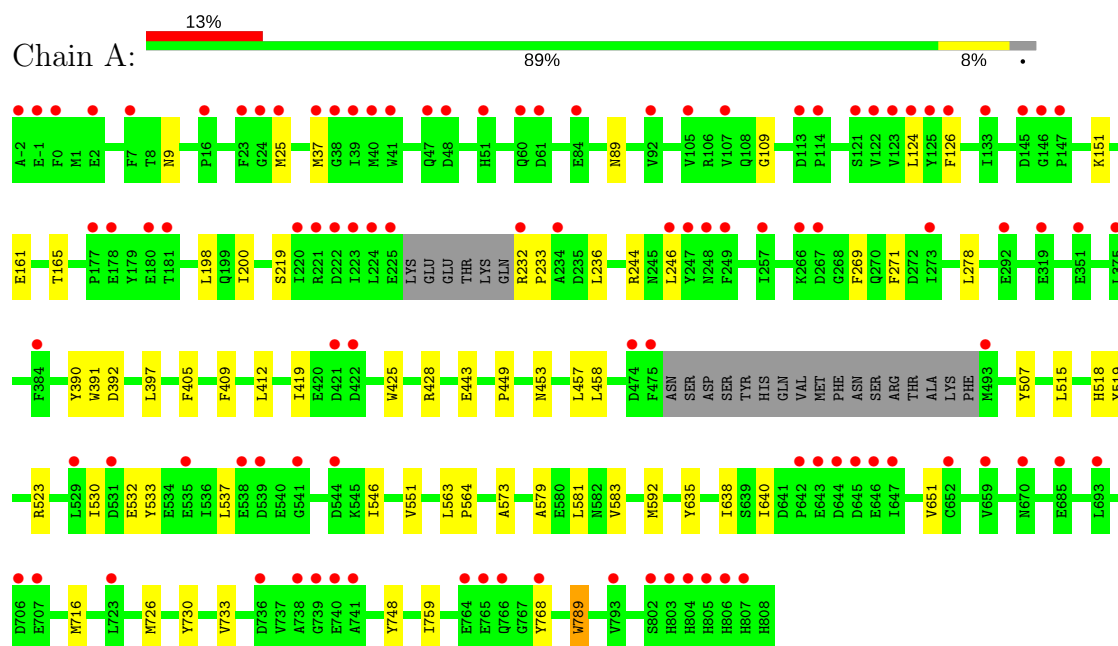
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	285	Total	O	0	0
			285	285		

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: Mannosyl-oligosaccharide glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 101.80Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.04 27.86 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.00-2.04) 97.8 (27.86-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.226 , 0.235 0.225 , 0.249	Depositor DCC
R_{free} test set	3176 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6838	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: NAG

