



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:28 AM UTC

PDB ID : 8FN5 / pdb_00008fn5
Title : Structure of the truncated catalytic domain of Streptococcus mutans GtfD
Authors : Schormann, N.; Deivanayagam, C.
Deposited on : 2022-12-27
Resolution : 1.92 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
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

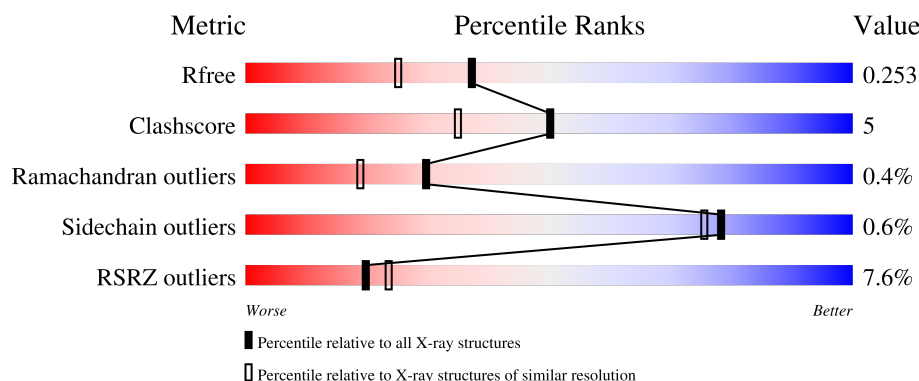
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 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	A	632	5% 87% 6% • 6%
1	B	632	9% 87% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9769 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 Glucosyltransferase-S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	1	0
			4690	2940	794	943	13			
1	B	595	Total	C	N	O	S	0	1	0
			4688	2939	793	943	13			

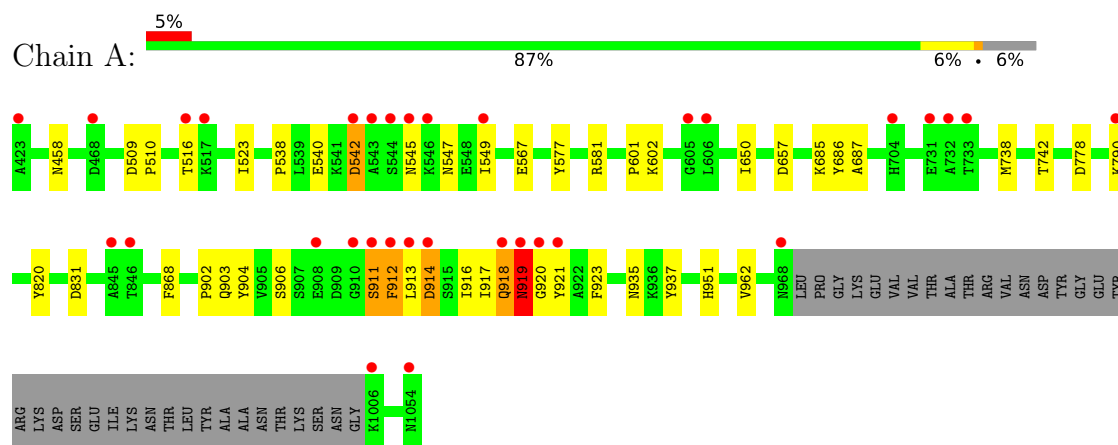
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	210	Total	O	0	0
			210	210		
2	B	181	Total	O	0	0
			181	181		

