



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:12 AM UTC

PDB ID : 6GGY / pdb_00006ggy
Title : Paenibacillus sp. YM1 laminaribiose phosphorylase with sulphate bound
Authors : Kuhaudomlarp, S.; Walpole, S.; Stevenson, C.E.M.; Nepogodiev, S.A.; Lawson, D.M.; Angulo, J.; Field, R.A.
Deposited on : 2018-05-04
Resolution : 1.95 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)
Validation Pipeline (wwPDB-VP)	:	2.49

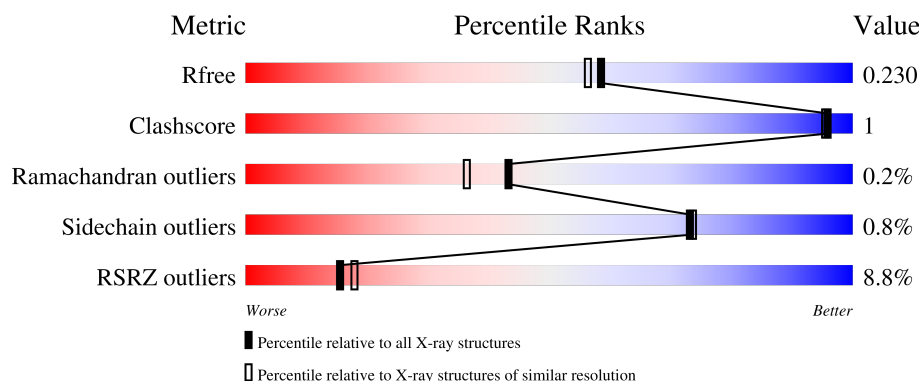
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	913	13% 95% ..
1	B	913	4% 96% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15063 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 Laminaribiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	908	Total	C	N	O	S	0	7	0
			6976	4421	1211	1321	23			
1	B	905	Total	C	N	O	S	0	7	0
			7087	4489	1241	1333	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP D7UT17
A	0	PRO	-	expression tag	UNP D7UT17
B	-1	GLY	-	expression tag	UNP D7UT17
B	0	PRO	-	expression tag	UNP D7UT17

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		

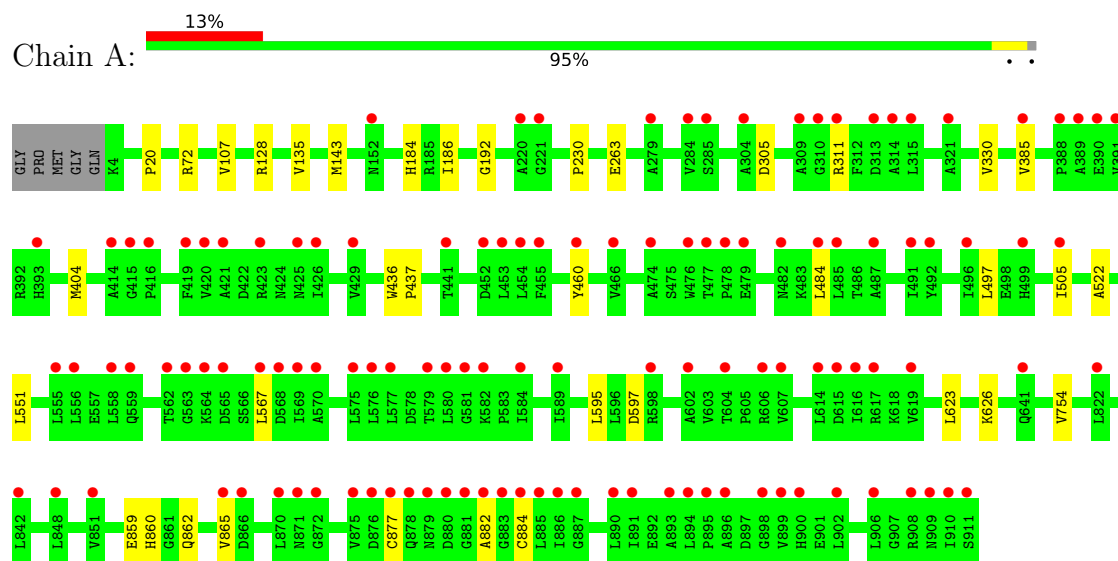
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	329	Total	O	0	19
			348	348		
5	B	563	Total	O	0	25
			588	588		

