



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:55 AM UTC

PDB ID : 5PZ5 / pdb_00005pz5
Title : PanDDA analysis group deposition – Crystal Structure of SP100 after initial refinement with no ligand modelled (structure 101)
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Deposited on : 2017-02-08
Resolution : 2.64 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)

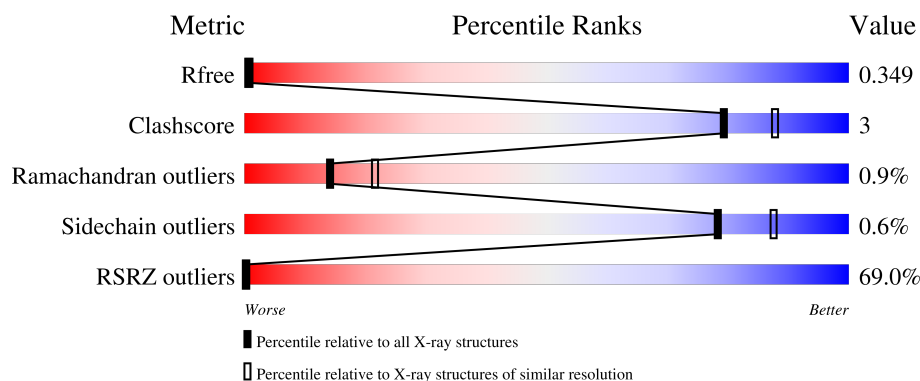
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	60% 91% 7% ..
1	B	180	76% 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
3	EDO	A	904	-	-	-	X
4	MES	B	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.

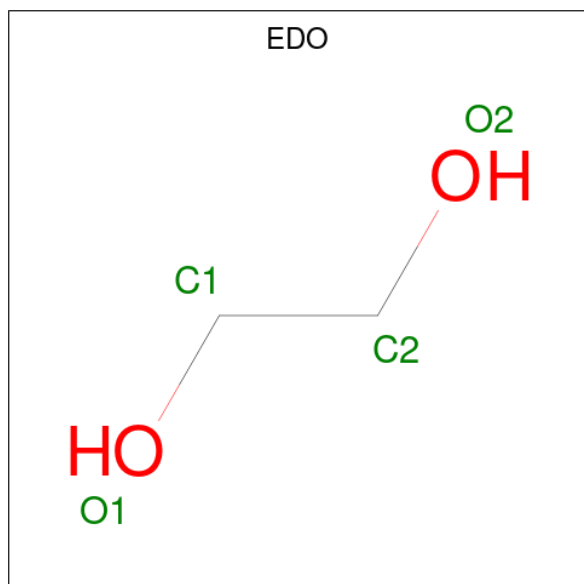
- Molecule 1 is a protein called Nuclear autoantigen Sp-100.

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).

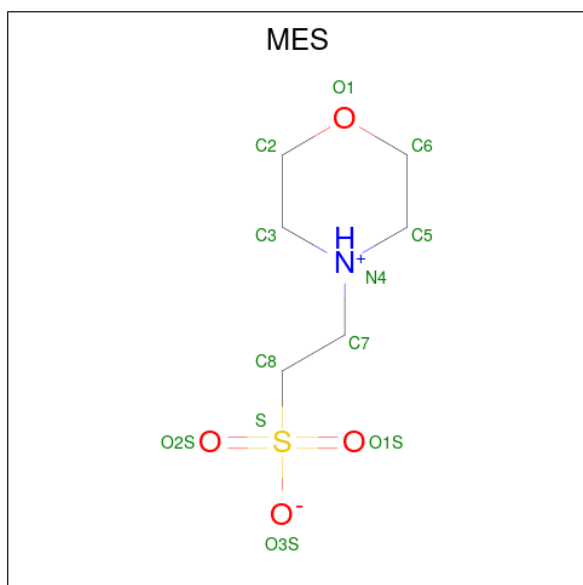
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

