



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 3PS0 / pdb_00003ps0
Title : The structure of the CRISPR-associated protein, csa2, from *Sulfolobus solfataricus*
Authors : Lintner, N.G.; Sdano, M.; Young, M.J.; Lawrence, C.M.
Deposited on : 2010-11-30
Resolution : 2.00 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

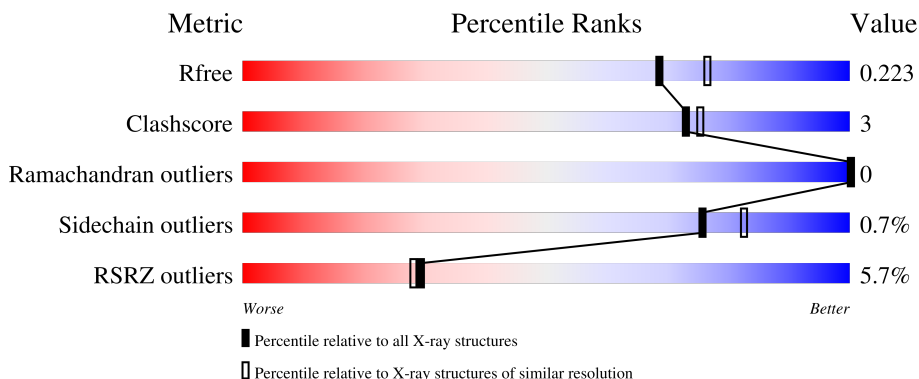
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	328	6% 83% 6% 11%
1	B	328	8% 74% 9% 17%
1	C	328	2% 83% 6% 11%
1	D	328	3% 78% 5% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9340 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 CRISPR-Associated protein, CSA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	1	0
			2290	1471	381	430	8			
1	B	272	Total	C	N	O	S	0	0	0
			2108	1349	354	397	8			
1	C	292	Total	C	N	O	S	0	2	0
			2287	1465	381	433	8			
1	D	272	Total	C	N	O	S	0	0	0
			2110	1351	352	399	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q97Y91
A	-5	HIS	-	expression tag	UNP Q97Y91
A	-4	HIS	-	expression tag	UNP Q97Y91
A	-3	HIS	-	expression tag	UNP Q97Y91
A	-2	HIS	-	expression tag	UNP Q97Y91
A	-1	HIS	-	expression tag	UNP Q97Y91
A	0	HIS	-	expression tag	UNP Q97Y91
B	-6	MET	-	expression tag	UNP Q97Y91
B	-5	HIS	-	expression tag	UNP Q97Y91
B	-4	HIS	-	expression tag	UNP Q97Y91
B	-3	HIS	-	expression tag	UNP Q97Y91
B	-2	HIS	-	expression tag	UNP Q97Y91
B	-1	HIS	-	expression tag	UNP Q97Y91
B	0	HIS	-	expression tag	UNP Q97Y91
C	-6	MET	-	expression tag	UNP Q97Y91
C	-5	HIS	-	expression tag	UNP Q97Y91
C	-4	HIS	-	expression tag	UNP Q97Y91
C	-3	HIS	-	expression tag	UNP Q97Y91
C	-2	HIS	-	expression tag	UNP Q97Y91
C	-1	HIS	-	expression tag	UNP Q97Y91
C	0	HIS	-	expression tag	UNP Q97Y91

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	expression tag	UNP Q97Y91
D	-5	HIS	-	expression tag	UNP Q97Y91
D	-4	HIS	-	expression tag	UNP Q97Y91
D	-3	HIS	-	expression tag	UNP Q97Y91
D	-2	HIS	-	expression tag	UNP Q97Y91
D	-1	HIS	-	expression tag	UNP Q97Y91
D	0	HIS	-	expression tag	UNP Q97Y91

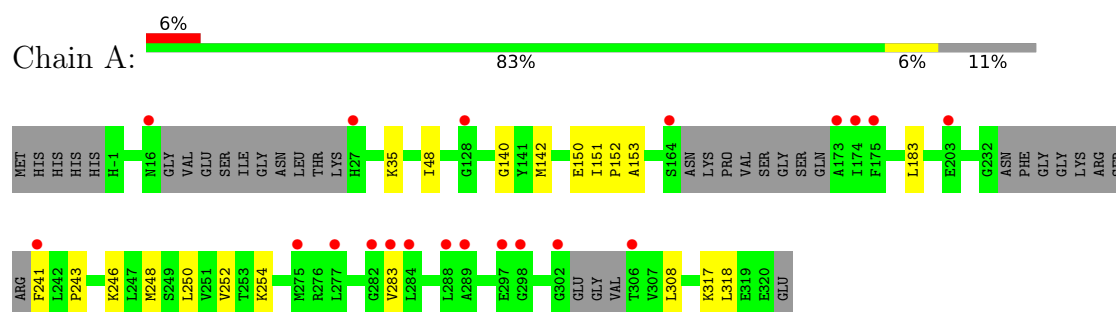
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total 126	O 126	0	0
2	B	60	Total 60	O 60	0	0
2	C	181	Total 181	O 181	0	0
2	D	178	Total 178	O 178	0	0