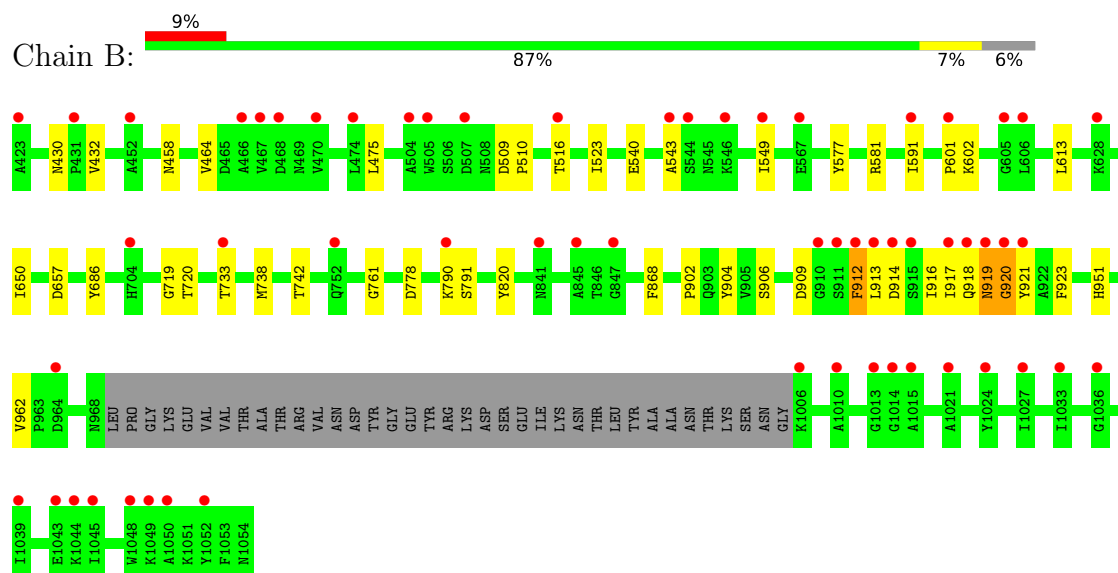
3 Residue-property plots [i](#)

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: Glucosyltransferase-S



• Molecule 1: Glucosyltransferase-S



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.62Å 126.77Å 173.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.83 – 1.92 86.83 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.1 (86.83-1.92) 95.1 (86.83-1.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.251 0.231 , 0.253	Depositor DCC
R_{free} test set	4821 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.2	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	0.94	EDS
Total number of atoms	9769	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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](#)

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	1.01	0/4778	1.34	1/6471 (0.0%)
1	B	1.01	0/4776	1.34	3/6468 (0.0%)
All	All	1.01	0/9554	1.34	4/12939 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	THR	N-CA-C	-5.66	103.06	110.53
1	B	516	THR	N-CA-C	-5.61	103.51	110.41
1	B	719	GLY	CA-C-O	-5.29	118.00	122.29
1	B	761	GLY	CA-C-O	-5.26	118.80	122.22

