



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:23 PM UTC

PDB ID : 5PYT / pdb_00005pyt
Title : PanDDA analysis group deposition – Crystal Structure of SP100 after initial refinement with no ligand modelled (structure 89)
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Deposited on : 2017-02-08
Resolution : 2.13 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

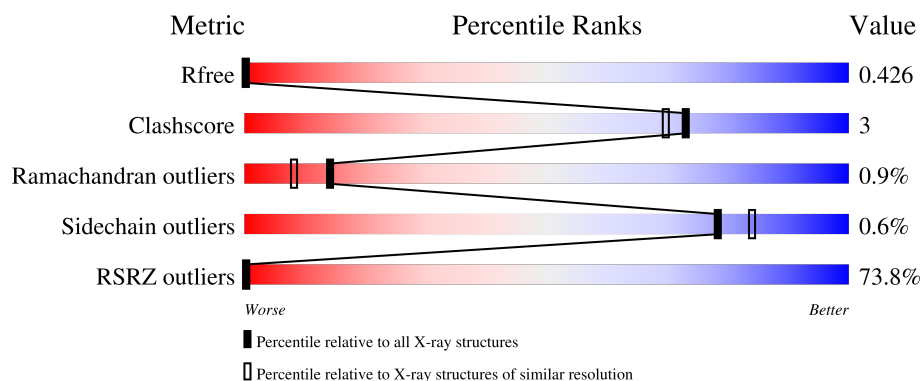
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	180	65% 92%7%
1	B	180	81% 92%6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	903	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3620 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 Nuclear autoantigen Sp-100.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	10	0
			1536	971	268	278	19			
1	B	177	Total	C	N	O	S	0	7	0
			1480	940	258	263	19			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	3
			314	314		
5	B	265	Total	O	0	0
			265	265		

- Molecule 1: Nuclear autoantigen Sp-100



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.59Å 45.41Å 83.50Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	38.97 – 2.13 38.97 – 2.13	Depositor EDS
% Data completeness (in resolution range)	87.3 (38.97-2.13) 87.3 (38.97-2.13)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.394 , 0.418 0.401 , 0.426	Depositor DCC
R_{free} test set	1289 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	-13.3	Xtriage
Anisotropy	-0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.38	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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](#)

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

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	0.93	0/1603	0.96	1/2154 (0.0%)
1	B	0.95	1/1538 (0.1%)	1.01	0/2071
All	All	0.94	1/3141 (0.0%)	0.98	1/4225 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	801	TYR	CA-C	8.56	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	ILE	CB-CA-C	-5.55	104.87	111.97

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	1536	0	1497	9	0
1	B	1480	0	1414	7	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	13	2	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
5	A	314	0	0	5	1
5	B	265	0	0	5	1
All	All	3620	0	2936	19	2

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 (19) 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:803[B]:ARG:NH1	5:A:1001:HOH:O	2.06	0.81
1:A:829[A]:ARG:NH1	5:A:1002:HOH:O	2.15	0.79
1:B:750:ILE:HD11	5:B:1001:HOH:O	1.88	0.74
3:A:904:MES:H81	5:A:1154:HOH:O	1.95	0.67
4:B:903:EDO:O2	5:B:1001:HOH:O	2.14	0.65
1:B:820:THR:OG1	5:B:1003:HOH:O	2.18	0.55
1:A:774[A]:GLU:HG2	1:A:778[A]:LYS:NZ	2.24	0.52
3:A:904:MES:C8	5:A:1154:HOH:O	2.55	0.50
1:B:757:SER:O	1:B:759:SER:N	2.42	0.50
1:B:826[B]:MET:HE2	5:B:1194:HOH:O	2.12	0.48
1:A:748:LYS:HE3	5:A:1270:HOH:O	2.16	0.46
1:A:701:ASN:ND2	1:A:716:CYS:HB3	2.32	0.45
1:A:774[A]:GLU:HG2	1:A:778[A]:LYS:HZ2	1.82	0.45
1:B:854[A]:THR:OG1	5:B:1002:HOH:O	2.16	0.44
1:A:803[A]:ARG:HB3	1:A:847:PHE:CZ	2.53	0.43
1:A:849:ARG:O	1:A:854[B]:THR:HG21	2.19	0.43
1:A:772:LEU:HB3	1:A:773:PRO:HD2	2.02	0.41
1:B:757:SER:C	1:B:759:SER:N	2.79	0.41
1:B:849:ARG:O	1:B:854[B]:THR:HG21	2.21	0.40

