



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:31 AM EDT

PDB ID : 4FRF / pdb_00004frf
Title : Structural Studies and Protein Engineering of Inositol Phosphate Multikinase
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Deposited on : 2012-06-26
Resolution : 2.90 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

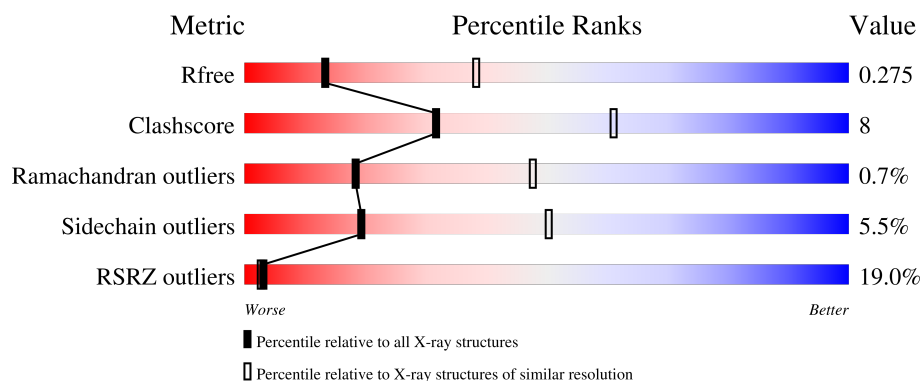
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	275	9% 58% 20% 22%
1	B	275	20% 64% 12% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3474 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 Inositol polyphosphate multikinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1726	1106	285	327	8			
1	B	213	Total	C	N	O	S	0	0	0
			1718	1100	284	326	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP Q9LY23
A	13	SER	-	expression tag	UNP Q9LY23
A	14	HIS	-	expression tag	UNP Q9LY23
A	15	MET	-	expression tag	UNP Q9LY23
B	12	GLY	-	expression tag	UNP Q9LY23
B	13	SER	-	expression tag	UNP Q9LY23
B	14	HIS	-	expression tag	UNP Q9LY23
B	15	MET	-	expression tag	UNP Q9LY23

