



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 AM UTC

PDB ID : 4U4J / pdb_00004u4j
Title : Crystal structure of Salmonella alpha-2-macroglobulin mutant Y1175G
Authors : Wong, S.G.; Dessen, A.
Deposited on : 2014-07-23
Resolution : 2.90 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
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

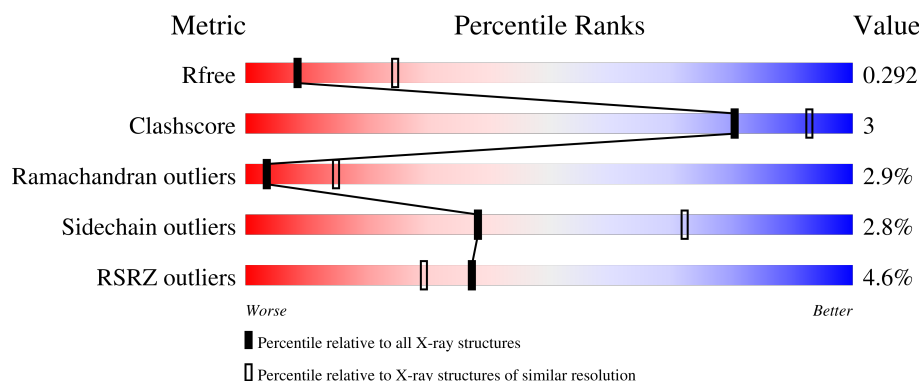
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1647	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23627 atoms, of which 11754 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 Putative inner membrane lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1538	23627	7480	11754	2091	2279	23	0	0	0

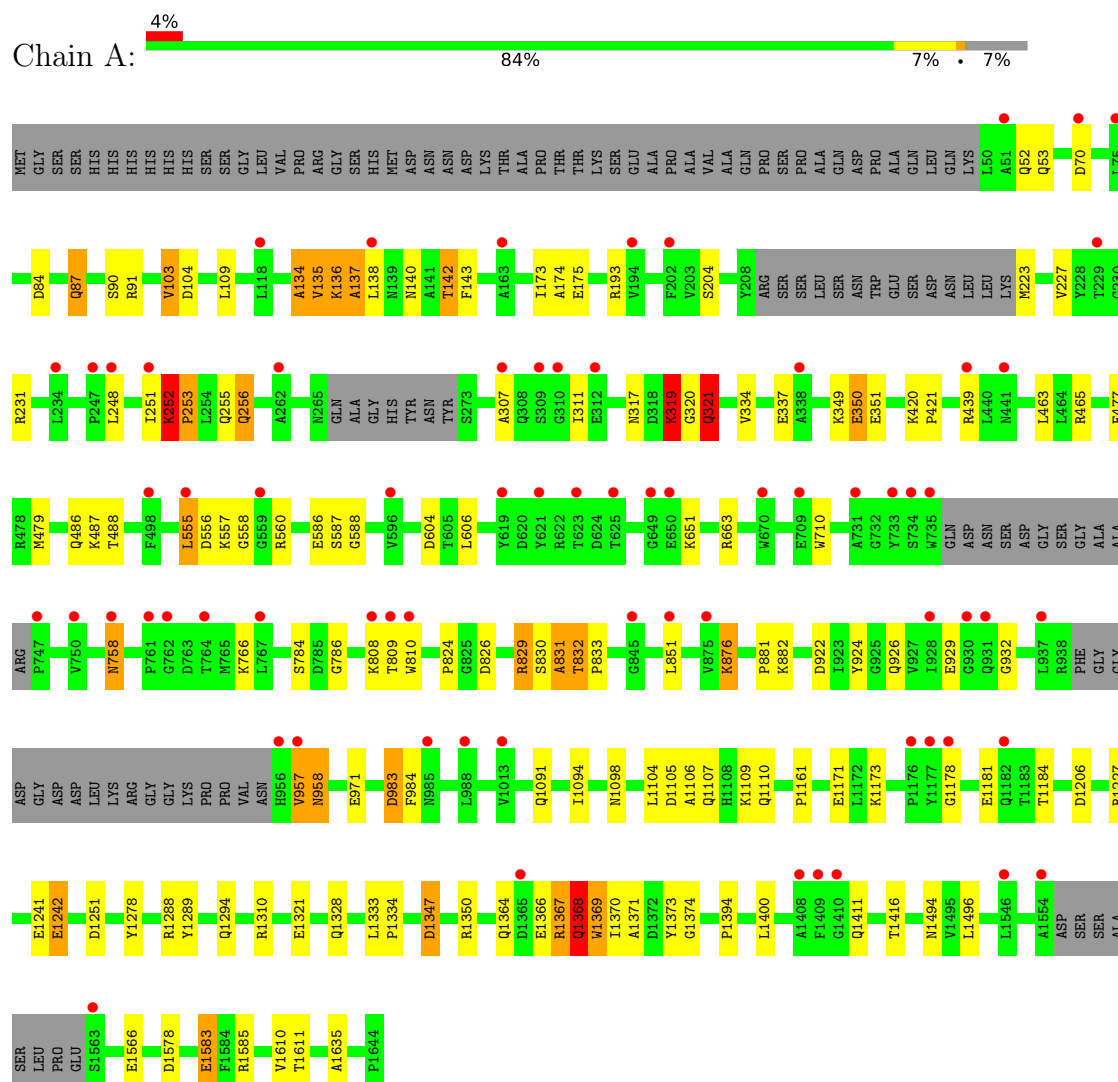
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q8ZN46
A	-1	GLY	-	expression tag	UNP Q8ZN46
