



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:59 PM UTC

PDB ID : 2QTW / pdb_00002qtw
Title : The Crystal Structure of PCSK9 at 1.9 Angstroms Resolution Reveals structural homology to Resistin within the C-terminal domain
Authors : Hampton, E.N.; Knuth, M.W.; Li, J.; Harris, J.L.; Lesley, S.A.; Spraggon, G.
Deposited on : 2007-08-02
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

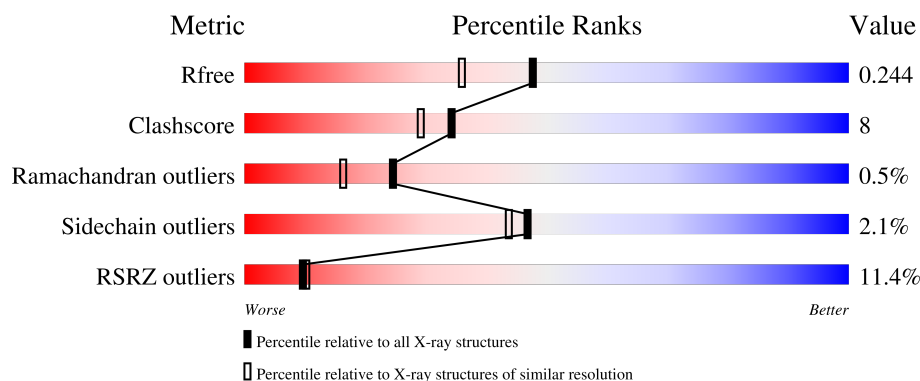
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	124	4% 69% 6% 26%
2	B	546	11% 73% 15% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4697 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 Proprotein convertase subtilisin/kexin type 9 Propeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	1	0
			748	479	136	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total	C	N	O	S	0	1	0
			3614	2229	668	685	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	693	HIS	-	expression tag	UNP Q8NBP7
B	694	HIS	-	expression tag	UNP Q8NBP7
B	695	HIS	-	expression tag	UNP Q8NBP7
B	696	HIS	-	expression tag	UNP Q8NBP7
B	697	HIS	-	expression tag	UNP Q8NBP7
B	698	HIS	-	expression tag	UNP Q8NBP7

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

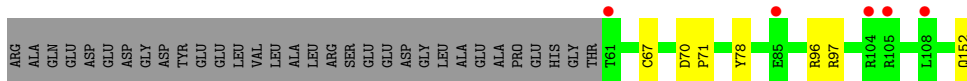
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	254	Total	O	0	0
			254	254		

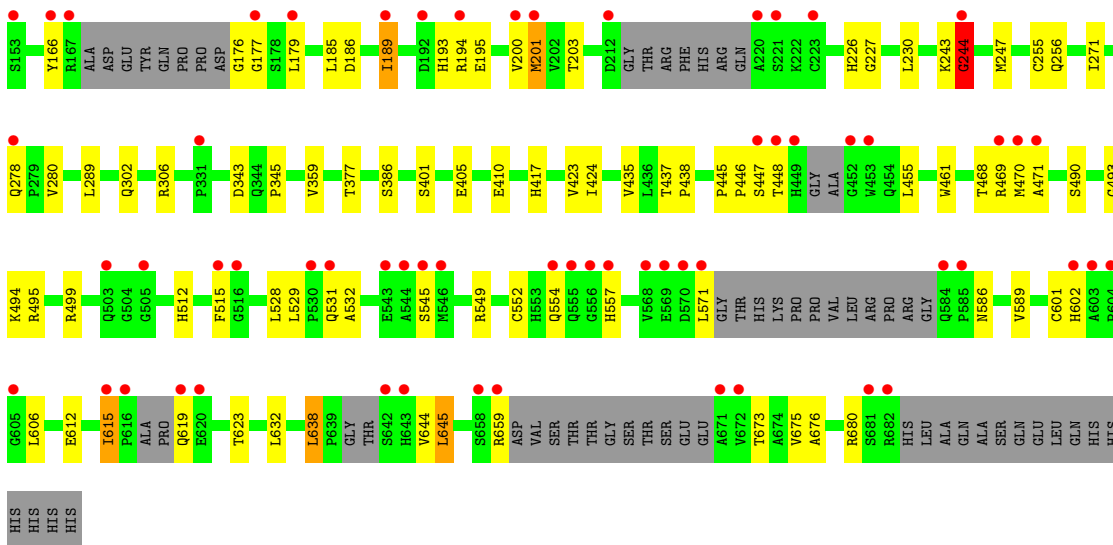
3 Residue-property plots [i](#)

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: Proprotein convertase subtilisin/kexin type 9 Propeptide



- Molecule 2: Proprotein convertase subtilisin/kexin type 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.43Å 70.15Å 148.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.90) 99.8 (50.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.239 0.197 , 0.244	Depositor DCC
R_{free} test set	2654 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4697	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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: CA, 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	0.97	0/768	0.87	0/1037
2	B	0.92	4/3682 (0.1%)	0.88	0/4996
All	All	0.93	4/4450 (0.1%)	0.88	0/6033

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
2	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	255	CYS	C-N	-8.72	1.21	1.33
2	B	256	GLN	C-N	-7.59	1.23	1.33
2	B	445	PRO	CA-C	5.58	1.55	1.52
2	B	189	ILE	C-N	-5.15	1.26	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	B	494	LYS	Peptide

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	748	0	763	4	1
2	B	3614	0	3522	63	1
3	B	14	0	13	1	0
4	B	1	0	0	0	0
5	A	66	0	0	1	0
5	B	254	0	0	7	0
All	All	4697	0	4298	66	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 8.

