



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:44 PM UTC

PDB ID : 8AY2 / pdb_00008ay2
Title : Crystal structure of the C-terminal part of rat Sec8
Authors : Dong, G.; Lesigang, J.
Deposited on : 2022-09-01
Resolution : 2.50 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
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)
Validation Pipeline (wwPDB-VP)	:	2.49

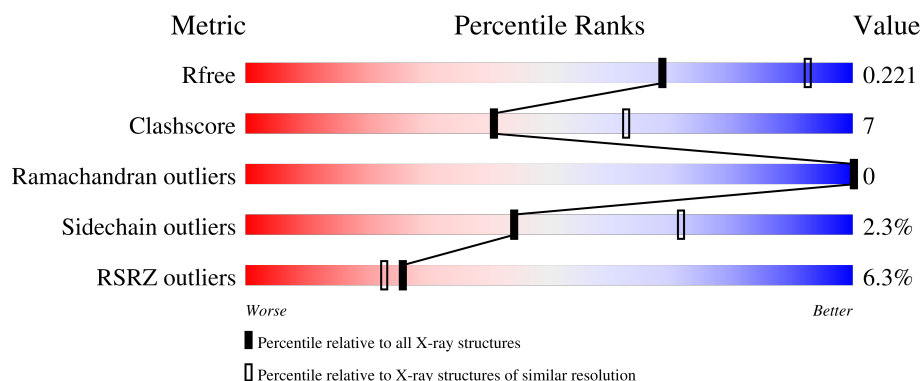
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

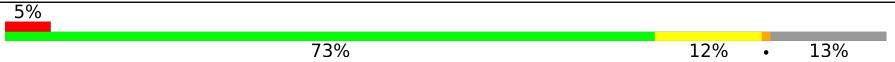
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	424	
1	B	424	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6184 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 Exocyst complex component 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3167	1999	538	607	23			
1	B	367	Total	C	N	O	S	0	0	0
			2927	1855	497	554	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	HIS	-	expression tag	UNP Q62824
A	553	MET	-	expression tag	UNP Q62824
B	552	HIS	-	expression tag	UNP Q62824
B	553	MET	-	expression tag	UNP Q62824

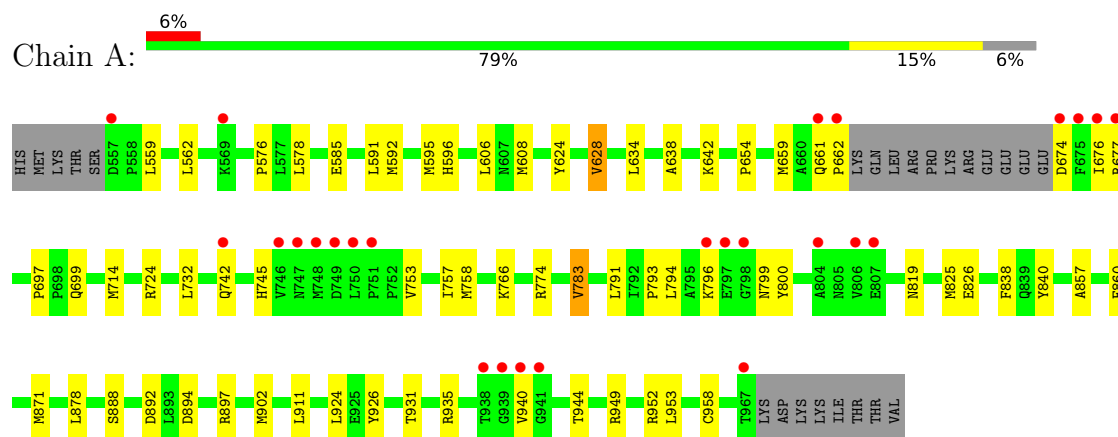
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	35	Total	O	0	0
			35	35		

