Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:13 AM EST

PDB ID	:	3PS0
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:

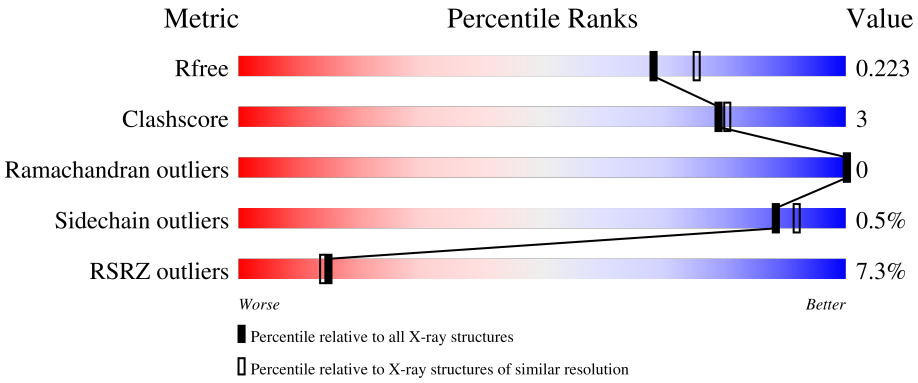
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	11% 74% 9% 17%
1	C	328	2% 84% 5% 11%
1	D	328	5% 79% 17%

2 Entry composition (i)

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

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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.

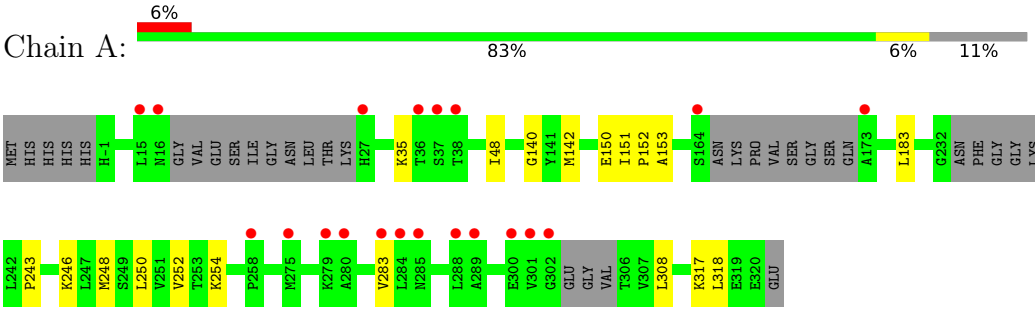
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	126	Total O 126 126	0	0
2	B	60	Total O 60 60	0	0
2	C	181	Total O 181 181	0	0
2	D	178	Total O 178 178	0	0

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.

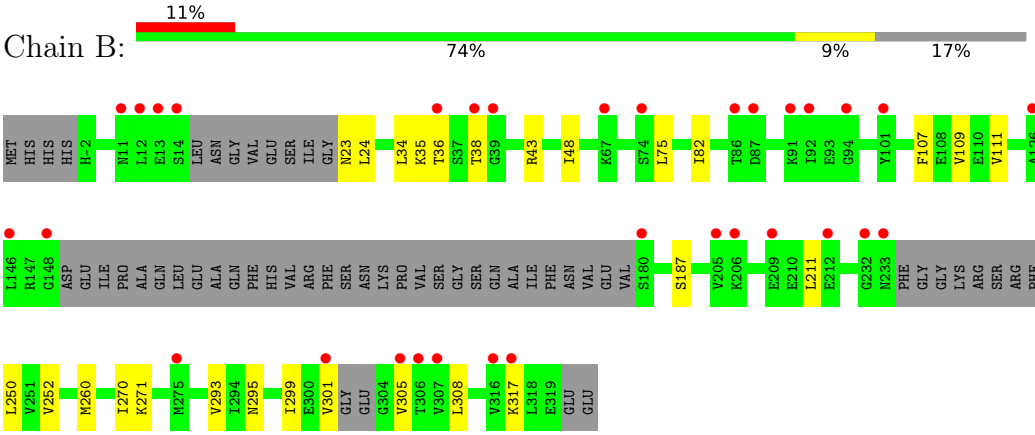
• Molecule 1: CRISPR-Associated protein, CSA2

