



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 PM UTC

PDB ID : 5PYI / pdb_00005pyi
Title : PanDDA analysis group deposition – Crystal Structure of SP100 after initial refinement with no ligand modelled (structure 78)
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Deposited on : 2017-02-08
Resolution : 2.29 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)

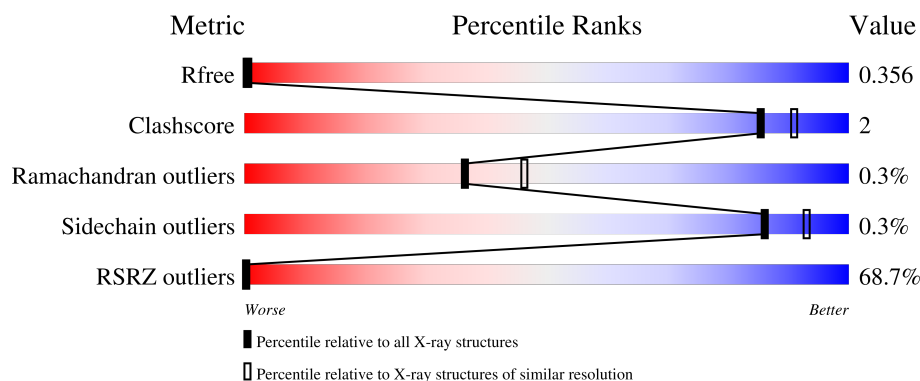
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	66% 94%
1	B	180	70% 91% 7%

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.

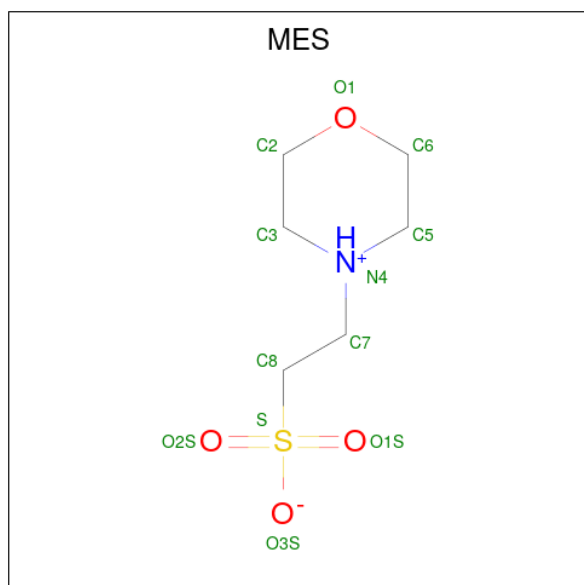
- Molecule 1 is a protein called Nuclear autoantigen Sp-100.

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).

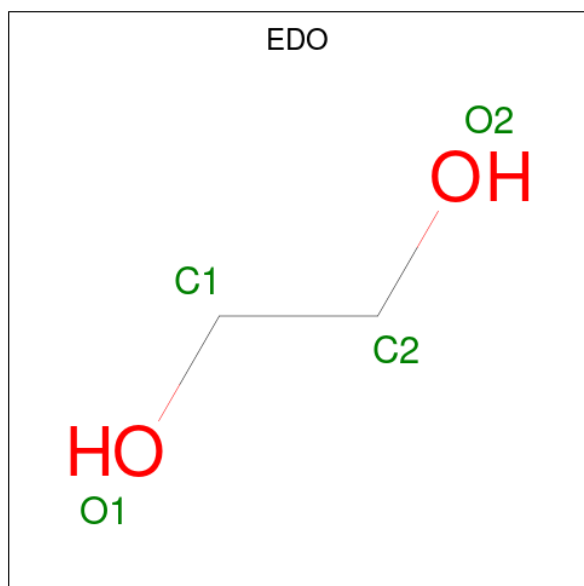
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	2	Total	Zn	0	0
			2	2		

