



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:42 AM UTC

PDB ID : 1QLW / pdb_00001qlw
Title : The Atomic Resolution Structure of a Novel Bacterial Esterase
Authors : Bourne, P.C.; Isupov, M.N.; Littlechild, J.A.
Deposited on : 1999-09-17
Resolution : 1.09 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

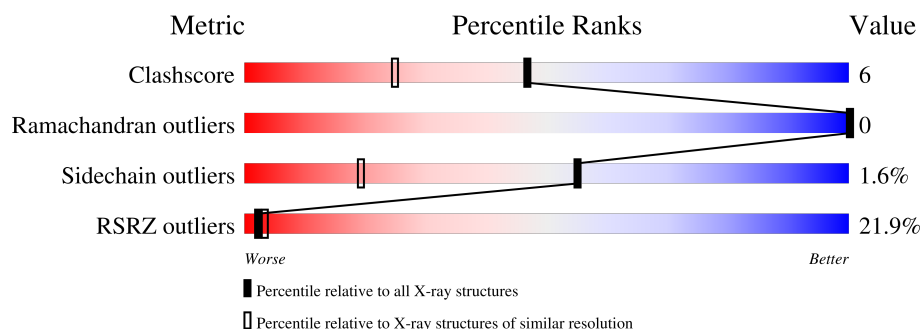
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.09 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	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	328	 19% 88% 6% ...
1	B	328	 23% 86% 9% ...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5599 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 ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	1	0
			2436	1554	420	448	14			
1	B	317	Total	C	N	O	S	0	4	0
			2433	1552	418	449	14			

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



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

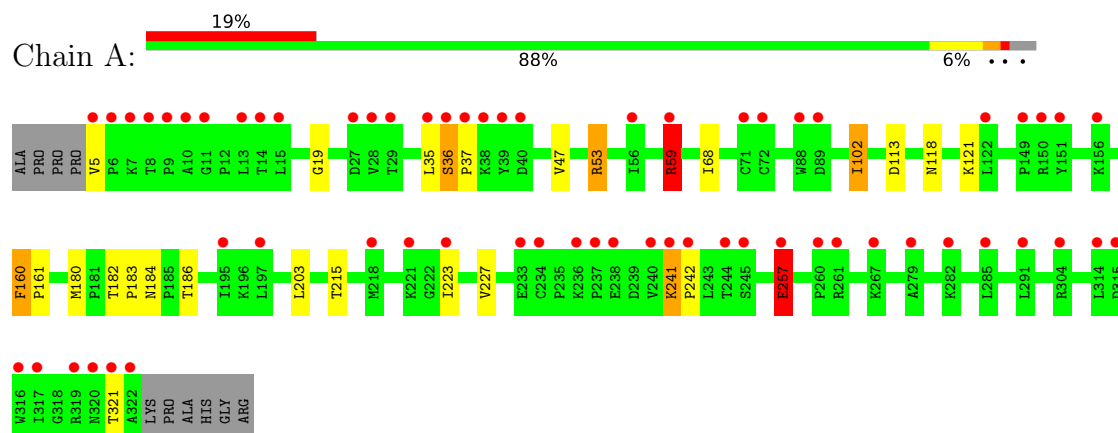
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	369	Total 369	O 369	0	0
3	B	346	Total 346	O 346	0	0

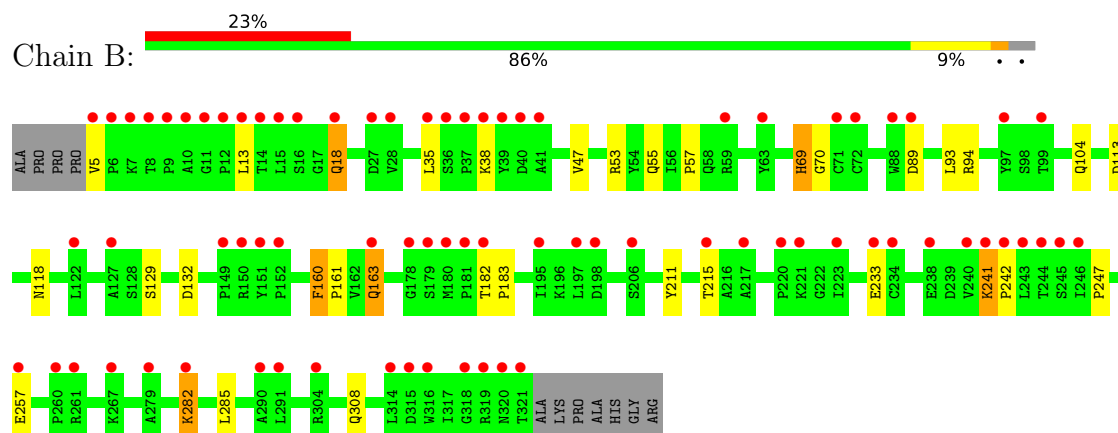
3 Residue-property plots [i](#)