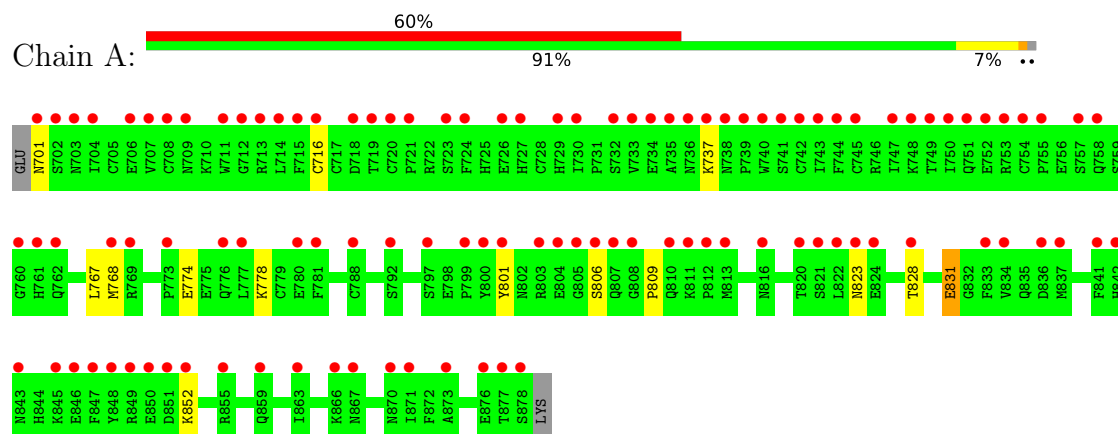
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	304	Total	O	0	3
			304	304		
5	B	275	Total	O	0	0
			275	275		

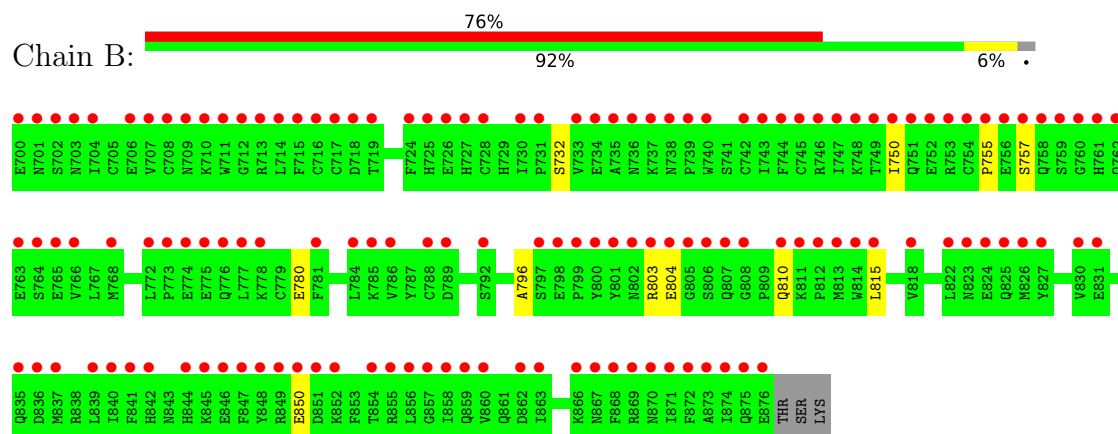
3 Residue-property plots

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	127.74Å 45.73Å 83.21Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	40.68 – 2.64 40.68 – 2.64	Depositor EDS
% Data completeness (in resolution range)	92.4 (40.68-2.64) 92.4 (40.68-2.64)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.293 , 0.347 0.298 , 0.349	Depositor DCC
R_{free} test set	671 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: EDO, MES, 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	0.72	0/1603	0.87	0/2154
1	B	0.72	0/1538	0.94	0/2071
All	All	0.72	0/3141	0.90	0/4225

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	1536	0	1497	11	0
1	B	1480	0	1414	5	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	12	0	0
4	B	12	0	13	1	0
5	A	304	0	0	7	1
5	B	275	0	0	2	1
All	All	3620	0	2936	16	1

