



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:45 AM UTC

PDB ID : 5AWS / pdb\_00005aws  
Title : Crystal structure of the SGIP1 mu homology domain in the P1 space group  
Authors : Shimada, A.; Yamaguchi, A.; Kohda, D.  
Deposited on : 2015-07-08  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

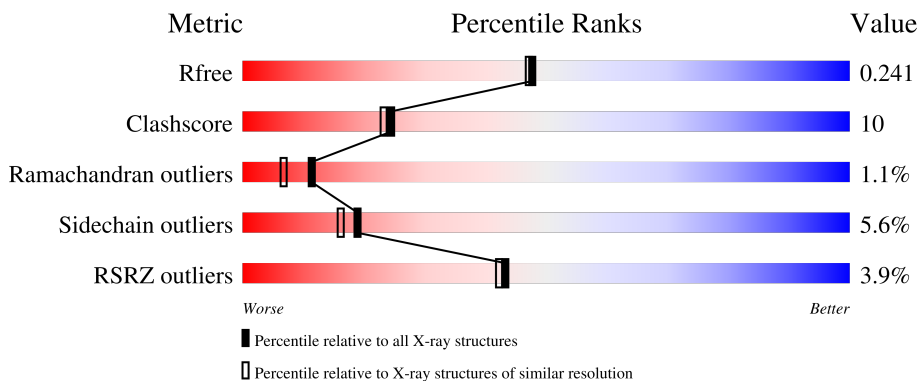
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

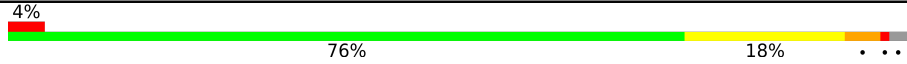
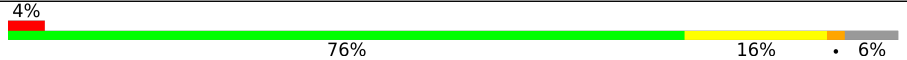
The reported resolution of this entry is 2.00 Å.

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  $\geq 3$ , 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	282	 4% 76% 18% • • •
1	B	282	 4% 76% 16% • 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4375 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 SH3-containing GRB2-like protein 3-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2123	1350	362	400	11	0	0	0
1	B	265	2052	1311	348	383	10	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	GLY	-	expression tag	UNP Q9BQI5
A	548	PRO	-	expression tag	UNP Q9BQI5
A	549	LEU	-	expression tag	UNP Q9BQI5
A	550	GLY	-	expression tag	UNP Q9BQI5
A	551	SER	-	expression tag	UNP Q9BQI5
B	547	GLY	-	expression tag	UNP Q9BQI5
B	548	PRO	-	expression tag	UNP Q9BQI5
B	549	LEU	-	expression tag	UNP Q9BQI5
B	550	GLY	-	expression tag	UNP Q9BQI5
B	551	SER	-	expression tag	UNP Q9BQI5

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	7	7	7	0	0
2	B	5	5	5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	102	102	102	0	0

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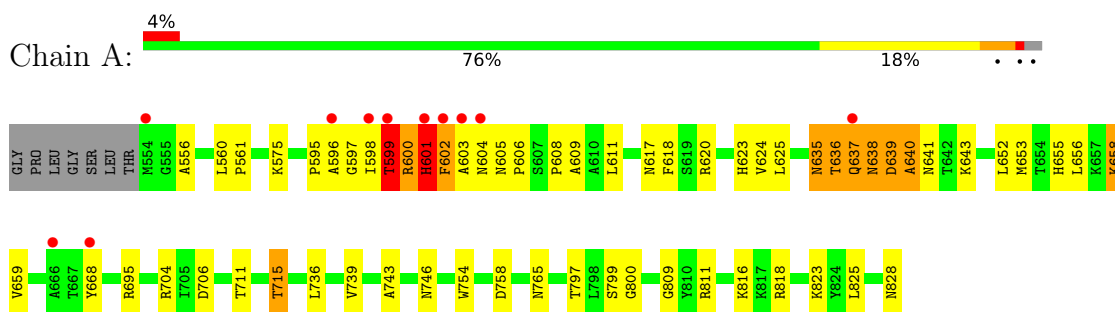
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	86	Total	O	0	0
			86	86		