Chain A:



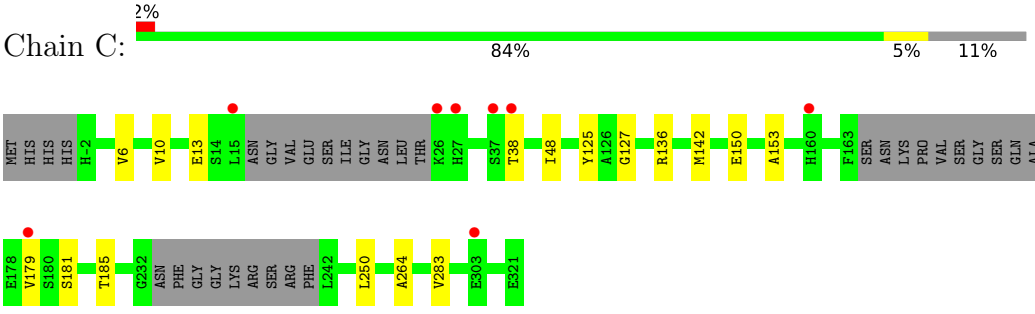
• Molecule 1: CRISPR-Associated protein, CSA2

Chain B:



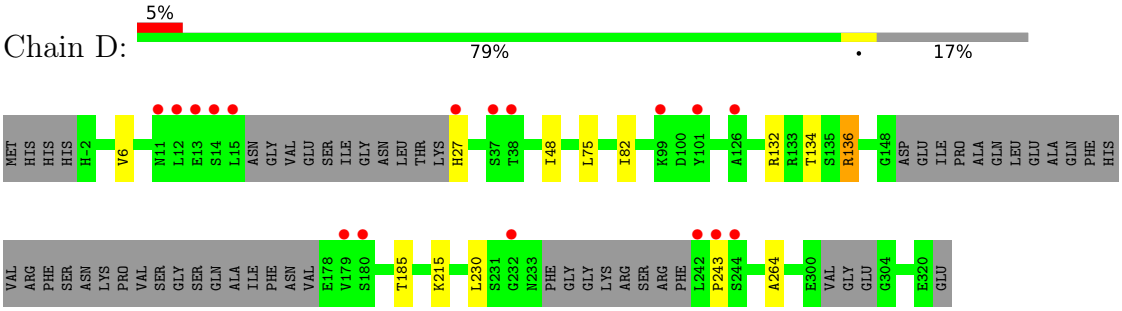
• Molecule 1: CRISPR-Associated protein, CSA2

Chain C:



• Molecule 1: CRISPR-Associated protein, CSA2

Chain D:


5%
79%
17%
MET HIS HIS HIS H-2 V6 N11 L12 E13 S14 L15 ASN GLY VAL GLU SER ILE GLY ASN LEU THR LYS H27 S37 T38 I48 L75 I82 K99 D100 Y101 A126 R132 R133 T134 S135 R136 G148 ASP GLU ILE PRO ALA GLN LEU GLU ALA GLN PHE HIS
VAL ARG PHE SER ASN LYS PRO VAL SER GLY SER GLN ALA ILE PHE ASN VAL E178 V179 S180 T185 K215 L230 S231 G232 N233 PHE GLY GLY LYS ARG SER ARG PHE L242 P243 S244 A264 E300 VAL GLY GLU G304 E320 GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	A	0.34	0/2332	0.51	0/3143
1	B	0.31	0/2141	0.48	0/2882
1	C	0.35	0/2332	0.51	0/3142
1	D	0.35	0/2143	0.54	2/2886 (0.1%)
All	All	0.34	0/8948	0.51	2/12053 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	136	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	136	ARG	NE-CZ-NH2	-5.13	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2290	0	2336	14	0
1	B	2108	0	2168	22	0
1	C	2287	0	2334	9	0
1	D	2110	0	2164	9	0
2	A	126	0	0	0	0
2	B	60	0	0	1	0
2	C	181	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	178	0	0	3	0
All	All	9340	0	9002	50	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 (50) 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:A:246:LYS:HD2	1:A:248:MET:HE3	1.86	0.58
1:B:38:THR:O	1:B:38:THR:HG22	2.07	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: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: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:293:VAL:HG23	1:B:305:VAL:HG11	1.93	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: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:187:SER:HB3	1:B:260:MET:HE2	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:250:LEU:C	1:B:250:LEU:HD12	2.38	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: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:C:10:VAL:HG21	1:C:142:MET:HE2	2.01	0.41
1:A:250:LEU:HD13	1:A:252:VAL:HG23	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: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
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%)	91 93
1	B	231/278 (83%)	231 (100%)	0	100 100
1	C	250/278 (90%)	247 (99%)	3 (1%)	71 76
1	D	231/278 (83%)	230 (100%)	1 (0%)	91 93
All	All	962/1112 (86%)	957 (100%)	5 (0%)	88 92

