



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2016 – 04:36 PM EDT

PDB ID : 4ZMH
Title : Crystal structure of a five-domain GH115 alpha-Glucuronidase from the Marine Bacterium *Saccharophagus degradans* 2-40T
Authors : Nocek, B.; Cui, H.; Wang, W.; Savchenko, A.
Deposited on : 2015-05-04
Resolution : 1.93 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

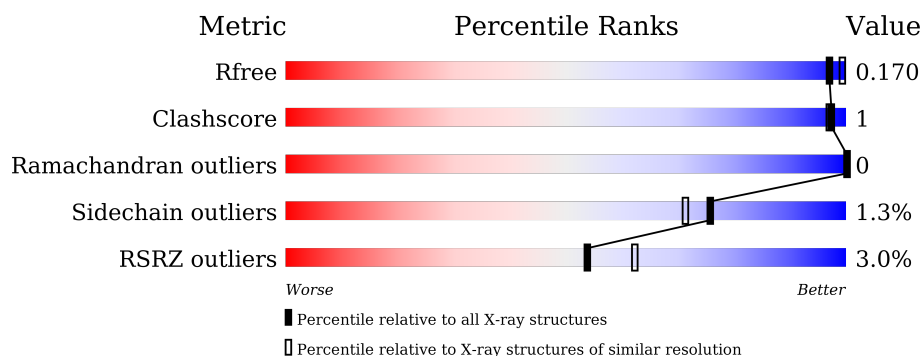
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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	939	<div> <div style="width: 97%;"></div> <div>97%</div> </div>
1	B	939	<div> <div style="width: 96%;"></div> <div>96%</div> </div>

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
2	PO4	A	1002	-	-	-	X
4	GOL	A	1005	-	-	-	X
5	ACT	A	1007	-	-	-	X

2 Entry composition [i](#)

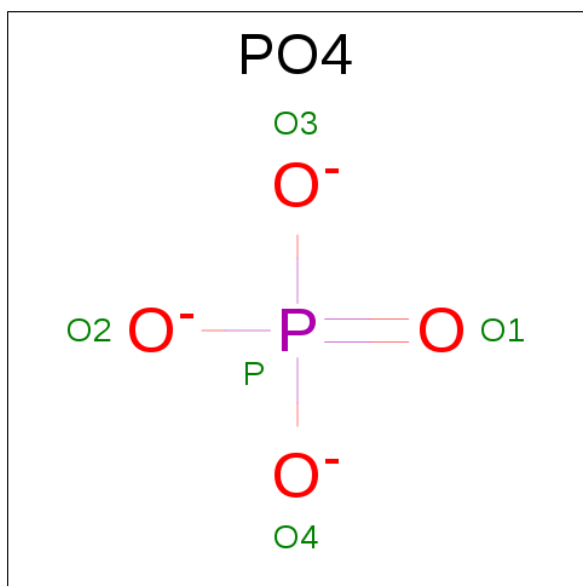
There are 6 unique types of molecules in this entry. The entry contains 31867 atoms, of which 14657 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	935	Total	C	H	N	O	S	Se		0	14	0
			14825	4785	7324	1300	1390	1	25				
1	B	931	Total	C	H	N	O	S	Se		0	17	0
			14804	4775	7314	1301	1389	1	24				

