



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:15 AM UTC

PDB ID : 9N2W / pdb_00009n2w
Title : Dienelactone hydrolase family protein SaDLH from Solimonas aquatica
Authors : Schnettler Fernandez, J.D.F.; Campbell, E.C.; Hollfelder, F.
Deposited on : 2025-01-29
Resolution : 1.90 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

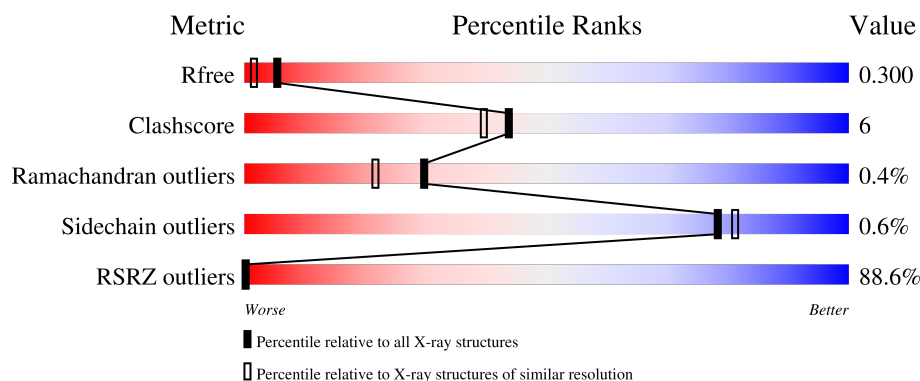
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	238	<div> <div>85%</div> <div>87%13%</div> </div>
1	B	238	<div> <div>90%</div> <div>86%13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3772 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 Dienelactone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	1	0
			1815	1139	335	331	10			
1	B	237	Total	C	N	O	S	0	1	0
			1815	1139	335	331	10			

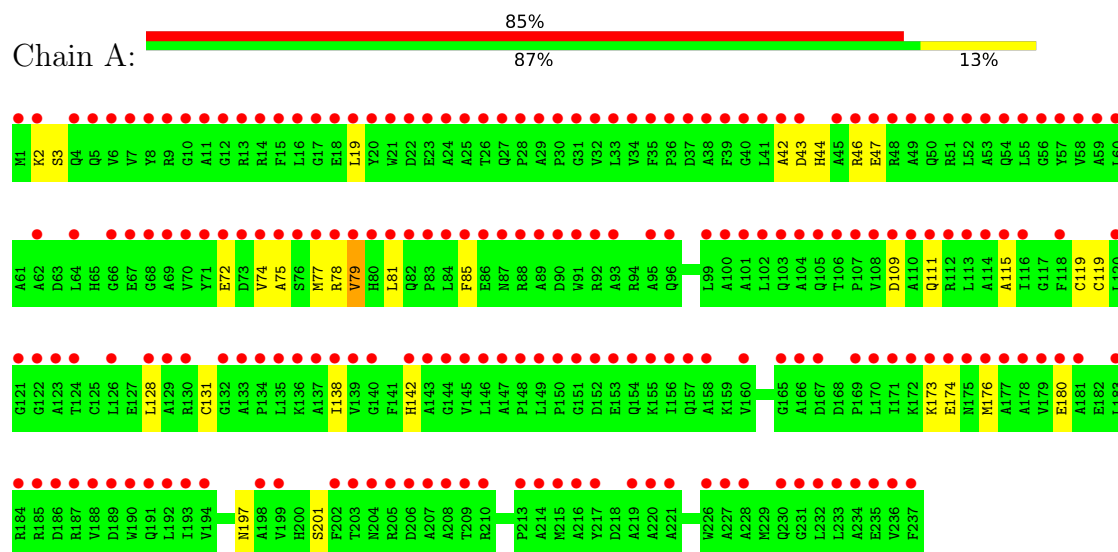
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	58	Total	O	0	0
			58	58		

