



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:33 PM UTC

PDB ID : 2H0Q / pdb_00002h0q
Title : Crystal Structure of the PGM domain of the Suppressor of T-Cell receptor (Sts-1)
Authors : Nassar, N.; Ford, B.; Carpino, N.
Deposited on : 2006-05-15
Resolution : 1.82 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

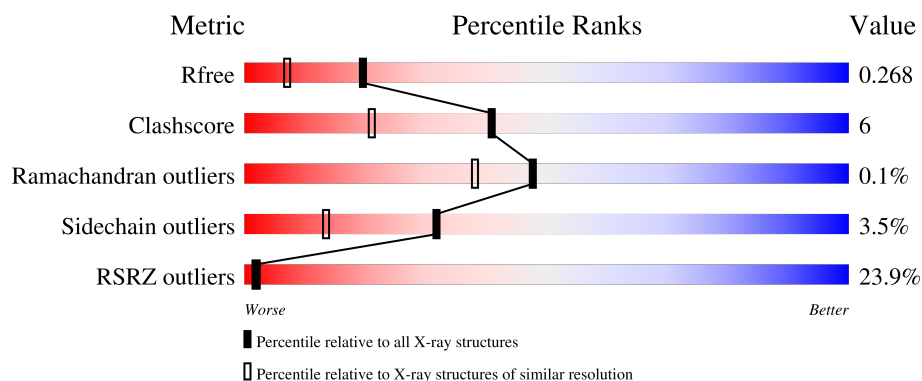
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	261	13% 87% 12% .
1	B	261	23% 79% 18% ..
1	C	261	35% 85% 13% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6472 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 Suppressor of T-cell receptor signaling 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	6	0
			2066	1311	361	375	19			
1	B	256	Total	C	N	O	S	0	9	0
			2032	1287	356	372	17			
1	C	261	Total	C	N	O	S	0	2	0
			2071	1314	363	377	17			

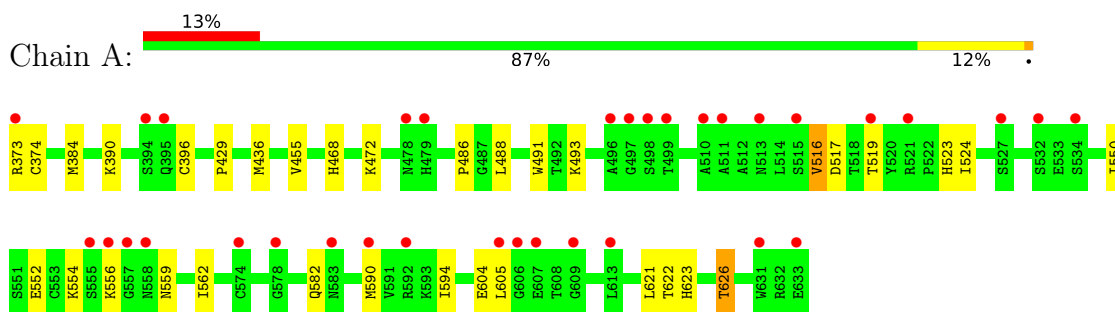
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	109	Total	O	0	0
			109	109		
2	C	62	Total	O	0	0
			62	62		

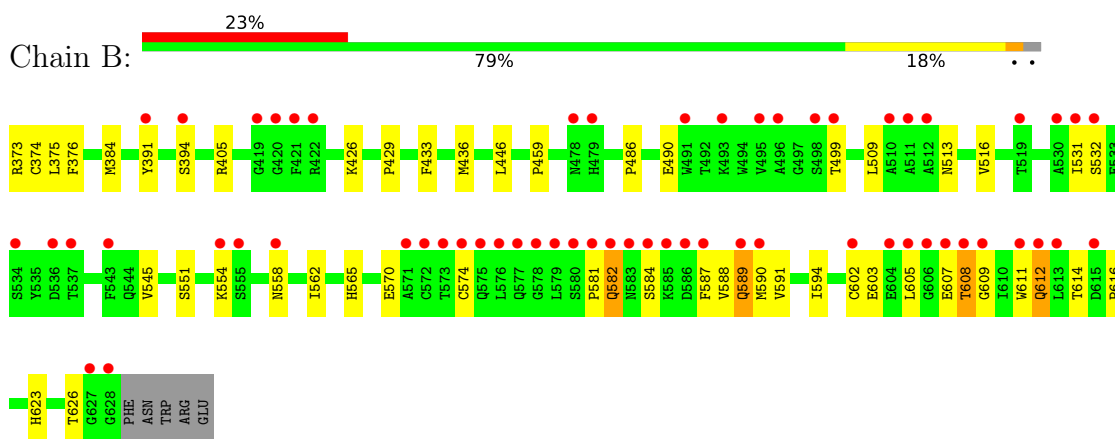
3 Residue-property plots [i](#)

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.