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

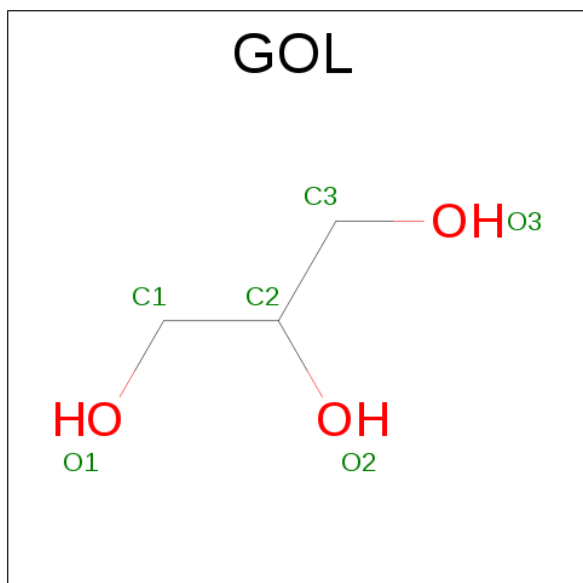


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			7	2	3	2		

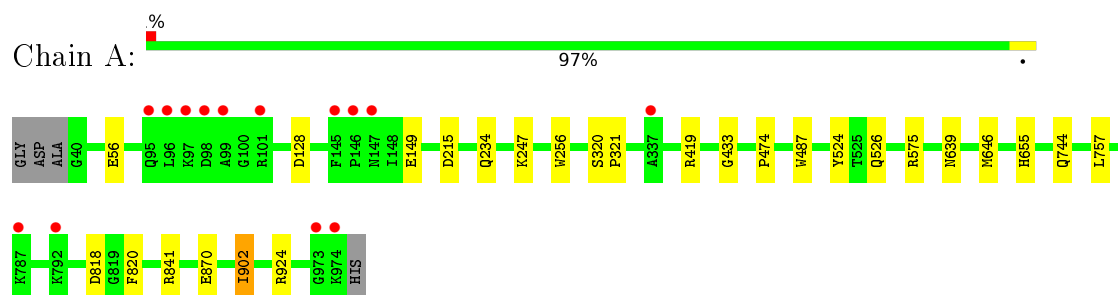
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1172	Total	O	0	0
			1172	1172		
6	B	1009	Total	O	0	0
			1009	1009		

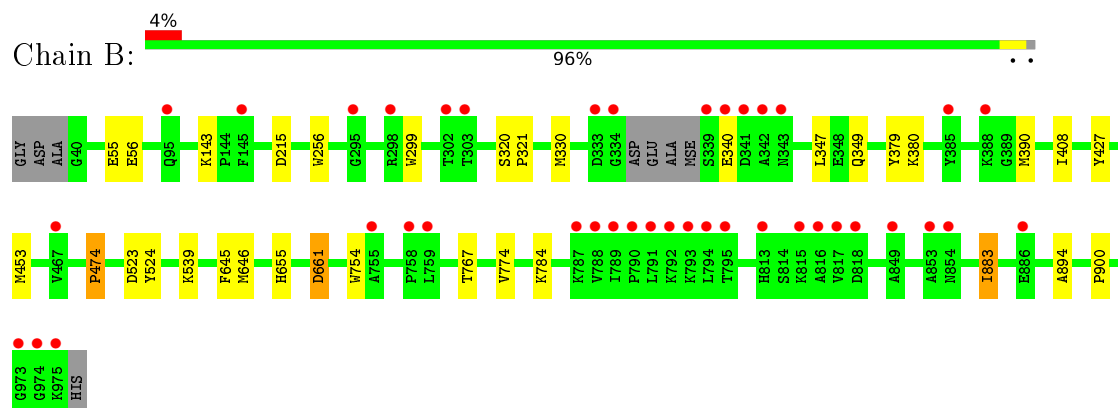
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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: Uncharacterized protein



• Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.44Å 124.29Å 180.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.15 – 1.93 38.15 – 1.93	Depositor EDS
% Data completeness (in resolution range)	93.7 (38.15-1.93) 93.7 (38.15-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1834)	Depositor
R, R_{free}	0.138 , 0.170 0.138 , 0.170	Depositor DCC
R_{free} test set	9189 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31867	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, PO4, ACT, NA

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	0.49	0/7730	0.60	2/10484 (0.0%)
1	B	0.46	0/7732	0.57	0/10485
All	All	0.48	0/15462	0.58	2/20969 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	419	ARG	NE-CZ-NH2	-5.39	117.60	120.30

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	7501	7324	7269	12	0
1	B	7490	7314	7236	21	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	16	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	3	3	0	0
6	A	1172	0	0	5	0
6	B	1009	0	0	6	0
All	All	17210	14657	14524	34	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 1.