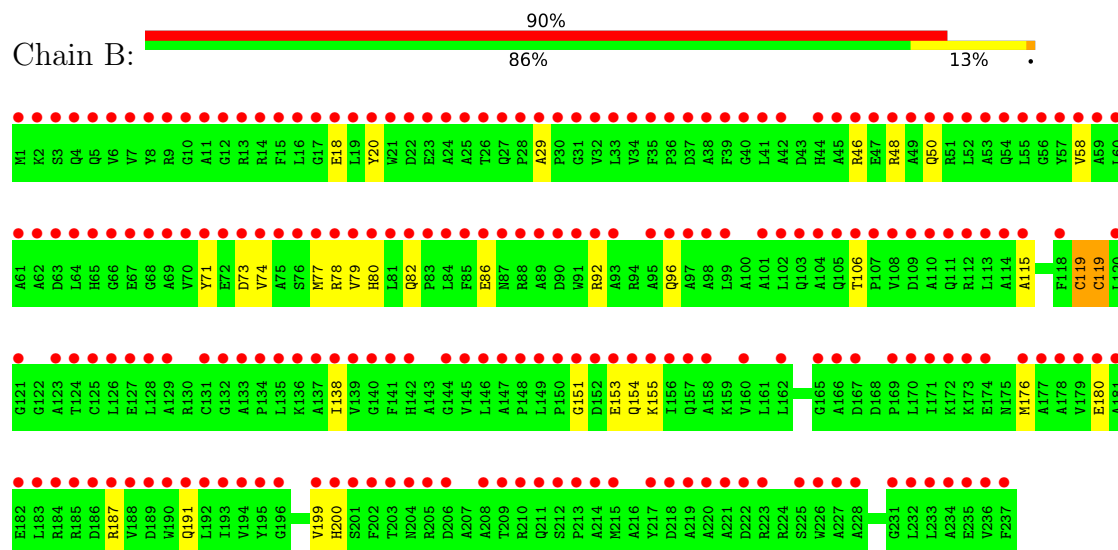
3 Residue-property plots [i](#)

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: Dienelactone hydrolase



• Molecule 1: Dienelactone hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.45Å 76.41Å 72.46Å 90.00° 107.77° 90.00°	Depositor
Resolution (Å)	69.00 – 1.90 69.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (69.00-1.90) 95.5 (69.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.243 , 0.298 0.248 , 0.300	Depositor DCC
R_{free} test set	2114 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3772	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.83% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CSD

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	0.36	0/1842	0.56	0/2496
1	B	0.36	0/1842	0.56	0/2496
All	All	0.36	0/3684	0.56	0/4992

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	1815	0	1791	20	0
1	B	1815	0	1792	22	0
2	A	84	0	0	0	0
2	B	58	0	0	2	0
All	All	3772	0	3583	41	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 6.

All (41) 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:173:LYS:HD2	1:A:173:LYS:H	1.28	0.97
1:B:119[A]:CSD:OD2	1:B:200:HIS:NE2	2.26	0.67
1:B:119[A]:CSD:SG	1:B:200:HIS:NE2	2.61	0.63
1:B:71:TYR:CZ	1:B:80:HIS:HD2	2.19	0.61
1:B:74:VAL:O	1:B:78:ARG:HG3	2.02	0.60
1:A:2:LYS:HD2	1:A:3:SER:H	1.71	0.56
1:A:43:ASP:O	1:A:47:GLU:HG2	2.06	0.55
1:A:173:LYS:HD2	1:A:173:LYS:N	2.11	0.54
1:A:72:GLU:H	1:A:72:GLU:CD	2.17	0.53
1:A:174:GLU:H	1:A:174:GLU:CD	2.17	0.53
1:A:197:ASN:OD1	1:B:187:ARG:HD3	2.10	0.52
1:B:46:ARG:O	1:B:50:GLN:HG3	2.11	0.51
1:B:82:GLN:O	1:B:86:GLU:HG2	2.11	0.51
1:A:173:LYS:H	1:A:173:LYS:CD	2.10	0.50
1:A:176:MET:O	1:A:180:GLU:HG3	2.11	0.49
1:A:74:VAL:O	1:A:78:ARG:HG3	2.13	0.48
1:B:151:GLY:O	1:B:155:LYS:NZ	2.46	0.48
1:A:81:LEU:HD11	1:A:85:PHE:CZ	2.49	0.48
1:B:79:VAL:HG12	1:B:80:HIS:ND1	2.29	0.48
1:B:79:VAL:HG12	1:B:80:HIS:CE1	2.49	0.48
1:B:119[A]:CSD:OD2	1:B:200:HIS:CE1	2.66	0.48
1:A:128:LEU:O	1:A:131:CYS:HB2	2.13	0.47
1:B:29:ALA:HB3	1:B:58:VAL:HG23	1.97	0.46
1:A:42:ALA:O	1:A:46:ARG:HG3	2.16	0.46
1:B:18:GLU:HG2	1:B:20:TYR:CZ	2.50	0.46
1:B:96:GLN:NE2	2:B:307:HOH:O	2.48	0.46
1:B:153:GLU:H	1:B:153:GLU:CD	2.22	0.46
1:B:92:ARG:O	1:B:96:GLN:HG3	2.16	0.45
1:A:75:ALA:O	1:A:79:VAL:HG13	2.18	0.44
1:B:77:MET:SD	1:B:77:MET:C	3.00	0.44
1:A:44:HIS:O	1:A:47:GLU:HG3	2.19	0.42
1:A:109:ASP:OD1	1:A:111:GLN:HB2	2.20	0.42
1:B:73:ASP:OD2	1:B:73:ASP:C	2.62	0.42
1:B:176:MET:O	1:B:180:GLU:HG3	2.19	0.42
1:A:142:HIS:CE1	1:A:201:SER:HA	2.54	0.42
1:A:3:SER:HA	1:A:19:LEU:O	2.20	0.41
1:B:191:GLN:HG3	2:B:343:HOH:O	2.21	0.40
1:A:77:MET:C	1:A:77:MET:SD	3.04	0.40
1:B:48:ARG:HD3	1:B:48:ARG:HA	1.79	0.40
1:B:115:ALA:O	1:B:138:ILE:HA	2.22	0.40
1:A:115:ALA:O	1:A:138:ILE:HA	2.21	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	234/238 (98%)	228 (97%)	6 (3%)	0	100	100
1	B	234/238 (98%)	223 (95%)	9 (4%)	2 (1%)	14	6
All	All	468/476 (98%)	451 (96%)	15 (3%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	GLN
1	B	199	VAL