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	4690	0	4551	57	0
1	B	4688	0	4550	45	0
2	A	210	0	0	5	0
2	B	181	0	0	0	0
All	All	9769	0	9101	98	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 (98) 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:913:LEU:HD13	1:A:921:TYR:HB3	1.40	1.03
1:A:540:GLU:HA	1:A:549:ILE:HD12	1.54	0.90
1:B:902:PRO:HG2	1:B:919:ASN:O	1.74	0.87
1:A:906:SER:HB3	1:A:917:ILE:HG23	1.54	0.86
1:A:913:LEU:HD22	1:A:918:GLN:NE2	1.91	0.85
1:B:906:SER:HB3	1:B:917:ILE:HG23	1.58	0.85
1:B:720:THR:O	1:B:733:THR:HG22	1.78	0.83
1:A:686:TYR:HB2	1:A:738:MET:HE2	1.64	0.79
1:B:913:LEU:HD22	1:B:918:GLN:OE1	1.83	0.78
1:A:906:SER:CB	1:A:917:ILE:HG23	2.15	0.76
1:B:540:GLU:HA	1:B:549:ILE:HD12	1.71	0.73
1:A:904:TYR:O	1:A:919:ASN:ND2	2.22	0.73
1:B:430:ASN:OD1	1:B:432:VAL:HG12	1.90	0.70
1:B:919:ASN:C	1:B:920:GLY:O	2.33	0.70
1:B:913:LEU:HD13	1:B:921:TYR:HB3	1.74	0.69
1:A:902:PRO:O	1:A:919:ASN:HB3	1.93	0.69
1:B:902:PRO:HB2	1:B:920:GLY:HA3	1.75	0.67
1:B:906:SER:CB	1:B:917:ILE:HG23	2.25	0.67
1:B:868:PHE:CZ	1:B:912:PHE:HZ	2.14	0.66
1:A:545:ASN:HD22	1:A:547:ASN:H	1.42	0.65
1:A:918:GLN:O	1:A:919:ASN:HB2	1.96	0.64
1:A:913:LEU:HG	2:A:1284:HOH:O	1.97	0.63
1:B:904:TYR:HD2	1:B:920:GLY:HA3	1.62	0.63
1:A:903:GLN:C	1:A:919:ASN:ND2	2.56	0.63
1:B:686:TYR:HB2	1:B:738:MET:HE2	1.82	0.60
1:B:720:THR:O	1:B:733:THR:CG2	2.51	0.59
1:A:919:ASN:C	1:A:920:GLY:O	2.45	0.58
1:A:902:PRO:HB2	1:A:920:GLY:HA3	1.86	0.56
1:B:904:TYR:HD2	1:B:920:GLY:CA	2.19	0.56
1:A:868:PHE:HE1	1:A:912:PHE:CZ	2.24	0.56
1:A:919:ASN:OD1	1:A:935:ASN:HB2	2.05	0.55
1:B:917:ILE:C	1:B:919:ASN:N	2.65	0.55
1:B:962:VAL:O	1:B:962:VAL:HG23	2.07	0.54
1:A:567:GLU:OE2	1:A:567:GLU:N	2.34	0.53
1:A:962:VAL:HG23	1:A:962:VAL:O	2.08	0.53
1:A:790:LYS:O	1:B:778:ASP:OD1	2.27	0.52
1:A:581:ARG:HD3	1:A:657:ASP:OD1	2.09	0.52
1:B:543:ALA:CB	1:B:549:ILE:HD13	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ARG:HD3	1:B:657:ASP:OD1	2.10	0.52
1:A:919:ASN:HB2	1:A:937:TYR:HE2	1.73	0.52
1:A:919:ASN:CG	2:A:1101:HOH:O	2.53	0.52
1:A:790:LYS:O	1:B:778:ASP:CG	2.53	0.51
1:A:917:ILE:O	1:A:917:ILE:HG22	2.09	0.51
1:A:902:PRO:O	1:A:919:ASN:CB	2.59	0.51
1:A:601:PRO:O	1:A:602:LYS:HB2	2.11	0.51