- 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		

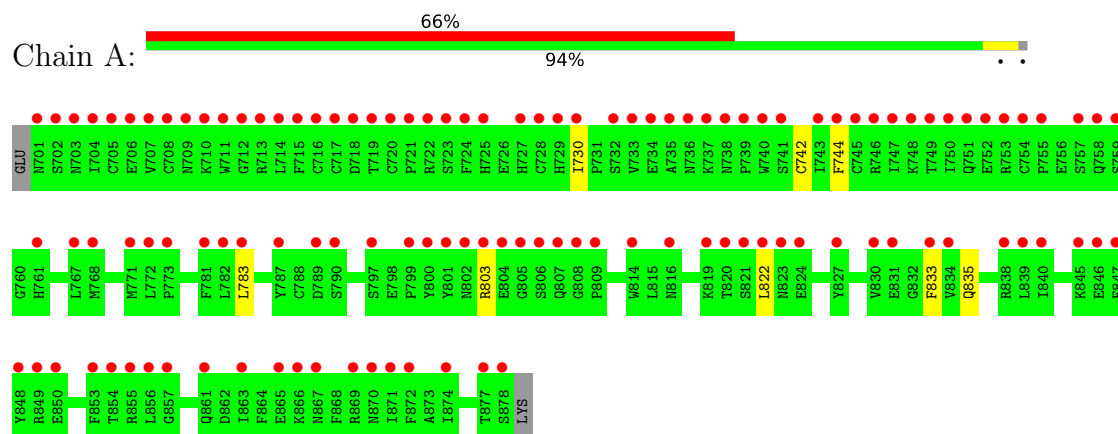
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	317	Total	O	0	3
			317	317		
5	B	262	Total	O	0	0
			262	262		

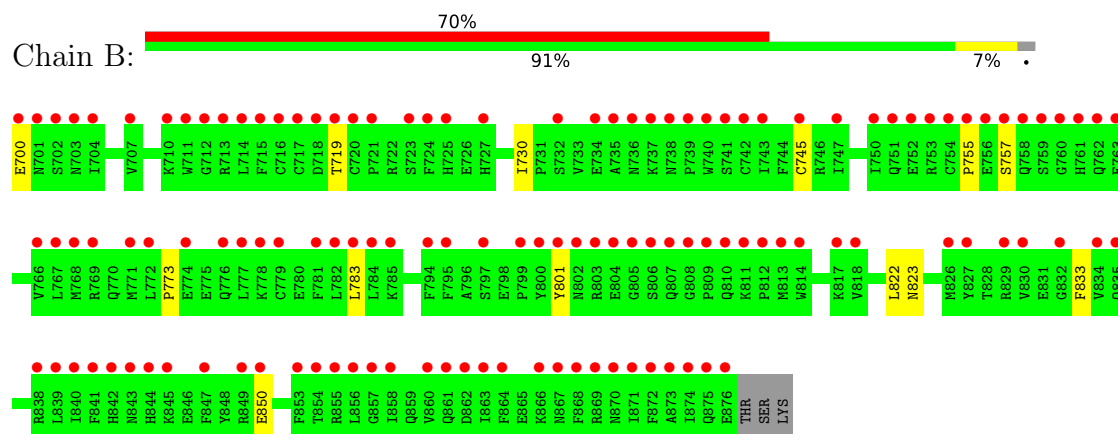
3 Residue-property plots

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: Nuclear autoantigen Sp-100



• 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	127.67Å 45.54Å 83.60Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	39.06 – 2.29 39.06 – 2.29	Depositor EDS
% Data completeness (in resolution range)	89.7 (39.06-2.29) 89.7 (39.06-2.29)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.286 , 0.349 0.298 , 0.356	Depositor DCC
R_{free} test set	1042 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: ZN, EDO, MES

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	0.79	0/1603	0.93	0/2154
1	B	0.80	1/1538 (0.1%)	0.96	0/2071
All	All	0.79	1/3141 (0.0%)	0.95	0/4225

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	801	TYR	CA-C	6.75	1.55	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	755	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	1536	0	1497	6	0
1	B	1480	0	1414	6	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	13	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	317	0	0	5	0
5	B	262	0	0	2	2
All	All	3620	0	2936	13	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 2.