All (2) 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)
5:B:1183:HOH:O	5:B:1183:HOH:O[2_555]	0.92	1.28
5:A:1034:HOH:O	5:A:1221:HOH:O[1_545]	1.72	0.48

5.3 Torsion angles

5.3.1 Protein backbone

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	186/180 (103%)	182 (98%)	4 (2%)	0	100	100
1	B	182/180 (101%)	175 (96%)	4 (2%)	3 (2%)	7	2
All	All	368/360 (102%)	357 (97%)	8 (2%)	3 (1%)	14	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	757	SER
1	B	758	GLN
1	B	755	PRO

5.3.2 Protein sidechains

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	178/171 (104%)	178 (100%)	0	100	100
1	B	165/171 (96%)	161 (98%)	4 (2%)	43	45
All	All	343/342 (100%)	339 (99%)	4 (1%)	78	69

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	850[A]	GLU
1	B	850[B]	GLU
1	B	862[A]	ASP

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Mol	Chain	Res	Type
1	B	862[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	ASN
1	A	727	HIS
1	A	758	GLN
1	A	761	HIS
1	B	701	ASN
1	B	738	ASN
1	B	842	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	B	903	-	3,3,3	0.47	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	A	904	-	12,12,12	1.97	1 (8%)	15,16,16	2.38	7 (46%)
4	EDO	A	905	-	3,3,3	0.45	0	2,2,2	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	903	-	-	0/1/1/1	-
3	MES	A	904	-	-	4/6/14/14	0/1/1/1
4	EDO	A	905	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	904	MES	C8-S	-6.37	1.68	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	MES	C6-C5-N4	5.29	118.16	110.12
3	A	904	MES	O1S-S-C8	3.79	112.46	106.73
3	A	904	MES	O2S-S-C8	3.67	112.27	106.73
3	A	904	MES	O1-C6-C5	2.97	118.16	111.77
3	A	904	MES	O1-C2-C3	-2.28	106.86	111.77
3	A	904	MES	O2S-S-O1S	-2.23	106.58	113.82
3	A	904	MES	C6-O1-C2	2.12	116.73	109.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	904	MES	C7-C8-S-O1S
4	A	905	EDO	O1-C1-C2-O2
3	A	904	MES	C7-C8-S-O2S
3	A	904	MES	C8-C7-N4-C3
3	A	904	MES	C7-C8-S-O3S