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	0.45	0/6675	0.47	0/9047

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	A	6497	0	6192	49	0
2	A	56	0	52	4	0
3	A	285	0	0	1	0
All	All	6838	0	6244	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 distance (Å)	Clash overlap (Å)
1:A:9:ASN:HD21	2:A:1001:NAG:C1	1.46	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:HD21	2:A:1003:NAG:C1	1.68	1.06
1:A:581:LEU:HD12	1:A:638:ILE:HD11	1.57	0.87
1:A:9:ASN:ND2	2:A:1001:NAG:O5	2.13	0.80
1:A:392:ASP:OD1	1:A:789:TRP:CZ3	2.45	0.69
1:A:532:GLU:OE1	1:A:579:ALA:HB2	1.96	0.66
1:A:428:ARG:HB3	1:A:453:ASN:OD1	1.99	0.63
1:A:151:LYS:HD3	1:A:165:THR:HG22	1.82	0.62
1:A:89:ASN:HD21	2:A:1003:NAG:C2	2.13	0.61
1:A:537:LEU:HD13	1:A:546:ILE:HD13	1.83	0.60
1:A:458:LEU:HD21	1:A:515:LEU:HD22	1.85	0.57
1:A:530:ILE:O	1:A:532:GLU:O	2.24	0.56
1:A:25:MET:HG3	1:A:37:MET:HE1	1.88	0.55
1:A:37:MET:HG3	1:A:126:PHE:CE1	2.43	0.53
1:A:530:ILE:HB	1:A:551:VAL:HG21	1.91	0.52
1:A:397:LEU:HD13	1:A:412[A]:LEU:HG	1.92	0.51
1:A:532:GLU:OE1	1:A:579:ALA:CB	2.59	0.51
1:A:425:TRP:CE2	1:A:449:PRO:HA	2.46	0.51
1:A:161:GLU:OE1	1:A:278:LEU:CD2	2.60	0.50
1:A:573:ALA:HB2	1:A:651:VAL:HG21	1.94	0.50
1:A:532:GLU:O	1:A:533:TYR:HB2	2.12	0.48
1:A:519:TYR:CZ	1:A:523:ARG:HD2	2.50	0.47
1:A:405:PHE:CE2	1:A:409:PHE:HE1	2.33	0.47
1:A:405:PHE:CE2	1:A:409:PHE:CE1	3.03	0.46
1:A:198:LEU:CD1	1:A:200:ILE:HG12	2.45	0.46
1:A:390:TYR:OH	1:A:518:HIS:NE2	2.38	0.45
1:A:458:LEU:HD12	1:A:592:MET:HE3	1.98	0.45
1:A:198:LEU:HD11	1:A:200:ILE:HD11	1.97	0.45
1:A:563:LEU:N	1:A:564:PRO:CD	2.80	0.44
1:A:161:GLU:OE1	1:A:278:LEU:HD22	2.17	0.44
1:A:532:GLU:HB3	1:A:640:ILE:HD11	2.00	0.44
1:A:412[A]:LEU:HD23	1:A:457:LEU:HD22	2.01	0.43
1:A:458:LEU:HD12	1:A:592:MET:CE	2.48	0.43
1:A:458:LEU:HD12	1:A:592:MET:HG2	1.99	0.43
1:A:233:PRO:HD2	1:A:236:LEU:HD12	2.01	0.43
1:A:37:MET:HG3	1:A:126:PHE:CD1	2.53	0.43
1:A:232:ARG:N	1:A:233:PRO:CD	2.82	0.43
1:A:419:ILE:HD11	1:A:518:HIS:HB2	2.00	0.42
1:A:716:MET:HE2	1:A:759:ILE:CD1	2.49	0.42
1:A:726[B]:MET:HE1	1:A:748:TYR:N	2.35	0.41
1:A:583:VAL:HG21	1:A:635:TYR:HB3	2.02	0.41
1:A:730:TYR:O	1:A:733:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HA	1:A:246:LEU:HD22	2.02	0.41
1:A:25:MET:HE2	1:A:25:MET:HB3	1.72	0.41
1:A:453:ASN:ND2	3:A:3272:HOH:O	2.49	0.41
1:A:109:GLY:HA3	1:A:269:PHE:CZ	2.56	0.41
1:A:244:ARG:CZ	1:A:246:LEU:HD13	2.51	0.41
1:A:409:PHE:HD2	1:A:507:TYR:CZ	2.40	0.40
1:A:124:LEU:HD11	1:A:271:PHE:CE1	2.56	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	789/811 (97%)	770 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	708/726 (98%)	703 (99%)	5 (1%)	85	86

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

Mol	Chain	Res	Type
1	A	391	TRP
1	A	443[A]	GLU
1	A	443[B]	GLU
1	A	768	TYR
1	A	789	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	ASN
1	A	89	ASN
1	A	807	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](#)

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	NAG	A	1001	1,2	14,14,15	0.63	0	17,19,21	1.73	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1002	2	14,14,15	0.59	0	17,19,21	1.03	1 (5%)
2	NAG	A	1003	1,2	14,14,15	0.62	0	17,19,21	1.24	2 (11%)
2	NAG	A	1004	2	14,14,15	0.55	0	17,19,21	1.32	2 (11%)

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	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	NAG	O5-C1-C2	-3.96	106.06	111.52
2	A	1001	NAG	O5-C1-C2	-3.88	106.17	111.52
2	A	1002	NAG	O5-C1-C2	-2.68	107.82	111.52
2	A	1003	NAG	O5-C1-C2	-2.54	108.01	111.52
2	A	1004	NAG	C3-C4-C5	2.36	114.47	110.24
2	A	1003	NAG	C3-C4-C5	3.03	115.66	110.24
2	A	1001	NAG	C3-C4-C5	4.61	118.49	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	2	0
2	A	1003	NAG	2	0