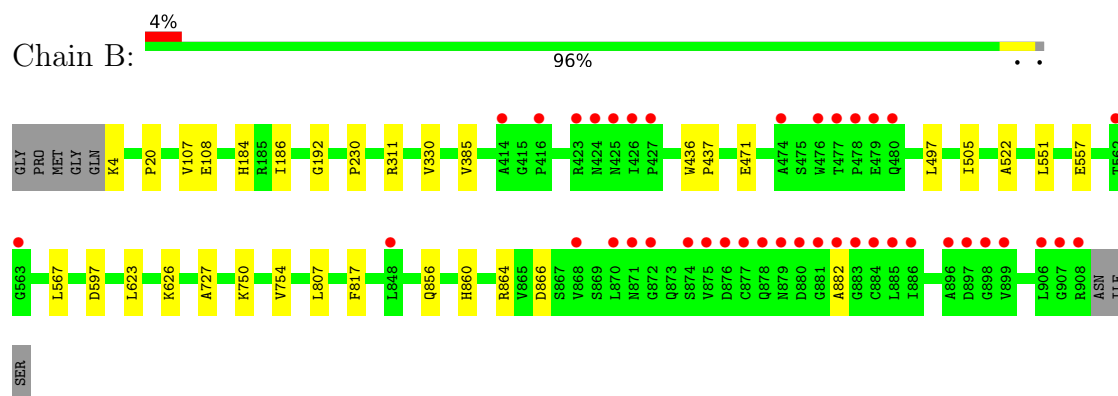
3 Residue-property plots [i](#)

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: Laminaribiose phosphorylase



• Molecule 1: Laminaribiose phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.70Å 146.70Å 222.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.74 – 1.95 103.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (103.74-1.95) 100.0 (103.74-1.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.223 0.208 , 0.230	Depositor DCC
R_{free} test set	8729 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15063	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2028e-03.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, EDO

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	0.69	0/7142	0.84	2/9710 (0.0%)
1	B	0.72	0/7252	0.84	1/9837 (0.0%)
All	All	0.71	0/14394	0.84	3/19547 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	VAL	CB-CA-C	-5.51	103.88	111.65
1	A	192	GLY	N-CA-C	5.06	117.41	110.58
1	B	192	GLY	N-CA-C	5.05	117.39	110.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6976	0	6524	19	0
1	B	7087	0	6786	12	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	A	16	0	24	0	0
3	B	24	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	348	0	0	0	0
5	B	588	0	0	1	0
All	All	15063	0	13370	30	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 1.