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	172/172 (100%)	171 (99%)	1 (1%)	78	81
1	B	172/172 (100%)	171 (99%)	1 (1%)	78	81
All	All	344/344 (100%)	342 (99%)	2 (1%)	78	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	B	106	THR

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	5	GLN
1	A	50	GLN
1	A	54	GLN
1	A	65	HIS
1	A	105	GLN
1	A	157	GLN
1	B	44	HIS
1	B	80	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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
1	CSD	B	119[A]	1	4,7,8	0.53	0	1,8,10	2.33	1 (100%)
1	CSD	A	119[A]	1	4,7,8	0.80	0	1,8,10	4.14	1 (100%)

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
1	CSD	B	119[A]	1	-	1/2/6/8	-
1	CSD	A	119[A]	1	-	1/2/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119[A]	CSD	OD1-SG-CB	4.14	113.23	105.60
1	B	119[A]	CSD	OD1-SG-CB	2.33	109.89	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	119[A]	CSD	N-CA-CB-SG
1	B	119[A]	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	119[A]	CSD	3	0

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	236/238 (99%)	3.34	203 (86%)  	25, 38, 64, 80	0
1	B	236/238 (99%)	3.51	215 (91%)  	25, 39, 69, 89	0
All	All	472/476 (99%)	3.43	418 (88%)  	25, 38, 66, 89	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	10.3
1	B	1	MET	8.6
1	B	85	PHE	8.1
1	A	1	MET	7.9
1	A	25	ALA	7.9
1	B	150	PRO	7.4
1	A	21	TRP	7.4
1	B	23	GLU	7.3
1	A	26	THR	7.1
1	A	24	ALA	7.0
1	B	83	PRO	7.0
1	A	81	LEU	6.9
1	B	79	VAL	6.9
1	B	82	GLN	6.9
1	A	150	PRO	6.7
1	B	21	TRP	6.6
1	B	26	THR	6.6
1	B	84	LEU	6.6
1	A	71	TYR	6.5
1	B	25	ALA	6.4
1	B	76	SER	6.3
1	B	149	LEU	6.2
1	B	74	VAL	6.1
1	A	23	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	79	VAL	6.0
1	A	85	PHE	5.9
1	A	75	ALA	5.9
1	B	146	LEU	5.9
1	A	76	SER	5.8
1	A	74	VAL	5.8
1	B	22	ASP	5.8
1	B	91	TRP	5.7
1	A	82	GLN	5.7
1	A	80	HIS	5.6
1	A	27	GLN	5.5
1	A	237	PHE	5.5
1	A	86	GLU	5.5
1	A	236	VAL	5.4
1	A	89	ALA	5.4
1	B	24	ALA	5.4
1	B	86	GLU	5.4
1	A	47	GLU	5.3
1	B	27	GLN	5.3
1	B	53	ALA	5.3
1	A	70	VAL	5.2
1	A	151	GLY	5.2
1	A	28	PRO	5.2
1	A	149	LEU	5.2
1	B	106	THR	5.0
1	B	151	GLY	5.0
1	B	75	ALA	5.0
1	B	80	HIS	4.9
1	B	47	GLU	4.9