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: ESTERASE



• Molecule 1: ESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.73Å 55.60Å 110.20Å 90.00° 125.06° 90.00°	Depositor
Resolution (Å)	30.00 – 1.09 30.00 – 1.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.09) 98.8 (30.00-1.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.143 , 0.158 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5599	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: 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	0.60	4/2510 (0.2%)	1.41	10/3423 (0.3%)
1	B	0.53	0/2522	1.10	12/3441 (0.3%)
All	All	0.57	4/5032 (0.1%)	1.26	22/6864 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ARG	NE-CZ	-10.21	1.21	1.33
1	A	59	ARG	CZ-NH2	8.96	1.45	1.33
1	A	180	MET	SD-CE	-6.51	1.63	1.79
1	A	59	ARG	CD-NE	-5.42	1.38	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	NE-CZ-NH2	-48.94	75.15	119.20
1	A	59	ARG	NE-CZ-NH1	23.30	144.80	121.50
1	A	59	ARG	NH1-CZ-NH2	14.90	138.68	119.30
1	B	257	GLU	CB-CG-CD	13.14	134.95	112.60
1	B	89	ASP	CA-CB-CG	12.33	124.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NH1-CZ-NH2	11.23	133.90	119.30
1	B	53	ARG	NE-CZ-NH2	-10.37	109.87	119.20
1	A	59	ARG	CD-NE-CZ	-9.04	111.75	124.40
1	B	18	GLN	OE1-CD-NE2	7.47	130.07	122.60
1	A	257	GLU	CB-CG-CD	6.97	124.45	112.60
1	B	18	GLN	CA-CB-CG	6.63	127.37	114.10
1	A	257	GLU	CG-CD-OE2	6.26	132.79	118.40
1	B	69	HIS	CB-CG-CD2	-6.08	123.29	131.20
1	B	233	GLU	CA-CB-CG	6.00	126.10	114.10
1	B	69	HIS	CB-CG-ND1	5.71	131.26	122.70
1	A	321	THR	N-CA-C	-5.58	105.07	113.89
1	B	160	PHE	CA-CB-CG	-5.56	108.24	113.80
1	B	53	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	53	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	282	LYS	CA-CB-CG	5.31	124.71	114.10
1	A	160	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	180	MET	CG-SD-CE	-5.10	89.69	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ARG	Sidechain
1	B	38	LYS	Mainchain