All (13) 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:1002:HOH:O	2.28	0.67
1:B:823:ASN:ND2	5:B:1003:HOH:O	2.39	0.51
1:A:822:LEU:HD11	1:A:833:PHE:CE1	2.48	0.48
1:A:742:CYS:SG	1:A:744:PHE:HB2	2.54	0.47
1:B:700:GLU:N	5:B:1014:HOH:O	2.49	0.46
1:A:835:GLN:O	5:A:1001:HOH:O	2.21	0.45
1:B:730:ILE:HD13	1:B:783:LEU:HD23	1.97	0.45
5:A:1016:HOH:O	1:B:773:PRO:HG2	2.18	0.44
1:A:803[A]:ARG:NH2	5:A:1016:HOH:O	2.50	0.43
1:B:719:THR:OG1	1:B:745:CYS:SG	2.70	0.42
3:A:904:MES:H31	5:A:1116:HOH:O	2.20	0.42
1:B:822:LEU:HD11	1:B:833:PHE:CE1	2.55	0.41
1:A:730:ILE:HD13	1:A:783:LEU:HD23	2.03	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:1014:HOH:O	5:B:1014:HOH:O[2_556]	1.68	0.52
5:B:1009:HOH:O	5:B:1052:HOH:O[2_556]	2.10	0.10

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	186/180 (103%)	180 (97%)	6 (3%)	0	100	100
1	B	182/180 (101%)	172 (94%)	9 (5%)	1 (0%)	24	31
All	All	368/360 (102%)	352 (96%)	15 (4%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	757	SER

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	178/171 (104%)	178 (100%)	0	100	100
1	B	165/171 (96%)	163 (99%)	2 (1%)	63	79
All	All	343/342 (100%)	341 (99%)	2 (1%)	86	89

All (2) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	701	ASN
1	B	762	GLN
1	B	870	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 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$
3	MES	A	904	-	12,12,12	2.40	1 (8%)	15,16,16	1.90	5 (33%)
4	EDO	B	903	-	3,3,3	0.52	0	2,2,2	0.20	0
4	EDO	A	905	-	3,3,3	0.62	0	2,2,2	0.20	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
3	MES	A	904	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	903	-	-	1/1/1/1	-
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	-7.96	1.66	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	MES	O2S-S-C8	3.53	112.06	106.73
3	A	904	MES	C6-C5-N4	3.47	115.39	110.12
3	A	904	MES	C2-C3-N4	3.04	114.74	110.12
3	A	904	MES	C5-N4-C3	2.91	115.10	108.84
3	A	904	MES	O1-C2-C3	-2.22	107.00	111.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	904	MES	C8-C7-N4-C3
3	A	904	MES	C7-C8-S-O3S
3	A	904	MES	C7-C8-S-O1S
3	A	904	MES	C7-C8-S-O2S
4	B	903	EDO	O1-C1-C2-O2
4	A	905	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	MES	1	0