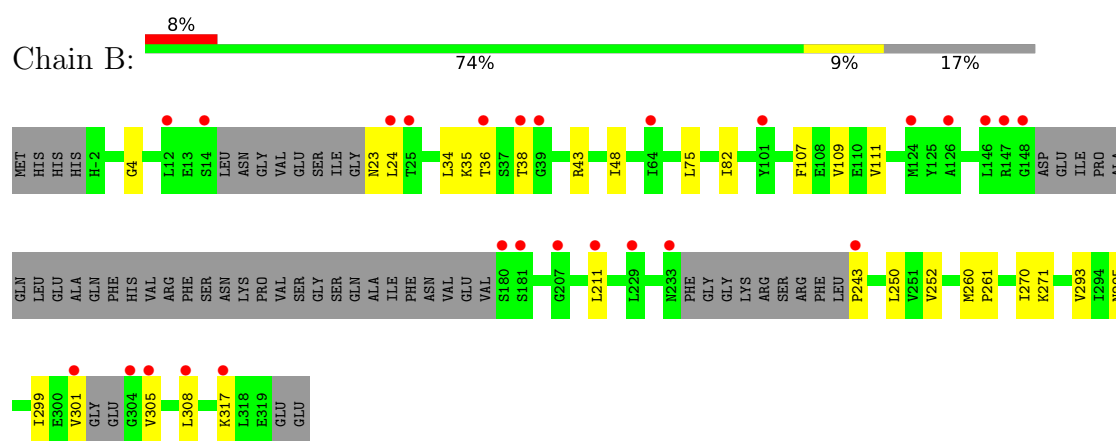
3 Residue-property plots [i](#)

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.

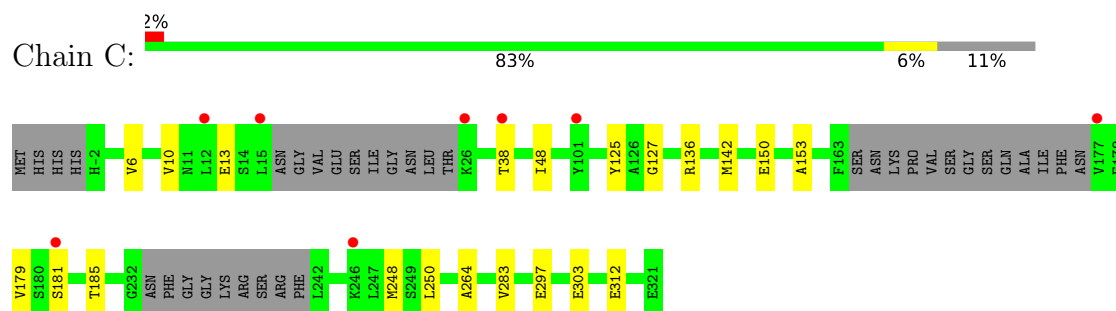
- Molecule 1: CRISPR-Associated protein, CSA2



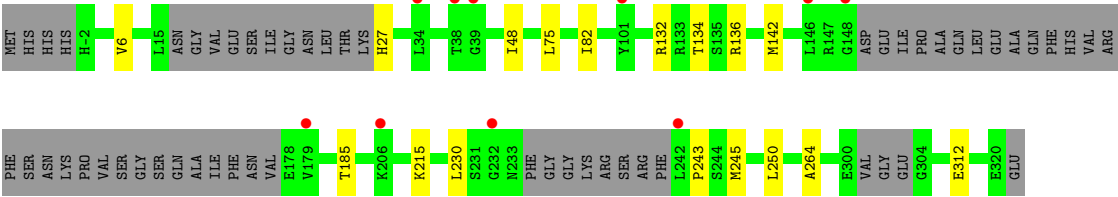
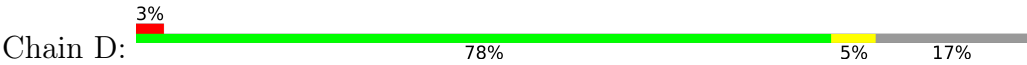
- Molecule 1: CRISPR-Associated protein, CSA2