A	0	SER	-	expression tag	UNP Q8ZN46
A	1	SER	-	expression tag	UNP Q8ZN46
A	2	HIS	-	expression tag	UNP Q8ZN46
A	3	HIS	-	expression tag	UNP Q8ZN46
A	4	HIS	-	expression tag	UNP Q8ZN46
A	5	HIS	-	expression tag	UNP Q8ZN46
A	6	HIS	-	expression tag	UNP Q8ZN46
A	7	HIS	-	expression tag	UNP Q8ZN46
A	8	SER	-	expression tag	UNP Q8ZN46
A	9	SER	-	expression tag	UNP Q8ZN46
A	10	GLY	-	expression tag	UNP Q8ZN46
A	11	LEU	-	expression tag	UNP Q8ZN46
A	12	VAL	-	expression tag	UNP Q8ZN46
A	13	PRO	-	expression tag	UNP Q8ZN46
A	14	ARG	-	expression tag	UNP Q8ZN46
A	15	GLY	-	expression tag	UNP Q8ZN46
A	16	SER	-	expression tag	UNP Q8ZN46
A	17	HIS	-	expression tag	UNP Q8ZN46
A	18	MET	-	expression tag	UNP Q8ZN46
A	98	ALA	LYS	engineered mutation	UNP Q8ZN46
A	99	ALA	LYS	engineered mutation	UNP Q8ZN46
A	1175	GLY	TYR	engineered mutation	UNP Q8ZN46