1:B:543:ALA:HB3	1:B:549:ILE:HD13	1.93	0.50
1:A:685:LYS:NZ	1:A:831:ASP:O	2.43	0.50
1:B:601:PRO:O	1:B:602:LYS:HB2	2.12	0.49
1:B:920:GLY:O	1:B:921:TYR:HB2	2.12	0.49
1:A:920:GLY:O	1:A:921:TYR:HB2	2.12	0.49
1:A:921:TYR:HA	2:A:1291:HOH:O	2.11	0.49
1:B:917:ILE:HG22	1:B:917:ILE:O	2.12	0.49
1:B:909:ASP:HB2	1:B:914:ASP:OD2	2.13	0.48
1:A:458:ASN:O	1:A:951:HIS:HE1	1.97	0.48
1:A:778:ASP:OD1	1:B:790:LYS:O	2.32	0.48
1:A:919:ASN:OD1	2:A:1101:HOH:O	2.20	0.47
1:B:920:GLY:HA2	1:B:923:PHE:CD2	2.49	0.47
1:A:904:TYR:HD2	1:A:920:GLY:HA3	1.79	0.47
1:A:911:SER:HB3	1:A:914:ASP:OD2	2.15	0.47
1:A:918:GLN:H	1:A:918:GLN:HG3	1.51	0.47
1:A:919:ASN:OD1	1:A:937:TYR:CE2	2.67	0.47
1:B:458:ASN:O	1:B:951:HIS:HE1	1.98	0.46
1:A:919:ASN:OD1	1:A:937:TYR:CD2	2.69	0.46
1:B:920:GLY:HA2	1:B:923:PHE:HD2	1.80	0.46
1:B:916:ILE:HD12	1:B:918:GLN:H	1.80	0.46
1:B:591:ILE:CD1	1:B:613:LEU:CD2	2.93	0.46
1:B:509:ASP:N	1:B:510:PRO:CD	2.79	0.46
1:A:509:ASP:N	1:A:510:PRO:CD	2.79	0.46
1:A:917:ILE:C	1:A:919:ASN:N	2.74	0.45
1:B:464:VAL:HG11	1:B:475:LEU:CD2	2.46	0.45
1:B:913:LEU:HD22	1:B:918:GLN:CD	2.41	0.45
1:A:904:TYR:N	1:A:919:ASN:HD22	2.14	0.45
1:B:523:ILE:HG12	1:B:577:TYR:CZ	2.50	0.45
1:A:919:ASN:HB3	1:A:920:GLY:H	1.51	0.45
1:A:919:ASN:HA	2:A:1101:HOH:O	2.17	0.45
1:B:917:ILE:C	1:B:919:ASN:H	2.25	0.45
1:A:920:GLY:HA2	1:A:923:PHE:HD2	1.82	0.44
1:A:778:ASP:CG	1:B:790:LYS:O	2.60	0.44
1:A:687:ALA:HB2	1:A:738:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:GLN:O	1:A:919:ASN:CB	2.65	0.43
1:A:918:GLN:NE2	1:A:921:TYR:HD2	2.15	0.43
1:B:742:THR:HA	1:B:820:TYR:O	2.19	0.43
1:A:523:ILE:HG12	1:A:577:TYR:CZ	2.54	0.42
1:A:601:PRO:O	1:A:602:LYS:CB	2.67	0.42
1:A:538:PRO:HB2	1:A:542:ASP:O	2.20	0.42
1:A:742:THR:HA	1:A:820:TYR:O	2.20	0.42
1:B:601:PRO:O	1:B:602:LYS:CB	2.68	0.42
1:B:918:GLN:OE1	1:B:921:TYR:CD2	2.73	0.41
1:A:685:LYS:HD2	1:A:686:TYR:CE2	2.56	0.41
1:A:902:PRO:HG3	1:A:921:TYR:CE2	2.56	0.41
1:A:918:GLN:OE1	1:A:921:TYR:HB2	2.21	0.41
1:B:868:PHE:CE1	1:B:912:PHE:HZ	2.37	0.41
1:B:790:LYS:O	1:B:791:SER:CB	2.68	0.41
1:B:912:PHE:O	1:B:916:ILE:HG13	2.21	0.41
1:A:577:TYR:HA	1:A:650:ILE:O	2.21	0.41
1:A:920:GLY:O	1:A:921:TYR:CB	2.68	0.41
1:A:918:GLN:NE2	1:A:921:TYR:CD2	2.89	0.41
1:B:577:TYR:HA	1:B:650:ILE:O	2.21	0.41

