



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 10:39 PM UTC

PDB ID : 2W2D / pdb_00002w2d
Title : Crystal Structure of a Catalytically Active, Non-toxic Endopeptidase Derivative of Clostridium botulinum Toxin A
Authors : Masuyer, G.; Thiyagarajan, N.; James, P.L.; Marks, P.M.H.; Chaddock, J.A.; Acharya, K.R.
Deposited on : 2008-10-29
Resolution : 2.59 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	:	FAILED
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)
Validation Pipeline (wwPDB-VP)	:	2.49

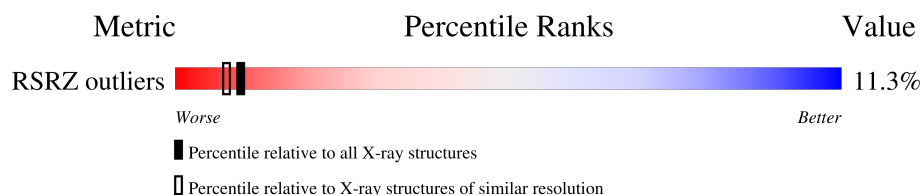
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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))
RSRZ outliers	180081	4008 (2.60-2.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	1436	-	X	-	-
6	GOL	A	1437	-	X	-	-
6	GOL	A	1438	-	X	-	-
6	GOL	B	1873	-	X	-	-
6	GOL	B	1874	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14160 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 BOTULINUM NEUROTOXIN A LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	1
			3534	2281	574	669	10			
1	C	436	Total	C	N	O	S	0	0	1
			3522	2273	573	666	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	PRO	conflict	UNP A5HZZ9
A	432	ASP	ARG	conflict	UNP A5HZZ9
C	2	GLU	PRO	conflict	UNP A5HZZ9
C	432	ASP	ARG	conflict	UNP A5HZZ9

- Molecule 2 is a protein called BOTULINUM NEUROTOXIN A HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3429	2195	550	674	10			
2	D	408	Total	C	N	O	S	0	0	1
			3308	2119	529	650	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	452	LEU	ASP	conflict	UNP A5HZZ9
B	453	GLN	LEU	conflict	UNP A5HZZ9
D	452	LEU	ASP	conflict	UNP A5HZZ9
D	453	GLN	LEU	conflict	UNP A5HZZ9

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

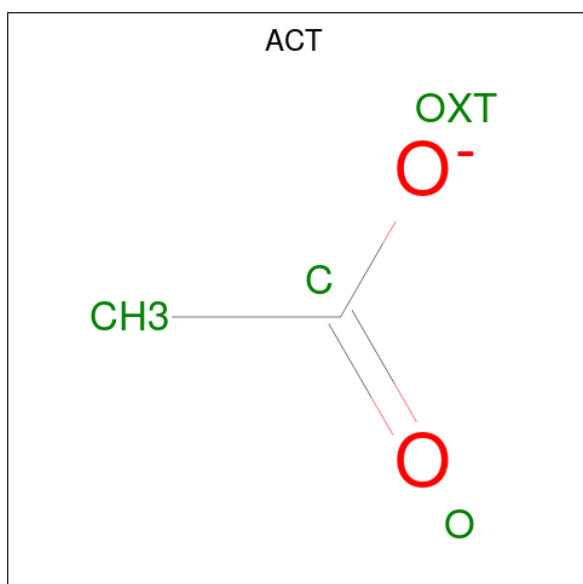
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	110	Total	O	0	0
			110	110		
8	B	49	Total	O	0	0
			49	49		
8	C	118	Total	O	0	0
			118	118		
8	D	31	Total	O	0	0
			31	31		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.36Å 156.91Å 211.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.59 49.11 – 2.59	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.11-2.59) 91.1 (49.11-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.58Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.253 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.6	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	0.92	EDS
Total number of atoms	14160	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	SO4	B	1872	-	4,4,4	0.38	0	6,6,6	0.10	0
6	GOL	A	1437	-	5,5,5	4.72	5 (100%)	5,5,5	6.15	3 (60%)
3	SO4	C	1437	-	4,4,4	0.36	0	6,6,6	0.07	0
6	GOL	B	1873	-	5,5,5	4.72	5 (100%)	5,5,5	6.12	3 (60%)
3	SO4	C	1436	-	4,4,4	0.41	0	6,6,6	0.06	0
6	GOL	B	1874	-	5,5,5	4.79	5 (100%)	5,5,5	6.11	3 (60%)
3	SO4	A	1433	-	4,4,4	0.41	0	6,6,6	0.11	0
7	ACT	C	1435	-	3,3,3	1.03	0	3,3,3	0.83	0
6	GOL	A	1436	-	5,5,5	4.81	5 (100%)	5,5,5	6.15	3 (60%)
6	GOL	A	1438	-	5,5,5	4.81	5 (100%)	5,5,5	6.09	3 (60%)