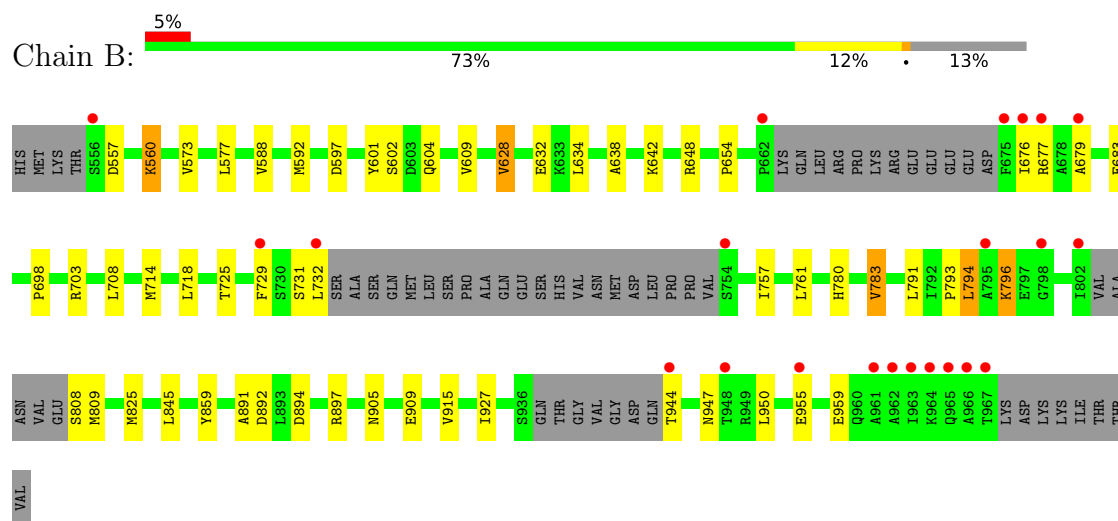
3 Residue-property plots [i](#)

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: Exocyst complex component 4



• Molecule 1: Exocyst complex component 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	190.00Å 190.00Å 175.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.6 (19.99-2.50) 89.2 (19.99-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.189 , 0.215 0.195 , 0.221	Depositor DCC
R_{free} test set	1999 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6184	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

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	0.18	0/3216	0.43	0/4347
1	B	0.16	0/2969	0.47	0/4003
All	All	0.17	0/6185	0.45	0/8350

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	3167	0	3190	49	0
1	B	2927	0	2963	34	0
2	A	55	0	0	2	0
2	B	35	0	0	3	0
All	All	6184	0	6153	80	0

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 7.

