



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 06:27 PM EDT

PDB ID : 2Q52 / pdb_00002q52
Title : Ensemble refinement of the crystal structure of a glycolipid transfer-like protein from *Galdieria sulphuraria*
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.38 Å(reported)

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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:

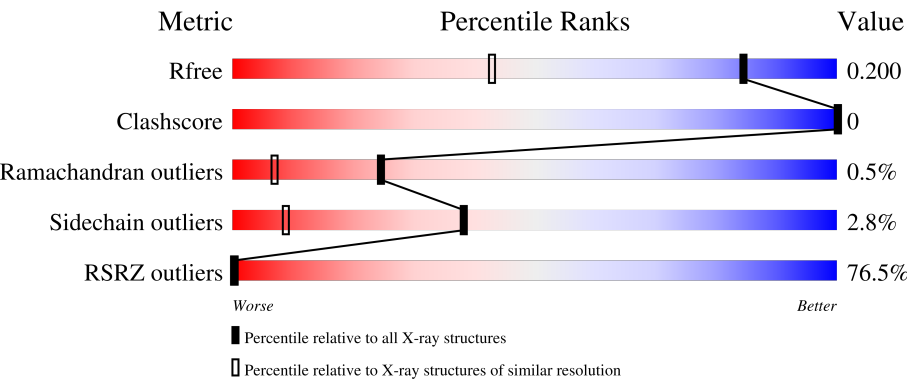
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	1-A	224	73% 89% 8%
1	1-B	224	68% 89% 8%
1	2-A	224	88% 8%
1	2-B	224	90% 8%
1	3-A	224	89% 8%

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Mol	Chain	Length	Quality of chain
1	3-B	224	 90% • 8%
1	4-A	224	 88% • 8%
1	4-B	224	 90% • 8%
1	5-A	224	 89% • 8%
1	5-B	224	 90% • 8%
1	6-A	224	 89% • 8%
1	6-B	224	 90% • 8%
1	7-A	224	 89% • 8%
1	7-B	224	 89% • 8%
1	8-A	224	 88% • 8%
1	8-B	224	 90% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29856 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 Glycolipid transfer-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	2-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	3-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	4-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	5-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	6-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	7-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	8-A	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	1-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	2-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	3-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	4-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	5-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	6-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	7-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			
1	8-B	206	Total	C	N	O	S	0	0	0
			1674	1085	287	296	6			

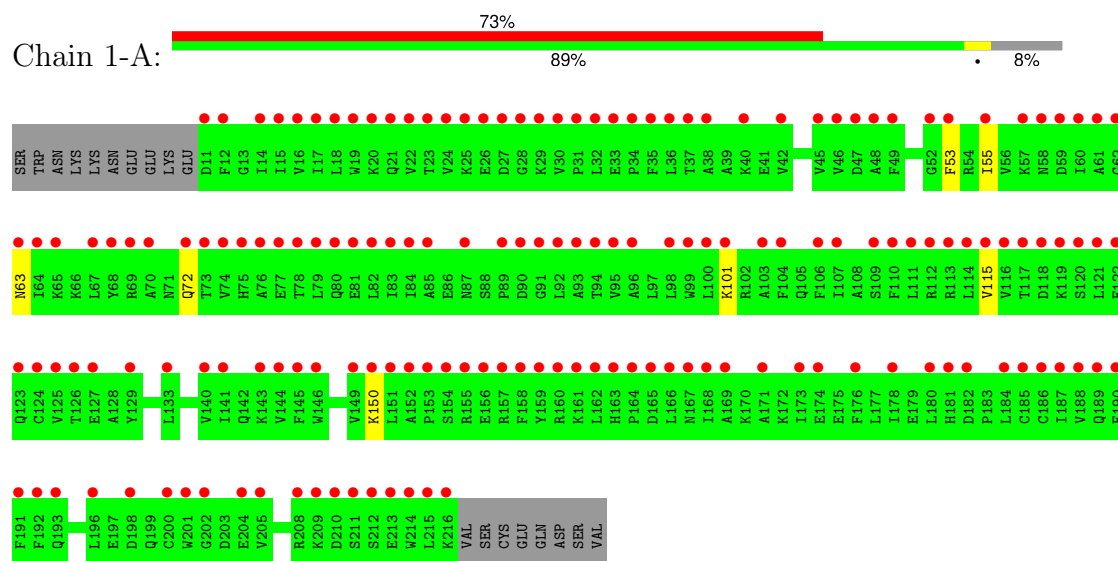
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	201	Total 201	O 201	0	0
2	2-A	206	Total 206	O 206	0	0
2	3-A	212	Total 212	O 212	0	0
2	4-A	202	Total 202	O 202	0	0
2	5-A	201	Total 201	O 201	0	0
2	6-A	202	Total 202	O 202	0	0
2	7-A	204	Total 204	O 204	0	0
2	8-A	206	Total 206	O 206	0	0
2	1-B	183	Total 183	O 183	0	0
2	2-B	178	Total 178	O 178	0	0
2	3-B	172	Total 172	O 172	0	0
2	4-B	182	Total 182	O 182	0	0
2	5-B	183	Total 183	O 183	0	0
2	6-B	182	Total 182	O 182	0	0
2	7-B	180	Total 180	O 180	0	0
2	8-B	178	Total 178	O 178	0	0