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	2436	0	2398	21	0
1	B	2433	0	2387	35	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	369	0	0	7	0
3	B	346	0	0	3	0
All	All	5599	0	4785	55	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 (55) 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:59:ARG:CZ	3:A:2090:HOH:O	1.85	1.18
1:A:59:ARG:NH2	3:A:2090:HOH:O	1.87	1.06
1:B:13:LEU:HD11	1:B:93[B]:LEU:HD12	1.41	0.96
1:B:55:GLN:HE21	1:B:93[A]:LEU:HD11	1.46	0.80
1:A:35:LEU:HD11	3:A:2187:HOH:O	1.83	0.79
1:B:69:HIS:CE1	1:B:104:GLN:H	2.04	0.75
1:B:69:HIS:HE1	1:B:104:GLN:H	1.32	0.74
1:B:13:LEU:HD11	1:B:93[B]:LEU:CD1	2.20	0.71
1:B:55:GLN:NE2	1:B:93[A]:LEU:HD11	2.07	0.70
1:B:247:PRO:HG3	1:B:282:LYS:HE3	1.73	0.70
1:A:257:GLU:CD	3:A:2312:HOH:O	2.37	0.67
1:B:247:PRO:HB3	1:B:282:LYS:HD2	1.76	0.67
1:B:241:LYS:HD3	1:B:241:LYS:H	1.62	0.64
1:B:247:PRO:HA	1:B:282:LYS:HG3	1.81	0.62
1:A:184:ASN:HD22	1:A:186:THR:H	1.48	0.60
1:B:57:PRO:HB3	1:B:93[B]:LEU:HD13	1.82	0.60
1:A:121:LYS:HE2	1:B:132[A]:ASP:OD1	2.01	0.60
1:B:241:LYS:H	1:B:241:LYS:CD	2.13	0.59
1:B:55:GLN:NE2	1:B:93[A]:LEU:CD1	2.66	0.59
1:A:184:ASN:ND2	1:A:186:THR:H	2.03	0.57
1:B:13:LEU:CD1	1:B:93[B]:LEU:HD12	2.25	0.56
1:A:59:ARG:NH1	3:A:2090:HOH:O	2.18	0.55
1:B:211:TYR:O	1:B:215:THR:HG23	2.07	0.54
1:B:13:LEU:HD21	1:B:93[B]:LEU:HG	1.89	0.52
1:B:282:LYS:HG2	3:B:2288:HOH:O	2.08	0.52
1:B:69:HIS:HD2	1:B:70:GLY:O	1.94	0.50
1:A:5:VAL:HG13	3:A:2350:HOH:O	2.12	0.50
1:A:118:ASN:ND2	3:A:2187:HOH:O	2.45	0.49
1:B:247:PRO:HG3	1:B:282:LYS:CE	2.43	0.48
1:B:241:LYS:HB2	1:B:242:PRO:HD3	1.95	0.48
1:A:215:THR:HG22	1:A:223:ILE:HD11	1.96	0.46
1:B:163:GLN:H	1:B:163:GLN:HG3	1.61	0.45
1:A:19:GLY:O	1:A:53:ARG:HD2	2.16	0.45
1:B:129:SER:HB3	3:B:2167:HOH:O	2.16	0.45
1:B:182:THR:HA	1:B:183:PRO:C	2.41	0.45
1:A:36:SER:HB2	1:A:37:PRO:HD2	1.99	0.44
1:A:47:VAL:HG11	1:A:113:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HG22	1:B:308:GLN:HB2	1.98	0.44
1:A:182:THR:HA	1:A:183:PRO:C	2.42	0.43
1:B:47:VAL:HG11	1:B:113:ASP:HB2	1.99	0.43
1:B:13:LEU:HD21	1:B:93[B]:LEU:HD12	2.01	0.43
1:B:13:LEU:HD21	1:B:93[B]:LEU:CG	2.49	0.43
1:A:241:LYS:HB2	1:A:242:PRO:HD3	2.01	0.42
1:A:241:LYS:H	1:A:241:LYS:HD3	1.85	0.42
1:B:13:LEU:HD13	1:B:94:ARG:HG2	2.01	0.42
1:A:160:PHE:CD1	1:A:161:PRO:HD2	2.55	0.41
1:A:68:ILE:HG23	1:A:102:ILE:HD11	2.02	0.41
1:B:160:PHE:CD1	1:B:161:PRO:HD2	2.55	0.41
1:A:203:LEU:HA	1:A:227:VAL:O	2.21	0.41
1:A:203:LEU:C	1:A:203:LEU:HD23	2.46	0.41
1:B:13:LEU:HD21	1:B:93[B]:LEU:CD1	2.50	0.41
1:B:241:LYS:HD3	1:B:241:LYS:N	2.33	0.40
1:B:285:LEU:C	1:B:285:LEU:HD23	2.46	0.40
1:B:118:ASN:ND2	3:B:2169:HOH:O	2.53	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	317/328 (97%)	311 (98%)	6 (2%)	0	100	100
1	B	319/328 (97%)	313 (98%)	6 (2%)	0	100	100
All	All	636/656 (97%)	624 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	260/267 (97%)	256 (98%)	4 (2%)	57	20
1	B	261/267 (98%)	257 (98%)	4 (2%)	57	20
All	All	521/534 (98%)	513 (98%)	8 (2%)	55	20

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	102	ILE
1	A	241	LYS
1	A	257	GLU
1	B	18	GLN
1	B	35	LEU
1	B	163	GLN
1	B	241	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	55	GLN
1	A	118	ASN
1	A	159	GLN
1	A	171	GLN
1	A	184	ASN
1	A	308	GLN
1	B	18	GLN
1	B	55	GLN
1	B	69	HIS
1	B	104	GLN
1	B	118	ASN
1	B	163	GLN
1	B	308	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z > 2$
2	SO4	A	576	-	4,4,4	0.85	0	6,6,6	0.47	0
2	SO4	A	575	-	4,4,4	0.89	0	6,6,6	0.81	0
2	SO4	B	575	-	4,4,4	0.69	0	6,6,6	0.18	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.

No monomer is involved in short contacts.

