Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:26 PM GMT

PDB ID	:	1TML
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF A THERMOPHILIC ENDOCELLULASE
Authors	:	Spezio, M.; Wilson, D.B.; Karplus, P.A.
Deposited on	:	1993-06-08
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

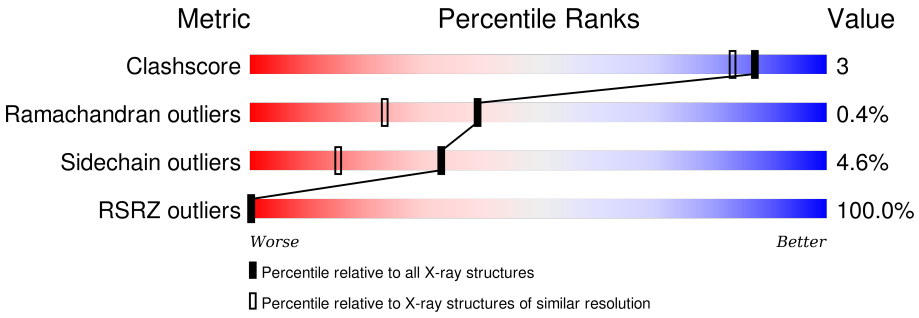
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	286	100% 86% 12% •

2 Entry composition

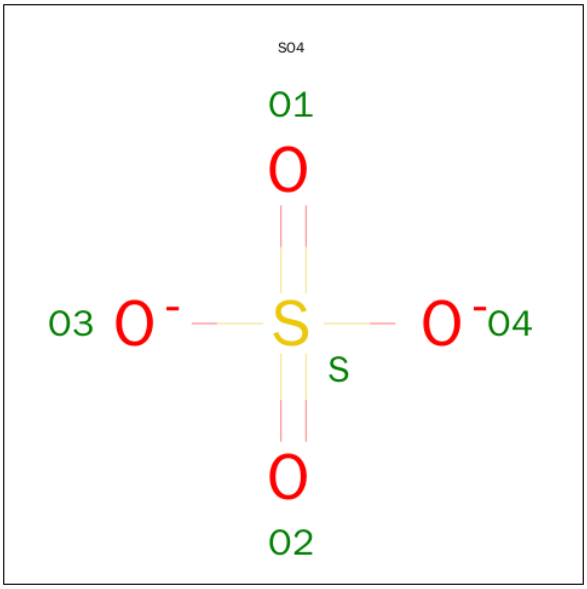
There are 3 unique types of molecules in this entry. The entry contains 2843 atoms, of which 625 are hydrogens and 0 are deuteriums.

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 ENDO-1,4-BETA-D-GLUCANASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	286	2619	1332	479	383	413	12	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

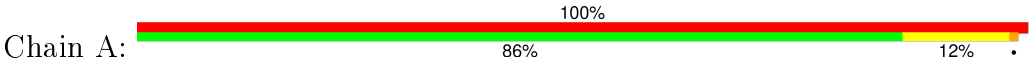
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	73	219	146	73	0	0

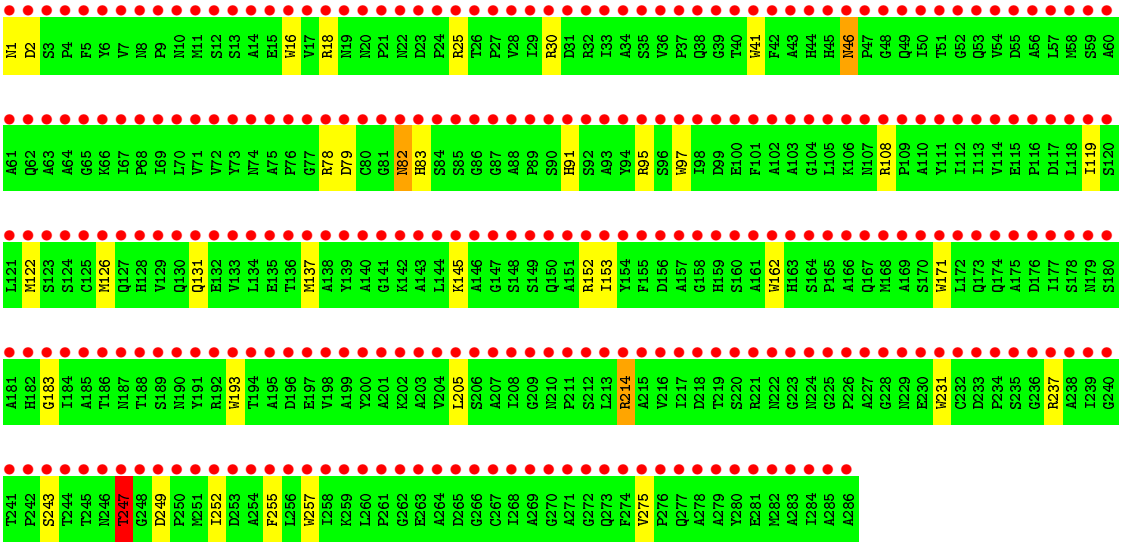
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ENDO-1,4-BETA-D-GLUCANASE