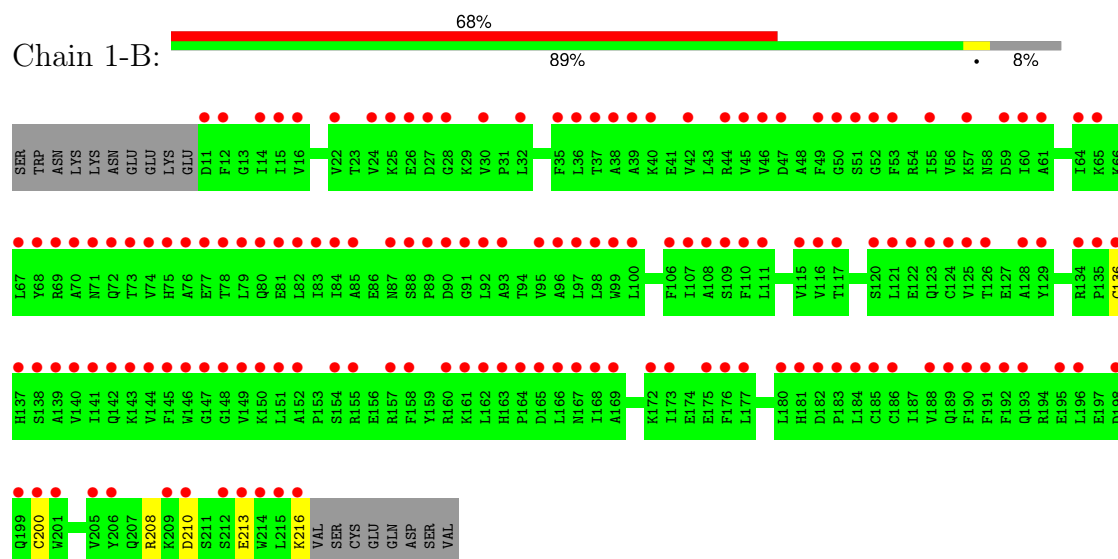
3 Residue-property plots [i](#)

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: Glycolipid transfer-like protein



- Molecule 1: Glycolipid transfer-like protein



- Molecule 1: Glycolipid transfer-like protein

Chain 2-A:  88% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 2-B:  90% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 3-A:  89% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 3-B:  90% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 4-A:  88% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 4-B:  90% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 5-A:  89% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 5-B:  90% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 6-A:  89% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 6-B:  90% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 7-A:  89% 8%



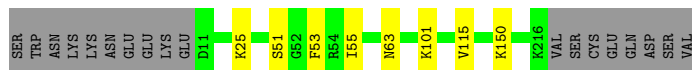
- Molecule 1: Glycolipid transfer-like protein

Chain 7-B:  89% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 8-A:  88% 8%



- Molecule 1: Glycolipid transfer-like protein

Chain 8-B:  90% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.44Å 48.20Å 89.41Å 90.00° 115.06° 90.00°	Depositor
Resolution (Å)	41.99 – 1.38 41.99 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.99-1.38) 99.0 (41.99-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.38Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.166 , 0.202 0.165 , 0.200	Depositor DCC
R_{free} test set	4669 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 42.0	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	0.90	EDS
Total number of atoms	29856	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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

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	1-A	0.27	0/1711	0.31	0/2315
1	1-B	0.29	0/1711	0.32	0/2315
1	2-A	0.27	0/1711	0.31	0/2315
1	2-B	0.29	0/1711	0.32	0/2315
1	3-A	0.27	0/1711	0.31	0/2315
1	3-B	0.29	0/1711	0.32	0/2315
1	4-A	0.27	0/1711	0.31	0/2315
1	4-B	0.29	0/1711	0.32	0/2315
1	5-A	0.27	0/1711	0.31	0/2315
1	5-B	0.29	0/1711	0.32	0/2315
1	6-A	0.27	0/1711	0.31	0/2315
1	6-B	0.29	0/1711	0.32	0/2315
1	7-A	0.27	0/1711	0.31	0/2315
1	7-B	0.29	0/1711	0.32	0/2315
1	8-A	0.27	0/1711	0.31	0/2315
1	8-B	0.29	0/1711	0.32	0/2315
All	All	0.28	0/27376	0.31	0/37040