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
6	GOL	A	1437	-	-	2/4/4/4	-
6	GOL	B	1873	-	-	2/4/4/4	-
6	GOL	B	1874	-	-	2/4/4/4	-
6	GOL	A	1436	-	-	3/4/4/4	-
6	GOL	A	1438	-	-	2/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1438	GOL	C3-C2	-8.09	1.20	1.51
6	B	1873	GOL	C3-C2	-8.08	1.21	1.51
6	B	1874	GOL	C3-C2	-8.04	1.21	1.51
6	A	1436	GOL	C3-C2	-8.01	1.21	1.51
6	A	1437	GOL	C3-C2	-7.97	1.21	1.51
6	B	1874	GOL	O1-C1	-4.74	1.22	1.42
6	A	1438	GOL	O1-C1	-4.68	1.22	1.42
6	A	1436	GOL	O1-C1	-4.63	1.23	1.42
6	A	1437	GOL	O1-C1	-4.44	1.23	1.42
6	B	1873	GOL	O1-C1	-4.38	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1436	GOL	O3-C3	3.44	1.56	1.42
6	B	1873	GOL	O3-C3	3.42	1.56	1.42
6	A	1437	GOL	O3-C3	3.34	1.56	1.42
6	B	1874	GOL	O3-C3	3.31	1.56	1.42
6	A	1438	GOL	O3-C3	3.28	1.56	1.42
6	A	1436	GOL	C1-C2	-3.10	1.39	1.51
6	A	1438	GOL	C1-C2	-3.07	1.40	1.51
6	B	1874	GOL	C1-C2	-2.99	1.40	1.51
6	A	1437	GOL	C1-C2	-2.96	1.40	1.51
6	A	1436	GOL	O2-C2	-2.92	1.34	1.43
6	A	1438	GOL	O2-C2	-2.88	1.35	1.43
6	B	1873	GOL	O2-C2	-2.86	1.35	1.43
6	A	1437	GOL	O2-C2	-2.84	1.35	1.43
6	B	1874	GOL	O2-C2	-2.76	1.35	1.43
6	B	1873	GOL	C1-C2	-2.66	1.41	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1437	GOL	O3-C3-C2	11.25	161.04	110.38
6	A	1436	GOL	O3-C3-C2	11.24	160.97	110.38
6	B	1873	GOL	O3-C3-C2	11.12	160.43	110.38
6	A	1438	GOL	O3-C3-C2	11.02	160.00	110.38
6	B	1874	GOL	O3-C3-C2	11.00	159.91	110.38
6	B	1874	GOL	O2-C2-C3	7.25	139.21	109.18
6	A	1438	GOL	O2-C2-C3	7.19	138.96	109.18
6	A	1436	GOL	O2-C2-C3	7.15	138.76	109.18
6	B	1873	GOL	O2-C2-C3	7.03	138.28	109.18
6	A	1437	GOL	O2-C2-C3	7.01	138.19	109.18
6	B	1873	GOL	O1-C1-C2	3.68	126.93	110.38
6	A	1437	GOL	O1-C1-C2	3.57	126.45	110.38
6	B	1874	GOL	O1-C1-C2	3.44	125.89	110.38
6	A	1438	GOL	O1-C1-C2	3.42	125.77	110.38
6	A	1436	GOL	O1-C1-C2	3.40	125.66	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1436	GOL	O1-C1-C2-C3
6	A	1436	GOL	C1-C2-C3-O3
6	A	1437	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	1438	GOL	O1-C1-C2-C3
6	A	1438	GOL	C1-C2-C3-O3
6	B	1873	GOL	O1-C1-C2-C3
6	B	1873	GOL	C1-C2-C3-O3
6	B	1874	GOL	O1-C1-C2-C3
6	B	1874	GOL	C1-C2-C3-O3
6	A	1437	GOL	O1-C1-C2-O2
6	A	1436	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	437/450 (97%)	-0.04	20 (4%) 37 32	12, 27, 54, 98	0