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, 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	318/328 (96%)	1.26	62 (19%) 3 4	10, 17, 29, 70	1 (0%)
1	B	317/328 (96%)	1.42	77 (24%) 2 3	11, 18, 30, 81	4 (1%)
All	All	635/656 (96%)	1.34	139 (21%) 2 3	10, 17, 30, 81	5 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	15.3
1	A	5	VAL	13.0
1	A	322	ALA	10.0
1	B	6	PRO	9.1
1	A	6	PRO	7.6
1	B	39	TYR	6.6
1	B	37	PRO	6.5
1	B	35	LEU	6.0
1	B	13	LEU	5.9
1	A	37	PRO	5.4
1	B	282	LYS	5.3
1	A	321	THR	5.2
1	B	321	THR	5.0
1	B	257	GLU	4.9
1	A	241	LYS	4.9
1	B	315	ASP	4.8
1	B	7	LYS	4.8
1	B	38	LYS	4.7
1	A	8	THR	4.7
1	A	7	LYS	4.7
1	B	150	ARG	4.6
1	A	237	PRO	4.6
1	A	35	LEU	4.5
1	A	315	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	36	SER	4.5
1	A	39	TYR	4.4
1	A	9	PRO	4.3
1	A	10	ALA	4.3
1	B	241	LYS	4.2
1	B	10	ALA	4.1
1	B	8	THR	4.0
1	A	36	SER	3.8
1	B	304	ARG	3.8
1	B	15	LEU	3.8
1	B	197	LEU	3.8
1	B	89	ASP	3.7
1	A	238	GLU	3.7
1	B	59	ARG	3.6
1	A	234	CYS	3.6
1	A	11	GLY	3.5
1	B	9	PRO	3.4
1	A	282	LYS	3.4
1	A	59	ARG	3.4
1	B	215	THR	3.3
1	A	319	ARG	3.3
1	A	38	LYS	3.3
1	B	163	GLN	3.3
1	B	72	CYS	3.2
1	B	11	GLY	3.1
1	A	240	VAL	3.1
1	B	195	ILE	3.1
1	A	291	LEU	3.1
1	B	178	GLY	3.0
1	A	71	CYS	3.0
1	B	71	CYS	3.0
1	A	257	GLU	2.9
1	A	236	LYS	2.9
1	B	319	ARG	2.9
1	A	151	TYR	2.9
1	A	242	PRO	2.9
1	B	12	PRO	2.9
1	B	242	PRO	2.9
1	A	56	ILE	2.9
1	A	15	LEU	2.9
1	B	234	CYS	2.9
1	A	245	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	260	PRO	2.9
1	B	149	PRO	2.8
1	B	223	ILE	2.8
1	A	261	ARG	2.8
1	B	179	SER	2.7
1	A	197	LEU	2.7
1	B	28	VAL	2.7
1	A	72	CYS	2.7
1	B	27	ASP	2.7
1	A	150	ARG	2.7
1	B	238	GLU	2.7
1	A	267	LYS	2.7
1	B	240	VAL	2.7
1	B	88	TRP	2.7
1	A	149	PRO	2.6
1	A	13	LEU	2.6
1	A	40	ASP	2.6
1	B	97	TYR	2.6
1	A	304	ARG	2.6
1	B	244	THR	2.6
1	B	151	TYR	2.6
1	B	261	ARG	2.5
1	B	318	GLY	2.5
1	A	156	LYS	2.5
1	A	221	LYS	2.5
1	B	40	ASP	2.5
1	B	320	ASN	2.5
1	B	221	LYS	2.5
1	A	29	THR	2.4
1	A	28	VAL	2.4
1	A	88	TRP	2.4
1	B	18	GLN	2.4
1	B	314	LEU	2.4
1	B	127	ALA	2.4
1	B	181	PRO	2.4
1	A	195	ILE	2.4
1	A	320	ASN	2.4
1	A	233	GLU	2.4
1	B	220	PRO	2.4
1	A	244	THR	2.4
1	B	246	ILE	2.4
1	B	182	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	317	ILE	2.3
1	A	314	LEU	2.3
1	B	233	GLU	2.3
1	A	218	MET	2.3
1	B	245	SER	2.3
1	B	122	LEU	2.3
1	B	198	ASP	2.3
1	B	63	TYR	2.2
1	A	260	PRO	2.2
1	B	217	ALA	2.2
1	B	243	LEU	2.2
1	A	223	ILE	2.2
1	B	316	TRP	2.2
1	B	206	SER	2.2
1	A	14	THR	2.1
1	B	99	THR	2.1
1	A	279	ALA	2.1
1	B	290	ALA	2.1
1	A	122	LEU	2.1
1	B	267	LYS	2.1
1	A	27	ASP	2.1
1	B	291	LEU	2.1
1	A	89	ASP	2.1
1	B	16	SER	2.1
1	B	152	PRO	2.1
1	A	316	TRP	2.1
1	B	180	MET	2.1
1	A	285	LEU	2.0
1	B	14	THR	2.0
1	B	41	ALA	2.0
1	B	279	ALA	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
2	SO4	B	575	5/5	0.87	0.17	30,31,32,32	0
2	SO4	A	576	5/5	0.88	0.24	23,24,24,25	0
2	SO4	A	575	5/5	0.94	0.20	18,21,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.