



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:34 am BST

PDB ID : 5AWS
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

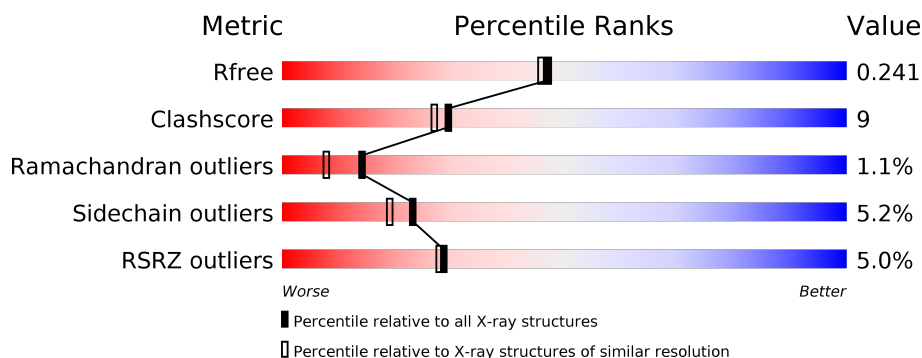
1 Overall quality at a glance

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}	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 on 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	282	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>•••</div> </div> </div>
1	B	282	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

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
1	A	275	Total	C	N	O	S	0	0	0
			2123	1350	362	400	11			
1	B	265	Total	C	N	O	S	0	0	0
			2052	1311	348	383	10			

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

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

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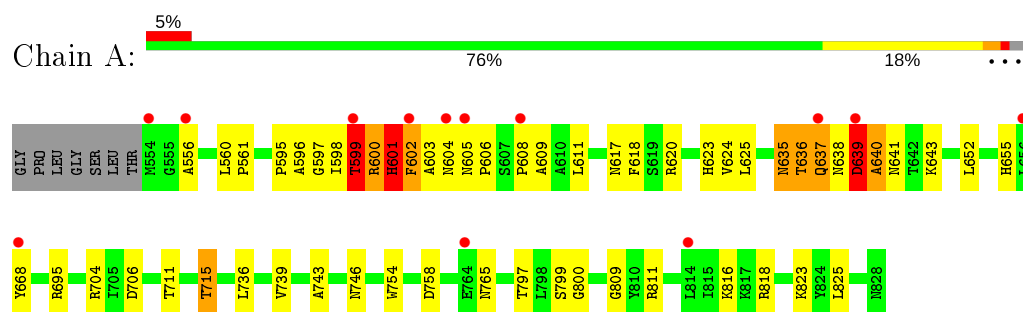
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	86	Total	O	0	0
			86	86		

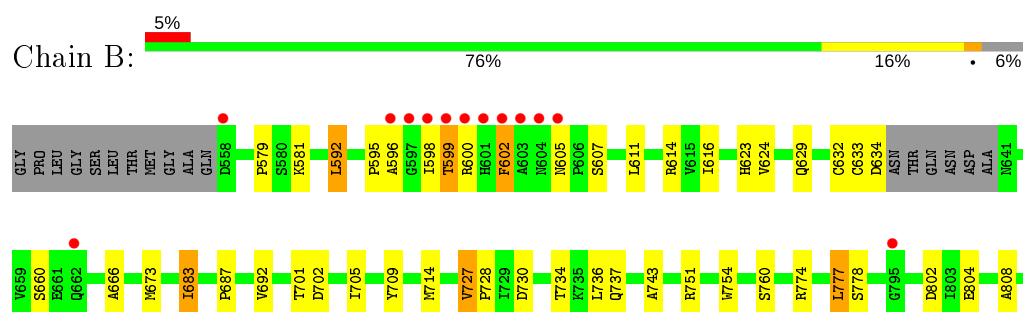
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, α , β , γ	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) 89.1 (39.05-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.199 , 0.241 0.199 , 0.241	Depositor DCC
R_{free} test set	1716 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4375	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	0.42	0/2171	0.67	0/2956
1	B	0.37	0/2099	0.63	0/2857
All	All	0.40	0/4270	0.65	0/5813

There are no bond length outliers.

There are no bond angle outliers.

