Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 04:59 PM EST

PDB ID	:	2NYD
Title	:	Crystal structure of Staphylococcus aureus hypothetical protein SA1388
Authors	:	Singh, K.S.; Zhang, X.; Zhang, H.
Deposited on	:	2006-11-20
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 (i) 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 (1)) were used in the production of this report:

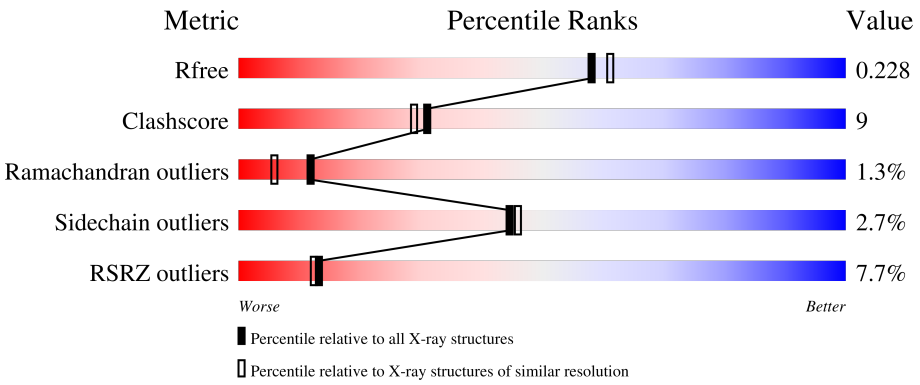
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	370	5% 69% 11% • 19%
1	B	370	9% 79% 13% • • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5932 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 UPF0135 protein SA1388.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2361	1507	388	454	12	0	1	0
1	B	348	2718	1739	441	524	14	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	cloning artifact	UNP P67273
A	-2	MET	-	cloning artifact	UNP P67273
A	-1	ASP	-	cloning artifact	UNP P67273
A	0	PRO	-	cloning artifact	UNP P67273
A	32	GLU	GLY	SEE REMARK 999	UNP P67273
A	115	VAL	ALA	SEE REMARK 999	UNP P67273
B	-3	ALA	-	cloning artifact	UNP P67273
B	-2	MET	-	cloning artifact	UNP P67273
B	-1	ASP	-	cloning artifact	UNP P67273
B	0	PRO	-	cloning artifact	UNP P67273
B	32	GLU	GLY	SEE REMARK 999	UNP P67273
B	115	VAL	ALA	SEE REMARK 999	UNP P67273

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is water.

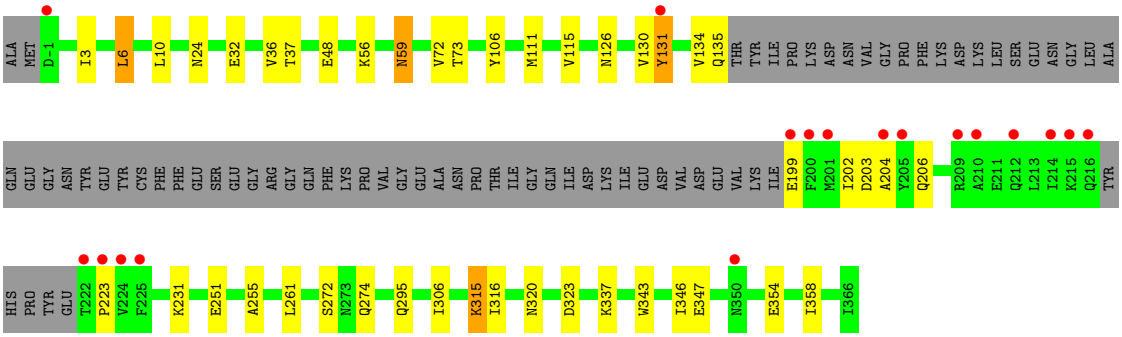
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	419	419	419	0	0
			Total	O		
3	B	430	430	430	0	0

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.