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

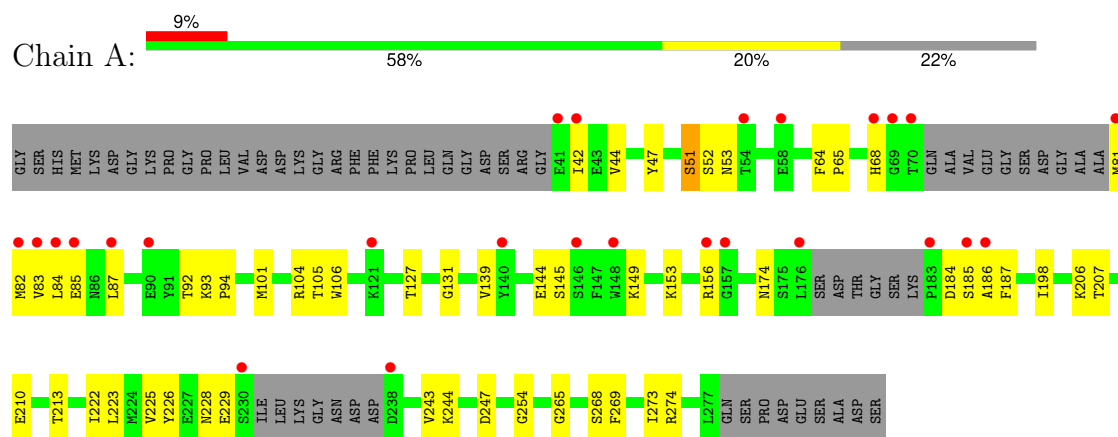


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

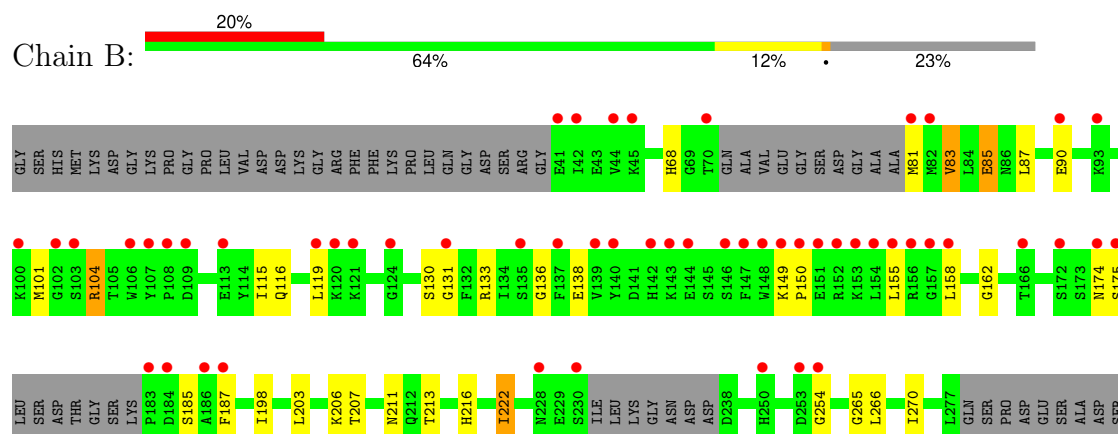
3 Residue-property plots

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: Inositol polyphosphate multikinase alpha



- Molecule 1: Inositol polyphosphate multikinase alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.79Å 130.79Å 129.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.90 46.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.00-2.90) 99.4 (46.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.239 , 0.251 0.262 , 0.275	Depositor DCC
R_{free} test set	1420 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3474	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.73	2/1767 (0.1%)	0.79	2/2384 (0.1%)
1	B	0.68	0/1759	0.77	2/2373 (0.1%)
All	All	0.70	2/3526 (0.1%)	0.78	4/4757 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	HIS	CB-CG	7.06	1.60	1.50
1	A	68	HIS	ND1-CE1	-6.50	1.26	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	PHE	N-CA-C	-5.88	105.30	112.88
1	A	187	PHE	N-CA-C	-5.72	106.19	112.72
1	B	83	VAL	N-CA-C	5.23	114.28	106.85
1	A	68	HIS	CE1-NE2-CD2	5.18	114.18	109.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ALA	Peptide

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	1726	0	1669	36	0
1	B	1718	0	1658	22	0
2	A	10	0	0	1	0
2	B	20	0	0	1	0
All	All	3474	0	3327	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 8.