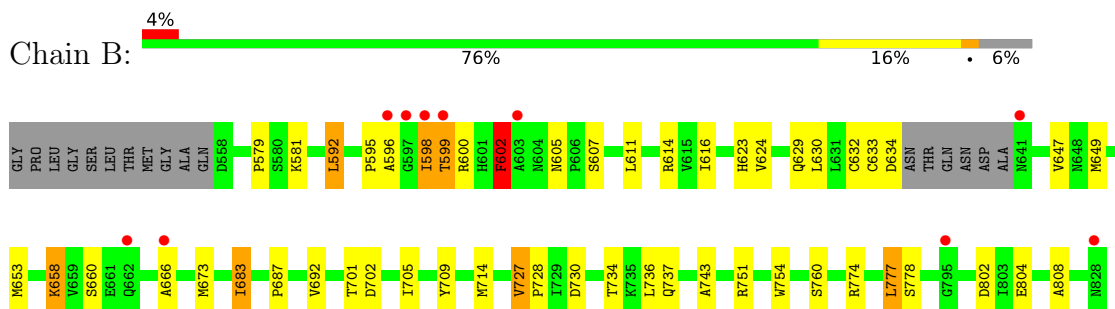
### 3 Residue-property plots [i](#)

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: SH3-containing GRB2-like protein 3-interacting protein 1



- Molecule 1: SH3-containing GRB2-like protein 3-interacting protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.55Å 53.63Å 75.20Å 101.87° 86.91° 95.61°	Depositor
Resolution (Å)	39.05 – 2.00 39.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (39.05-2.00) 89.0 (39.05-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.199 , 0.241 0.200 , 0.241	Depositor DCC
$R_{free}$ test set	1716 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtrriage
Anisotropy	0.818	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.51	0/2171	0.92	3/2956 (0.1%)
1	B	0.47	0/2099	0.87	1/2857 (0.0%)
All	All	0.49	0/4270	0.90	4/5813 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	601	HIS	N-CA-C	6.17	123.94	110.80
1	B	602	PHE	N-CA-C	-5.41	106.52	113.23
1	A	599	THR	N-CA-C	5.09	121.65	110.80
1	A	638	ASN	N-CA-C	-5.06	99.72	108.52

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	2123	0	2117	45	1
1	B	2052	0	2056	40	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
3	A	102	0	0	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	86	0	0	8	2
All	All	4375	0	4173	83	3

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 10.