All (80) 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:753:VAL:HG11	1:A:758:MET:HE3	1.47	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:PRO:HG3	1:B:796:LYS:HE3	1.54	0.89
1:B:642:LYS:NZ	2:B:1001:HOH:O	2.16	0.79
1:A:800:TYR:HE2	1:A:871:MET:HE2	1.51	0.75
1:B:677:ARG:NH2	2:B:1003:HOH:O	2.19	0.74
1:B:894:ASP:OD1	1:B:897:ARG:NH2	2.22	0.73
1:B:944:THR:OG1	1:B:947:ASN:OD1	2.11	0.68
1:B:677:ARG:HH12	1:B:891:ALA:HB3	1.58	0.67
1:B:796:LYS:HD2	1:B:859:TYR:O	1.97	0.65
1:A:888:SER:OG	2:A:1001:HOH:O	2.15	0.64
1:A:642:LYS:HA	1:A:774:ARG:HH12	1.64	0.62
1:B:892:ASP:OD2	2:B:1002:HOH:O	2.16	0.61
1:A:911:LEU:HD22	1:A:953:LEU:HD13	1.81	0.60
1:A:860:PHE:O	1:A:935:ARG:NH2	2.33	0.59
1:B:905:ASN:HB3	1:B:909:GLU:HB2	1.83	0.59
1:B:808:SER:O	1:B:809:MET:HE2	2.02	0.59
1:A:591:LEU:HD21	1:A:608:MET:HE2	1.85	0.58
1:A:677:ARG:NH1	1:A:892:ASP:OD2	2.36	0.58
1:A:628:VAL:HG22	1:A:638:ALA:HB2	1.87	0.56
1:B:592:MET:HE3	1:B:609:VAL:HG21	1.88	0.56
1:A:799:ASN:C	1:A:800:TYR:HD1	2.14	0.56
1:A:606:LEU:HB3	1:A:757:ILE:HG21	1.88	0.55
1:A:595:MET:HE1	1:A:606:LEU:HG	1.87	0.55
1:A:766:LYS:NZ	2:A:1004:HOH:O	2.38	0.55
1:A:783:VAL:HG22	1:A:825:MET:SD	2.47	0.53
1:B:588:VAL:HG22	1:B:609:VAL:HG13	1.89	0.53
1:A:940:VAL:CG2	1:A:949:ARG:HH12	2.22	0.52
1:B:676:ILE:HD12	1:B:679:ALA:HB3	1.91	0.52
1:A:624:TYR:HB2	1:A:714:MET:HE1	1.92	0.52
1:B:601:TYR:HD1	1:B:604:GLN:OE1	1.94	0.51
1:A:753:VAL:CG1	1:A:758:MET:HE3	2.32	0.49
1:A:742:GLN:HA	1:A:745:HIS:ND1	2.27	0.49
1:B:729:PHE:CE2	1:B:761:LEU:HG	2.48	0.49
1:B:783:VAL:HG13	1:B:825:MET:SD	2.53	0.49
1:A:931:THR:HG22	1:A:935:ARG:NH1	2.28	0.48
1:B:698:PRO:O	1:B:703:ARG:NH1	2.46	0.48
1:B:791:LEU:O	1:B:794:LEU:HB2	2.12	0.48
1:B:628:VAL:HG13	1:B:634:LEU:HD22	1.94	0.48
1:B:955:GLU:O	1:B:959:GLU:N	2.31	0.48
1:A:642:LYS:HA	1:A:774:ARG:NH1	2.28	0.48
1:B:714:MET:O	1:B:718:LEU:HD13	2.13	0.48
1:A:606:LEU:HA	1:A:606:LEU:HD23	1.74	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:VAL:HG22	1:B:638:ALA:HB2	1.95	0.47
1:A:894:ASP:OD1	1:A:897:ARG:NH1	2.46	0.47
1:A:796:LYS:HE2	1:B:793:PRO:CG	2.45	0.46
1:A:902:MET:HE1	1:A:926:TYR:CE1	2.50	0.46
1:B:955:GLU:OE1	1:B:955:GLU:N	2.46	0.46
1:A:562:LEU:HD13	1:A:576:PRO:HB3	1.97	0.46
1:B:708:LEU:CD1	1:B:825:MET:HE2	2.45	0.46
1:A:791:LEU:O	1:A:794:LEU:HB2	2.15	0.46
1:B:677:ARG:NH1	1:B:891:ALA:HB3	2.28	0.45
1:A:857:ALA:HA	1:A:860:PHE:HD2	1.80	0.45
1:B:683:GLU:OE2	1:B:780:HIS:NE2	2.37	0.45
1:A:732:LEU:CD1	1:A:758:MET:HE1	2.47	0.45
1:A:674:ASP:HB2	1:A:677:ARG:HB3	1.99	0.45
1:A:628:VAL:HG13	1:A:634:LEU:HD22	1.99	0.44
1:A:742:GLN:HA	1:A:745:HIS:HD1	1.81	0.44
1:A:902:MET:HE1	1:A:926:TYR:HE1	1.83	0.44
1:B:654:PRO:HD2	1:B:679:ALA:HB1	1.99	0.44
1:B:573:VAL:HG11	1:B:577:LEU:HD11	2.00	0.44
1:A:826:GLU:HG2	1:A:838:PHE:HZ	1.82	0.44
1:A:819:ASN:OD1	1:A:878:LEU:HD23	2.18	0.44
1:A:562:LEU:HD23	1:A:578:LEU:HD23	2.00	0.43
1:B:725:THR:HB	1:B:729:PHE:CE2	2.53	0.43
1:A:911:LEU:HD12	1:A:952:ARG:NH2	2.33	0.43
1:A:559:LEU:HD21	1:A:714:MET:SD	2.59	0.42
1:B:731:SER:OG	1:B:732:LEU:HD22	2.19	0.42
1:A:659:MET:HE2	1:A:840:TYR:CG	2.54	0.42
1:A:654:PRO:HB2	1:A:676:ILE:HG12	2.02	0.42
1:A:826:GLU:HG2	1:A:838:PHE:CZ	2.55	0.42
1:A:585:GLU:OE2	1:A:724:ARG:NH1	2.53	0.41
1:A:697:PRO:HB2	1:A:699:GLN:OE1	2.19	0.41
1:A:800:TYR:CE2	1:A:871:MET:HE2	2.42	0.41
1:B:927:ILE:HG23	1:B:950:LEU:HD11	2.01	0.41
1:A:758:MET:HA	1:A:758:MET:HE2	2.01	0.41
1:A:796:LYS:HE2	1:B:793:PRO:HG3	2.03	0.41
1:A:661:GLN:HA	1:A:662:PRO:HD3	1.89	0.41
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.87	0.41
1:A:592:MET:O	1:A:596:HIS:ND1	2.53	0.40
1:B:557:ASP:HB3	1:B:560:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