All (66) 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)
2:B:201:MET:HE1	2:B:203:THR:HG22	1.44	0.99
2:B:615:ILE:HD12	2:B:619:GLN:HE21	1.34	0.91
2:B:615:ILE:HD12	2:B:619:GLN:NE2	1.95	0.81
2:B:446:PRO:HB2	2:B:448:THR:HG22	1.63	0.78
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.65	0.77
2:B:186:ASP:OD2	2:B:230:LEU:HD12	1.85	0.76
2:B:302:GLN:HE21	2:B:306:ARG:HH21	1.34	0.76
2:B:201:MET:HE1	2:B:203:THR:CG2	2.22	0.69
2:B:529:LEU:HG	2:B:532:ALA:HB2	1.75	0.68
2:B:435:VAL:HG23	5:B:1061:HOH:O	1.94	0.68
2:B:343:ASP:HB3	2:B:423:VAL:HG12	1.76	0.66
2:B:437:THR:O	5:B:1167:HOH:O	2.15	0.64
2:B:612:GLU:HG2	2:B:675:VAL:HG22	1.81	0.62
2:B:176:GLY:O	2:B:244:GLY:HA3	2.00	0.61
2:B:343:ASP:OD2	2:B:423:VAL:HG11	2.00	0.61
2:B:343:ASP:CB	2:B:423:VAL:HG12	2.31	0.59
2:B:552:CYS:HB3	2:B:557[B]:HIS:CE1	2.39	0.58
2:B:615:ILE:CD1	2:B:619:GLN:HE21	2.13	0.58
2:B:638:LEU:HD13	2:B:675:VAL:HG21	1.86	0.56
2:B:189:ILE:CD1	2:B:200:VAL:HG11	2.37	0.55
2:B:638:LEU:HD22	2:B:673:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:ARG:HD2	2:B:515:PHE:CD1	2.44	0.53
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.91	0.53
1:A:97:ARG:CZ	5:A:202:HOH:O	2.57	0.53
2:B:201:MET:CE	2:B:203:THR:HG22	2.29	0.52
2:B:345:PRO:HD3	2:B:424:ILE:HG23	1.91	0.52
1:A:67:CYS:SG	5:B:1256:HOH:O	2.04	0.52
1:A:152:GLN:C	2:B:386:SER:OG	2.54	0.51
2:B:179:LEU:HD22	2:B:401:SER:HA	1.93	0.51
2:B:343:ASP:CB	2:B:423:VAL:CG1	2.88	0.51
2:B:468:THR:OG1	2:B:471:ALA:HB2	2.11	0.50
2:B:177:GLY:HA2	2:B:401:SER:OG	2.12	0.50
2:B:632:LEU:HD13	2:B:676:ALA:HB1	1.95	0.49
2:B:193:HIS:HD2	2:B:195:GLU:H	1.61	0.49
2:B:531:GLN:O	3:B:1001:NAG:H82	2.13	0.49
2:B:632:LEU:CD1	2:B:676:ALA:HB1	2.43	0.48
2:B:455:LEU:HD22	2:B:606:LEU:HD11	1.96	0.47
2:B:186:ASP:OD1	2:B:226:HIS:ND1	2.36	0.47
2:B:201:MET:CE	2:B:203:THR:CG2	2.91	0.46
2:B:289:LEU:HD12	2:B:289:LEU:C	2.41	0.46
2:B:554:GLN:HB2	2:B:557[B]:HIS:CE1	2.51	0.46
2:B:435:VAL:HG12	2:B:461:TRP:CZ2	2.51	0.46
2:B:469:ARG:C	2:B:470:MET:HE2	2.40	0.46
2:B:243:LYS:O	2:B:244:GLY:C	2.58	0.45
2:B:557[A]:HIS:CE1	2:B:602:HIS:HB2	2.52	0.45
2:B:410:GLU:HA	2:B:528:LEU:HD11	1.99	0.44
2:B:469:ARG:O	2:B:470:MET:HE2	2.16	0.44
2:B:493:GLY:CA	2:B:645:LEU:HD12	2.48	0.44
2:B:200:VAL:HG22	2:B:247:MET:HB2	2.00	0.44
2:B:493:GLY:HA3	2:B:645:LEU:HD12	1.99	0.43
2:B:189:ILE:HG22	2:B:227:GLY:C	2.44	0.43
2:B:417:HIS:ND1	5:B:1181:HOH:O	2.36	0.42
2:B:495:ARG:CG	5:B:1133:HOH:O	2.66	0.42
2:B:194:ARG:HG3	2:B:377:THR:HG22	2.02	0.42
2:B:557[B]:HIS:HB2	2:B:601:CYS:O	2.20	0.42
2:B:166:TYR:HA	2:B:447:SER:OG	2.20	0.41
2:B:302:GLN:O	2:B:306:ARG:HG3	2.19	0.41
2:B:359:VAL:O	2:B:438:PRO:HG2	2.20	0.41
2:B:495:ARG:HG2	5:B:1133:HOH:O	2.19	0.41
1:A:70:ASP:N	1:A:71:PRO:CD	2.83	0.41
2:B:552:CYS:HB2	2:B:586:ASN:HB3	2.02	0.41
2:B:490:SER:OG	2:B:493:GLY:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:GLN:H	2:B:557[B]:HIS:CE1	2.39	0.41
2:B:201:MET:HE2	2:B:201:MET:HB3	1.96	0.41
2:B:680:ARG:NE	5:B:1185:HOH:O	2.52	0.40
2:B:499:ARG:HD3	2:B:512:HIS:NE2	2.36	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:A:78:TYR:OH	2:B:405:GLU:OE2[3_655]	2.17	0.03