All (34) 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:870:GLU:OE1	6:A:1101:HOH:O	2.04	0.75
1:B:661:ASP:OD1	6:B:1101:HOH:O	2.08	0.71
1:B:523:ASP:OD2	6:B:1102:HOH:O	2.10	0.68
1:B:453:MSE:SE	6:B:1856:HOH:O	2.62	0.68
1:A:575:ARG:NH1	6:A:1106:HOH:O	2.29	0.64
1:B:347:LEU:CB	1:B:390:MSE:HE1	2.29	0.63
1:A:526:GLN:OE1	6:A:1102:HOH:O	2.16	0.62
1:B:427:TYR:CE1	1:B:453:MSE:HE3	2.36	0.60
1:B:539:LYS:NZ	6:B:1108:HOH:O	2.37	0.57
1:B:767[A]:THR:HG23	6:B:1206:HOH:O	2.07	0.55
1:B:347:LEU:HB2	1:B:390:MSE:HE1	1.90	0.54
1:B:347:LEU:HB3	1:B:390:MSE:HE1	1.91	0.52
1:B:408:ILE:HD11	1:B:453:MSE:HE1	1.94	0.50
1:B:408:ILE:HD11	1:B:453:MSE:CE	2.42	0.50
1:A:215:ASP:HA	1:A:256:TRP:CZ2	2.49	0.47
1:B:453:MSE:N	1:B:453:MSE:HE2	2.30	0.46
1:B:427:TYR:CE1	1:B:453:MSE:CE	2.99	0.46
1:A:902:ILE:HD11	6:A:2239:HOH:O	2.18	0.44
1:A:247:LYS:HE2	1:A:487:TRP:CD2	2.54	0.43
1:B:883:ILE:H	1:B:883:ILE:HD13	1.84	0.43
1:B:299:TRP:NE1	1:B:330:MSE:HE3	2.33	0.43
1:A:820:PHE:CE1	1:A:841:ARG:HG2	2.55	0.42
1:B:754:TRP:O	1:B:784:LYS:NZ	2.51	0.41
1:A:639[B]:ASN:ND2	6:A:1145:HOH:O	2.53	0.41
1:A:320:SER:N	1:A:321:PRO:CD	2.84	0.41
1:A:474:PRO:HG3	1:A:646:MSE:HE1	2.02	0.41
1:B:379:TYR:CD2	1:B:380:LYS:HG3	2.56	0.41
1:B:215:ASP:HA	1:B:256:TRP:CZ2	2.56	0.41
1:B:894:ALA:HB2	1:B:900:PRO:HA	2.03	0.40
1:A:433:GLY:HA2	4:A:1006:GOL:H11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:SER:N	1:B:321:PRO:CD	2.84	0.40
1:B:474:PRO:HG3	1:B:646:MSE:HE1	2.03	0.40
1:A:128:ASP:OD1	1:A:128:ASP:N	2.53	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	947/939 (101%)	918 (97%)	29 (3%)	0	100	100
1	B	944/939 (100%)	909 (96%)	35 (4%)	0	100	100
All	All	1891/1878 (101%)	1827 (97%)	64 (3%)	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	795/762 (104%)	786 (99%)	9 (1%)	80	76
1	B	797/762 (105%)	785 (98%)	12 (2%)	72	66
All	All	1592/1524 (104%)	1571 (99%)	21 (1%)	76	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	149	GLU
1	A	234	GLN
1	A	524	TYR
1	A	655	HIS
1	A	744	GLN
1	A	757	LEU
1	A	818	ASP
1	A	902	ILE
1	B	55	GLU
1	B	56	GLU
1	B	143	LYS
1	B	340	GLU
1	B	349	GLN
1	B	474	PRO
1	B	524	TYR
1	B	645	PHE
1	B	655	HIS
1	B	661	ASP
1	B	774	VAL
1	B	883	ILE