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	129	TYR	Sidechain

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	1-A	1674	0	1701	0	0
1	1-B	1674	0	1701	0	0
1	2-A	1674	0	1701	0	0
1	2-B	1674	0	1701	0	0
1	3-A	1674	0	1701	0	0
1	3-B	1674	0	1701	0	0
1	4-A	1674	0	1701	0	0
1	4-B	1674	0	1701	0	0
1	5-A	1674	0	1701	0	0
1	5-B	1674	0	1701	0	0
1	6-A	1674	0	1701	0	0
1	6-B	1674	0	1701	0	0
1	7-A	1674	0	1701	0	0
1	7-B	1674	0	1701	0	0
1	8-A	1674	0	1701	0	0
1	8-B	1674	0	1701	0	0
2	1-A	201	0	0	0	0
2	1-B	183	0	0	0	0
2	2-A	206	0	0	0	0
2	2-B	178	0	0	0	0
2	3-A	212	0	0	0	0
2	3-B	172	0	0	0	0
2	4-A	202	0	0	0	0
2	4-B	182	0	0	0	0
2	5-A	201	0	0	0	0
2	5-B	183	0	0	0	0
2	6-A	202	0	0	0	0
2	6-B	182	0	0	0	0
2	7-A	204	0	0	0	0
2	7-B	180	0	0	0	0
2	8-A	206	0	0	0	0
2	8-B	178	0	0	0	0
All	All	29856	0	27216	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1-A	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	24	7
1	1-B	204/224 (91%)	194 (95%)	8 (4%)	2 (1%)	12	2
1	2-A	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	24	7
1	2-B	204/224 (91%)	194 (95%)	9 (4%)	1 (0%)	24	7
1	3-A	204/224 (91%)	198 (97%)	6 (3%)	0	100	100
1	3-B	204/224 (91%)	192 (94%)	11 (5%)	1 (0%)	24	7
1	4-A	204/224 (91%)	189 (93%)	11 (5%)	4 (2%)	6	0
1	4-B	204/224 (91%)	199 (98%)	5 (2%)	0	100	100
1	5-A	204/224 (91%)	198 (97%)	6 (3%)	0	100	100
1	5-B	204/224 (91%)	197 (97%)	7 (3%)	0	100	100
1	6-A	204/224 (91%)	200 (98%)	4 (2%)	0	100	100
1	6-B	204/224 (91%)	195 (96%)	9 (4%)	0	100	100
1	7-A	204/224 (91%)	193 (95%)	11 (5%)	0	100	100
1	7-B	204/224 (91%)	195 (96%)	6 (3%)	3 (2%)	8	1
1	8-A	204/224 (91%)	189 (93%)	13 (6%)	2 (1%)	12	2
1	8-B	204/224 (91%)	193 (95%)	10 (5%)	1 (0%)	24	7
All	All	3264/3584 (91%)	3110 (95%)	138 (4%)	16 (0%)	24	7

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	8-A	25	LYS
1	1-B	200	CYS
1	8-A	51	SER
1	8-B	53	PHE
1	1-A	72	GLN

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	1-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	1-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	2-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	2-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	3-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	3-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	4-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	4-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	5-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	5-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	6-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	6-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	7-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	7-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
1	8-A	181/199 (91%)	175 (97%)	6 (3%)	33 6
1	8-B	181/199 (91%)	177 (98%)	4 (2%)	45 14
All	All	2896/3184 (91%)	2816 (97%)	80 (3%)	38 9

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6-B	210	ASP

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Mol	Chain	Res	Type
1	8-A	55	ILE
1	6-B	216	LYS
1	7-A	150	LYS
1	8-A	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-B	167	ASN
1	7-B	167	ASN
1	5-B	123	GLN
1	7-B	75	HIS
1	8-A	199	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1-A	206/224 (91%)	3.21	163 (79%) 0 0	1, 2, 3, 4	206 (100%)
1	1-B	206/224 (91%)	3.03	152 (73%) 0 0	1, 2, 3, 5	206 (100%)
1	2-A	0/224	-	-	-	-
1	2-B	0/224	-	-	-	-
1	3-A	0/224	-	-	-	-
1	3-B	0/224	-	-	-	-
1	4-A	0/224	-	-	-	-
1	4-B	0/224	-	-	-	-
1	5-A	0/224	-	-	-	-
1	5-B	0/224	-	-	-	-
1	6-A	0/224	-	-	-	-
1	6-B	0/224	-	-	-	-
1	7-A	0/224	-	-	-	-
1	7-B	0/224	-	-	-	-
1	8-A	0/224	-	-	-	-
1	8-B	0/224	-	-	-	-
All	All	412/3584 (11%)	3.12	315 (76%) 0 0	1, 2, 3, 5	412 (100%)

The worst 5 of 315 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	73	THR	12.1
1	1-B	166	LEU	10.3
1	1-A	74	VAL	10.0
1	1-B	200	CYS	8.5
1	1-B	185	CYS	8.4

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 [i](#)

There are no such residues in this entry.