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	EDO	1	0
3	A	904	MES	2	0

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	178/180 (98%)	3.08	117 (65%) 0 0	8, 21, 50, 94	10 (5%)
1	B	177/180 (98%)	3.58	145 (81%) 0 0	8, 22, 73, 123	7 (3%)
All	All	355/360 (98%)	3.33	262 (73%) 0 0	8, 21, 68, 123	17 (4%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	ALA	14.3
1	B	757	SER	12.3
1	B	800	TYR	10.9
1	B	805	GLY	10.7
1	A	738	ASN	10.6
1	A	736	ASN	10.3
1	A	737	LYS	10.3
1	B	806	SER	9.7
1	B	756	GLU	9.5
1	B	758	GLN	9.4
1	B	759	SER	8.7
1	A	807	GLN	8.3
1	B	755	PRO	8.1
1	B	735	ALA	8.1
1	B	711	TRP	8.0
1	B	804	GLU	7.8
1	A	753	ARG	7.8
1	A	734	GLU	7.7
1	B	760	GLY	7.7
1	A	877	THR	7.7
1	B	801	TYR	7.6
1	B	803	ARG	7.5
1	B	876	GLU	7.4
1	A	733	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	802	ASN	7.0
1	B	736	ASN	6.8
1	B	810	GLN	6.8
1	A	752	GLU	6.8
1	A	800	TYR	6.4
1	A	739	PRO	6.4
1	A	740	TRP	6.3
1	B	762	GLN	6.1
1	A	701	ASN	6.0
1	B	712	GLY	6.0
1	B	809	PRO	5.9
1	B	761	HIS	5.7
1	B	738	ASN	5.7
1	A	750	ILE	5.7
1	B	875	GLN	5.7
1	B	737	LYS	5.5
1	B	839	LEU	5.4
1	B	808	GLY	5.4
1	A	703	ASN	5.4
1	B	754	CYS	5.2
1	B	807	GLN	5.2
1	A	748	LYS	5.1
1	B	772	LEU	5.1
1	B	811	LYS	5.1
1	B	830	VAL	5.1
1	A	755	PRO	5.1
1	A	758	GLN	5.0
1	B	872	PHE	4.9
1	A	768	MET	4.9
1	A	878	SER	4.9
1	B	850[A]	GLU	4.8
1	B	714	LEU	4.8
1	A	751	GLN	4.8
1	B	713	ARG	4.8
1	A	719	THR	4.8
1	A	711	TRP	4.7
1	A	714	LEU	4.7
1	B	716[A]	CYS	4.7
1	A	718	ASP	4.6
1	A	846	GLU	4.6
1	B	734	GLU	4.6
1	A	845[A]	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	703	ASN	4.5
1	A	849	ARG	4.4
1	B	858	ILE	4.4
1	B	868	PHE	4.4
1	A	715	PHE	4.3
1	A	810	GLN	4.3
1	B	845	LYS	4.3
1	B	753	ARG	4.3
1	A	716	CYS	4.3
1	B	739	PRO	4.2
1	A	874	ILE	4.2
1	B	751	GLN	4.2
1	A	756	GLU	4.2
1	B	701	ASN	4.2
1	A	723	SER	4.1
1	A	712	GLY	4.1
1	A	702	SER	4.1
1	A	754[A]	CYS	4.1
1	A	781	PHE	4.1
1	A	704	ILE	4.1
1	A	720	CYS	4.1
1	B	752	GLU	4.1
1	B	769	ARG	4.1
1	A	824	GLU	4.1
1	A	850	GLU	4.0
1	A	713	ARG	4.0
1	A	710	LYS	4.0
1	B	833	PHE	4.0
1	B	750	ILE	4.0
1	B	788	CYS	3.9
1	A	809	PRO	3.9
1	B	740	TRP	3.9
1	B	873	ALA	3.8
1	B	799	PRO	3.8
1	A	747	ILE	3.8
1	A	766	VAL	3.8
1	B	710	LYS	3.8
1	A	717	CYS	3.7
1	A	709	ASN	3.7
1	A	732	SER	3.7
1	B	747	ILE	3.7
1	A	848	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	721	PRO	3.7
1	B	857	GLY	3.7
1	B	847	PHE	3.7
1	A	804	GLU	3.7
1	B	874	ILE	3.7
1	B	766	VAL	3.6
1	A	726	GLU	3.6
1	B	864	PHE	3.6
1	A	741	SER	3.6
1	B	790	SER	3.6
1	B	748	LYS	3.6
1	B	777	LEU	3.6
1	A	801	TYR	3.6
1	B	871	ILE	3.6
1	A	707	VAL	3.5
1	B	846	GLU	3.5
1	B	866	LYS	3.5
1	A	777	LEU	3.5
1	B	744	PHE	3.5
1	A	806	SER	3.5
1	A	840	ILE	3.5
1	B	768	MET	3.5
1	B	764[A]	SER	3.4
1	A	876	GLU	3.4
1	B	718	ASP	3.4
1	B	781	PHE	3.4