All (30) 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:404:MET:HE1	1:A:460:TYR:CE2	2.36	0.60
1:B:557:GLU:HG2	1:B:817:PHE:CZ	2.44	0.51
1:B:311[B]:ARG:NH2	5:B:1553[B]:HOH:O	2.44	0.49
1:A:877:CYS:HB3	1:A:884:CYS:HB2	1.95	0.49
1:A:404:MET:HE3	1:A:484:LEU:CD2	2.43	0.49
1:A:186:ILE:HG21	1:A:230:PRO:HB2	1.97	0.47
1:A:551:LEU:HB3	1:A:623:LEU:HD13	1.96	0.47
1:B:186:ILE:HG21	1:B:230:PRO:HB2	1.97	0.47
1:B:864:ARG:NH1	1:B:866:ASP:OD1	2.49	0.46
1:A:865:VAL:O	1:A:865:VAL:HG23	2.15	0.46
1:A:754:VAL:HG21	1:A:860:HIS:CE1	2.52	0.45
1:A:859:GLU:H	1:A:862:GLN:HE21	1.64	0.45
1:A:305:ASP:O	1:A:311[A]:ARG:NE	2.50	0.45
1:A:135:VAL:O	1:A:135:VAL:CG1	2.65	0.44
1:B:551:LEU:HB3	1:B:623:LEU:HD13	1.98	0.44
1:A:263[A]:GLU:HG3	1:B:727:ALA:HB1	1.99	0.44
1:A:595:LEU:C	1:A:595:LEU:HD23	2.42	0.44
1:B:20:PRO:HG3	1:B:107:VAL:HG23	2.00	0.43
1:A:20:PRO:HG3	1:A:107:VAL:HG23	1.99	0.43
1:A:497:LEU:HD23	1:A:567:LEU:HD22	2.01	0.43
1:B:754:VAL:HG21	1:B:860:HIS:CE1	2.54	0.43
1:B:436:TRP:N	1:B:437:PRO:CD	2.82	0.43
1:B:497:LEU:HD23	1:B:567:LEU:HD22	2.01	0.42
1:A:436:TRP:N	1:A:437:PRO:CD	2.82	0.42
1:A:128:ARG:NH1	2:A:1002:SO4:O3	2.53	0.41
1:B:505[A]:ILE:HG23	1:B:626:LYS:HE2	2.03	0.41
1:A:404:MET:CE	1:A:460:TYR:CD2	3.03	0.41
1:A:72:ARG:HB3	1:A:143:MET:HE1	2.02	0.41
1:A:505:ILE:HG23	1:A:626:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:VAL:HG11	1:B:807:LEU:HD23	2.03	0.40

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	913/913 (100%)	886 (97%)	25 (3%)	2 (0%)	43	36
1	B	910/913 (100%)	881 (97%)	27 (3%)	2 (0%)	43	36
All	All	1823/1826 (100%)	1767 (97%)	52 (3%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522	ALA
1	B	522	ALA
1	A	882	ALA
1	B	882	ALA