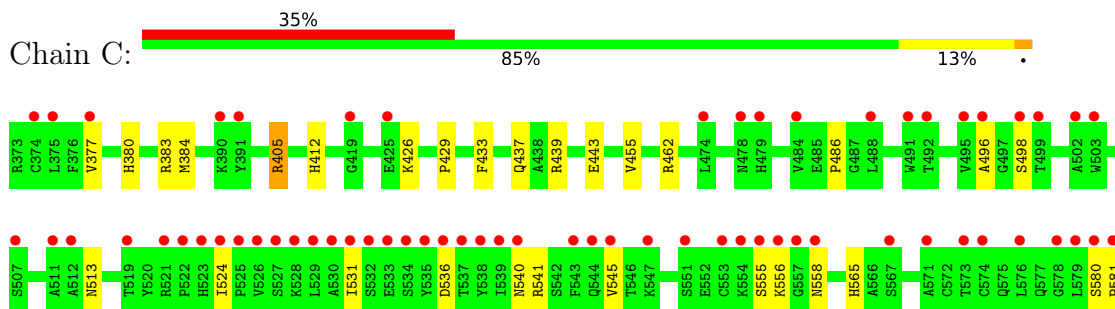
- Molecule 1: Suppressor of T-cell receptor signaling 1

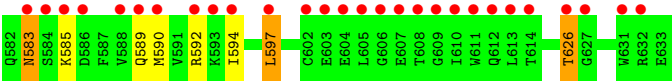


- Molecule 1: Suppressor of T-cell receptor signaling 1



- Molecule 1: Suppressor of T-cell receptor signaling 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.23Å 74.34Å 100.11Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	98.06 – 1.82 98.06 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.2 (98.06-1.82) 96.3 (98.06-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.236 0.234 , 0.268	Depositor DCC
R_{free} test set	3653 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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	0.78	0/2154	0.92	1/2924 (0.0%)
1	B	0.78	0/2128	0.91	2/2889 (0.1%)
1	C	0.62	0/2140	0.87	2/2905 (0.1%)
All	All	0.73	0/6422	0.90	5/8718 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	ILE	N-CA-C	6.24	114.06	107.76
1	C	498	SER	N-CA-C	-5.33	106.36	112.92
1	A	516	VAL	N-CA-C	5.18	117.00	108.97
1	C	597	LEU	CA-CB-CG	-5.18	98.17	116.30
1	B	616	PRO	O-C-N	5.03	123.62	121.31

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	2066	0	2038	28	0
1	B	2032	0	2023	42	1
1	C	2071	0	2051	23	1
2	A	132	0	0	0	0
2	B	109	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	62	0	0	3	0
All	All	6472	0	6112	80	1

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 6.