- Molecule 1: CRISPR-Associated protein, CSA2



- Molecule 1: CRISPR-Associated protein, CSA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.64Å 120.88Å 158.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.75 – 2.00 33.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.75-2.00) 98.7 (33.75-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.221 0.190 , 0.223	Depositor DCC
R_{free} test set	4790 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.4	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	0.96	EDS
Total number of atoms	9340	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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	0.46	0/2332	0.67	0/3143
1	B	0.41	0/2141	0.68	0/2882
1	C	0.46	0/2332	0.70	1/3142 (0.0%)
1	D	0.45	0/2143	0.66	0/2886
All	All	0.45	0/8948	0.68	1/12053 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	GLU	N-CA-C	5.97	117.58	111.14

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	2290	0	2336	14	0
1	B	2108	0	2168	25	0
1	C	2287	0	2334	10	0
1	D	2110	0	2164	11	0
2	A	126	0	0	0	0
2	B	60	0	0	1	0
2	C	181	0	0	0	0
2	D	178	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9340	0	9002	56	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 (56) 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:B:34:LEU:HD11	1:B:43:ARG:HD2	1.78	0.64
1:B:270:ILE:HG22	1:B:301:VAL:HG11	1.80	0.64
1:D:136:ARG:NH2	2:D:460:HOH:O	2.35	0.59
1:D:215:LYS:HE3	2:D:463:HOH:O	2.01	0.58
1:B:295:ASN:ND2	1:B:299:ILE:HG22	2.17	0.58
1:A:140:GLY:HA2	1:B:24:LEU:HA	1.86	0.58
1:B:38:THR:O	1:B:38:THR:HG22	2.07	0.54
1:D:142:MET:HE1	1:D:245:MET:HE1	1.89	0.54
1:B:250:LEU:HD13	1:B:252:VAL:HG23	1.90	0.54
1:D:215:LYS:CE	2:D:463:HOH:O	2.54	0.54
1:A:246:LYS:HD2	1:A:248:MET:HE1	1.89	0.53
1:B:75:LEU:HD13	1:B:82:ILE:HG21	1.90	0.53
1:A:35:LYS:CE	1:B:34:LEU:HD22	2.39	0.52
1:B:260:MET:HE3	1:B:261:PRO:HD2	1.92	0.52
1:C:150:GLU:HG2	1:C:153:ALA:HB3	1.92	0.52
1:B:48:ILE:HD11	1:B:243:PRO:HG3	1.91	0.51
1:B:250:LEU:C	1:B:250:LEU:HD12	2.38	0.49
1:B:293:VAL:HG23	1:B:305:VAL:HG11	1.93	0.49
1:B:4:GLY:O	1:B:260:MET:HE1	2.12	0.49
1:B:35:LYS:HE3	1:B:36:THR:O	2.11	0.49
1:D:6:VAL:HG21	1:D:230:LEU:HD22	1.93	0.49
1:A:308:LEU:HD21	1:A:317:LYS:HE2	1.95	0.49
1:B:271:LYS:H	1:B:301:VAL:HG21	1.78	0.48
1:A:48:ILE:HD11	1:A:243:PRO:HG3	1.95	0.48
1:B:260:MET:HE3	1:B:261:PRO:CD	2.43	0.48
1:B:75:LEU:HD13	1:B:82:ILE:CG2	2.44	0.47
1:B:271:LYS:N	1:B:301:VAL:HG21	2.28	0.47
1:B:23:ASN:N	2:B:423:HOH:O	2.45	0.47
1:A:48:ILE:HB	1:A:142:MET:HB3	1.95	0.47
1:A:254:LYS:HD2	1:A:318:LEU:HD23	1.96	0.47
1:A:183:LEU:HD21	1:A:248:MET:HG3	1.97	0.46
1:A:283:VAL:HA	1:C:283:VAL:HG13	1.98	0.46
1:A:246:LYS:HD2	1:A:248:MET:CE	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HB	1:C:142:MET:HB3	1.99	0.45
1:A:283:VAL:HA	1:C:283:VAL:CG1	2.47	0.45
1:B:107:PHE:O	1:B:111:VAL:HG23	2.16	0.44
1:D:132:ARG:NH1	1:D:134:THR:HG22	2.31	0.44
1:B:308:LEU:HD11	1:B:317:LYS:HD2	1.99	0.44
1:C:185:THR:OG1	1:C:264:ALA:HB3	2.18	0.44
1:A:150:GLU:HG2	1:A:153:ALA:HB3	1.99	0.44