All (5) 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	D	27	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.23	21 (7%) 15 14	24, 42, 71, 88	0
1	B	272/328 (82%)	0.60	36 (13%) 3 2	35, 57, 88, 104	0
1	C	292/328 (89%)	0.10	8 (2%) 54 53	21, 35, 64, 90	0
1	D	272/328 (82%)	0.15	17 (6%) 20 19	21, 35, 64, 84	0
All	All	1129/1312 (86%)	0.27	82 (7%) 15 14	21, 42, 76, 104	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	9.3
1	B	101	TYR	8.7
1	A	283	VAL	6.3
1	B	126	ALA	6.1
1	D	13	GLU	5.7
1	B	38	THR	5.6
1	B	13	GLU	5.5
1	B	127	GLY	5.2
1	C	160	HIS	4.5
1	B	305	VAL	4.5
1	B	180	SER	4.4
1	A	285	ASN	4.2
1	D	242	LEU	4.1
1	B	12	LEU	4.1
1	B	301	VAL	4.1
1	A	280	ALA	4.0
1	C	303	GLU	4.0
1	B	233	ASN	4.0
1	D	232	GLY	3.8
1	B	317	LYS	3.8
1	C	26	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	15	LEU	3.8
1	B	128	GLY	3.7
1	D	14	SER	3.6
1	B	129	ALA	3.5
1	A	279	LYS	3.4
1	D	101	TYR	3.4
1	A	275	MET	3.3
1	A	258	PRO	3.3
1	B	91	LYS	3.2
1	B	14	SER	3.2
1	C	37	SER	3.2
1	A	289	ALA	3.2
1	B	316	VAL	3.1
1	D	37	SER	3.1
1	A	301	VAL	3.1
1	C	179	VAL	3.0
1	D	244	SER	3.0
1	A	16	ASN	3.0
1	B	206	LYS	2.9
1	B	11	ASN	2.9
1	B	94	GLY	2.9
1	B	307	VAL	2.9
1	A	37	SER	2.9
1	D	38	THR	2.9
1	B	209	GLU	2.8
1	B	36	THR	2.8
1	D	11	ASN	2.8
1	D	12	LEU	2.8
1	B	39	GLY	2.8
1	C	15	LEU	2.8
1	A	288	LEU	2.7
1	C	27	HIS	2.7
1	B	275	MET	2.6
1	D	180	SER	2.5
1	D	99	LYS	2.5
1	A	15	LEU	2.5
1	A	302	GLY	2.5
1	B	87	ASP	2.5
1	B	244	SER	2.5
1	D	27	HIS	2.5
1	B	205	VAL	2.4
1	B	148	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	146	LEU	2.4
1	A	27	HIS	2.4
1	A	241	PHE	2.3
1	B	86	THR	2.3
1	C	38	THR	2.3
1	B	92	ILE	2.2
1	B	306	THR	2.2
1	A	173	ALA	2.2
1	B	212	GLU	2.1
1	B	67	LYS	2.1
1	B	74	SER	2.1
1	D	126	ALA	2.1
1	D	179	VAL	2.1
1	D	243	PRO	2.1
1	A	300	GLU	2.1
1	A	164	SER	2.1
1	B	232	GLY	2.1
1	A	36	THR	2.0
1	A	38	THR	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 monosaccharides 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.