Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 11:15 AM EDT

PDB ID	:	3B01
Title	:	Crystal structure of the laminarinase catalytic domain from Thermotoga maritima MSB8
Authors	:	Jeng, W.Y.; Wang, N.C.; Wang, A.H.J.
Deposited on	:	2011-06-03
Resolution	:	1.87 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.87 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.
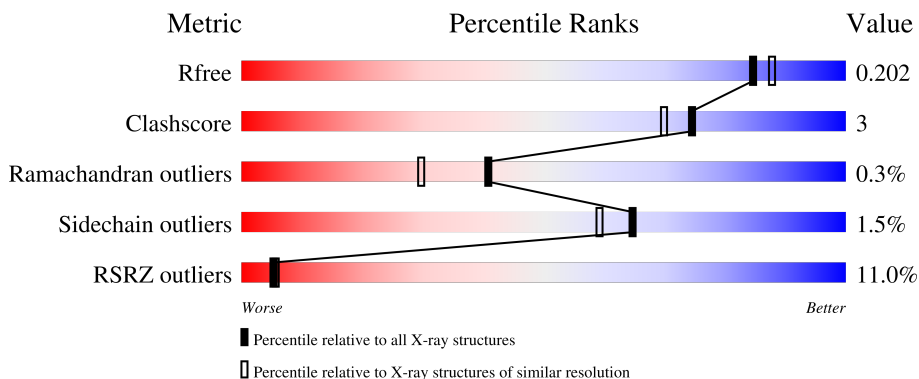
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	272	
1	B	272	
1	C	272	
1	D	272	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8937 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 Laminarinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			2036	1315	320	393	8			
1	B	250	Total	C	N	O	S	0	5	0
			2051	1324	324	395	8			
1	C	251	Total	C	N	O	S	0	7	0
			2072	1337	328	399	8			
1	D	251	Total	C	N	O	S	0	6	0
			2067	1334	327	398	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9WXN1
A	265	VAL	-	expression tag	UNP Q9WXN1
A	266	GLU	-	expression tag	UNP Q9WXN1
A	267	HIS	-	expression tag	UNP Q9WXN1
A	268	HIS	-	expression tag	UNP Q9WXN1
A	269	HIS	-	expression tag	UNP Q9WXN1
A	270	HIS	-	expression tag	UNP Q9WXN1
A	271	HIS	-	expression tag	UNP Q9WXN1
A	272	HIS	-	expression tag	UNP Q9WXN1
B	1	MET	-	expression tag	UNP Q9WXN1
B	265	VAL	-	expression tag	UNP Q9WXN1
B	266	GLU	-	expression tag	UNP Q9WXN1
B	267	HIS	-	expression tag	UNP Q9WXN1
B	268	HIS	-	expression tag	UNP Q9WXN1
B	269	HIS	-	expression tag	UNP Q9WXN1
B	270	HIS	-	expression tag	UNP Q9WXN1
B	271	HIS	-	expression tag	UNP Q9WXN1
B	272	HIS	-	expression tag	UNP Q9WXN1
C	1	MET	-	expression tag	UNP Q9WXN1
C	265	VAL	-	expression tag	UNP Q9WXN1
C	266	GLU	-	expression tag	UNP Q9WXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP Q9WXN1
C	268	HIS	-	expression tag	UNP Q9WXN1
C	269	HIS	-	expression tag	UNP Q9WXN1
C	270	HIS	-	expression tag	UNP Q9WXN1
C	271	HIS	-	expression tag	UNP Q9WXN1
C	272	HIS	-	expression tag	UNP Q9WXN1
D	1	MET	-	expression tag	UNP Q9WXN1
D	265	VAL	-	expression tag	UNP Q9WXN1
D	266	GLU	-	expression tag	UNP Q9WXN1
D	267	HIS	-	expression tag	UNP Q9WXN1
D	268	HIS	-	expression tag	UNP Q9WXN1
D	269	HIS	-	expression tag	UNP Q9WXN1
D	270	HIS	-	expression tag	UNP Q9WXN1
D	271	HIS	-	expression tag	UNP Q9WXN1
D	272	HIS	-	expression tag	UNP Q9WXN1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total 183	O 183	0	0
5	B	137	Total 137	O 137	0	0
5	C	146	Total 146	O 146	0	0
5	D	198	Total 198	O 198	0	0