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	21	13
All	All	562/670 (84%)	549 (98%)	10 (2%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	GLY
2	B	545	SER
2	B	280	VAL

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	80/104 (77%)	79 (99%)	1 (1%)	61	61
2	B	389/437 (89%)	380 (98%)	9 (2%)	44	40
All	All	469/541 (87%)	459 (98%)	10 (2%)	47	44

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
2	B	201	MET
2	B	278	GLN
2	B	571	LEU
2	B	615	ILE
2	B	623	THR
2	B	638	LEU
2	B	644	VAL
2	B	645	LEU
2	B	659	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	116	HIS
2	B	302	GLN
2	B	449	HIS
2	B	602	HIS
2	B	619	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	NAG	B	1001	2	14,14,15	0.52	0	17,19,21	1.02	1 (5%)

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
3	NAG	B	1001	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NAG	C3-C4-C5	2.13	114.10	110.23

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
3	B	1001	NAG	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	92/124 (74%)	0.10	5 (5%) 31 33	17, 23, 36, 44	1 (1%)
2	B	486/546 (89%)	0.50	61 (12%) 8 8	13, 26, 53, 74	1 (0%)
All	All	578/670 (86%)	0.44	66 (11%) 10 10	13, 25, 52, 74	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	ALA	6.8
2	B	571	LEU	6.2
2	B	449	HIS	6.1
2	B	515	PHE	6.1
2	B	616	PRO	5.1
2	B	448	THR	4.1
2	B	221	SER	4.1
2	B	447	SER	4.1
2	B	544	ALA	4.0
2	B	557[A]	HIS	3.9
2	B	546	MET	3.5
2	B	469	ARG	3.5
2	B	453	TRP	3.4
2	B	212	ASP	3.3
2	B	615	ILE	3.3
1	A	61	THR	3.2
2	B	671	ALA	3.2
2	B	659	ARG	3.2
2	B	331	PRO	3.1
2	B	605	GLY	3.0
2	B	167	ARG	2.9
2	B	244	GLY	2.9
2	B	604	PRO	2.9
2	B	223	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	177	GLY	2.9
2	B	585	PRO	2.8
2	B	543	GLU	2.8
2	B	503	GLN	2.7
2	B	470	MET	2.7
2	B	682	ARG	2.7
2	B	568	VAL	2.7
2	B	530	PRO	2.7
1	A	85	GLU	2.7
2	B	452	GLY	2.6
2	B	569	GLU	2.6
2	B	643	HIS	2.6
2	B	584	GLN	2.6
2	B	153	SER	2.6
2	B	516	GLY	2.6
2	B	603	ALA	2.6
2	B	556	GLY	2.5
2	B	189	ILE	2.5
2	B	531	GLN	2.5
2	B	555	GLN	2.5
2	B	194	ARG	2.4
2	B	620	GLU	2.4
2	B	545	SER	2.4
2	B	672	VAL	2.4
2	B	602	HIS	2.4
2	B	200	VAL	2.4
1	A	105[A]	ARG	2.3
1	A	108	LEU	2.3
2	B	471	ALA	2.3
2	B	642	SER	2.3
2	B	681	SER	2.3
2	B	554	GLN	2.3
1	A	104	ARG	2.2
2	B	619	GLN	2.2
2	B	192	ASP	2.2
2	B	658	SER	2.2
2	B	505	GLY	2.1
2	B	179	LEU	2.1
2	B	278	GLN	2.1
2	B	570	ASP	2.1
2	B	201	MET	2.0
2	B	166	TYR	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](#)

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($\text{\AA}^2$)	Q<0.9
3	NAG	B	1001	14/15	0.71	0.17	57,62,65,69	0
4	CA	B	1	1/1	0.90	0.13	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.