All (80) 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:436[B]:MET:CE	1:B:436[B]:MET:HE2	1.61	1.31
1:B:570:GLU:HG2	2:B:738:HOH:O	1.36	1.22
1:A:436[B]:MET:CE	1:B:436[B]:MET:CE	2.16	1.15
1:C:462[B]:ARG:HH12	1:C:565:HIS:CE1	1.74	1.04
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE3	1.61	0.99
1:A:622:THR:HA	1:B:626[B]:THR:HG21	1.47	0.96
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE1	0.38	0.88
1:A:436[B]:MET:SD	1:B:436[B]:MET:CE	0.92	0.88
1:C:405:ARG:NH2	2:C:692:HOH:O	2.07	0.86
1:B:626[B]:THR:HG23	2:B:663:HOH:O	1.78	0.82
1:B:607:GLU:HG3	1:B:608:THR:N	1.98	0.76
1:A:436[B]:MET:HE1	1:B:436[B]:MET:HE2	1.70	0.73
1:A:468:HIS:NE2	1:A:472:LYS:HE3	2.05	0.72
1:C:462[B]:ARG:NH1	1:C:565:HIS:CE1	2.56	0.72
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE2	1.30	0.71
1:A:582:GLN:NE2	1:A:590[A]:MET:SD	2.64	0.70
1:A:468:HIS:CD2	1:A:472:LYS:HE3	2.30	0.67
1:B:374[B]:CYS:SG	1:B:376:PHE:CE1	2.83	0.67
1:C:439:ARG:NH1	1:C:443:GLU:OE2	2.33	0.62
1:B:426:LYS:NZ	1:B:499:THR:HG23	2.16	0.59
1:C:384:MET:HG3	1:C:429:PRO:HG2	1.85	0.58
1:A:523:HIS:HE1	1:A:552:GLU:OE2	1.87	0.57
1:B:426:LYS:HZ1	1:B:499:THR:HG23	1.69	0.57
1:C:583:ASN:HD21	1:C:585:LYS:HD2	1.71	0.56
1:A:384:MET:HG3	1:A:429:PRO:HG2	1.89	0.55
1:C:462[B]:ARG:HH12	1:C:565:HIS:HE1	1.49	0.54
1:C:626:THR:HA	2:C:685:HOH:O	2.08	0.54
1:C:380:HIS:CE1	1:C:462[B]:ARG:HD2	2.45	0.51
1:B:459:PRO:HD3	1:B:486:PRO:HA	1.93	0.51
1:A:554:LYS:NZ	1:A:604:GLU:OE1	2.42	0.50
1:B:603:GLU:HB2	1:B:614:THR:HG21	1.93	0.49
1:B:587:PHE:O	1:B:591:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:GLU:HG3	1:B:608:THR:H	1.74	0.48
1:C:486:PRO:HB2	1:C:524:ILE:O	2.14	0.48
1:A:491:TRP:CE2	1:A:493:LYS:HG3	2.49	0.48
1:A:590[B]:MET:HE1	1:A:594:ILE:HD11	1.96	0.47
1:A:621[A]:LEU:HD11	1:B:433:PHE:HE1	1.79	0.47
1:B:375:LEU:HD11	1:B:562:ILE:HD12	1.96	0.47
1:B:446:LEU:HD12	2:B:679:HOH:O	2.14	0.46
1:C:405:ARG:HD3	1:C:412:HIS:HA	1.97	0.46
1:C:555:SER:HB3	1:C:556:LYS:HG3	1.97	0.46
1:B:373:ARG:N	1:B:558:ASN:O	2.49	0.45
1:B:513:ASN:HB2	1:C:513:ASN:CG	2.41	0.45
1:B:607:GLU:C	1:B:609:GLY:H	2.25	0.45
1:A:626:THR:HG23	1:B:623:HIS:CD2	2.52	0.45
1:B:607:GLU:O	1:B:609:GLY:N	2.44	0.45
1:C:462[A]:ARG:NH2	2:C:660:HOH:O	2.48	0.44
1:B:509:LEU:HB2	1:B:516[A]:VAL:HG21	1.97	0.44
1:C:426:LYS:NZ	1:C:496:ALA:HB3	2.32	0.44
1:B:384:MET:HG3	1:B:429:PRO:HG2	1.99	0.44
1:A:517:ASP:OD1	1:A:519:THR:HB	2.17	0.44
1:C:590:MET:CE	1:C:594:ILE:HD11	2.47	0.44
1:A:436[B]:MET:HE1	1:B:436[B]:MET:CE	2.31	0.44
1:C:580:SER:HA	1:C:581:PRO:HD3	1.91	0.43
1:A:623:HIS:CD2	1:B:626[A]:THR:HG23	2.54	0.43
1:C:383:ARG:HG2	1:C:462[B]:ARG:HD3	2.01	0.43
1:A:486:PRO:HB2	1:A:524:ILE:O	2.19	0.43
1:B:490:GLU:HB3	1:B:565:HIS:CG	2.54	0.43
1:B:582:GLN:NE2	1:B:590[B]:MET:SD	2.91	0.42
1:A:374:CYS:HB2	1:A:559:ASN:OD1	2.18	0.42
1:C:433:PHE:O	1:C:437:GLN:HG3	2.19	0.42
1:B:605:LEU:HD21	1:B:612:GLN:NE2	2.34	0.42
1:C:541:ARG:O	1:C:545:VAL:HG23	2.19	0.42
1:B:426:LYS:NZ	1:B:499:THR:CG2	2.83	0.42
1:A:488:LEU:HD13	1:A:562:ILE:HG23	2.02	0.41
1:B:374[B]:CYS:SG	1:B:376:PHE:CZ	3.10	0.41
1:B:551:SER:HA	1:B:554:LYS:HG3	2.02	0.41
1:C:536:ASP:O	1:C:540:ASN:ND2	2.54	0.41
1:A:468:HIS:HE2	1:A:472:LYS:HE3	1.82	0.41
1:A:550:ILE:O	1:A:554:LYS:HG2	2.20	0.41
1:C:589:GLN:HG3	1:C:592:ARG:NH1	2.35	0.41
1:C:462[B]:ARG:NH1	1:C:565:HIS:ND1	2.60	0.41
1:B:574:CYS:SG	1:B:581:PRO:HA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:CYS:HB3	1:B:611:TRP:HB3	2.03	0.41
1:B:584:SER:O	1:B:588:VAL:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TYR:OH	1:C:540:ASN:ND2[3_555]	2.16	0.04