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.
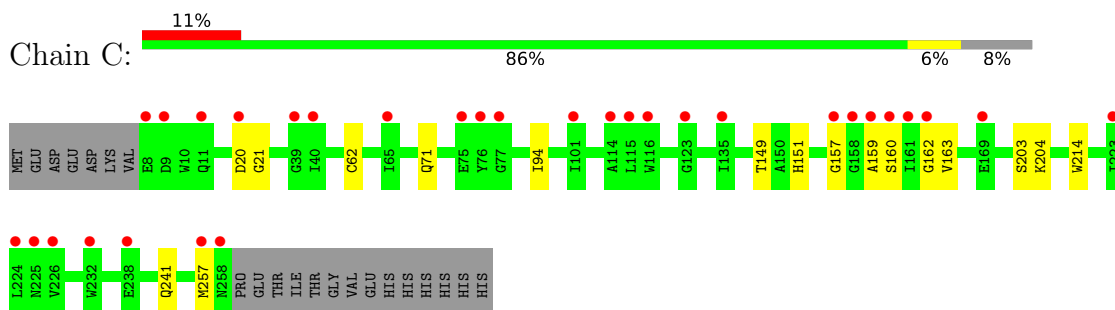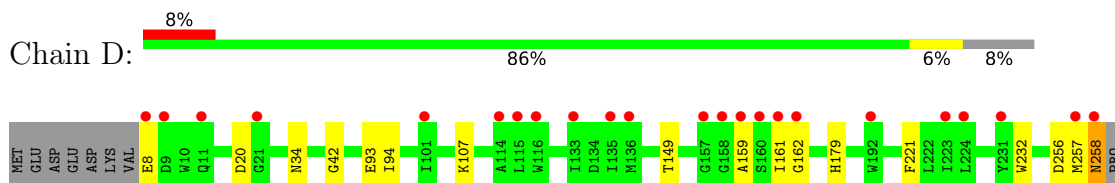
- Molecule 1: Laminarinase
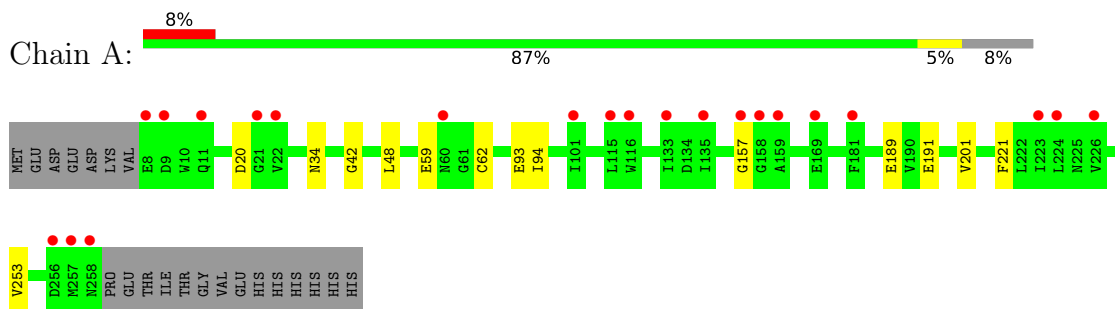
Chain A:

- Molecule 1: Laminarinase

Chain B:

- Molecule 1: Laminarinase

Chain C:

- Molecule 1: Laminarinase

Chain D:
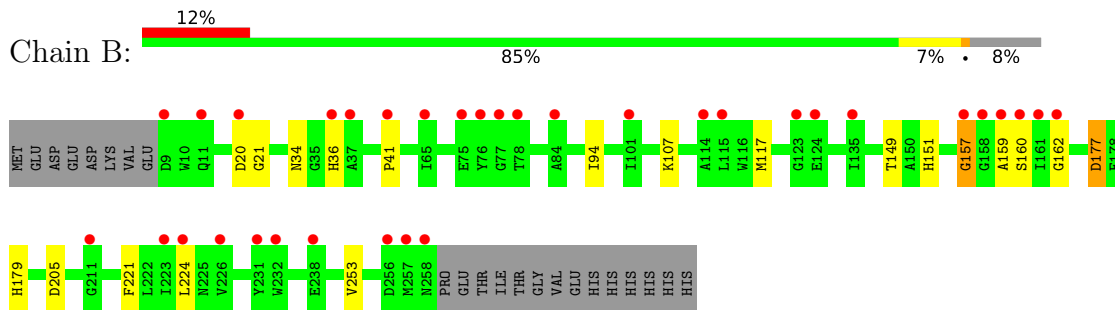
GLU THR ILE THR GLY VAL GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	120.31Å　120.31Å　107.15Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	27.50　–　1.87 27.41　–　1.87	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.50-1.87) 99.6 (27.41-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.152　,　0.188 0.169　,　0.202	Depositor DCC
R_{free} test set	6303 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8937	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, CL, 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	0.38	0/2106	0.69	0/2868
1	B	0.34	0/2118	0.67	0/2884
1	C	0.36	0/2146	0.70	0/2922
1	D	0.40	0/2138	0.72	0/2911
All	All	0.37	0/8508	0.70	0/11585