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, 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%)	2.76	118 (66%) 0 0	16, 32, 70, 114	10 (5%)
1	B	177/180 (98%)	3.02	126 (71%) 0 0	16, 35, 97, 128	7 (3%)
All	All	355/360 (98%)	2.89	244 (68%) 0 0	16, 33, 84, 128	17 (4%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	807	GLN	8.2
1	B	800	TYR	8.2
1	B	758	GLN	7.7
1	A	736	ASN	7.2
1	A	737	LYS	7.1
1	A	715	PHE	7.0
1	B	736	ASN	6.7
1	B	759	SER	6.5
1	A	703	ASN	6.4
1	A	847	PHE	6.3
1	A	719	THR	6.3
1	A	751	GLN	6.0
1	B	805	GLY	6.0
1	B	753	ARG	6.0
1	B	757	SER	6.0
1	B	766	VAL	5.9
1	B	761	HIS	5.9
1	B	756	GLU	5.9
1	A	721	PRO	5.8
1	B	760	GLY	5.8
1	A	735	ALA	5.6
1	B	737	LYS	5.6
1	B	801	TYR	5.5
1	B	711	TRP	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	874	ILE	5.4
1	B	814	TRP	5.4
1	A	805	GLY	5.4
1	B	806	SER	5.3
1	B	747	ILE	5.3
1	A	806	SER	5.1
1	A	752	GLU	5.1
1	B	762	GLN	5.0
1	B	804	GLU	5.0
1	B	875	GLN	5.0
1	B	839	LEU	4.9
1	B	807	GLN	4.9
1	B	854[A]	THR	4.9
1	B	834	VAL	4.9
1	A	743	ILE	4.9
1	A	714	LEU	4.8
1	B	719	THR	4.8
1	A	733	VAL	4.8
1	B	701	ASN	4.6
1	B	810	GLN	4.6
1	B	752	GLU	4.6
1	A	738	ASN	4.5
1	B	862[A]	ASP	4.5
1	A	740	TRP	4.5
1	B	738	ASN	4.4
1	A	877	THR	4.4
1	B	872	PHE	4.4
1	B	809	PRO	4.3
1	A	822	LEU	4.3
1	A	750	ILE	4.3
1	A	772	LEU	4.3
1	A	712	GLY	4.3
1	B	802	ASN	4.2
1	B	735	ALA	4.2
1	A	808	GLY	4.2
1	A	824	GLU	4.2
1	B	700	GLU	4.2
1	B	754	CYS	4.2
1	A	739	PRO	4.2
1	A	781	PHE	4.2
1	B	704	ILE	4.2
1	B	864	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	863	ILE	4.1
1	B	724	PHE	4.1
1	B	755	PRO	4.1
1	A	857	GLY	4.1
1	A	707	VAL	4.1
1	B	876	GLU	4.1
1	B	845	LYS	4.0
1	B	856	LEU	4.0
1	A	768	MET	4.0
1	A	755	PRO	3.9
1	A	711	TRP	3.9
1	A	710	LYS	3.9
1	A	800	TYR	3.9
1	B	866	LYS	3.9
1	A	849	ARG	3.9
1	B	783	LEU	3.9
1	A	722	ARG	3.9
1	A	790	SER	3.8
1	B	743	ILE	3.8
1	A	702	SER	3.8
1	A	732	SER	3.8
1	A	846	GLU	3.8
1	A	758	GLN	3.8
1	B	740	TRP	3.8
1	B	847	PHE	3.8
1	A	848	TYR	3.7
1	A	748	LYS	3.7
1	A	804	GLU	3.7
1	B	769	ARG	3.7
1	B	844	HIS	3.7
1	B	734	GLU	3.7
1	B	826[A]	MET	3.6
1	B	785	LYS	3.6
1	A	871	ILE	3.5
1	A	834	VAL	3.5
1	A	724	PHE	3.5
1	B	868	PHE	3.5
1	B	808	GLY	3.5
1	B	803	ARG	3.5
1	B	742	CYS	3.5
1	B	702	SER	3.4
1	A	704	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	870	ASN	3.4
1	A	797	SER	3.4
1	B	741	SER	3.4
1	B	812	PRO	3.4
1	A	854[A]	THR	3.3
1	A	866	LYS	3.3
1	A	803[A]	ARG	3.3
1	A	734	GLU	3.3
1	A	741	SER	3.3
1	B	750	ILE	3.3
1	A	801	TYR	3.3
1	A	718	ASP	3.2
1	B	772	LEU	3.2
1	A	856	LEU	3.2
1	A	773	PRO	3.2
1	A	730	ILE	3.2