1	B	700	GLU	3.4
1	B	817	LYS	3.4
1	B	722	ARG	3.3
1	B	715	PHE	3.3
1	B	863	ILE	3.3
1	B	849	ARG	3.2
1	B	853	PHE	3.2
1	B	815	LEU	3.2
1	B	749	THR	3.2
1	A	774[A]	GLU	3.1
1	A	759	SER	3.1
1	A	847	PHE	3.1
1	A	705	CYS	3.1
1	A	855	ARG	3.1
1	B	798	GLU	3.1
1	B	827	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	773	PRO	3.1
1	A	749	THR	3.1
1	B	797	SER	3.1
1	A	814	TRP	3.0
1	A	799	PRO	3.0
1	B	793	CYS	3.0
1	B	767	LEU	3.0
1	B	848	TYR	3.0
1	B	733	VAL	3.0
1	B	704	ILE	3.0
1	B	840	ILE	3.0
1	A	808	GLY	3.0
1	B	854[A]	THR	3.0
1	B	844	HIS	3.0
1	A	830	VAL	2.9
1	A	842	HIS	2.9
1	B	860	VAL	2.9
1	B	855	ARG	2.9
1	B	814	TRP	2.9
1	B	742	CYS	2.8
1	A	731	PRO	2.8
1	B	794	PHE	2.8
1	B	707	VAL	2.8
1	B	720	CYS	2.8
1	B	818	VAL	2.8
1	B	821	SER	2.8
1	A	725	HIS	2.8
1	B	812	PRO	2.8
1	A	858	ILE	2.8
1	B	745	CYS	2.8
1	B	709	ASN	2.7
1	A	724	PHE	2.7
1	A	794	PHE	2.7
1	A	875	GLN	2.7
1	B	870	ASN	2.7
1	B	826[A]	MET	2.7
1	A	743	ILE	2.7
1	A	793	CYS	2.7
1	A	744	PHE	2.7
1	A	856	LEU	2.7
1	B	743	ILE	2.7
1	A	742	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	842	HIS	2.6
1	B	706	GLU	2.6
1	A	844	HIS	2.6
1	A	862[A]	ASP	2.6
1	B	823	ASN	2.6
1	A	868	PHE	2.5
1	B	841	PHE	2.5
1	B	770	GLN	2.5
1	B	776	GLN	2.5
1	A	708	CYS	2.5
1	A	829[A]	ARG	2.5
1	B	829[A]	ARG	2.5
1	B	702	SER	2.5
1	A	727	HIS	2.5
1	B	862[A]	ASP	2.5
1	B	730	ILE	2.5
1	A	745	CYS	2.5
1	A	805	GLY	2.5
1	A	730	ILE	2.5
1	A	770	GLN	2.4
1	B	824	GLU	2.4
1	A	782	LEU	2.4
1	B	717	CYS	2.4
1	B	723	SER	2.4
1	A	773	PRO	2.4
1	A	795	PHE	2.4
1	A	764	SER	2.4
1	A	826[A]	MET	2.4
1	B	859	GLN	2.4
1	B	786	VAL	2.4
1	A	852	LYS	2.4
1	B	719	THR	2.4
1	B	867	ASN	2.3
1	A	757	SER	2.3
1	B	825	GLN	2.3
1	A	822	LEU	2.3
1	A	722	ARG	2.3
1	A	812	PRO	2.3
1	B	820	THR	2.3
1	B	708	CYS	2.3
1	B	843	ASN	2.3
1	A	728	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	832	GLY	2.3
1	A	706	GLU	2.2
1	B	727	HIS	2.2
1	B	851	ASP	2.2
1	B	822	LEU	2.2
1	B	732	SER	2.2
1	A	762	GLN	2.2
1	A	851	ASP	2.2
1	B	774	GLU	2.1
1	B	791	LYS	2.1
1	B	763	GLU	2.1
1	A	820	THR	2.1
1	A	825	GLN	2.1
1	A	873	ALA	2.1
1	A	788	CYS	2.1
1	B	813	MET	2.1
1	B	775	GLU	2.1
1	B	787	TYR	2.1
1	B	869	ARG	2.1
1	A	860	VAL	2.1
1	A	771	MET	2.1
1	A	865	GLU	2.1
1	B	765	GLU	2.1
1	A	746	ARG	2.1
1	A	853	PHE	2.0
1	B	792	SER	2.0
1	B	796	ALA	2.0
1	B	856	LEU	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, 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	903	1/1	0.55	0.43	63,63,63,63	1
4	EDO	A	905	4/4	0.59	0.35	44,49,51,51	0
4	EDO	B	903	4/4	0.71	0.28	31,32,33,33	0
3	MES	A	904	12/12	0.77	0.26	22,24,27,27	12
2	ZN	B	902	1/1	0.92	0.07	20,20,20,20	0
2	ZN	A	902	1/1	0.95	0.03	25,25,25,25	0
2	ZN	A	901	1/1	0.95	0.05	19,19,19,19	0
2	ZN	B	901	1/1	0.98	0.03	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.