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	2036	0	1871	9	0
1	B	2051	0	1886	22	0
1	C	2072	0	1905	11	0
1	D	2067	0	1899	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	183	0	0	2	0
5	B	137	0	0	3	0
5	C	146	0	0	1	0
5	D	198	0	0	3	0
All	All	8937	0	7561	50	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 (50) 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:B:151:HIS:CE1	1:B:160[A]:SER:HB2	1.77	1.18
1:B:177:ASP:OD1	5:B:418:HOH:O	1.72	1.06
1:A:62:CYS:SG	5:A:530:HOH:O	2.20	0.97
1:C:62:CYS:SG	5:C:571:HOH:O	2.23	0.97
1:B:20:ASP:CG	1:B:21:GLY:H	1.75	0.90
1:B:151:HIS:HE1	1:B:160[A]:SER:HB2	1.37	0.90
1:C:20:ASP:CG	1:C:21:GLY:H	1.78	0.85
1:B:151:HIS:ND1	1:B:160[A]:SER:HB2	1.94	0.81
1:B:151:HIS:CE1	1:B:160[A]:SER:CB	2.66	0.76
1:C:157:GLY:C	1:C:159[A]:ALA:H	1.97	0.67
1:B:20:ASP:CG	1:B:21:GLY:N	2.47	0.66
1:D:149:THR:OG1	1:D:162[B]:GLY:HA3	1.96	0.66
1:D:257:MET:O	1:D:258:ASN:HB3	1.96	0.64
1:C:20:ASP:OD1	1:C:21:GLY:N	2.16	0.63
1:C:149:THR:OG1	1:C:162[B]:GLY:HA3	1.99	0.63
1:C:151:HIS:ND1	1:C:160[A]:SER:HB3	2.14	0.63
1:D:107:LYS:HE3	5:D:588:HOH:O	2.00	0.60
1:C:20:ASP:CG	1:C:21:GLY:N	2.48	0.60
1:B:151:HIS:HE1	1:B:160[A]:SER:CB	2.08	0.59
1:D:161[B]:ILE:HD11	1:D:232:TRP:HB3	1.84	0.59
1:D:107:LYS:NZ	5:D:404:HOH:O	2.37	0.57
1:B:36:HIS:CE1	1:B:41:PRO:HB3	2.40	0.56
1:C:157:GLY:C	1:C:159[A]:ALA:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD22	1:B:205:ASP:HB3	1.88	0.56
1:B:149:THR:OG1	1:B:162[B]:GLY:HA3	2.08	0.54
1:D:179:HIS:HE1	5:D:596:HOH:O	1.90	0.53
1:A:94:ILE:HD12	1:A:253:VAL:HG11	1.92	0.51
1:A:94:ILE:HD12	1:A:253:VAL:CG1	2.41	0.50
1:B:36:HIS:ND1	3:B:304:SO4:O1	2.43	0.50
1:B:36:HIS:NE2	1:B:41:PRO:HB3	2.26	0.50
1:A:189:GLU:OE2	5:A:549:HOH:O	2.19	0.48
1:C:151:HIS:ND1	1:C:160[A]:SER:CB	2.78	0.47
1:A:48:LEU:CD2	1:B:205:ASP:HB3	2.44	0.46
1:C:162[A]:GLY:O	1:C:163:VAL:HG23	2.15	0.46
1:B:20:ASP:OD1	1:B:21:GLY:N	2.27	0.45
1:A:34:ASN:ND2	1:A:42:GLY:H	2.14	0.45
1:B:34:ASN:HD22	1:B:36:HIS:HE1	1.65	0.44
1:B:159[A]:ALA:HB3	5:B:651:HOH:O	2.18	0.43
1:B:157:GLY:O	1:B:160[A]:SER:HB3	2.18	0.43
1:A:191:GLU:HG2	1:A:201:VAL:HG22	2.01	0.42
1:C:204:LYS:HG3	1:C:214:TRP:CG	2.55	0.42
1:B:94:ILE:HD13	1:B:253:VAL:HG11	2.01	0.42
1:A:93:GLU:HG2	1:A:221:PHE:HB3	2.02	0.42
1:D:93:GLU:HG2	1:D:221:PHE:HB3	2.02	0.41
1:D:161[B]:ILE:HD12	1:D:161[B]:ILE:HG21	1.71	0.41
1:B:179:HIS:HE1	5:B:605:HOH:O	2.03	0.41
1:B:117:MET:HA	1:B:221:PHE:O	2.21	0.41
1:D:8:GLU:HG2	1:D:256:ASP:OD2	2.20	0.40
1:B:34:ASN:HD22	1:B:36:HIS:CE1	2.39	0.40
1:D:34:ASN:ND2	1:D:42:GLY:H	2.20	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	250/272 (92%)	243 (97%)	6 (2%)	1 (0%)	34	22
1	B	253/272 (93%)	244 (96%)	8 (3%)	1 (0%)	34	22
1	C	256/272 (94%)	244 (95%)	12 (5%)	0	100	100
1	D	255/272 (94%)	242 (95%)	11 (4%)	2 (1%)	19	9
All	All	1014/1088 (93%)	973 (96%)	37 (4%)	4 (0%)	41	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	GLY
1	D	159[A]	ALA
1	D	159[B]	ALA
1	B	157	GLY