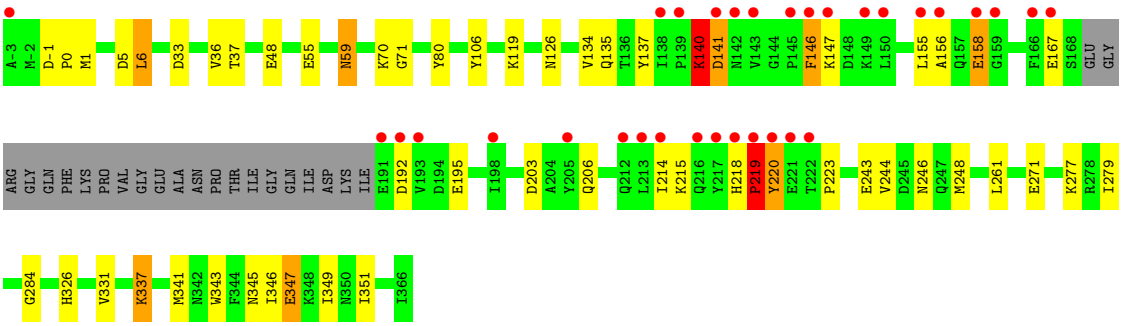
- Molecule 1: UPF0135 protein SA1388

Chain A:



- Molecule 1: UPF0135 protein SA1388

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	132.55Å 132.55Å 125.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.51 – 2.00 33.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (84.51-2.00) 94.8 (33.14-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.231 0.172 , 0.228	Depositor DCC
R_{free} test set	2675 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5932	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.81	1/2401 (0.0%)	0.76	0/3250
1	B	0.80	1/2769 (0.0%)	0.74	0/3751
All	All	0.80	2/5170 (0.0%)	0.75	0/7001

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	GLU	CG-CD	6.04	1.61	1.51
1	A	255	ALA	CA-CB	5.28	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	PRO	Peptide

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	2361	0	2343	42	0
1	B	2718	0	2668	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	419	0	0	17	0
3	B	430	0	0	17	0
All	All	5932	0	5011	92	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 9.