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	2123	0	2117	43	1
1	B	2052	0	2056	38	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
3	A	102	0	0	10	1
3	B	86	0	0	8	2
All	All	4375	0	4173	79	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 9.

All (79) 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:611:LEU:HB3	1:B:649:MET:HE1	1.67	0.76
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:A:600:ARG:O	1:A:602:PHE:N	2.23	0.69
1:B:701:THR:OG1	3:B:1001:HOH:O	2.10	0.68
1:B:737:GLN:HE21	1:B:774:ARG:HD3	1.58	0.67
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: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:596:ALA:O	1:A:598:ILE:N	2.38	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:B:611:LEU:H	1:B:649:MET:HE3	1.71	0.54
1:A:560:LEU:HD21	1:A:601:HIS:HB3	1.89	0.53
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:HB	1:A:637:GLN:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:602:PHE:HD2	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:HE2	1:A:658:LYS:HB2	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: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:658:LYS:N	3:A:1002:HOH:O	2.51	0.42
1:A:624:VAL:O	1:B:623:HIS:HB3	2.20	0.42
1:A:711:THR:HG22	3:A:1030:HOH:O	2.19	0.42
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:A:657:LYS:O	1:A:660:SER:OG	2.27	0.41
1:B:728:PRO:HA	1:B:751:ARG:HB3	2.03	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%)	6	2
1	B	261/282 (93%)	252 (97%)	9 (3%)	0	100	100
All	All	534/564 (95%)	508 (95%)	20 (4%)	6 (1%)	14	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	GLY
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%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	227/239 (95%)	216 (95%)	11 (5%)	25	22
All	All	461/478 (96%)	437 (95%)	24 (5%)	23	19

All (24) 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	639	ASP
1	A	643	LYS
1	A	652	LEU
1	A	715	THR
1	A	765	ASN
1	B	581	LYS
1	B	592	LEU
1	B	599	THR
1	B	600	ARG
1	B	602	PHE
1	B	634	ASP
1	B	683	ILE
1	B	727	VAL
1	B	736	LEU
1	B	777	LEU
1	B	811	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	737	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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, 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	275/282 (97%)	0.10	14 (5%) 28 27	27, 51, 106, 136	0
1	B	265/282 (93%)	0.16	13 (4%) 29 28	30, 52, 95, 135	0
All	All	540/564 (95%)	0.13	27 (5%) 28 28	27, 52, 105, 136	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	605	ASN	6.2
1	A	637	GLN	5.9
1	A	604	ASN	5.0
1	A	602	PHE	4.5
1	A	605	ASN	4.5
1	A	668	TYR	4.3
1	B	597	GLY	3.9
1	B	599	THR	3.7
1	B	662	GLN	3.6
1	B	600	ARG	3.5
1	B	604	ASN	3.3
1	B	596	ALA	3.2
1	A	764	GLU	3.1
1	B	603	ALA	3.1
1	B	602	PHE	3.0
1	A	639	ASP	2.9
1	B	558	ASP	2.8
1	A	657	LYS	2.7
1	A	599	THR	2.7
1	A	556	ALA	2.7
1	B	598	ILE	2.5
1	A	608	PRO	2.3
1	A	554	MET	2.2
1	A	656	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	795	GLY	2.1
1	A	814	LEU	2.0
1	B	601	HIS	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 carbohydrates 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	B	903	1/1	0.66	0.06	128,128,128,128	0
2	ZN	A	906	1/1	0.79	0.10	169,169,169,169	0
2	ZN	B	905	1/1	0.85	0.16	202,202,202,202	0
2	ZN	A	902	1/1	0.88	0.14	91,91,91,91	0
2	ZN	B	902	1/1	0.90	0.14	134,134,134,134	0
2	ZN	A	905	1/1	0.97	0.03	62,62,62,62	0
2	ZN	B	904	1/1	0.97	0.04	131,131,131,131	0
2	ZN	A	901	1/1	0.98	0.05	97,97,97,97	0
2	ZN	A	907	1/1	0.98	0.14	40,40,40,40	0
2	ZN	A	904	1/1	0.99	0.14	41,41,41,41	0
2	ZN	B	901	1/1	0.99	0.14	72,72,72,72	0
2	ZN	A	903	1/1	0.99	0.13	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.