1	A	708	CYS	3.2
1	B	778	LYS	3.2
1	B	811	LYS	3.2
1	A	747	ILE	3.2
1	B	732	SER	3.1
1	B	857	GLY	3.1
1	A	701	ASN	3.1
1	A	761	HIS	3.1
1	B	703	ASN	3.1
1	B	873	ALA	3.1
1	B	784	LEU	3.1
1	B	841	PHE	3.1
1	A	744	PHE	3.0
1	B	843	ASN	3.0
1	B	832	GLY	3.0
1	B	745	CYS	3.0
1	A	745	CYS	3.0
1	B	776	GLN	3.0
1	B	718	ASP	3.0
1	B	781	PHE	2.9
1	B	855	ARG	2.9
1	A	709	ASN	2.9
1	A	759	SER	2.9
1	B	723	SER	2.9
1	B	739	PRO	2.9
1	A	845[A]	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	717	CYS	2.9
1	A	867	ASN	2.9
1	A	809	PRO	2.9
1	B	795	PHE	2.8
1	A	874	ILE	2.8
1	A	723	SER	2.8
1	B	842	HIS	2.8
1	B	716[A]	CYS	2.8
1	B	797	SER	2.8
1	A	767	LEU	2.8
1	A	746	ARG	2.8
1	B	860	VAL	2.8
1	A	840	ILE	2.7
1	B	871	ILE	2.7
1	B	850[A]	GLU	2.7
1	B	768	MET	2.7
1	B	813	MET	2.7
1	B	713	ARG	2.7
1	B	717	CYS	2.7
1	B	774	GLU	2.7
1	B	869	ARG	2.7
1	A	787	TYR	2.7
1	A	853	PHE	2.7
1	B	715	PHE	2.7
1	A	831	GLU	2.7
1	B	763	GLU	2.7
1	A	782	LEU	2.7
1	B	767	LEU	2.7
1	B	751	GLN	2.6
1	B	853	PHE	2.6
1	A	749	THR	2.6
1	B	721	PRO	2.6
1	B	799	PRO	2.6
1	A	754[A]	CYS	2.6
1	B	710	LYS	2.6
1	A	850	GLU	2.5
1	A	720	CYS	2.5
1	B	858	ILE	2.5
1	A	869	ARG	2.5
1	B	849	ARG	2.5
1	A	870	ASN	2.5
1	A	820	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	706	GLU	2.4
1	A	728	CYS	2.4
1	A	878	SER	2.4
1	A	814	TRP	2.4
1	A	783	LEU	2.4
1	A	839	LEU	2.4
1	B	714	LEU	2.4
1	B	827	TYR	2.4
1	B	838	ARG	2.4
1	A	827	TYR	2.4
1	A	830	VAL	2.4
1	B	725	HIS	2.4
1	A	753	ARG	2.4
1	A	802	ASN	2.4
1	B	830	VAL	2.4
1	B	861	GLN	2.4
1	A	819	LYS	2.3
1	A	872	PHE	2.3
1	B	840	ILE	2.3
1	A	757	SER	2.3
1	A	861	GLN	2.3
1	B	818	VAL	2.3
1	A	816	ASN	2.3
1	B	771	MET	2.3
1	A	713	ARG	2.3
1	A	705	CYS	2.3
1	A	821	SER	2.3
1	B	727	HIS	2.2
1	B	817	LYS	2.2
1	A	833	PHE	2.2
1	B	777	LEU	2.2
1	B	794	PHE	2.2
1	A	771	MET	2.2
1	A	865	GLU	2.2
1	A	716	CYS	2.2
1	B	867	ASN	2.1
1	B	720	CYS	2.1
1	B	707	VAL	2.1
1	A	855	ARG	2.1
1	A	727	HIS	2.1
1	B	712	GLY	2.1
1	B	829[A]	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	725	HIS	2.1
1	A	823	ASN	2.1
1	A	729	HIS	2.0
1	B	835	GLN	2.0
1	A	789	ASP	2.0
1	B	782	LEU	2.0
1	A	799	PRO	2.0
1	B	779	CYS	2.0
1	A	838	ARG	2.0
1	A	863	ILE	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
4	EDO	A	905	4/4	0.54	0.31	43,47,48,50	0
2	ZN	A	903	1/1	0.72	0.16	66,66,66,66	1
3	MES	A	904	12/12	0.75	0.30	29,32,34,34	12
4	EDO	B	903	4/4	0.75	0.24	42,47,47,47	0
2	ZN	A	901	1/1	0.95	0.08	36,36,36,36	0
2	ZN	B	901	1/1	0.96	0.05	26,26,26,26	0
2	ZN	A	902	1/1	0.97	0.04	37,37,37,37	0
2	ZN	B	902	1/1	0.98	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.