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.35Å 65.94Å 43.41Å 90.00° 107.69° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 41.36 – 2.58	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 94.1 (41.36-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.99 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available) 0.137 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 30.7	EDS
Estimated twinning fraction	0.031 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 6973 reflections	Xtriage
F_o,F_c correlation	0.28	EDS
Total number of atoms	2843	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	0.80	0/2198	1.43	38/3002 (1.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	A	16	TRP	CD1-CG-CD2	8.73	113.28	106.30
1	A	97	TRP	CD1-CG-CD2	8.53	113.13	106.30
1	A	171	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	A	247	THR	N-CA-CB	-8.14	94.84	110.30
1	A	18	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	152	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	193	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	A	237	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	231	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	257	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	152	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	16	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	171	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	231	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	193	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	41	TRP	CD1-CG-CD2	6.73	111.69	106.30
1	A	162	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	41	TRP	CE2-CD2-CG	-6.34	102.22	107.30
1	A	97	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	A	30	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	78	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	97	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	257	TRP	CE2-CD2-CG	-6.04	102.47	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	162	TRP	CD1-CG-CD2	5.99	111.09	106.30
1	A	16	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	A	231	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	A	78	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	231	TRP	CG-CD2-CE3	5.72	139.05	133.90
1	A	231	TRP	CB-CG-CD1	-5.60	119.72	127.00
1	A	162	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	A	171	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	A	193	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	A	25	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	30	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	214	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	16	TRP	CB-CG-CD1	-5.12	120.34	127.00

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	2140	479	2029	11	0
2	A	5	0	0	1	0
3	A	73	146	0	0	0
All	All	2218	625	2029	11	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 3.

All (11) 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:119:ILE:HD11	1:A:137:MET:HG3	1.73	0.69
1:A:247:THR:HG21	1:A:252:ILE:O	1.93	0.68
1:A:46:ASN:H	1:A:46:ASN:HD22	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HG22	1:A:249:ASP:H	1.67	0.59
1:A:79:ASP:HB3	1:A:82:ASN:HD21	1.77	0.50
1:A:145:LYS:HG3	1:A:153:ILE:CD1	2.44	0.47
1:A:183:GLY:HA3	1:A:214:ARG:O	2.17	0.44
1:A:91:HIS:HB3	1:A:95:ARG:NH1	2.34	0.42
1:A:79:ASP:HB2	2:A:360:SO4:O1	2.21	0.41
1:A:79:ASP:HB3	1:A:82:ASN:ND2	2.35	0.41
1:A:243:SER:HA	1:A:255:PHE:O	2.21	0.41

There are no symmetry-related clashes.

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	284/286 (99%)	274 (96%)	9 (3%)	1 (0%)	39 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	HIS

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	219/219 (100%)	209 (95%)	10 (5%)	33 15

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	2	ASP
1	A	46	ASN
1	A	82	ASN
1	A	122	MET
1	A	126	MET
1	A	131	GLN
1	A	205	LEU
1	A	247	THR
1	A	275	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	46	ASN
1	A	49	GLN
1	A	53	GLN
1	A	82	ASN
1	A	83	HIS
1	A	107	ASN
1	A	131	GLN
1	A	273	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	A	360	-	4,4,4	1.71	1 (25%)	6,6,6	0.33	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
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	360	SO4	O1-S	-2.03	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	360	SO4	1	0