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	211/230 (92%)	209 (99%)	2 (1%)	78	76
1	B	211/230 (92%)	208 (99%)	3 (1%)	67	62
1	C	214/230 (93%)	209 (98%)	5 (2%)	50	41
1	D	213/230 (93%)	210 (99%)	3 (1%)	67	62
All	All	849/920 (92%)	836 (98%)	13 (2%)	65	59

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	59	GLU
1	B	107	LYS
1	B	177	ASP
1	B	224	LEU
1	C	71	GLN
1	C	94	ILE

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Mol	Chain	Res	Type
1	C	203	SER
1	C	241	GLN
1	C	257	MET
1	D	20	ASP
1	D	94	ILE
1	D	258	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	34	ASN
1	A	36	HIS
1	A	55	ASN
1	A	60	ASN
1	B	26	ASN
1	B	34	ASN
1	B	55	ASN
1	B	151	HIS
1	B	179	HIS
1	C	26	ASN
1	C	29	ASN
1	C	34	ASN
1	C	55	ASN
1	C	71	GLN
1	D	29	ASN
1	D	34	ASN
1	D	45	ASN
1	D	55	ASN
1	D	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	A	303	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	C	305	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	B	304	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	B	305	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	D	303	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	C	303	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	B	303	-	4,4,4	0.16	0	6,6,6	0.23	0
3	SO4	C	304	-	4,4,4	0.17	0	6,6,6	0.26	0

There are no bond length outliers.