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	682/740 (92%)	679 (100%)	3 (0%)	84	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	715/740 (97%)	707 (99%)	8 (1%)	65	64
All	All	1397/1480 (94%)	1386 (99%)	11 (1%)	73	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	HIS
1	A	330	VAL
1	A	597	ASP
1	B	4	LYS
1	B	108	GLU
1	B	184	HIS
1	B	330	VAL
1	B	471	GLU
1	B	597	ASP
1	B	750	LYS
1	B	856	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	318	GLN
1	A	718	GLN
1	A	862	GLN
1	A	909	ASN
1	B	67	ASN
1	B	318	GLN
1	B	718	GLN
1	B	773	ASN
1	B	828	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
2	SO4	A	1002	-	4,4,4	0.49	0	6,6,6	0.25	0
2	SO4	B	1001	-	4,4,4	0.45	0	6,6,6	0.45	0
2	SO4	B	1002	-	4,4,4	0.44	0	6,6,6	0.23	0
3	EDO	B	1007	-	3,3,3	0.55	0	2,2,2	0.01	0
3	EDO	B	1008	-	3,3,3	0.37	0	2,2,2	0.42	0
3	EDO	B	1005	-	3,3,3	0.43	0	2,2,2	0.60	0
3	EDO	A	1005	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	A	1003	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	B	1004	-	3,3,3	0.51	0	2,2,2	0.10	0
3	EDO	A	1006	-	3,3,3	0.43	0	2,2,2	0.47	0
3	EDO	B	1003	-	3,3,3	0.59	0	2,2,2	0.29	0
2	SO4	A	1001	-	4,4,4	0.44	0	6,6,6	0.36	0
3	EDO	B	1006	-	3,3,3	0.46	0	2,2,2	0.43	0
3	EDO	A	1004	-	3,3,3	0.46	0	2,2,2	0.53	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
3	EDO	B	1007	-	-	1/1/1/1	-
3	EDO	B	1008	-	-	0/1/1/1	-
3	EDO	B	1005	-	-	0/1/1/1	-
3	EDO	A	1005	-	-	1/1/1/1	-
3	EDO	A	1003	-	-	0/1/1/1	-
3	EDO	B	1004	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1006	-	-	0/1/1/1	-
3	EDO	B	1003	-	-	0/1/1/1	-
3	EDO	B	1006	-	-	1/1/1/1	-
3	EDO	A	1004	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1005	EDO	O1-C1-C2-O2
3	A	1004	EDO	O1-C1-C2-O2
3	B	1007	EDO	O1-C1-C2-O2
3	B	1006	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
2	A	1002	SO4	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	908/913 (99%)	0.73	120 (13%) 7 8	14, 44, 85, 100	7 (0%)
1	B	905/913 (99%)	0.05	40 (4%) 39 45	10, 26, 63, 92	7 (0%)
All	All	1813/1826 (99%)	0.39	160 (8%) 15 18	10, 35, 79, 100	14 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	882	ALA	6.1
1	A	910	ILE	5.7
1	B	882	ALA	5.4
1	A	569	ILE	5.2
1	B	879	ASN	5.1
1	A	562	THR	5.1
1	B	426	ILE	5.0
1	A	879	ASN	5.0
1	B	424	ASN	4.9
1	A	476[A]	TRP	4.8
1	B	479	GLU	4.5
1	A	880	ASP	4.3
1	A	492	TYR	4.2
1	A	885	LEU	4.1
1	A	871	ASN	4.1
1	A	883	GLY	4.0
1	A	881	GLY	4.0
1	B	897	ASP	3.9
1	A	389	ALA	3.8
1	B	425	ASN	3.8
1	A	909	ASN	3.8
1	B	906	LEU	3.6
1	B	478	PRO	3.6
1	A	414	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	423	ARG	3.5
1	B	871	ASN	3.5
1	A	877	CYS	3.4
1	A	309	ALA	3.4
1	B	876	ASP	3.4
1	A	911	SER	3.4
1	B	881	GLY	3.4
1	B	427	PRO	3.4
1	A	872	GLY	3.3
1	A	884	CYS	3.3
1	A	310	GLY	3.3
1	B	896	ALA	3.3
1	A	617	ARG	3.3
1	B	883	GLY	3.3
1	A	896	ALA	3.2
1	A	887	GLY	3.2
1	B	476	TRP	3.2
1	A	491	ILE	3.2
1	B	477	THR	3.2
1	A	581	GLY	3.2
1	A	388	PRO	3.2
1	A	870	LEU	3.2