5.7 Other polymers (i)

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, 95^{th} 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	286/286 (100%)	8.32	286 (100%)	0	0	3, 10, 26, 51	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	SER	26.5
1	A	42	PHE	22.8
1	A	85	SER	22.3
1	A	57	LEU	18.6
1	A	172	LEU	18.5
1	A	97	TRP	17.5
1	A	59	SER	17.1
1	A	144	LEU	16.9
1	A	86	GLY	16.4
1	A	268	ILE	16.3
1	A	89	PRO	16.0
1	A	266	GLY	15.7
1	A	258	ILE	15.7
1	A	48	GLY	15.6
1	A	180	SER	15.6
1	A	5	PHE	15.3
1	A	29	ILE	15.2
1	A	134	LEU	14.7
1	A	70	LEU	14.5
1	A	231	TRP	14.2
1	A	228	GLY	14.1
1	A	127	GLN	14.1
1	A	41	TRP	13.9
1	A	276	PRO	13.8
1	A	185	ALA	13.6
1	A	174	GLN	13.5
1	A	129	VAL	13.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	PHE	13.3
1	A	157	ALA	13.2
1	A	279	ALA	13.0
1	A	88	ALA	12.9
1	A	188	THR	12.9
1	A	162	TRP	12.8
1	A	18	ARG	12.7
1	A	168	MET	12.6
1	A	19	ASN	12.6
1	A	179	ASN	12.4
1	A	73	TYR	12.1
1	A	208	ILE	12.0
1	A	50	ILE	12.0
1	A	198	VAL	12.0
1	A	220	SER	12.0
1	A	125	CYS	11.9
1	A	139	TYR	11.9
1	A	161	ALA	11.6
1	A	62	GLN	11.6
1	A	164	SER	11.6
1	A	90	SER	11.6
1	A	191	TYR	11.6
1	A	7	VAL	11.5
1	A	23	ASP	11.5
1	A	56	ALA	11.4
1	A	166	ALA	11.4
1	A	167	GLN	11.3
1	A	103	ALA	11.3
1	A	130	GLN	11.3
1	A	275	VAL	11.2
1	A	4	PRO	11.1
1	A	82	ASN	11.1
1	A	286	ALA	11.1
1	A	246	ASN	10.9
1	A	265	ASP	10.9
1	A	173	GLN	10.8
1	A	171	TRP	10.7
1	A	61	ALA	10.6
1	A	109	PRO	10.5
1	A	238	ALA	10.4
1	A	155	PHE	10.4
1	A	54	VAL	10.3