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	PO4	A	1001	-	4,4,4	0.92	0	6,6,6	0.24	0
2	PO4	A	1002	-	4,4,4	0.59	0	6,6,6	0.24	0
2	PO4	A	1003	-	4,4,4	0.69	0	6,6,6	0.24	0
4	GOL	A	1005	-	5,5,5	0.31	0	5,5,5	0.28	0
4	GOL	A	1006	-	5,5,5	0.40	0	5,5,5	0.28	0
5	ACT	A	1007	-	0,3,3	0.00	-	0,3,3	0.00	-
2	PO4	B	1001	-	4,4,4	0.42	0	6,6,6	0.22	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	PO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
5	ACT	A	1007	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1001	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1006	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 ⓘ

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	910/939 (96%)	-0.27	14 (1%) 76 82	10, 22, 48, 84	0
1	B	907/939 (96%)	-0.09	40 (4%) 38 47	11, 26, 53, 82	0
All	All	1817/1878 (96%)	-0.18	54 (2%) 54 62	10, 24, 50, 84	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	GLY	5.8
1	B	974	GLY	5.8
1	B	342	ALA	5.2
1	B	333	ASP	4.5
1	A	146	PRO	4.3
1	A	101	ARG	4.2
1	B	794	LEU	4.0
1	B	339	SER	4.0
1	A	337	ALA	4.0
1	B	792	LYS	3.9
1	B	787	LYS	3.9
1	B	816	ALA	3.4
1	A	973	GLY	3.4
1	B	975	LYS	3.3
1	B	793	LYS	3.3
1	A	98	ASP	3.3
1	A	96	LEU	3.2
1	B	973	GLY	3.1
1	B	791	LEU	3.1
1	A	95	GLN	3.1
1	B	341	ASP	3.1
1	B	817	VAL	3.0
1	B	789	ILE	3.0
1	B	340	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	792	LYS	2.8
1	A	145	PHE	2.8
1	B	813	HIS	2.8
1	B	759	LEU	2.7
1	B	788	VAL	2.7
1	B	95	GLN	2.7
1	A	787	LYS	2.7
1	A	147	ASN	2.7
1	B	385	TYR	2.7
1	B	758	PRO	2.7
1	B	849	ALA	2.6
1	B	388	LYS	2.6
1	B	818	ASP	2.6
1	B	853	ALA	2.5
1	A	99	ALA	2.5
1	B	295	GLY	2.5
1	B	298	ARG	2.5
1	B	755	ALA	2.4
1	B	795	THR	2.4
1	B	886	GLU	2.4
1	A	974	LYS	2.4
1	B	302	THR	2.3
1	B	854	ASN	2.3
1	A	97	LYS	2.3
1	B	343	ASN	2.2
1	B	815	LYS	2.2
1	B	467	VAL	2.2
1	B	790	PRO	2.1
1	B	303	THR	2.1
1	B	145	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 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
4	GOL	A	1005	6/6	0.79	0.24	10.36	67,80,84,88	0
2	PO4	A	1002	5/5	0.95	0.13	3.18	58,59,63,68	0
5	ACT	A	1007	4/4	0.95	0.15	2.41	28,29,45,45	0
3	NA	B	1002	1/1	0.94	0.14	1.26	30,30,30,30	0
4	GOL	A	1006	6/6	0.86	0.12	0.91	56,69,81,84	0
3	NA	A	1004	1/1	0.97	0.13	0.81	28,28,28,28	0
2	PO4	B	1001	5/5	0.99	0.12	-0.77	17,21,24,32	0
2	PO4	A	1001	5/5	0.99	0.09	-0.84	13,20,22,27	5
2	PO4	A	1003	5/5	0.94	0.11	-0.91	75,78,80,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.