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 (16) 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:806:SER:OG	5:A:1001:HOH:O	2.13	0.65
4:B:903:MES:C2	5:B:1007:HOH:O	2.49	0.59
1:A:701:ASN:N	5:A:1003:HOH:O	2.36	0.59
1:B:796:ALA:HA	1:B:815:LEU:HB2	1.94	0.50
1:A:737:LYS:CB	5:A:1186:HOH:O	2.60	0.50
1:A:768:MET:HE1	5:A:1117:HOH:O	2.15	0.47
1:A:767:LEU:O	1:A:831:GLU:HB2	2.16	0.46
1:A:852:LYS:NZ	1:B:780:GLU:OE2	2.48	0.46
5:A:1016:HOH:O	1:B:750:ILE:HD11	2.17	0.45
1:A:801:TYR:CD2	1:A:809:PRO:HD2	2.52	0.45
1:A:701:ASN:CG	1:A:716:CYS:HB3	2.42	0.45
1:A:823:ASN:ND2	5:A:1007:HOH:O	2.50	0.44
1:A:774[A]:GLU:HG2	1:A:778[A]:LYS:NZ	2.34	0.43
1:A:828:THR:HG22	5:A:1166:HOH:O	2.19	0.41
1:B:803:ARG:HA	1:B:804:GLU:HA	1.84	0.40
1:B:732:SER:O	5:B:1001:HOH:O	2.22	0.40

All (1) 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:A:1047:HOH:O	5:B:1007:HOH:O[1_545]	2.16	0.04

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%)	178 (96%)	7 (4%)	1 (0%)	24	36
1	B	182/180 (101%)	171 (94%)	9 (5%)	2 (1%)	11	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	368/360 (102%)	349 (95%)	16 (4%)	3 (1%)	14	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	757	SER
1	A	831	GLU
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%)	162 (98%)	3 (2%)	51	71
All	All	343/342 (100%)	340 (99%)	3 (1%)	78	82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	810	GLN
1	B	850[A]	GLU
1	B	850[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	758	GLN
1	A	823	ASN
1	B	701	ASN
1	B	727	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	$\# Z > 2$
3	EDO	A	904	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	A	905	-	3,3,3	0.47	0	2,2,2	0.24	0
4	MES	B	903	-	12,12,12	2.28	1 (8%)	15,16,16	1.57	3 (20%)