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	265/261 (102%)	259 (98%)	6 (2%)	0	100	100
1	B	263/261 (101%)	252 (96%)	10 (4%)	1 (0%)	30	19
1	C	262/261 (100%)	252 (96%)	10 (4%)	0	100	100
All	All	790/783 (101%)	763 (97%)	26 (3%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	608	THR

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	234/229 (102%)	225 (96%)	9 (4%)	29	11
1	B	233/229 (102%)	224 (96%)	9 (4%)	28	11
1	C	232/229 (101%)	224 (97%)	8 (3%)	32	14
All	All	699/687 (102%)	673 (96%)	26 (4%)	32	12

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	ARG
1	A	390	LYS
1	A	396[A]	CYS
1	A	396[B]	CYS
1	A	455	VAL
1	A	516	VAL
1	A	556	LYS
1	A	605	LEU
1	A	626	THR
1	B	394	SER
1	B	405[A]	ARG
1	B	405[B]	ARG
1	B	531	ILE
1	B	532	SER
1	B	545	VAL
1	B	582	GLN
1	B	589	GLN
1	B	612	GLN
1	C	377	VAL
1	C	405	ARG
1	C	455	VAL
1	C	531	ILE
1	C	558	ASN
1	C	583	ASN
1	C	597	LEU
1	C	626	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	523	HIS
1	B	395	GLN
1	B	412	HIS

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Mol	Chain	Res	Type
1	B	416	GLN
1	B	612	GLN
1	C	416	GLN
1	C	540	ASN
1	C	558	ASN
1	C	583	ASN