All (83) 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:605:ASN:HB3	1:B:607:SER:H	1.28	0.98
1:A:604:ASN:ND2	3:A:1004:HOH:O	2.00	0.92
1:B:633:CYS:SG	3:B:1028:HOH:O	2.26	0.92
1:A:659:VAL:N	3:A:1002:HOH:O	2.07	0.86
1:A:638:ASN:O	1:A:640:ALA:N	2.10	0.84
1:A:655:HIS:O	3:A:1002:HOH:O	1.97	0.81
1:A:599:THR:HB	1:A:600:ARG:HD3	1.64	0.80
1:A:758:ASP:OD2	3:A:1003:HOH:O	1.99	0.79
1:B:605:ASN:HB3	1:B:607:SER:N	2.00	0.76
1:A:602:PHE:HE1	1:A:609:ALA:H	1.34	0.74
1:B:611:LEU:H	1:B:649:MET:HE3	1.56	0.69
1:A:600:ARG:O	1:A:602:PHE:N	2.23	0.69
1:B:737:GLN:HE21	1:B:774:ARG:HD3	1.58	0.67
1:B:611:LEU:HB3	1:B:649:MET:HE1	1.76	0.66
1:B:683:ILE:HD13	1:B:683:ILE:H	1.63	0.62
1:B:647:VAL:O	3:B:1002:HOH:O	2.16	0.62
1:B:632:CYS:HB3	3:B:1072:HOH:O	2.01	0.60
1:B:602:PHE:CE1	1:B:653:MET:HE1	2.36	0.59
1:B:701:THR:OG1	3:B:1001:HOH:O	2.10	0.59
1:B:595:PRO:O	1:B:598:ILE:HG22	2.04	0.58
1:A:746:ASN:ND2	3:A:1009:HOH:O	2.35	0.58
1:A:620:ARG:HG2	1:A:799:SER:O	2.05	0.57
1:A:575:LYS:NZ	1:A:828:ASN:O	2.33	0.56
1:A:596:ALA:O	1:A:598:ILE:N	2.38	0.56
1:A:636:THR:HB	1:A:637:GLN:C	2.31	0.56
1:B:629:GLN:OE1	3:B:1003:HOH:O	2.18	0.55
1:A:598:ILE:HG13	1:A:599:THR:H	1.71	0.54
1:B:592:LEU:HD22	1:B:673:MET:HG3	1.89	0.54
1:A:638:ASN:ND2	3:A:1011:HOH:O	2.40	0.54
1:A:659:VAL:HG22	3:A:1002:HOH:O	2.07	0.54
1:B:598:ILE:HG12	1:B:602:PHE:HB2	1.89	0.54
1:A:560:LEU:HD21	1:A:601:HIS:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ARG:NH1	1:A:706:ASP:OD1	2.39	0.53
1:A:823:LYS:HE2	1:A:825:LEU:HD11	1.90	0.52
1:B:702:ASP:OD1	1:B:774:ARG:NE	2.43	0.51
1:A:603:ALA:O	1:A:608:PRO:HD3	2.11	0.51
1:A:636:THR:HG22	1:A:637:GLN:HB3	1.91	0.51
1:B:599:THR:OG1	1:B:660:SER:HB2	2.10	0.51
1:B:743:ALA:HB2	1:B:754:TRP:CD1	2.46	0.50
1:A:715:THR:HG22	1:A:797:THR:O	2.13	0.49
1:B:737:GLN:NE2	1:B:774:ARG:HD3	2.26	0.49
1:B:760:SER:HB2	3:B:1052:HOH:O	2.12	0.48
1:A:605:ASN:HA	1:A:606:PRO:HA	1.71	0.48
1:A:560:LEU:N	1:A:809:GLY:O	2.35	0.48
1:A:635:ASN:N	1:A:635:ASN:OD1	2.47	0.48
1:A:811:ARG:NH2	3:A:1014:HOH:O	2.46	0.47
1:B:692:VAL:HG23	1:B:705:ILE:HG12	1.96	0.47
1:A:639:ASP:O	1:A:641:ASN:N	2.48	0.47
1:B:701:THR:OG1	1:B:777:LEU:HD21	2.14	0.46
1:A:736:LEU:HD12	1:A:739:VAL:HB	1.97	0.46
1:B:602:PHE:HD2	1:B:602:PHE:HA	1.63	0.46
1:A:816:LYS:CE	1:A:818:ARG:HH22	2.29	0.45
1:B:596:ALA:HB2	1:B:666:ALA:O	2.17	0.45
1:B:579:PRO:HB2	1:B:683:ILE:HD12	1.98	0.45
1:B:616:ILE:HD13	1:B:802:ASP:HB3	1.98	0.45
1:B:727:VAL:HA	1:B:728:PRO:HD3	1.73	0.45
1:A:600:ARG:O	1:A:603:ALA:N	2.37	0.45
1:B:808:ALA:O	3:B:1004:HOH:O	2.21	0.45
1:A:617:ASN:HA	1:A:641:ASN:OD1	2.17	0.44
1:A:658:LYS:HB2	1:A:658:LYS:HE2	1.71	0.44
1:A:743:ALA:HB2	1:A:754:TRP:CD1	2.52	0.44
1:A:560:LEU:HA	1:A:561:PRO:HD3	1.75	0.44
1:B:598:ILE:HD11	1:B:602:PHE:CD1	2.53	0.44
1:A:608:PRO:HG3	1:A:653:MET:HE1	2.00	0.44
1:B:709:TYR:CE1	1:B:760:SER:HA	2.53	0.44
1:B:614:ARG:NH1	1:B:804:GLU:OE2	2.52	0.43
1:A:618:PHE:N	1:A:641:ASN:O	2.42	0.43
1:B:658:LYS:HB2	1:B:658:LYS:HE2	1.67	0.43
1:A:715:THR:HG21	1:A:800:GLY:HA2	1.99	0.43
1:A:623:HIS:HB3	1:B:624:VAL:O	2.19	0.43
1:A:624:VAL:O	1:B:623:HIS:HB3	2.20	0.42
1:A:658:LYS:N	3:A:1002:HOH:O	2.51	0.42
1:A:711:THR:HG22	3:A:1030:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:LYS:HE3	1:A:818:ARG:HH22	1.84	0.42
1:B:709:TYR:CD1	1:B:760:SER:HA	2.54	0.42
1:B:730:ASP:HB2	3:B:1013:HOH:O	2.18	0.42
1:A:598:ILE:O	1:A:600:ARG:N	2.49	0.42
1:B:734:THR:CG2	1:B:778:SER:HB3	2.50	0.42
1:B:702:ASP:CG	1:B:774:ARG:HE	2.28	0.41
1:B:728:PRO:HA	1:B:751:ARG:HB3	2.03	0.40
1:A:656:LEU:C	3:A:1002:HOH:O	2.63	0.40
1:B:687:PRO:HB3	1:B:714:MET:SD	2.62	0.40
1:A:595:PRO:HA	1:A:668:TYR:CD1	2.57	0.40