1	A	890	LEU	3.2
1	A	419	PHE	3.2
1	B	423	ARG	3.2
1	A	479	GLU	3.1
1	A	878	GLN	3.1
1	A	460	TYR	3.1
1	B	880	ASP	3.1
1	A	421	ALA	3.1
1	B	885	LEU	3.1
1	B	878	GLN	3.1
1	A	416	PRO	3.1
1	B	884	CYS	3.0
1	A	221	GLY	3.0
1	A	842	LEU	3.0
1	A	604	THR	3.0
1	B	872	GLY	3.0
1	A	279	ALA	3.0
1	A	391	VAL	2.9
1	A	429	VAL	2.9
1	B	907	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	ASN	2.9
1	A	891	ILE	2.9
1	A	619	VAL	2.9
1	A	899	VAL	2.9
1	A	390	GLU	2.9
1	B	877	CYS	2.9
1	B	870	LEU	2.9
1	B	875	VAL	2.9
1	A	894	LEU	2.9
1	A	563	GLY	2.9
1	B	908	ARG	2.8
1	A	565	ASP	2.8
1	A	482	ASN	2.8
1	A	615	ASP	2.7
1	B	414	ALA	2.7
1	A	454	LEU	2.7
1	A	485	LEU	2.7
1	A	415	GLY	2.7
1	A	452	ASP	2.7
1	A	851	VAL	2.6
1	B	899	VAL	2.6
1	A	385	VAL	2.6
1	A	455	PHE	2.5
1	A	487	ALA	2.5
1	A	420	VAL	2.5
1	A	558	LEU	2.5
1	A	567	LEU	2.5
1	A	393	HIS	2.5
1	A	321	ALA	2.5
1	A	598	ARG	2.4
1	A	900	HIS	2.4
1	A	505	ILE	2.4
1	A	314	ALA	2.4
1	A	865	VAL	2.4
1	A	425	ASN	2.4
1	A	570	ALA	2.4
1	B	562	THR	2.4
1	A	886	ILE	2.4
1	A	893	ALA	2.4
1	A	607	VAL	2.4
1	A	484	LEU	2.3
1	A	614	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	564	LYS	2.3
1	A	466	VAL	2.3
1	A	822	LEU	2.3
1	A	477	THR	2.3
1	A	584	ILE	2.3
1	B	886	ILE	2.3
1	A	478	PRO	2.3
1	B	416	PRO	2.3
1	A	866	ASP	2.3
1	A	582	LYS	2.3
1	A	602	ALA	2.3
1	A	311[A]	ARG	2.3
1	B	563	GLY	2.3
1	A	568	ASP	2.3
1	A	555	LEU	2.3
1	A	556	LEU	2.3
1	A	474	ALA	2.2
1	A	575	LEU	2.2
1	A	577	LEU	2.2
1	A	898	GLY	2.2
1	A	576	LEU	2.2
1	A	313	ASP	2.2
1	B	898	GLY	2.2
1	A	895	PRO	2.2
1	B	474	ALA	2.2
1	A	496	ILE	2.2
1	A	908	ARG	2.2
1	A	579	THR	2.2
1	A	304	ALA	2.2
1	A	589	ILE	2.1
1	A	284	VAL	2.1
1	A	606	ARG	2.1
1	A	906	LEU	2.1
1	B	848	LEU	2.1
1	A	641	GLN	2.1
1	B	874	SER	2.1
1	A	875	VAL	2.1
1	A	902	LEU	2.1
1	A	220	ALA	2.1
1	A	285	SER	2.1
1	B	868	VAL	2.1
1	A	559	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	480	GLN	2.1
1	A	315	LEU	2.1
1	A	453	LEU	2.1
1	A	848	LEU	2.1
1	A	616	ILE	2.0
1	A	441	THR	2.0
1	A	499	HIS	2.0
1	A	580	LEU	2.0
1	A	876	ASP	2.0
1	A	426	ILE	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	B	1006	4/4	0.79	0.21	45,48,48,50	0
2	SO4	A	1002	5/5	0.82	0.10	56,57,60,64	0
3	EDO	A	1004	4/4	0.83	0.17	44,44,46,46	0
3	EDO	B	1005	4/4	0.87	0.16	39,40,40,41	0
3	EDO	B	1007	4/4	0.88	0.17	38,42,42,45	0
4	CL	B	1010	1/1	0.88	0.17	65,65,65,65	0
4	CL	A	1008	1/1	0.90	0.14	65,65,65,65	0
3	EDO	B	1004	4/4	0.91	0.15	49,49,49,49	0
3	EDO	A	1006	4/4	0.91	0.15	35,36,37,39	0
3	EDO	A	1005	4/4	0.92	0.12	35,36,36,36	0
3	EDO	B	1003	4/4	0.93	0.14	22,22,24,24	0
2	SO4	A	1001	5/5	0.94	0.12	32,33,36,37	0
3	EDO	B	1008	4/4	0.94	0.09	34,37,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1009	1/1	0.96	0.10	54,54,54,54	0
4	CL	A	1007	1/1	0.96	0.08	53,53,53,53	0
3	EDO	A	1003	4/4	0.97	0.09	23,25,25,26	0
2	SO4	B	1001	5/5	0.97	0.08	24,26,28,31	0
2	SO4	B	1002	5/5	0.98	0.10	35,38,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.