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: Putative inner membrane lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.24Å 82.16Å 98.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.99 – 2.90 58.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.99-2.90) 99.8 (58.99-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.244 , 0.284 0.252 , 0.292	Depositor DCC
R_{free} test set	2340 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.0	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	0.93	EDS
Total number of atoms	23627	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.30	0/12113	0.65	6/16503 (0.0%)

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	A	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	809	THR	N-CA-C	-7.45	103.93	113.16
1	A	932	GLY	N-CA-C	6.79	118.41	111.95
1	A	252	LYS	CA-C-N	-5.63	112.81	119.84
1	A	252	LYS	C-N-CA	-5.63	112.81	119.84
1	A	1374	GLY	N-CA-C	5.42	119.05	111.14
1	A	321	GLN	N-CA-C	5.05	121.56	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	LYS	Peptide
1	A	808	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	11873	11754	11772	61	0
All	All	11873	11754	11772	61	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 3.

All (61) 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:87:GLN:N	1:A:87:GLN:OE1	2.19	0.76
1:A:1366:GLU:O	1:A:1368:GLN:N	2.19	0.75
1:A:1368:GLN:OE1	1:A:1369:TRP:N	2.30	0.65
1:A:463:LEU:O	1:A:465:ARG:NH1	2.34	0.60
1:A:317:ASN:O	1:A:319:LYS:N	2.33	0.60
1:A:1091:GLN:NE2	1:A:1110:GLN:OE1	2.36	0.58
1:A:337:GLU:N	1:A:337:GLU:OE1	2.37	0.57
1:A:1181:GLU:OE1	1:A:1416:THR:OG1	2.22	0.57
1:A:829:ARG:O	1:A:831:ALA:N	2.38	0.57
1:A:1294:GLN:OE1	1:A:1328:GLN:NE2	2.38	0.57
1:A:555:LEU:HD23	1:A:555:LEU:C	2.32	0.55
1:A:1566:GLU:OE1	1:A:1566:GLU:N	2.40	0.55
1:A:84:ASP:HB2	1:A:136:LYS:HE3	1.89	0.55
1:A:922:ASP:OD2	1:A:924:TYR:N	2.40	0.54
1:A:349:LYS:O	1:A:351:GLU:N	2.41	0.53
1:A:663:ARG:NH2	1:A:710:TRP:O	2.40	0.53
1:A:784:SER:O	1:A:786:GLY:N	2.41	0.53
1:A:555:LEU:O	1:A:557:LYS:N	2.42	0.53
1:A:1105:ASP:OD1	1:A:1106:ALA:N	2.42	0.53
1:A:1181:GLU:O	1:A:1184:THR:N	2.42	0.52
1:A:1583:GLU:OE2	1:A:1585:ARG:NE	2.42	0.52
1:A:137:ALA:O	1:A:140:ASN:N	2.43	0.52
1:A:1241:GLU:OE2	1:A:1278:TYR:OH	2.19	0.51
1:A:758:ASN:O	1:A:758:ASN:ND2	2.42	0.51
1:A:320:GLY:O	1:A:321:GLN:NE2	2.45	0.49
1:A:1227:ARG:NH1	1:A:1241:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:ASP:OD2	1:A:1350:ARG:NH1	2.45	0.49
1:A:134:ALA:C	1:A:136:LYS:H	2.20	0.48
1:A:136:LYS:HE2	1:A:138:LEU:HA	1.96	0.48
1:A:1289:TYR:OH	1:A:1578:ASP:OD2	2.22	0.48
1:A:983:ASP:OD1	1:A:1109:LYS:NZ	2.47	0.47
1:A:1494:ASN:O	1:A:1496:LEU:N	2.47	0.47
1:A:320:GLY:C	1:A:321:GLN:CD	2.83	0.46
1:A:204:SER:OG	1:A:319:LYS:O	2.27	0.46
1:A:103:VAL:HG22	1:A:104:ASP:H	1.80	0.46
1:A:1368:GLN:N	1:A:1368:GLN:CD	2.73	0.45
1:A:1251:ASP:OD1	1:A:1310:ARG:NH1	2.50	0.45
1:A:136:LYS:HE2	1:A:137:ALA:C	2.42	0.45
1:A:486:GLN:O	1:A:488:THR:N	2.50	0.45
1:A:134:ALA:O	1:A:136:LYS:N	2.51	0.44
1:A:557:LYS:HG2	1:A:558:GLY:H	1.82	0.44
1:A:1610:VAL:HG23	1:A:1611:THR:N	2.33	0.44
1:A:251:ILE:HG23	1:A:253:PRO:HD2	2.00	0.44
1:A:136:LYS:HZ3	1:A:137:ALA:CA	2.31	0.43
1:A:1369:TRP:C	1:A:1371:ALA:H	2.26	0.43
1:A:84:ASP:HB2	1:A:136:LYS:HD3	2.01	0.43
1:A:1364:GLN:OE1	1:A:1364:GLN:N	2.49	0.42
1:A:604:ASP:N	1:A:604:ASP:OD1	2.52	0.42
1:A:420:LYS:HB2	1:A:421:PRO:HD2	2.01	0.42
1:A:957:VAL:O	1:A:958:ASN:CB	2.68	0.42
1:A:193:ARG:NH2	1:A:256:GLN:OE1	2.53	0.41
1:A:252:LYS:HG3	1:A:255:GLN:HB2	2.01	0.41
1:A:1094:ILE:HB	1:A:1107:GLN:HB2	2.01	0.41
1:A:1288:ARG:NH2	1:A:1289:TYR:OH	2.54	0.41
1:A:810:TRP:CD1	1:A:810:TRP:N	2.89	0.41
1:A:1242:GLU:OE1	1:A:1373:TYR:OH	2.31	0.41
1:A:173:ILE:CD1	1:A:175:GLU:HB2	2.51	0.41
1:A:477:GLU:O	1:A:479:MET:N	2.54	0.41
1:A:832:THR:HA	1:A:833:PRO:HD2	2.00	0.40
1:A:1333:LEU:HB3	1:A:1334:PRO:HD3	2.03	0.40
1:A:135:VAL:CG2	1:A:143:PHE:HB2	2.51	0.40

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	A	1526/1647 (93%)	1375 (90%)	106 (7%)	45 (3%)	3	15

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	A	556	ASP
1	A	587	SER
1	A	651	LYS
1	A	758	ASN
1	A	882	LYS
1	A	957	VAL
1	A	1098	ASN
1	A	1367	ARG
1	A	1368	GLN
1	A	1370	ILE
1	A	134	ALA
1	A	137	ALA
1	A	142	THR
1	A	231	ARG
1	A	829	ARG
1	A	830	SER
1	A	958	ASN
1	A	983	ASP
1	A	1347	ASP
1	A	1635	ALA
1	A	135	VAL
1	A	487	LYS
1	A	588	GLY
1	A	876	LYS
1	A	1369	TRP
1	A	1411	GLN
1	A	90	SER