All (92) 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:346:ILE:HD13	3:A:678:HOH:O	1.10	1.23
1:B:346:ILE:CD1	3:B:832:HOH:O	1.87	1.18
1:B:346:ILE:HD13	3:B:832:HOH:O	1.46	1.06
1:B:33:ASP:HB3	3:B:698:HOH:O	1.59	1.03
1:B:55:GLU:HB3	3:B:689:HOH:O	1.58	1.02
1:B:167:GLU:HB2	1:B:195:GLU:OE1	1.67	0.93
1:A:315:LYS:HE2	3:A:496:HOH:O	1.74	0.88
1:B:0:PRO:HD2	3:B:581:HOH:O	1.79	0.83
1:A:316:ILE:HD11	3:A:451:HOH:O	1.81	0.80
1:A:316:ILE:HD13	1:B:80:TYR:CE2	2.18	0.78
1:B:156:ALA:HB2	3:B:799:HOH:O	1.84	0.77
1:B:140:LYS:HG3	1:B:141:ASP:H	1.52	0.72
1:B:140:LYS:HG3	1:B:141:ASP:N	2.07	0.69
1:B:203:ASP:H	1:B:206:GLN:HE21	1.42	0.66
1:B:126:ASN:HD22	1:B:126:ASN:H	1.43	0.64
1:B:48:GLU:HG3	3:B:439:HOH:O	1.98	0.63
1:B:244:VAL:HG13	1:B:279:ILE:HD11	1.79	0.62
1:A:106:TYR:HD2	3:A:544:HOH:O	1.82	0.62
1:A:111:MET:O	1:A:115:VAL:HG23	1.99	0.62
1:B:218:HIS:HB3	3:B:734:HOH:O	2.00	0.60
1:B:203:ASP:H	1:B:206:GLN:NE2	2.00	0.60
1:A:316:ILE:CD1	1:B:80:TYR:CE2	2.85	0.60
1:A:204:ALA:HA	3:A:790:HOH:O	2.01	0.59
1:B:106:TYR:HE1	3:B:503:HOH:O	1.84	0.59
1:A:135:GLN:NE2	3:A:773:HOH:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:CD1	3:A:451:HOH:O	2.44	0.59
1:B:218:HIS:CG	1:B:219:PRO:HD3	2.37	0.59
1:B:347:GLU:HB3	1:B:349:ILE:HD12	1.84	0.58
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:HA	1.69	0.58
1:B:243:GLU:OE1	1:B:277:LYS:HE3	2.02	0.58
1:B:218:HIS:CG	1:B:219:PRO:CD	2.87	0.57
1:A:126:ASN:H	1:A:126:ASN:HD22	1.53	0.57
1:B:214:ILE:O	1:B:218:HIS:HB2	2.05	0.56
1:A:337:LYS:HD3	3:A:516:HOH:O	2.05	0.56
1:A:48:GLU:HB3	1:A:358:ILE:HD13	1.89	0.55
1:B:218:HIS:CD2	1:B:219:PRO:HD2	2.44	0.53
1:A:316:ILE:HG13	3:A:607:HOH:O	2.07	0.53
1:B:37:THR:H	1:B:59:ASN:ND2	2.07	0.52
1:B:135:GLN:HB2	3:B:765:HOH:O	2.10	0.52
1:A:202:ILE:HB	1:A:206:GLN:HB2	1.91	0.52
1:B:246:ASN:O	1:B:248:MET:HG3	2.09	0.51
1:A:56:LYS:HE3	1:A:354:GLU:OE1	2.11	0.51
1:A:37:THR:H	1:A:59:ASN:ND2	2.08	0.51
1:A:316:ILE:HD12	1:B:80:TYR:CZ	2.45	0.51
1:B:220:TYR:O	1:B:223:PRO:HD3	2.10	0.51
1:A:3:ILE:HB	1:A:32:GLU:HA	1.93	0.51
1:A:343:TRP:HA	1:A:346:ILE:HD12	1.92	0.51
1:A:295[B]:GLN:HA	1:A:295[B]:GLN:NE2	2.25	0.50
1:A:274:GLN:HE21	1:A:320:ASN:HD21	1.60	0.50
1:B:346:ILE:HG13	3:B:558:HOH:O	2.11	0.49
1:A:251:GLU:HB2	1:A:272:SER:HB2	1.94	0.49
1:A:72:VAL:HG13	3:A:772:HOH:O	2.14	0.48
1:A:24:ASN:ND2	3:A:797:HOH:O	2.42	0.48
1:A:316:ILE:CD1	1:B:80:TYR:CZ	2.97	0.47
1:A:130:VAL:HG22	1:A:231:LYS:HD3	1.96	0.47
1:A:115:VAL:HG11	1:A:261:LEU:HD23	1.95	0.47
1:A:306:ILE:HD12	1:A:323:ASP:HB2	1.97	0.46
1:B:48:GLU:HG3	3:B:521:HOH:O	2.14	0.46
1:A:36:VAL:HA	1:A:59:ASN:HD21	1.81	0.46
1:B:126:ASN:H	1:B:126:ASN:ND2	2.11	0.46
1:B:215:LYS:HA	3:B:734:HOH:O	2.15	0.46
1:B:146:PHE:HD1	3:B:709:HOH:O	1.98	0.45
1:B:55:GLU:HG3	3:B:508:HOH:O	2.16	0.45
1:A:131:TYR:C	3:A:786:HOH:O	2.55	0.45
1:B:218:HIS:CD2	1:B:219:PRO:CD	3.01	0.44
1:A:346:ILE:HG12	3:A:817:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:HD2	1:B:223:PRO:CB	2.31	0.44
1:A:315:LYS:CE	3:A:496:HOH:O	2.46	0.44
1:B:36:VAL:HA	1:B:59:ASN:HD21	1.84	0.43
1:A:316:ILE:HD12	1:B:80:TYR:OH	2.18	0.43
1:B:-1:ASP:OD2	1:B:-1:ASP:N	2.51	0.43
1:B:1:MET:HE2	1:B:351:ILE:HD13	1.99	0.43
1:B:337:LYS:HE3	1:B:341:MET:SD	2.58	0.43
1:A:134:VAL:O	1:A:199:GLU:HA	2.19	0.43
1:B:70:LYS:O	1:B:71:GLY:C	2.57	0.43
1:A:316:ILE:CG1	3:A:451:HOH:O	2.67	0.42
1:B:1:MET:HE3	1:B:6:LEU:HG	2.00	0.42
1:A:6:LEU:HD22	1:A:10:LEU:HG	2.01	0.42
1:A:72:VAL:CG1	3:A:772:HOH:O	2.66	0.42
1:A:316:ILE:HG12	3:A:451:HOH:O	2.20	0.42
1:B:343:TRP:HA	1:B:346:ILE:HD12	2.01	0.42
1:B:244:VAL:HG13	1:B:279:ILE:CD1	2.46	0.42
1:B:137:TYR:HE1	3:B:765:HOH:O	2.00	0.41
1:B:140:LYS:CG	1:B:141:ASP:H	2.20	0.41
1:B:119:LYS:HB3	3:B:706:HOH:O	2.21	0.41
1:B:1:MET:HG3	1:B:5:ASP:HB2	2.03	0.41
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:CA	2.32	0.41
1:B:261:LEU:CD2	1:B:331:VAL:HG11	2.50	0.41
1:B:345:ASN:O	1:B:346:ILE:C	2.60	0.40
1:B:284:GLY:HA2	1:B:326:HIS:CD2	2.56	0.40
1:A:202:ILE:HD12	1:A:203:ASP:O	2.22	0.40
1:B:1:MET:CE	1:B:351:ILE:HD13	2.52	0.40