1	A	42	ALA	4.9
1	B	166	ALA	4.9
1	B	173	LYS	4.9
1	B	42	ALA	4.9
1	A	54	GLN	4.8
1	B	71	TYR	4.8
1	B	28	PRO	4.8
1	A	157	GLN	4.7
1	A	84	LEU	4.7
1	A	110	ALA	4.7
1	B	64	LEU	4.7
1	B	78	ARG	4.7
1	A	144	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLY	4.6
1	B	39	PHE	4.6
1	A	146	LEU	4.6
1	B	16	LEU	4.6
1	B	113	LEU	4.6
1	A	2	LYS	4.6
1	B	206	ASP	4.6
1	B	174	GLU	4.5
1	B	49	ALA	4.5
1	A	6	VAL	4.5
1	A	209	THR	4.5
1	A	49	ALA	4.5
1	B	38	ALA	4.5
1	B	213	PRO	4.5
1	A	171	ILE	4.4
1	A	73	ASP	4.4
1	A	180	GLU	4.4
1	B	35	PHE	4.4
1	A	112	ARG	4.4
1	B	69	ALA	4.4
1	B	177	ALA	4.3
1	A	172	LYS	4.3
1	B	152	ASP	4.3
1	B	232	LEU	4.3
1	A	106	THR	4.3
1	A	29	ALA	4.3
1	A	177	ALA	4.3
1	B	18	GLU	4.3
1	A	19	LEU	4.2
1	B	157	GLN	4.2
1	A	78	ARG	4.2
1	A	205	ARG	4.2
1	B	236	VAL	4.2
1	B	169	PRO	4.2
1	B	170	LEU	4.2
1	B	72	GLU	4.2
1	A	206	ASP	4.2
1	B	55	LEU	4.2
1	A	118	PHE	4.2
1	B	58	VAL	4.2
1	B	179	VAL	4.2
1	A	22	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	109	ASP	4.2
1	A	69	ALA	4.2
1	B	124	THR	4.2
1	A	15	PHE	4.1
1	B	40	GLY	4.1
1	B	70	VAL	4.1
1	B	41	LEU	4.1
1	B	156	ILE	4.1
1	A	8	TYR	4.1
1	B	195	TYR	4.1
1	A	170	LEU	4.1
1	B	68	GLY	4.1
1	A	46	ARG	4.0
1	A	220	ALA	4.0
1	B	227	ALA	4.0
1	B	154	GLN	4.0
1	A	186	ASP	4.0
1	A	148	PRO	4.0
1	A	20	TYR	4.0
1	B	87	ASN	4.0
1	B	4	GLN	4.0
1	B	147	ALA	4.0
1	A	39	PHE	4.0
1	B	112	ARG	4.0
1	B	148	PRO	4.0
1	B	237	PHE	4.0
1	A	4	GLN	3.9
1	A	91	TRP	3.9
1	B	190	TRP	3.9
1	B	19	LEU	3.9
1	A	147	ALA	3.9
1	A	181	ALA	3.9
1	A	213	PRO	3.9
1	B	133	ALA	3.9
1	B	178	ALA	3.9
1	A	120	LEU	3.9
1	B	77	MET	3.9
1	B	192	LEU	3.9
1	B	153	GLU	3.9
1	A	123	ALA	3.9
1	B	110	ALA	3.9
1	B	2	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	56	GLY	3.8
1	B	15	PHE	3.8
1	A	183	LEU	3.8
1	A	90	ASP	3.8
1	B	123	ALA	3.8
1	A	43	ASP	3.8
1	B	208	ALA	3.8
1	B	226	TRP	3.8
1	B	88	ARG	3.8
1	B	73	ASP	3.7
1	B	111	GLN	3.7
1	B	61	ALA	3.7
1	B	171	ILE	3.7
1	B	194	VAL	3.7
1	B	99	LEU	3.7
1	A	133	ALA	3.7
1	A	219	ALA	3.7
1	B	29	ALA	3.7
1	B	214	ALA	3.7
1	B	33	LEU	3.7
1	A	234	ALA	3.7
1	B	59	ALA	3.7
1	A	16	LEU	3.6
1	A	64	LEU	3.6
1	A	192	LEU	3.6
1	B	65	HIS	3.6
1	A	87	ASN	3.6
1	A	204	ASN	3.6
1	B	140	GLY	3.6