All (3) 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)
3:B:1036:HOH:O	3:B:1080:HOH:O[1_455]	1.93	0.27
1:A:556:ALA:O	1:A:695:ARG:NH1[1_554]	2.15	0.05
3:A:1091:HOH:O	3:B:1081:HOH:O[1_666]	2.16	0.04

## 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	273/282 (97%)	256 (94%)	11 (4%)	6 (2%)	5 2
1	B	261/282 (93%)	252 (97%)	9 (3%)	0	100 100
All	All	534/564 (95%)	508 (95%)	20 (4%)	6 (1%)	11 7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	GLY

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Mol	Chain	Res	Type
1	A	601	HIS
1	A	602	PHE
1	A	639	ASP
1	A	599	THR
1	A	640	ALA

### 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	234/239 (98%)	221 (94%)	13 (6%)	19	16
1	B	227/239 (95%)	214 (94%)	13 (6%)	18	15
All	All	461/478 (96%)	435 (94%)	26 (6%)	19	16

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	599	THR
1	A	600	ARG
1	A	601	HIS
1	A	611	LEU
1	A	625	LEU
1	A	635	ASN
1	A	636	THR
1	A	637	GLN
1	A	643	LYS
1	A	652	LEU
1	A	658	LYS
1	A	715	THR
1	A	765	ASN
1	B	581	LYS
1	B	592	LEU
1	B	598	ILE
1	B	599	THR
1	B	600	ARG

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Mol	Chain	Res	Type
1	B	602	PHE
1	B	630	LEU
1	B	634	ASP
1	B	658	LYS
1	B	683	ILE
1	B	727	VAL
1	B	736	LEU
1	B	777	LEU

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	605	ASN
1	A	721	ASN
1	A	765	ASN
1	B	641	ASN
1	B	737	GLN
1	B	828	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](#)

Of 12 ligands modelled in this entry, 12 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/282 (97%)	0.24	11 (4%) 42 41	27, 51, 106, 136	0
1	B	265/282 (93%)	0.24	10 (3%) 44 43	30, 52, 95, 135	0
All	All	540/564 (95%)	0.24	21 (3%) 43 42	27, 52, 105, 136	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	GLY	4.8
1	A	598	ILE	3.4
1	A	554	MET	3.2
1	A	637	GLN	3.2
1	B	603	ALA	3.1
1	B	596	ALA	2.9
1	A	604	ASN	2.8
1	A	668	TYR	2.8
1	A	602	PHE	2.7
1	B	795	GLY	2.7
1	A	599	THR	2.7
1	B	666	ALA	2.6
1	B	662	GLN	2.6
1	B	641	ASN	2.3
1	A	603	ALA	2.2
1	B	828	ASN	2.2
1	B	598	ILE	2.1
1	A	596	ALA	2.1
1	A	666	ALA	2.1
1	A	601	HIS	2.1
1	B	599	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 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, 95<sup>th</sup> 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
2	ZN	A	906	1/1	0.74	0.09	169,169,169,169	0
2	ZN	B	905	1/1	0.78	0.13	202,202,202,202	0
2	ZN	B	902	1/1	0.84	0.09	134,134,134,134	0
2	ZN	B	904	1/1	0.85	0.08	131,131,131,131	0
2	ZN	B	903	1/1	0.89	0.08	128,128,128,128	0
2	ZN	A	902	1/1	0.93	0.08	91,91,91,91	0
2	ZN	A	905	1/1	0.97	0.13	62,62,62,62	0
2	ZN	A	901	1/1	0.98	0.04	97,97,97,97	0
2	ZN	A	907	1/1	0.98	0.03	40,40,40,40	0
2	ZN	A	903	1/1	0.99	0.02	42,42,42,42	0
2	ZN	B	901	1/1	0.99	0.06	72,72,72,72	0
2	ZN	A	904	1/1	0.99	0.02	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.