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
3	B	304	SO4	1	0

5.7　Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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	251/272 (92%)	0.15	22 (8%)	10	10	19, 25, 40, 59	0
1	B	250/272 (91%)	0.38	34 (13%)	3	3	19, 29, 44, 58	0
1	C	251/272 (92%)	0.36	31 (12%)	4	4	19, 26, 43, 57	0
1	D	251/272 (92%)	0.12	23 (9%)	9	9	18, 22, 38, 56	0
All	All	1003/1088 (92%)	0.25	110 (10%)	5	6	18, 25, 42, 59	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	ASN	7.2
1	C	258	ASN	7.0
1	D	161[A]	ILE	6.6
1	A	159	ALA	6.3
1	D	257	MET	6.0
1	B	161[A]	ILE	5.8
1	B	257	MET	5.7
1	B	258	ASN	5.6
1	C	161[A]	ILE	5.6
1	A	257	MET	5.4
1	A	9	ASP	4.9
1	C	257	MET	4.8
1	B	159[A]	ALA	4.6
1	D	258	ASN	4.6
1	B	76	TYR	4.2
1	D	162[A]	GLY	4.2
1	D	135	ILE	4.2
1	C	157	GLY	4.1
1	C	115	LEU	3.9
1	C	158[A]	GLY	3.9
1	B	78	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	3.9
1	A	21	GLY	3.8
1	B	9	ASP	3.8
1	D	159[A]	ALA	3.8
1	A	157	GLY	3.8
1	B	77	GLY	3.7
1	D	133	ILE	3.7
1	B	75	GLU	3.6
1	D	160[A]	SER	3.6
1	C	20	ASP	3.6
1	B	157	GLY	3.5
1	C	226	VAL	3.5
1	C	162[A]	GLY	3.5
1	D	9	ASP	3.4
1	B	20	ASP	3.3
1	A	60	ASN	3.3
1	A	115	LEU	3.3
1	C	9	ASP	3.2
1	D	223	ILE	3.2
1	C	232	TRP	3.1
1	C	224	LEU	3.1
1	B	231	TYR	3.1
1	A	22	VAL	3.1
1	C	8	GLU	3.0
1	A	8	GLU	3.0
1	C	159[A]	ALA	3.0
1	C	75	GLU	3.0
1	B	162[A]	GLY	2.9
1	C	114	ALA	2.9
1	D	115	LEU	2.9
1	A	135	ILE	2.9
1	B	223	ILE	2.9
1	C	135	ILE	2.9
1	A	101	ILE	2.9
1	A	116	TRP	2.8
1	C	76	TYR	2.8
1	D	116	TRP	2.8
1	C	223	ILE	2.7
1	A	158	GLY	2.7
1	B	36	HIS	2.7
1	D	157	GLY	2.7
1	B	84	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	11	GLN	2.7
1	B	41	PRO	2.6
1	B	224	LEU	2.6
1	C	65	ILE	2.6
1	D	8	GLU	2.6
1	D	158[A]	GLY	2.6
1	C	238	GLU	2.5
1	D	231	TYR	2.5
1	A	224	LEU	2.5
1	C	160[A]	SER	2.5
1	C	123	GLY	2.5
1	D	21	GLY	2.5
1	B	211	GLY	2.5
1	B	226	VAL	2.5
1	C	169	GLU	2.4
1	B	115	LEU	2.4
1	B	37	ALA	2.4
1	C	39	GLY	2.4
1	B	238	GLU	2.4
1	D	11	GLN	2.4
1	A	226	VAL	2.4
1	B	114	ALA	2.3
1	C	11	GLN	2.3
1	B	232	TRP	2.3
1	C	116	TRP	2.3
1	A	256	ASP	2.3
1	B	65	ILE	2.3
1	D	114	ALA	2.3
1	D	192	TRP	2.3
1	A	169	GLU	2.3
1	B	101	ILE	2.2
1	B	135	ILE	2.2
1	B	158[A]	GLY	2.2
1	C	40	ILE	2.1
1	C	225	ASN	2.1
1	D	136	MET	2.1
1	A	223	ILE	2.1
1	A	11	GLN	2.1
1	B	124	GLU	2.1
1	B	256	ASP	2.1
1	C	77	GLY	2.1
1	A	181	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	ILE	2.1
1	D	224	LEU	2.1
1	C	101	ILE	2.0
1	D	101	ILE	2.0
1	B	160[A]	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	SO4	C	305	5/5	0.82	0.20	92,93,93,93	0
3	SO4	B	305	5/5	0.92	0.22	66,67,68,69	0
3	SO4	A	303	5/5	0.92	0.28	65,67,67,67	0
3	SO4	C	303	5/5	0.94	0.22	58,59,60,61	0
3	SO4	D	303	5/5	0.95	0.24	55,56,57,57	0
3	SO4	B	303	5/5	0.96	0.14	55,56,57,57	0
3	SO4	C	304	5/5	0.97	0.23	41,41,41,43	0
2	CA	A	301	1/1	0.97	0.06	29,29,29,29	0
2	CA	C	301	1/1	0.97	0.05	23,23,23,23	0
2	CA	D	301	1/1	0.98	0.05	26,26,26,26	0
3	SO4	B	304	5/5	0.99	0.16	48,49,50,51	0
2	CA	B	301	1/1	0.99	0.04	26,26,26,26	0
4	CL	B	302	1/1	0.99	0.04	29,29,29,29	0
4	CL	D	302	1/1	0.99	0.10	35,35,35,35	0
4	CL	C	302	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.