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	788/811 (97%)	0.71	102 (12%) 3 3	26, 42, 73, 97	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	806	HIS	8.1
1	A	803	HIS	7.1
1	A	0	PHE	5.6
1	A	644	ASP	5.2
1	A	740	GLU	5.1
1	A	802	SER	5.1
1	A	247	TYR	5.1
1	A	178	GLU	5.1
1	A	224	LEU	4.8
1	A	145	ASP	4.6
1	A	-1	GLU	4.5
1	A	804	HIS	4.5
1	A	232	ARG	4.4
1	A	-2	ALA	4.2
1	A	122	VAL	4.1
1	A	807	HIS	3.9
1	A	114	PRO	3.9
1	A	181	THR	3.7
1	A	221	ARG	3.7
1	A	39	ILE	3.7
1	A	535	GLU	3.7
1	A	113	ASP	3.6
1	A	474	ASP	3.6
1	A	123	VAL	3.6
1	A	422	ASP	3.4
1	A	177	PRO	3.4
1	A	147	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	3.4
1	A	645	ASP	3.4
1	A	23	PHE	3.4
1	A	738	ALA	3.3
1	A	234	ALA	3.3
1	A	180	GLU	3.2
1	A	225	GLU	3.2
1	A	267	ASP	3.2
1	A	92	VAL	3.1
1	A	107	VAL	3.1
1	A	421	ASP	3.1
1	A	544	ASP	3.1
1	A	384	PHE	3.1
1	A	124	LEU	3.0
1	A	257	ILE	3.0
1	A	539	ASP	3.0
1	A	273	ILE	3.0
1	A	266	LYS	3.0
1	A	739	GLY	2.9
1	A	805	HIS	2.9
1	A	47	GLN	2.9
1	A	220	ILE	2.8
1	A	643	GLU	2.8
1	A	647	ILE	2.8
1	A	541	GLY	2.7
1	A	475	PHE	2.7
1	A	126	PHE	2.7
1	A	292	GLU	2.7
1	A	765	GLU	2.7
1	A	736	ASP	2.6
1	A	16	PRO	2.6
1	A	249	PHE	2.6
1	A	25	MET	2.6
1	A	222	ASP	2.6
1	A	7	PHE	2.6
1	A	61	ASP	2.6
1	A	2	GLU	2.6
1	A	646	GLU	2.6
1	A	538	GLU	2.5
1	A	125	TYR	2.5
1	A	319	GLU	2.5
1	A	146	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLY	2.5
1	A	706	ASP	2.5
1	A	84	GLU	2.5
1	A	223	ILE	2.5
1	A	41	TRP	2.4
1	A	105	VAL	2.4
1	A	51	HIS	2.4
1	A	659	VAL	2.3
1	A	37	MET	2.3
1	A	60	GLN	2.3
1	A	529	LEU	2.3
1	A	652	CYS	2.3
1	A	38	GLY	2.3
1	A	48	ASP	2.3
1	A	693	LEU	2.3
1	A	493	MET	2.3
1	A	685	GLU	2.3
1	A	741	ALA	2.2
1	A	375	LEU	2.2
1	A	531	ASP	2.2
1	A	133	ILE	2.2
1	A	248	ASN	2.2
1	A	351	GLU	2.1
1	A	642	PRO	2.1
1	A	121	SER	2.1
1	A	707	GLU	2.1
1	A	768	TYR	2.1
1	A	766	GLN	2.1
1	A	40	MET	2.1
1	A	670	ASN	2.0
1	A	723	LEU	2.0
1	A	793	VAL	2.0
1	A	764	GLU	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 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. 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(\AA^2)	Q<0.9
2	NAG	A	1004	14/15	0.63	0.34	72,84,92,93	0
2	NAG	A	1002	14/15	0.73	0.28	64,72,78,80	0
2	NAG	A	1001	14/15	0.86	0.17	43,48,57,58	0
2	NAG	A	1003	14/15	0.89	0.23	51,64,71,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.