1	B	108	VAL	3.6
1	A	83	PRO	3.6
1	A	152	ASP	3.6
1	A	179	VAL	3.6
1	A	41	LEU	3.6
1	A	174	GLU	3.6
1	A	138	ILE	3.6
1	B	36	PRO	3.6
1	A	185	ARG	3.6
1	A	122	GLY	3.5
1	B	3	SER	3.5
1	B	144	GLY	3.5
1	A	217	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	108	VAL	3.5
1	B	54	GLN	3.5
1	B	234	ALA	3.5
1	B	185	ARG	3.5
1	A	50	GLN	3.5
1	B	103	GLN	3.5
1	B	211	GLN	3.5
1	A	58	VAL	3.5
1	A	194	VAL	3.5
1	A	59	ALA	3.5
1	A	100	ALA	3.5
1	A	184	ARG	3.5
1	A	233	LEU	3.5
1	B	66	GLY	3.5
1	B	135	LEU	3.5
1	B	205	ARG	3.5
1	A	111	GLN	3.4
1	B	20	TYR	3.4
1	A	173	LYS	3.4
1	B	11	ALA	3.4
1	B	172	LYS	3.4
1	A	77	MET	3.4
1	A	176	MET	3.4
1	A	226	TRP	3.4
1	A	68	GLY	3.4
1	A	107	PRO	3.4
1	A	5	GLN	3.4
1	B	120	LEU	3.4
1	A	36	PRO	3.4
1	A	72	GLU	3.3
1	B	210	ARG	3.3
1	A	99	LEU	3.3
1	A	113	LEU	3.3
1	A	18	GLU	3.3
1	A	104	ALA	3.3
1	A	158	ALA	3.3
1	B	176	MET	3.3
1	B	162	LEU	3.3
1	A	67	GLU	3.3
1	B	180	GLU	3.3
1	B	193	ILE	3.3
1	A	207	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	3.3
1	B	209	THR	3.3
1	A	109	ASP	3.3
1	A	14	ARG	3.3
1	B	132	GLY	3.3
1	A	214	ALA	3.2
1	B	34	VAL	3.2
1	B	118	PHE	3.2
1	A	140	GLY	3.2
1	A	55	LEU	3.2
1	B	67	GLU	3.2
1	A	191	GLN	3.2
1	A	129	ALA	3.2
1	A	7	VAL	3.2
1	A	153	GLU	3.2
1	A	33	LEU	3.1
1	B	233	LEU	3.1
1	B	90	ASP	3.1
1	A	193	ILE	3.1
1	A	232	LEU	3.1
1	B	32	VAL	3.1
1	B	45	ALA	3.1
1	B	95	ALA	3.1
1	A	188	VAL	3.1
1	B	136	LYS	3.1
1	B	218	ASP	3.0
1	B	105	GLN	3.0
1	B	199	VAL	3.0
1	B	225	SER	3.0
1	A	132	GLY	3.0
1	B	93	ALA	3.0
1	B	167	ASP	3.0
1	B	101	ALA	3.0
1	B	188	VAL	3.0
1	B	184	ARG	3.0
1	B	215	MET	3.0
1	A	101	ALA	3.0
1	B	145	VAL	2.9
1	A	154	GLN	2.9
1	A	167	ASP	2.9
1	B	46	ARG	2.9
1	A	38	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	2.9
1	A	114	ALA	2.9
1	A	137	ALA	2.9
1	A	178	ALA	2.9
1	B	128	LEU	2.9
1	B	204	ASN	2.9
1	B	44	HIS	2.9
1	A	105	GLN	2.9
1	A	34	VAL	2.9
1	B	30	PRO	2.9
1	B	107	PRO	2.9
1	A	35	PHE	2.9
1	A	189	ASP	2.9
1	A	190	TRP	2.9
1	A	202	PHE	2.8
1	A	208	ALA	2.8
1	B	129	ALA	2.8
1	B	37	ASP	2.8
1	B	52	LEU	2.8
1	B	138	ILE	2.8
1	A	31	GLY	2.8
1	B	17	GLY	2.8
1	A	37	ASP	2.8
1	A	11	ALA	2.8
1	B	114	ALA	2.8
1	A	203	THR	2.8
1	A	169	PRO	2.8
1	B	6	VAL	2.8
1	B	92	ARG	2.8