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	396/424 (93%)	389 (98%)	7 (2%)	0	100	100
1	B	357/424 (84%)	349 (98%)	8 (2%)	0	100	100
All	All	753/848 (89%)	738 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	355/379 (94%)	351 (99%)	4 (1%)	65	84
1	B	327/379 (86%)	315 (96%)	12 (4%)	30	57
All	All	682/758 (90%)	666 (98%)	16 (2%)	44	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	628	VAL
1	A	783	VAL
1	A	944	THR
1	A	958	CYS
1	B	560	LYS
1	B	597	ASP
1	B	602	SER
1	B	628	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	632	GLU
1	B	648	ARG
1	B	757	ILE
1	B	783	VAL
1	B	794	LEU
1	B	796	LYS
1	B	845	LEU
1	B	915	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	GLN
1	A	604	GLN
1	A	769	GLN
1	A	835	GLN
1	A	905	ASN
1	A	928	HIS
1	B	855	ASN
1	B	928	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](#)

There are no ligands in this entry.

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	400/424 (94%)	0.10	26 (6%) 25 22	36, 61, 117, 159	0
1	B	367/424 (86%)	0.23	22 (5%) 27 24	42, 69, 125, 159	0
All	All	767/848 (90%)	0.16	48 (6%) 26 23	36, 64, 121, 159	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	966	ALA	6.5
1	A	748	MET	5.9
1	A	675	PHE	5.4
1	B	662	PRO	5.4
1	B	962	ALA	5.2
1	A	938	THR	5.2
1	B	802	ILE	5.2
1	A	676	ILE	5.1
1	A	677	ARG	5.0
1	B	944	THR	4.9
1	A	806	VAL	4.6
1	B	676	ILE	4.5
1	B	963	ILE	4.4
1	B	675	PHE	4.4
1	B	965	GLN	4.3
1	A	750	LEU	4.1
1	B	732	LEU	4.1
1	A	940	VAL	4.1
1	B	967	THR	4.0
1	B	964	LYS	3.5
1	A	746	VAL	3.5
1	A	941	GLY	3.3
1	A	662	PRO	3.1
1	A	749	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	557	ASP	2.9
1	A	798	GLY	2.8
1	B	677	ARG	2.8
1	B	729	PHE	2.8
1	B	948	THR	2.8
1	B	955	GLU	2.6
1	A	569	LYS	2.6
1	B	795	ALA	2.6
1	A	939	GLY	2.5
1	B	961	ALA	2.5
1	A	796	LYS	2.5
1	A	967	THR	2.5
1	B	556	SER	2.5
1	B	754	SER	2.4
1	B	679	ALA	2.4
1	B	798	GLY	2.4
1	A	674	ASP	2.4
1	A	797	GLU	2.3
1	A	751	PRO	2.3
1	A	661	GLN	2.2
1	A	747	ASN	2.1
1	A	807	GLU	2.1
1	A	742	GLN	2.1
1	A	804	ALA	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.