1:C:248:MET:HE3	1:C:297:GLU:HG3	2.00	0.43
1:B:260:MET:HE3	1:B:261:PRO:N	2.33	0.43
1:C:6:VAL:HG13	1:C:250:LEU:HB3	2.01	0.43
1:D:75:LEU:HD13	1:D:82:ILE:HG21	2.00	0.43
1:C:125:TYR:CZ	1:C:127:GLY:HA3	2.54	0.42
1:B:109:VAL:HG13	1:B:211:LEU:HD22	2.01	0.42
1:D:6:VAL:HG21	1:D:230:LEU:CD2	2.48	0.42
1:B:271:LYS:HB2	1:B:301:VAL:HG22	2.02	0.42
1:A:250:LEU:HD13	1:A:252:VAL:HG23	2.02	0.41
1:C:10:VAL:HG21	1:C:142:MET:HE2	2.02	0.41
1:D:185:THR:OG1	1:D:264:ALA:HB3	2.19	0.41
1:C:179:VAL:HG12	1:C:181:SER:H	1.84	0.41
1:D:250:LEU:HD12	1:D:250:LEU:C	2.45	0.41
1:B:270:ILE:CG2	1:B:301:VAL:HG11	2.50	0.41
1:D:48:ILE:HD11	1:D:243:PRO:HD3	2.03	0.41
1:A:151:ILE:HB	1:A:152:PRO:HD3	2.02	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	284/328 (87%)	277 (98%)	7 (2%)	0	100	100
1	B	262/328 (80%)	253 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	286/328 (87%)	280 (98%)	6 (2%)	0	100	100
1	D	262/328 (80%)	256 (98%)	6 (2%)	0	100	100
All	All	1094/1312 (83%)	1066 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	250/278 (90%)	249 (100%)	1 (0%)	84	89
1	B	231/278 (83%)	231 (100%)	0	100	100
1	C	250/278 (90%)	246 (98%)	4 (2%)	55	62
1	D	231/278 (83%)	229 (99%)	2 (1%)	70	78
All	All	962/1112 (86%)	955 (99%)	7 (1%)	76	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	PHE
1	C	13	GLU
1	C	38	THR
1	C	136	ARG
1	C	312	GLU
1	D	27	HIS
1	D	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	287	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	11	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	293/328 (89%)	0.39	20 (6%)	23 22	23, 42, 71, 88	1 (0%)
1	B	272/328 (82%)	0.85	26 (9%)	13 12	35, 57, 88, 104	0
1	C	292/328 (89%)	0.06	8 (2%)	56 55	19, 35, 64, 90	2 (0%)
1	D	272/328 (82%)	0.04	10 (3%)	45 44	21, 35, 64, 84	0
All	All	1129/1312 (86%)	0.33	64 (5%)	29 28	19, 42, 76, 104	3 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	ALA	6.1
1	B	301	VAL	6.0
1	B	38	THR	4.8
1	D	148	GLY	4.5
1	D	232	GLY	4.5
1	A	302	GLY	4.0
1	B	101	TYR	3.9
1	D	146	LEU	3.9
1	A	284	LEU	3.8
1	B	24	LEU	3.8
1	B	304	GLY	3.8
1	A	288	LEU	3.7
1	A	173	ALA	3.7
1	A	275	MET	3.6
1	A	283	VAL	3.5
1	B	148	GLY	3.4
1	A	174	ILE	3.4
1	B	14	SER	3.3
1	A	16	ASN	3.3
1	A	289	ALA	3.1
1	C	12	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	180	SER	3.1
1	A	164	SER	3.1
1	C	15	LEU	3.0
1	D	38	THR	3.0
1	A	241	PHE	3.0
1	C	177	VAL	2.9
1	B	146	LEU	2.8
1	D	179	VAL	2.8
1	C	181	SER	2.7
1	B	233	ASN	2.7
1	B	207	GLY	2.7
1	B	12	LEU	2.6
1	D	242	LEU	2.6
1	B	305	VAL	2.6
1	B	39	GLY	2.6
1	C	26	LYS	2.6
1	A	298	GLY	2.6
1	B	124	MET	2.6
1	D	206	LYS	2.6
1	A	128	GLY	2.5
1	B	36	THR	2.5
1	A	277	LEU	2.5
1	B	211	LEU	2.5
1	B	147	ARG	2.5
1	B	308	LEU	2.4
1	A	175	PHE	2.4
1	A	203	GLU	2.4
1	B	317	LYS	2.4
1	D	101	TYR	2.3
1	D	34	LEU	2.3
1	B	25	THR	2.3
1	A	27	HIS	2.2
1	A	306	THR	2.2
1	B	243	PRO	2.1
1	B	64	ILE	2.1
1	A	282	GLY	2.1
1	B	181	SER	2.1
1	C	246	LYS	2.1
1	B	229	LEU	2.1
1	C	38	THR	2.1
1	A	297	GLU	2.0
1	D	39	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	101	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.