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	261/261 (100%)	1.01	34 (13%)	7 8	16, 30, 43, 50	6 (2%)
1	B	256/261 (98%)	1.34	60 (23%)	2 2	17, 31, 45, 50	9 (3%)
1	C	261/261 (100%)	1.82	92 (35%)	1 1	20, 38, 49, 55	2 (0%)
All	All	778/783 (99%)	1.39	186 (23%)	2 2	16, 33, 46, 55	17 (2%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	ALA	9.0
1	B	499	THR	7.5
1	C	578	GLY	7.3
1	B	531	ILE	6.7
1	C	536	ASP	6.3
1	B	574	CYS	6.1
1	C	537	THR	6.0
1	A	479	HIS	5.2
1	A	478	ASN	5.2
1	C	534	SER	5.0
1	B	578	GLY	5.0
1	B	605	LEU	5.0
1	C	540	ASN	5.0
1	B	498	SER	4.9
1	C	631	TRP	4.9
1	C	605	LEU	4.8
1	B	391	TYR	4.7
1	B	495	VAL	4.7
1	A	519	THR	4.7
1	C	531	ILE	4.7
1	B	628	GLY	4.6
1	C	611	TRP	4.5
1	C	610	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	554	LYS	4.3
1	C	527	SER	4.3
1	C	538	TYR	4.3
1	C	581	PRO	4.3
1	C	579	LEU	4.2
1	B	555	SER	4.2
1	C	606	GLY	4.2
1	C	496	ALA	4.1
1	C	545	VAL	4.0
1	C	391	TYR	4.0
1	C	585	LYS	4.0
1	A	498	SER	4.0
1	C	602	CYS	4.0
1	C	547	LYS	3.9
1	C	499	THR	3.8
1	B	583	ASN	3.7
1	A	511	ALA	3.6
1	A	605	LEU	3.6
1	B	581	PRO	3.6
1	C	525	PRO	3.6
1	C	590	MET	3.6
1	C	555	SER	3.6
1	C	530	ALA	3.5
1	B	394	SER	3.5
1	B	478	ASN	3.5
1	C	576	LEU	3.5
1	C	632	ARG	3.5
1	C	574	CYS	3.5
1	A	497	GLY	3.5
1	C	519	THR	3.4
1	C	539	ILE	3.4
1	A	606	GLY	3.4
1	A	613	LEU	3.4
1	C	522	PRO	3.4
1	C	524	ILE	3.4
1	C	627	GLY	3.3
1	C	491	TRP	3.3
1	C	543	PHE	3.3
1	C	608	THR	3.3
1	C	557	GLY	3.3
1	B	573	THR	3.3
1	B	572	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	529	LEU	3.2
1	B	627	GLY	3.2
1	A	590[A]	MET	3.2
1	A	394	SER	3.2
1	B	580	SER	3.2
1	C	535	TYR	3.1
1	A	574[A]	CYS	3.1
1	A	499	THR	3.1
1	B	534	SER	3.1
1	C	479	HIS	3.1
1	C	580	SER	3.1
1	C	554	LYS	3.0
1	C	583	ASN	3.0
1	C	551	SER	3.0
1	B	589	GLN	3.0
1	C	612	GLN	2.9
1	B	602	CYS	2.9
1	C	374	CYS	2.9
1	C	588	VAL	2.9
1	A	557	GLY	2.9
1	B	607	GLU	2.9
1	B	512	ALA	2.9
1	C	592	ARG	2.9
1	C	584	SER	2.9
1	B	608	THR	2.8
1	B	422	ARG	2.8
1	C	586	ASP	2.8
1	B	582	GLN	2.8
1	A	532	SER	2.8
1	C	521	ARG	2.8
1	C	604	GLU	2.8
1	C	495	VAL	2.8
1	B	584	SER	2.8
1	C	532	SER	2.8
1	C	613	LEU	2.8
1	B	491	TRP	2.8
1	C	567	SER	2.7
1	B	571	ALA	2.7
1	C	528	LYS	2.7
1	C	614	THR	2.7
1	A	513	ASN	2.7
1	C	609	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	586	ASP	2.7
1	A	633	GLU	2.7
1	B	511	ALA	2.6
1	B	606	GLY	2.6
1	A	515	SER	2.6
1	B	579	LEU	2.6
1	B	420	GLY	2.6
1	A	510	ALA	2.6
1	C	593	LYS	2.6
1	A	527	SER	2.6
1	B	587	PHE	2.6
1	C	544	GLN	2.6
1	B	419	GLY	2.6
1	C	419	GLY	2.6
1	B	530	ALA	2.6
1	B	532	SER	2.6
1	B	421	PHE	2.5
1	B	612	GLN	2.5
1	B	576	LEU	2.5
1	A	583	ASN	2.5
1	C	571	ALA	2.5
1	C	498	SER	2.5
1	C	573	THR	2.5
1	C	626	THR	2.5
1	B	493	LYS	2.5
1	B	536	ASP	2.5
1	C	556	LYS	2.5
1	A	395	GLN	2.4
1	A	373	ARG	2.4
1	A	592	ARG	2.4
1	B	558	ASN	2.4
1	A	607	GLU	2.4
1	B	611	TRP	2.4
1	C	503	TRP	2.4
1	C	526	VAL	2.4
1	B	609	GLY	2.4
1	B	585	LYS	2.4
1	A	496	ALA	2.4
1	C	511	ALA	2.4
1	B	575	GLN	2.4
1	C	558	ASN	2.4
1	C	484	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	523	HIS	2.3
1	C	607	GLU	2.3
1	C	512	ALA	2.3
1	A	609	GLY	2.3
1	B	604	GLU	2.3
1	C	603	GLU	2.3
1	C	553	CYS	2.3
1	B	613	LEU	2.3
1	C	594	ILE	2.3
1	C	589	GLN	2.3
1	A	558	ASN	2.3
1	B	519[A]	THR	2.3
1	A	578	GLY	2.2
1	C	533	GLU	2.2
1	C	488	LEU	2.2
1	A	534	SER	2.2
1	A	555	SER	2.2
1	B	510	ALA	2.2
1	B	537	THR	2.2
1	C	375	LEU	2.2
1	A	556	LYS	2.2
1	C	377	VAL	2.2
1	B	615	ASP	2.2
1	C	492	THR	2.1
1	C	507	SER	2.1
1	A	521	ARG	2.1
1	C	390	LYS	2.1
1	B	590[A]	MET	2.1
1	C	474	LEU	2.1
1	C	478	ASN	2.1
1	C	597	LEU	2.1
1	B	577	GLN	2.1
1	A	631	TRP	2.1
1	C	425	GLU	2.0
1	B	479	HIS	2.0
1	C	502	ALA	2.0
1	B	543	PHE	2.0

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 [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.