1	A	165	GLY	2.8
1	B	126	LEU	2.8
1	B	182	GLU	2.8
1	A	30	PRO	2.8
1	B	7	VAL	2.8
1	B	219	ALA	2.7
1	B	202	PHE	2.7
1	B	200	HIS	2.7
1	A	10	GLY	2.7
1	A	52	LEU	2.7
1	A	156	ILE	2.7
1	A	199	VAL	2.7
1	A	230	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLN	2.7
1	B	127	GLU	2.7
1	B	104	ALA	2.7
1	A	56	GLY	2.7
1	B	196	GLY	2.7
1	A	227	ALA	2.6
1	B	10	GLY	2.6
1	B	155	LYS	2.6
1	B	60	LEU	2.6
1	A	215	MET	2.6
1	B	160	VAL	2.6
1	B	115	ALA	2.6
1	A	126	LEU	2.6
1	A	135	LEU	2.6
1	A	121	GLY	2.6
1	B	50	GLN	2.6
1	B	189	ASP	2.6
1	B	231	GLY	2.6
1	B	62	ALA	2.6
1	B	158	ALA	2.6
1	B	131	CYS	2.6
1	B	235	GLU	2.6
1	B	165	GLY	2.6
1	A	160	VAL	2.6
1	B	98	ALA	2.6
1	B	221	ALA	2.6
1	B	228	ALA	2.6
1	A	134	PRO	2.5
1	B	8	TYR	2.5
1	B	134	PRO	2.5
1	B	141	PHE	2.5
1	B	183	LEU	2.5
1	A	45	ALA	2.5
1	B	181	ALA	2.5
1	A	92	ARG	2.5
1	B	14	ARG	2.5
1	A	155	LYS	2.5
1	B	57	TYR	2.5
1	A	17	GLY	2.5
1	B	102	LEU	2.5
1	B	187	ARG	2.5
1	B	89	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	203	THR	2.5
1	A	51	ARG	2.4
1	B	212	SER	2.4
1	A	88	ARG	2.4
1	A	210	ARG	2.4
1	A	12	GLY	2.4
1	A	40	GLY	2.4
1	A	231	GLY	2.4
1	A	57	TYR	2.4
1	A	62	ALA	2.4
1	A	115	ALA	2.4
1	A	143	ALA	2.4
1	A	48	ARG	2.4
1	B	51	ARG	2.4
1	A	142	HIS	2.4
1	A	187	ARG	2.4
1	A	221	ALA	2.4
1	B	97	ALA	2.4
1	A	32	VAL	2.4
1	A	145	VAL	2.4
1	B	139	VAL	2.4
1	B	201	SER	2.4
1	A	136	LYS	2.4
1	B	223	ARG	2.3
1	A	103	GLN	2.3
1	B	137	ALA	2.3
1	B	13	ARG	2.3
1	B	63	ASP	2.3
1	A	124	THR	2.3
1	B	217	TYR	2.3
1	A	95	ALA	2.3
1	A	166	ALA	2.3
1	A	235	GLU	2.3
1	B	125	CYS	2.3
1	A	128	LEU	2.3
1	A	13	ARG	2.2
1	A	116	ILE	2.2
1	A	60	LEU	2.2
1	A	66	GLY	2.2
1	B	31	GLY	2.2
1	B	9	ARG	2.2
1	B	96	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	93	ALA	2.2
1	A	9	ARG	2.2
1	B	48	ARG	2.2
1	A	102	LEU	2.2
1	A	96	GLN	2.1
1	A	198	ALA	2.1
1	B	191	GLN	2.1
1	B	220	ALA	2.1
1	B	186	ASP	2.1
1	A	139	VAL	2.1
1	A	130	ARG	2.1
1	B	121	GLY	2.0
1	A	175	ASN	2.0
1	A	216	ALA	2.0
1	B	222	ASP	2.0
1	B	142	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CSD	A	119[A]	8/9	0.72	0.19	27,31,39,44	8
1	CSD	B	119[A]	8/9	0.73	0.17	28,31,43,43	8

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.