1	C	436/450 (96%)	0.02	19 (4%) 39 33	12, 30, 59, 75	0
2	B	424/431 (98%)	0.67	51 (12%) 9 7	20, 42, 78, 93	0
2	D	408/431 (94%)	1.31	103 (25%) 1 1	21, 48, 101, 117	0
All	All	1705/1762 (96%)	0.48	193 (11%) 10 8	12, 36, 78, 117	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	606	TRP	9.5
2	D	607	VAL	7.8
2	D	601	ALA	7.8
2	D	603	PHE	7.8
2	B	566	ILE	7.4
2	D	764	PHE	7.1
1	A	65	ALA	6.7
2	D	604	LEU	6.7
2	D	872	ASN	6.4
2	D	600	ALA	6.3
2	D	487	ILE	6.1
2	D	647	LEU	6.0
2	D	831	ILE	5.9
2	B	761	ASN	5.9
2	D	873	ILE	5.7
1	C	422	LEU	5.6
2	D	566	ILE	5.6
2	D	755	THR	5.5
2	D	576	LEU	5.3
1	A	-2	PHE	5.2
2	D	761	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	602	MET	5.1
1	A	423	PHE	5.1
2	D	649	LYS	5.1
2	D	605	GLY	5.1
2	D	594	VAL	5.0
2	B	577	LEU	5.0
2	B	563	LYS	4.9
1	A	200	LEU	4.9
2	D	561	HIS	4.9
2	B	565	ARG	4.8
2	D	747	ILE	4.7
2	D	537	PHE	4.7
1	C	0	SER	4.6
2	D	568	LEU	4.6
2	D	599	GLU	4.5
2	D	579	PRO	4.5
2	B	489	ALA	4.5
2	D	759	LYS	4.5
2	D	646	MET	4.5
2	D	754	TYR	4.4
2	B	568	LEU	4.4
1	C	434	ILE	4.4
2	D	489	ALA	4.4
1	C	423	PHE	4.4
2	B	760	ASN	4.4
2	D	830	LEU	4.4
1	A	1	MET	4.2
2	D	753	GLN	4.2
2	B	647	LEU	4.2
2	B	564	SER	4.1
2	D	871	LYS	4.1
2	D	869	TYR	4.0
2	B	534	ILE	4.0
2	D	766	ILE	4.0
1	A	202	VAL	4.0
2	D	650	ASP	3.9
2	D	611	VAL	3.9
2	D	651	ASP	3.9
2	D	449	ALA	3.9
2	B	762	ILE	3.8
2	D	534	ILE	3.8
2	D	532	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLU	3.8
2	D	569	THR	3.7
2	B	490	ALA	3.7
1	A	203	ASP	3.7
2	D	631	THR	3.6
2	B	537	PHE	3.6
2	D	644	GLY	3.6
2	D	591	VAL	3.6
2	D	833	GLN	3.5
1	C	64	GLU	3.5
2	D	609	GLN	3.5
2	B	567	ALA	3.5
2	B	530	LEU	3.4
1	C	203	ASP	3.3
2	D	645	ASN	3.3
1	A	425	PHE	3.2
2	B	561	HIS	3.2
2	D	515	ILE	3.2
2	D	575	ALA	3.2
1	A	-3	GLU	3.2
2	D	834	VAL	3.1
2	D	765	ASN	3.1
2	B	532	PRO	3.0
2	B	870	ILE	3.0
2	B	756	GLU	3.0
2	B	871	LYS	3.0
2	B	562	GLY	3.0
2	B	755	THR	3.0
2	B	533	ASN	3.0
2	B	572	VAL	2.9
2	D	565	ARG	2.9
2	D	530	LEU	2.9
1	A	-1	GLY	2.9
2	D	486	ASN	2.9
2	D	752	ASN	2.9
2	B	531	MET	2.9
1	C	1	MET	2.9
2	D	491	GLU	2.9
2	D	593	LYS	2.9
2	B	869	TYR	2.9
2	B	507	ASN	2.8
1	C	63	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	652	PHE	2.8
2	D	533	ASN	2.8
2	D	746	ILE	2.8
2	D	653	VAL	2.8
2	D	567	ALA	2.8