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	EDO	A	904	-	-	0/1/1/1	-
3	EDO	A	905	-	-	1/1/1/1	-
4	MES	B	903	-	-	3/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	903	MES	C8-S	-7.57	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	MES	O2S-S-C8	2.97	111.21	106.73
4	B	903	MES	C5-N4-C3	2.90	115.10	108.84
4	B	903	MES	C6-C5-N4	2.84	114.44	110.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	903	MES	C7-C8-S-O1S
4	B	903	MES	C7-C8-S-O3S
4	B	903	MES	C7-C8-S-O2S
3	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
4	B	903	MES	1	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%)	2.59	108 (60%) 0 0	16, 33, 76, 123	10 (5%)
1	B	177/180 (98%)	3.27	137 (77%) 0 0	16, 39, 132, 167	7 (3%)
All	All	355/360 (98%)	2.93	245 (69%) 0 0	16, 36, 93, 167	17 (4%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	806	SER	10.8
1	A	736	ASN	8.6
1	A	738	ASN	7.9
1	B	758	GLN	7.8
1	B	757	SER	7.8
1	B	803	ARG	7.7
1	B	759	SER	7.5
1	B	756	GLU	7.3
1	B	802	ASN	6.9
1	B	805	GLY	6.8
1	B	755	PRO	6.8
1	B	804	GLU	6.7
1	A	702	SER	6.5
1	A	701	ASN	6.5
1	B	876	GLU	6.4
1	B	736	ASN	6.4
1	B	753	ARG	6.3
1	A	878	SER	6.3
1	B	713	ARG	6.3
1	B	737	LYS	6.2
1	A	877	THR	6.1
1	B	735	ALA	6.1
1	B	762	GLN	5.9
1	B	711	TRP	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	800	TYR	5.7
1	A	703	ASN	5.7
1	A	735	ALA	5.7
1	A	733	VAL	5.6
1	B	849	ARG	5.5
1	B	702	SER	5.4
1	B	754	CYS	5.4
1	A	849	ARG	5.3
1	B	788	CYS	5.3
1	A	721	PRO	5.3
1	A	807	GLN	5.3
1	B	760	GLY	5.2
1	B	851	ASP	5.1
1	B	807	GLN	5.1
1	B	850[A]	GLU	5.1
1	B	855	ARG	5.0
1	B	701	ASN	4.9
1	B	704	ILE	4.9
1	B	738	ASN	4.8
1	B	761	HIS	4.8
1	B	716[A]	CYS	4.8
1	A	750	ILE	4.8
1	B	866	LYS	4.8
1	A	737	LYS	4.7
1	B	700	GLU	4.6
1	B	750	ILE	4.6
1	B	845	LYS	4.6
1	A	719	THR	4.5
1	A	716	CYS	4.5
1	B	875	GLN	4.5
1	B	826[A]	MET	4.4
1	A	855	ARG	4.3
1	A	752	GLU	4.3
1	B	825	GLN	4.3
1	A	800	TYR	4.2
1	A	739	PRO	4.2
1	B	810	GLN	4.1
1	A	846	GLU	4.1
1	B	712	GLY	4.0
1	A	851	ASP	4.0
1	B	749	THR	4.0
1	A	753	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	852	LYS	4.0
1	B	808	GLY	3.9
1	A	848	TYR	3.9
1	B	714	LEU	3.9
1	B	747	ILE	3.9
1	B	868	PHE	3.9
1	A	751	GLN	3.9
1	A	732	SER	3.9
1	B	768	MET	3.8
1	B	801	TYR	3.8
1	A	741	SER	3.8
1	A	734	GLU	3.8
1	B	831	GLU	3.8
1	A	805	GLY	3.8
1	B	734	GLU	3.8
1	A	804	GLU	3.7
1	A	797	SER	3.7
1	B	823	ASN	3.7
1	A	788	CYS	3.6
1	B	874	ILE	3.6
1	B	863	ILE	3.6
1	A	799	PRO	3.6
1	B	715	PHE	3.5
1	B	818	VAL	3.5
1	A	713	ARG	3.5
1	A	704	ILE	3.5
1	B	731	PRO	3.5
1	B	797	SER	3.4
1	B	717	CYS	3.4
1	B	867	ASN	3.4
1	B	870	ASN	3.4
1	B	841	PHE	3.4
1	B	740	TRP	3.4
1	B	827	TYR	3.4
1	A	836	ASP	3.4
1	A	744	PHE	3.4
1	A	811	LYS	3.3
1	B	726	GLU	3.3
1	B	774	GLU	3.3
1	A	742	CYS	3.3
1	A	850	GLU	3.3
1	A	808	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	739	PRO	3.3
1	A	715	PHE	3.3