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	295/370 (80%)	285 (97%)	9 (3%)	1 (0%)	41	37
1	B	344/370 (93%)	322 (94%)	15 (4%)	7 (2%)	7	3
All	All	639/740 (86%)	607 (95%)	24 (4%)	8 (1%)	12	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	LYS
1	B	219	PRO
1	B	141	ASP
1	B	155	LEU
1	B	192	ASP
1	B	158	GLU
1	A	223	PRO
1	B	220	TYR

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	259/322 (80%)	253 (98%)	6 (2%)	50	53
1	B	294/322 (91%)	285 (97%)	9 (3%)	40	40
All	All	553/644 (86%)	538 (97%)	15 (3%)	44	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	59	ASN
1	A	73	THR
1	A	131	TYR
1	A	315	LYS
1	A	347	GLU
1	B	6	LEU
1	B	59	ASN

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Mol	Chain	Res	Type
1	B	134	VAL
1	B	140	LYS
1	B	146	PHE
1	B	147	LYS
1	B	158	GLU
1	B	337	LYS
1	B	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	59	ASN
1	A	126	ASN
1	A	128	GLN
1	A	206	GLN
1	A	274	GLN
1	A	317	HIS
1	B	24	ASN
1	B	59	ASN
1	B	126	ASN
1	B	206	GLN
1	B	218	HIS

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 (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	300/370 (81%)	-0.10	18 (6%)	21	20	12, 21, 80, 80	0
1	B	348/370 (94%)	0.17	32 (9%)	9	8	11, 21, 76, 80	0
All	All	648/740 (87%)	0.05	50 (7%)	13	12	11, 21, 78, 80	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	TYR	10.6
1	B	142	ASN	10.3
1	A	223	PRO	8.7
1	B	222	THR	8.4
1	A	224	VAL	8.4
1	B	155	LEU	7.7
1	B	143	VAL	7.1
1	B	221	GLU	6.6
1	B	146	PHE	5.9
1	B	141	ASP	5.7
1	B	145	PRO	5.6
1	A	212	GLN	5.5
1	A	131	TYR	5.5
1	B	191	GLU	5.3
1	A	222	THR	5.3
1	B	166	PHE	5.1
1	B	-3	ALA	4.8
1	B	216	GLN	4.7
1	B	217	TYR	4.6
1	B	219	PRO	4.5
1	A	215	LYS	4.4
1	A	216	GLN	4.4
1	B	150	LEU	4.2
1	B	158	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	3.9
1	A	205	TYR	3.8
1	B	218	HIS	3.6
1	A	201	MET	3.6
1	B	167	GLU	3.5
1	A	225	PHE	3.2
1	A	-1	ASP	3.2
1	A	214	ILE	3.1
1	B	159	GLY	3.0
1	B	198	ILE	2.9
1	A	200	PHE	2.8
1	A	209	ARG	2.7
1	B	147	LYS	2.7
1	B	149	LYS	2.7
1	A	210	ALA	2.7
1	B	212	GLN	2.6
1	B	192	ASP	2.6
1	B	139	PRO	2.6
1	A	204	ALA	2.4
1	B	214	ILE	2.4
1	B	156	ALA	2.3
1	A	199	GLU	2.3
1	A	350	ASN	2.3
1	B	213	LEU	2.3
1	B	138	ILE	2.2
1	B	205	TYR	2.1

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)

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(Å^2)	Q<0.9
2	ZN	A	401	1/1	0.98	0.05	50,50,50,50	0
2	ZN	A	402	1/1	0.98	0.06	48,48,48,48	0
2	ZN	B	401	1/1	0.99	0.09	41,41,41,41	0
2	ZN	B	402	1/1	0.99	0.08	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.