2	B	861	ARG	2.8
2	D	573	ASN	2.7
2	D	630	ILE	2.7
1	A	64	GLU	2.7
2	D	612	TYR	2.7
2	D	584	THR	2.7
2	D	868	GLU	2.7
2	D	581	ARG	2.6
2	D	632	ILE	2.6
2	D	658	PHE	2.6
2	D	751	TYR	2.6
1	A	433	GLY	2.6
2	B	764	PHE	2.6
2	B	757	GLU	2.6
2	B	626	LYS	2.6
2	B	574	GLU	2.5
2	D	450	LEU	2.5
2	D	760	ASN	2.5
2	D	768	ASP	2.5
2	D	685	ILE	2.5
2	D	610	LEU	2.5
1	A	66	LYS	2.5
1	C	387	TYR	2.4
2	B	859	ASN	2.4
2	D	771	SER	2.4
2	D	643	ILE	2.4
2	D	657	ILE	2.4
2	D	671	ILE	2.4
2	B	450	LEU	2.4
2	D	582	VAL	2.4
2	D	531	MET	2.4
2	B	584	THR	2.4
2	B	536	ARG	2.4
2	B	629	ASP	2.4
2	B	493	ASN	2.4
2	D	743	THR	2.3
1	C	435	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	860	GLN	2.3
2	D	613	ASP	2.3
1	C	425	PHE	2.3
2	B	763	ASN	2.3
1	A	201	GLU	2.3
2	D	490	ALA	2.3
2	D	829	THR	2.3
2	B	759	LYS	2.3
1	C	431	VAL	2.3
1	C	433	GLY	2.3
2	D	750	GLN	2.3
2	D	492	GLU	2.3
2	B	573	ASN	2.3
2	B	623	THR	2.3
1	A	311	GLN	2.3
2	D	769	LEU	2.3
2	D	488	GLU	2.3
1	A	27	ALA	2.2
2	B	872	ASN	2.2
2	D	574	GLU	2.2
1	C	65	ALA	2.2
2	B	628	ALA	2.2
1	C	172	VAL	2.2
2	B	765	ASN	2.2
1	C	57	GLY	2.2
2	D	580	SER	2.2
2	D	770	SER	2.2
2	D	656	LEU	2.1
2	D	870	ILE	2.1
2	D	538	PRO	2.1
1	A	204	THR	2.1
1	A	411	MET	2.1
2	D	621	VAL	2.1
2	B	597	ALA	2.1
2	D	452	LEU	2.1
1	A	0	SER	2.1
2	B	858	ASP	2.1
2	D	586	PHE	2.1
1	C	54	PRO	2.1
1	C	27	ALA	2.0
2	B	449	ALA	2.0
2	B	627	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	803	TYR	2.0
1	C	411	MET	2.0
2	D	571	SER	2.0
2	D	535	GLU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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
6	GOL	B	1873	6/6	0.77	0.19	51,53,55,56	0
3	SO4	C	1436	5/5	0.81	0.19	82,83,85,85	0
6	GOL	A	1438	6/6	0.87	0.16	54,55,56,58	0
6	GOL	A	1436	6/6	0.87	0.15	54,55,56,58	0
7	ACT	C	1435	4/4	0.88	0.14	49,50,51,52	0
3	SO4	A	1433	5/5	0.89	0.14	68,69,70,72	0
3	SO4	C	1437	5/5	0.89	0.12	69,69,70,70	0
6	GOL	B	1874	6/6	0.92	0.13	55,59,59,60	0
6	GOL	A	1437	6/6	0.93	0.14	44,46,47,49	0
3	SO4	B	1872	5/5	0.94	0.09	47,48,50,51	0
5	CL	A	1435	1/1	0.97	0.08	44,44,44,44	0
5	CL	A	1439	1/1	0.97	0.12	44,44,44,44	0
5	CL	D	1872	1/1	0.97	0.15	47,47,47,47	0
4	ZN	C	1438	1/1	1.00	0.04	29,29,29,29	0
4	ZN	A	1434	1/1	1.00	0.02	23,23,23,23	0

5.5 Other polymers [i](#)

There are no such residues in this entry.