1	A	730	ILE	3.3
1	B	743	ILE	3.3
1	B	822	LEU	3.2
1	A	806	SER	3.2
1	B	703	ASN	3.2
1	B	751	GLN	3.2
1	B	873	ALA	3.2
1	A	812	PRO	3.2
1	A	740	TRP	3.2
1	A	768	MET	3.1
1	B	789	ASP	3.1
1	B	812	PRO	3.1
1	B	844	HIS	3.1
1	A	870	ASN	3.1
1	B	836	ASP	3.1
1	B	856	LEU	3.1
1	A	706	GLU	3.1
1	B	728	CYS	3.1
1	B	752	GLU	3.1
1	B	746	ARG	3.1
1	A	748	LYS	3.0
1	B	744	PHE	3.0
1	B	772	LEU	3.0
1	A	843	ASN	3.0
1	B	710	LYS	3.0
1	A	828	THR	3.0
1	A	821	SER	3.0
1	A	876	GLU	3.0
1	B	813	MET	3.0
1	A	743	ILE	3.0
1	B	763	GLU	2.9
1	B	814	TRP	2.9
1	A	720	CYS	2.9
1	B	848	TYR	2.9
1	A	847	PHE	2.9
1	B	725	HIS	2.9
1	B	798	GLU	2.9
1	A	758	GLN	2.9
1	A	754[A]	CYS	2.9
1	A	824	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	757	SER	2.9
1	A	727	HIS	2.9
1	B	824	GLU	2.9
1	A	837	MET	2.9
1	A	803[A]	ARG	2.9
1	B	764[A]	SER	2.9
1	A	749	THR	2.9
1	B	719	THR	2.9
1	B	811	LYS	2.9
1	A	708	CYS	2.8
1	B	776	GLN	2.8
1	A	873	ALA	2.8
1	A	842	HIS	2.8
1	A	813	MET	2.8
1	A	712	GLY	2.8
1	A	781	PHE	2.8
1	B	786	VAL	2.8
1	B	792	SER	2.8
1	A	834	VAL	2.8
1	B	724	PHE	2.8
1	B	766	VAL	2.8
1	A	866	LYS	2.7
1	A	723	SER	2.7
1	A	780	GLU	2.7
1	B	854[A]	THR	2.7
1	A	776	GLN	2.7
1	B	840	ILE	2.7
1	B	709	ASN	2.7
1	B	846	GLU	2.7
1	A	707	VAL	2.7
1	B	777	LEU	2.7
1	B	765	GLU	2.7
1	A	841	PHE	2.7
1	B	745	CYS	2.6
1	A	845[A]	LYS	2.6
1	B	706	GLU	2.6
1	B	733	VAL	2.6
1	B	872	PHE	2.6
1	B	718	ASP	2.6
1	A	747	ILE	2.5
1	B	860	VAL	2.5
1	B	778	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	859	GLN	2.5
1	B	815	LEU	2.5
1	B	862[A]	ASP	2.5
1	A	867	ASN	2.4
1	A	714	LEU	2.4
1	A	792	SER	2.4
1	A	711	TRP	2.4
1	A	718	ASP	2.4
1	B	837	MET	2.4
1	A	822	LEU	2.4
1	A	762	GLN	2.4
1	B	835	GLN	2.4
1	A	724	PHE	2.4
1	B	869	ARG	2.4
1	B	730	ILE	2.4
1	B	784	LEU	2.4
1	A	761	HIS	2.4
1	A	709	ASN	2.3
1	A	773	PRO	2.3
1	B	742	CYS	2.3
1	A	769	ARG	2.3
1	B	839	LEU	2.3
1	B	858	ILE	2.3
1	A	833	PHE	2.3
1	A	820	THR	2.3
1	A	852	LYS	2.3
1	B	775	GLU	2.3
1	A	755	PRO	2.3
1	A	745	CYS	2.3
1	B	799	PRO	2.3
1	A	760	GLY	2.3
1	A	816	ASN	2.2
1	B	773	PRO	2.2
1	B	707	VAL	2.2
1	B	847	PHE	2.2
1	A	801	TYR	2.2
1	B	781	PHE	2.2
1	A	729	HIS	2.2
1	B	727	HIS	2.2
1	B	871	ILE	2.2
1	A	726	GLU	2.1
1	A	823	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	748	LYS	2.1
1	B	708	CYS	2.1
1	A	863	ILE	2.1
1	B	842	HIS	2.1
1	B	857	GLY	2.1
1	B	785	LYS	2.1
1	A	810	GLN	2.0
1	A	777	LEU	2.0
1	B	859	GLN	2.0
1	A	871	ILE	2.0
1	B	830	VAL	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
3	EDO	A	904	4/4	0.53	0.63	121,123,126,129	0
2	ZN	A	903	1/1	0.55	0.27	83,83,83,83	1
4	MES	B	903	12/12	0.58	0.47	90,94,101,103	12
3	EDO	A	905	4/4	0.75	0.27	65,68,69,69	0
2	ZN	B	901	1/1	0.97	0.04	29,29,29,29	0
2	ZN	A	901	1/1	0.97	0.06	26,26,26,26	0
2	ZN	A	902	1/1	0.98	0.03	33,33,33,33	0
2	ZN	B	902	1/1	1.00	0.02	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.