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Mol	Chain	Res	Type	RSRZ
1	A	71	VAL	10.3
1	A	176	ASP	10.3
1	A	261	PRO	10.2
1	A	156	ASP	10.2
1	A	83	HIS	10.2
1	A	80	CYS	10.2
1	A	51	THR	10.1
1	A	133	VAL	10.1
1	A	205	LEU	10.0
1	A	108	ARG	10.0
1	A	34	ALA	9.9
1	A	165	PRO	9.9
1	A	33	ILE	9.9
1	A	40	THR	9.8
1	A	112	ILE	9.8
1	A	26	THR	9.7
1	A	118	LEU	9.7
1	A	116	PRO	9.5
1	A	16	TRP	9.5
1	A	146	ALA	9.5
1	A	227	ALA	9.4
1	A	201	ALA	9.4
1	A	69	ILE	9.3
1	A	267	CYS	9.1
1	A	269	ALA	9.1
1	A	160	SER	9.1
1	A	1	ASN	9.1
1	A	195	ALA	9.1
1	A	260	LEU	9.0
1	A	91	HIS	9.0
1	A	241	THR	9.0
1	A	60	ALA	8.9
1	A	177	ILE	8.9
1	A	15	GLU	8.8
1	A	143	ALA	8.8
1	A	55	ASP	8.8
1	A	124	SER	8.7
1	A	216	VAL	8.7
1	A	123	SER	8.6
1	A	206	SER	8.6
1	A	98	ILE	8.5
1	A	8	ASN	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLY	8.4
1	A	150	GLN	8.3
1	A	224	ASN	8.3
1	A	44	HIS	8.3
1	A	113	ILE	8.3
1	A	149	SER	8.3
1	A	36	VAL	8.2
1	A	11	MET	8.2
1	A	3	SER	8.2
1	A	285	ALA	8.2
1	A	193	TRP	8.2
1	A	256	LEU	8.2
1	A	175	ALA	8.1
1	A	64	ALA	8.1
1	A	114	VAL	8.1
1	A	67	ILE	8.0
1	A	236	GLY	8.0
1	A	226	PRO	8.0
1	A	24	PRO	7.9
1	A	43	ALA	7.8
1	A	28	VAL	7.8
1	A	31	ASP	7.8
1	A	22	ASN	7.7
1	A	245	THR	7.7
1	A	140	ALA	7.7
1	A	119	ILE	7.7
1	A	104	GLY	7.7
1	A	204	VAL	7.7
1	A	126	MET	7.7
1	A	178	SER	7.6
1	A	257	TRP	7.6
1	A	274	PHE	7.6
1	A	158	GLY	7.5
1	A	14	ALA	7.5
1	A	250	PRO	7.4
1	A	154	TYR	7.4
1	A	234	PRO	7.4
1	A	66	LYS	7.3
1	A	122	MET	7.3
1	A	9	PRO	7.3
1	A	106	LYS	7.2
1	A	186	THR	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	THR	7.2
1	A	99	ASP	7.2
1	A	251	MET	7.2
1	A	58	MET	7.2
1	A	280	TYR	7.2
1	A	121	LEU	7.2
1	A	135	GLU	7.1
1	A	96	SER	7.1
1	A	81	GLY	7.1
1	A	233	ASP	7.1
1	A	21	PRO	7.1
1	A	212	SER	7.1
1	A	221	ARG	7.0
1	A	230	GLU	6.9
1	A	49	GLN	6.9
1	A	284	ILE	6.9
1	A	17	VAL	6.8
1	A	232	CYS	6.7
1	A	72	VAL	6.7
1	A	153	ILE	6.7
1	A	169	ALA	6.7
1	A	200	TYR	6.7
1	A	94	TYR	6.6
1	A	111	TYR	6.6
1	A	45	HIS	6.6
1	A	264	ALA	6.6
1	A	131	GLN	6.6
1	A	152	ARG	6.6
1	A	214	ARG	6.6
1	A	278	ALA	6.6
1	A	213	LEU	6.5
1	A	52	GLY	6.5
1	A	210	ASN	6.5
1	A	53	GLN	6.5
1	A	229	ASN	6.5
1	A	254	ALA	6.5
1	A	100	GLU	6.5
1	A	137	MET	6.4
1	A	259	LYS	6.3
1	A	107	ASN	6.2
1	A	47	PRO	6.2
1	A	184	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	ILE	6.1
1	A	151	ALA	6.1
1	A	37	PRO	6.1
1	A	202	LYS	6.1
1	A	142	LYS	6.1
1	A	190	ASN	6.1
1	A	170	SER	6.0
1	A	283	ALA	5.9
1	A	32	ARG	5.9
1	A	75	ALA	5.9
1	A	27	PRO	5.9
1	A	271	ALA	5.8
1	A	92	SER	5.8
1	A	132	GLU	5.8
1	A	163	HIS	5.8
1	A	136	THR	5.8
1	A	203	ALA	5.8
1	A	87	GLY	5.7
1	A	247	THR	5.7
1	A	30	ARG	5.7
1	A	117	ASP	5.7
1	A	282	MET	5.7
1	A	159	HIS	5.7
1	A	197	GLU	5.6
1	A	76	PRO	5.6
1	A	281	GLU	5.6
1	A	79	ASP	5.5
1	A	78	ARG	5.5
1	A	10	ASN	5.5
1	A	145	LYS	5.5
1	A	46	ASN	5.5
1	A	225	GLY	5.4
1	A	240	GLY	5.4
1	A	68	PRO	5.4
1	A	273	GLN	5.3
1	A	101	PHE	5.3
1	A	2	ASP	5.3
1	A	102	ALA	5.3
1	A	272	GLY	5.3
1	A	211	PRO	5.3
1	A	196	ASP	5.2
1	A	192	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	115	GLU	5.2
1	A	249	ASP	5.2
1	A	141	GLY	5.1
1	A	6	TYR	5.1
1	A	105	LEU	5.0
1	A	128	HIS	4.9
1	A	65	GLY	4.9
1	A	237	ARG	4.8
1	A	194	THR	4.8
1	A	147	GLY	4.8
1	A	95	ARG	4.7
1	A	215	ALA	4.7
1	A	252	ILE	4.6
1	A	12	SER	4.6
1	A	110	ALA	4.6
1	A	182	HIS	4.6
1	A	63	ALA	4.6
1	A	207	ALA	4.6
1	A	263	GLU	4.5
1	A	248	GLY	4.4
1	A	277	GLN	4.3
1	A	120	SER	4.3
1	A	239	ILE	4.3
1	A	242	PRO	4.3
1	A	25	ARG	4.2
1	A	74	ASN	4.2
1	A	77	GLY	4.2
1	A	199	ALA	4.1
1	A	183	GLY	4.0
1	A	209	GLY	4.0
1	A	189	SER	4.0
1	A	223	GLY	3.8
1	A	39	GLY	3.8
1	A	187	ASN	3.8
1	A	235	SER	3.8
1	A	222	ASN	3.7
1	A	35	SER	3.7
1	A	13	SER	3.7
1	A	138	ALA	3.6
1	A	20	ASN	3.5
1	A	243	SER	3.5
1	A	219	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	181	ALA	3.4
1	A	148	SER	3.3
1	A	253	ASP	3.2
1	A	270	GLY	3.0
1	A	38	GLN	3.0
1	A	218	ASP	2.6
1	A	93	ALA	2.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	360	5/5	0.79	0.33	-0.92	18,18,18,19	0

6.5 Other polymers (i)

There are no such residues in this entry.