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Mol	Chain	Res	Type
1	A	307	ALA
1	A	319	LYS
1	A	350	GLU
1	A	832	THR
1	A	1104	LEU
1	A	174	ALA
1	A	253	PRO
1	A	831	ALA
1	A	881	PRO
1	A	984	PHE
1	A	1178	GLY
1	A	1206	ASP
1	A	1394	PRO
1	A	929	GLU
1	A	1161	PRO
1	A	103	VAL
1	A	824	PRO

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	1259/1347 (94%)	1224 (97%)	35 (3%)	38 72

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	53	GLN
1	A	70	ASP
1	A	87	GLN
1	A	91	ARG
1	A	109	LEU
1	A	136	LYS
1	A	142	THR
1	A	223	MET

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Mol	Chain	Res	Type
1	A	227	VAL
1	A	248	LEU
1	A	256	GLN
1	A	311	ILE
1	A	319	LYS
1	A	334	VAL
1	A	350	GLU
1	A	439	ARG
1	A	555	LEU
1	A	560	ARG
1	A	586	GLU
1	A	606	LEU
1	A	766	LYS
1	A	826	ASP
1	A	851	LEU
1	A	876	LYS
1	A	926	GLN
1	A	971	GLU
1	A	1171	GLU
1	A	1173	LYS
1	A	1242	GLU
1	A	1321	GLU
1	A	1367	ARG
1	A	1368	GLN
1	A	1400	LEU
1	A	1583	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	185	ASN
1	A	186	HIS
1	A	235	ASN
1	A	274	ASN
1	A	758	ASN
1	A	791	GLN
1	A	841	HIS
1	A	956	HIS
1	A	1091	GLN
1	A	1164	ASN
1	A	1328	GLN

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Mol	Chain	Res	Type
1	A	1398	ASN
1	A	1430	GLN
1	A	1551	GLN
1	A	1568	GLN
1	A	1575	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	1538/1647 (93%)	0.42	70 (4%) 37 29	54, 99, 150, 216	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	GLY	4.5
1	A	1176	PRO	4.4
1	A	1554	ALA	4.3
1	A	649	GLY	4.2
1	A	70	ASP	4.1
1	A	1178	GLY	3.9
1	A	956	HIS	3.9
1	A	229	THR	3.7
1	A	851	LEU	3.6
1	A	735	TRP	3.5
1	A	1563	SER	3.3
1	A	623	THR	3.2
1	A	937	LEU	3.0
1	A	118	LEU	3.0
1	A	764	THR	2.9
1	A	596	VAL	2.8
1	A	309	SER	2.8
1	A	625	THR	2.8
1	A	621	TYR	2.8
1	A	762	GLY	2.7
1	A	1177	TYR	2.7
1	A	734	SER	2.6
1	A	1408	ALA	2.6
1	A	262	ALA	2.6
1	A	758	ASN	2.6
1	A	761	PRO	2.5
1	A	650	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	957	VAL	2.5
1	A	1013	VAL	2.5
1	A	498	PHE	2.5
1	A	441	ASN	2.5
1	A	234	LEU	2.4
1	A	767	LEU	2.4
1	A	985	ASN	2.4
1	A	138	LEU	2.4
1	A	1365	ASP	2.3
1	A	248	LEU	2.3
1	A	1182	GLN	2.3
1	A	247	PRO	2.3
1	A	251	ILE	2.3
1	A	194	VAL	2.3
1	A	988	LEU	2.3
1	A	555	LEU	2.2
1	A	930	GLY	2.2
1	A	1410	GLY	2.2
1	A	928	ILE	2.2
1	A	75	LEU	2.2
1	A	709	GLU	2.2
1	A	310	GLY	2.2
1	A	808	LYS	2.2
1	A	1409	PHE	2.2
1	A	51	ALA	2.2
1	A	731	ALA	2.2
1	A	750	VAL	2.1
1	A	845	GLY	2.1
1	A	307	ALA	2.1
1	A	338	ALA	2.1
1	A	747	PRO	2.1
1	A	202	PHE	2.1
1	A	670	TRP	2.1
1	A	163	ALA	2.1
1	A	931	GLN	2.1
1	A	875	VAL	2.1
1	A	1546	LEU	2.1
1	A	810	TRP	2.1
1	A	619	TYR	2.1
1	A	439	ARG	2.0
1	A	809	THR	2.0
1	A	733	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	312	GLU	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 [i](#)

There are no such residues in this entry.