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	592/632 (94%)	565 (95%)	25 (4%)	2 (0%)	36	26
1	B	592/632 (94%)	569 (96%)	20 (3%)	3 (0%)	24	14
All	All	1184/1264 (94%)	1134 (96%)	45 (4%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	911	SER
1	A	919	ASN
1	B	920	GLY
1	B	912	PHE
1	B	919	ASN

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	A	507/537 (94%)	501 (99%)	6 (1%)	63	57
1	B	507/537 (94%)	507 (100%)	0	100	100
All	All	1014/1074 (94%)	1008 (99%)	6 (1%)	78	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	ASP
1	A	912	PHE
1	A	914	ASP
1	A	916	ILE
1	A	918	GLN
1	A	919	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
1	A	513	ASN
1	A	545	ASN
1	A	615	GLN
1	A	626	GLN
1	A	766	ASN
1	A	832	ASN
1	A	941	GLN

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Mol	Chain	Res	Type
1	B	476	GLN
1	B	513	ASN
1	B	615	GLN
1	B	888	GLN

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](#)

There are no ligands in this entry.

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	595/632 (94%)	0.37	32 (5%)	31 35	12, 28, 52, 86	1 (0%)
1	B	595/632 (94%)	0.61	59 (9%)	13 16	18, 32, 59, 77	1 (0%)
All	All	1190/1264 (94%)	0.49	91 (7%)	20 23	12, 30, 58, 86	2 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	919	ASN	8.2
1	B	919	ASN	7.4
1	A	920	GLY	6.3
1	B	920	GLY	5.9
1	A	921	TYR	5.7
1	A	606	LEU	5.2
1	B	606	LEU	5.1
1	B	912	PHE	5.0
1	B	467	VAL	4.9
1	B	910	GLY	4.7
1	A	912	PHE	4.6
1	A	704	HIS	4.3
1	B	921	TYR	4.0
1	A	543	ALA	3.9
1	A	542	ASP	3.7
1	A	911	SER	3.6
1	B	917	ILE	3.6
1	B	911	SER	3.5
1	B	1033	ILE	3.5
1	B	470	VAL	3.4
1	A	732	ALA	3.1
1	A	733	THR	3.1
1	A	544	SER	3.1
1	A	910	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	914	ASP	3.0
1	B	913	LEU	3.0
1	B	918	GLN	3.0
1	A	468	ASP	3.0
1	A	549	ILE	3.0
1	B	1052	TYR	3.0
1	B	546	LYS	2.9
1	B	423	ALA	2.9
1	B	1010	ALA	2.9
1	A	546	LYS	2.9
1	B	549	ILE	2.9
1	B	507	ASP	2.8
1	A	545	ASN	2.8
1	B	1049	LYS	2.8
1	B	567	GLU	2.7
1	B	1048	TRP	2.7
1	B	1044	LYS	2.7
1	B	1036	GLY	2.7
1	B	543	ALA	2.6
1	B	601	PRO	2.6
1	B	452	ALA	2.6
1	B	474	LEU	2.6
1	B	468	ASP	2.6
1	A	423	ALA	2.6
1	B	1015	ALA	2.6
1	B	1050	ALA	2.6
1	A	968	ASN	2.5
1	A	605	GLY	2.5
1	A	1006	LYS	2.5
1	A	845	ALA	2.5
1	B	605	GLY	2.4
1	B	1027	ILE	2.4
1	B	845	ALA	2.4
1	A	918	GLN	2.4
1	A	790	LYS	2.4
1	B	591	ILE	2.4
1	B	505	TRP	2.3
1	A	516	THR	2.3
1	A	1054	ASN	2.3
1	B	790	LYS	2.3
1	B	1006	LYS	2.3
1	B	504	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	908	GLU	2.3
1	A	517	LYS	2.3
1	A	846	THR	2.3
1	B	847	GLY	2.2
1	B	841	ASN	2.2
1	B	1043	GLU	2.2
1	B	431	PRO	2.2
1	B	1039	ILE	2.2
1	A	731	GLU	2.2
1	B	544	SER	2.2
1	A	913	LEU	2.2
1	B	752	GLN	2.1
1	B	1021	ALA	2.1
1	B	1024	TYR	2.1
1	B	914	ASP	2.1
1	B	733	THR	2.1
1	B	1014	GLY	2.1
1	B	628	LYS	2.1
1	B	704	HIS	2.1
1	B	964	ASP	2.1
1	B	1045	ILE	2.1
1	B	1013	GLY	2.1
1	B	915[A]	SER	2.0
1	B	516	THR	2.0
1	B	466	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](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.