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:B:138:GLU:HG3	1:B:149:LYS:HB2	1.59	0.82
1:A:47:TYR:O	1:A:51:SER:OG	1.99	0.80
1:B:131:GLY:HA3	1:B:265:GLY:HA2	1.66	0.78
1:A:131:GLY:HA3	1:A:265:GLY:HA2	1.67	0.77
1:A:274:ARG:NH2	1:B:211:ASN:OD1	2.23	0.68
1:A:213:THR:O	1:A:254:GLY:O	2.11	0.68
1:B:213:THR:O	1:B:254:GLY:O	2.12	0.66
1:A:81:MET:O	1:A:81:MET:HG3	1.97	0.65
1:B:104:ARG:NH2	2:B:504:SO4:O2	2.29	0.65
1:A:101:MET:HE3	1:A:222:ILE:HD12	1.78	0.64
1:B:81:MET:O	1:B:81:MET:HG3	2.00	0.61
1:B:101:MET:HE3	1:B:222:ILE:HD12	1.84	0.60
1:A:106:TRP:H	1:A:106:TRP:CD1	2.22	0.58
1:A:131:GLY:CA	1:A:265:GLY:HA2	2.34	0.57
1:A:81:MET:O	1:A:81:MET:CG	2.53	0.56
1:A:269:PHE:CE2	1:A:273:ILE:HD11	2.40	0.56
1:A:104:ARG:NH2	2:A:302:SO4:O3	2.40	0.54
1:B:203:LEU:HD23	1:B:270:ILE:HD13	1.89	0.54
1:B:116:GLN:HA	1:B:116:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PHE:CE2	1:A:273:ILE:CD1	2.93	0.52
1:B:216:HIS:CD2	1:B:254:GLY:HA3	2.45	0.51
1:A:210:GLU:OE2	1:B:206:LYS:CE	2.59	0.50
1:A:42:ILE:HD12	1:A:42:ILE:O	2.12	0.50
1:B:68:HIS:HB2	1:B:83:VAL:HG12	1.92	0.50
1:A:92:THR:HG22	1:A:93:LYS:HG3	1.93	0.49
1:A:225:VAL:HG22	1:A:226:TYR:N	2.28	0.48
1:A:82:MET:HE3	1:A:84:LEU:HD11	1.95	0.48
1:A:223:LEU:C	1:A:223:LEU:HD23	2.39	0.48
1:A:243:VAL:O	1:A:244:LYS:HG2	2.13	0.48
1:A:64:PHE:O	1:A:65:PRO:C	2.57	0.48
1:A:206:LYS:O	1:A:207:THR:C	2.57	0.47
1:A:53:ASN:OD1	1:A:53:ASN:C	2.58	0.45
1:A:101:MET:HE1	1:A:269:PHE:CB	2.47	0.45
1:B:266:LEU:O	1:B:270:ILE:HG13	2.16	0.45
1:B:81:MET:O	1:B:81:MET:CG	2.62	0.44
1:A:83:VAL:O	1:A:83:VAL:HG12	2.18	0.44
1:A:206:LYS:O	1:A:210:GLU:HG3	2.18	0.44
1:B:68:HIS:HB2	1:B:83:VAL:CG1	2.48	0.44
1:A:225:VAL:CG2	1:A:226:TYR:N	2.80	0.44
1:A:268:SER:O	1:A:269:PHE:C	2.61	0.43
1:A:144:GLU:O	1:A:145:SER:C	2.61	0.43
1:B:174:ASN:O	1:B:175:SER:CB	2.66	0.42
1:A:153:LYS:O	1:A:156:ARG:HB2	2.19	0.42
1:B:206:LYS:O	1:B:207:THR:C	2.61	0.42
1:A:94:PRO:HA	1:A:226:TYR:O	2.20	0.41
1:A:101:MET:HE1	1:A:269:PHE:HB2	2.01	0.41
1:A:210:GLU:OE2	1:B:206:LYS:HE2	2.20	0.41
1:A:101:MET:HE1	1:A:269:PHE:CG	2.56	0.41
1:A:52:SER:O	1:A:53:ASN:C	2.63	0.41
1:A:243:VAL:O	1:A:244:LYS:CG	2.68	0.41
1:B:136:GLY:HA2	1:B:155:LEU:HD12	2.03	0.40
1:B:149:LYS:HA	1:B:150:PRO:HD3	1.90	0.40
1:B:85:GLU:O	1:B:85:GLU:HG2	2.21	0.40
1:B:158:LEU:HD22	1:B:162:GLY:C	2.47	0.40
1:A:228:ASN:O	1:A:229:GLU:C	2.63	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	206/275 (75%)	181 (88%)	23 (11%)	2 (1%)	12	39
1	B	205/275 (74%)	192 (94%)	12 (6%)	1 (0%)	24	54
All	All	411/550 (75%)	373 (91%)	35 (8%)	3 (1%)	18	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	B	185	SER
1	A	44	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	193/240 (80%)	182 (94%)	11 (6%)	18	49
1	B	192/240 (80%)	182 (95%)	10 (5%)	21	52
All	All	385/480 (80%)	364 (94%)	21 (6%)	19	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	85	GLU
1	A	87	LEU

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Mol	Chain	Res	Type
1	A	105	THR
1	A	127	THR
1	A	139	VAL
1	A	149	LYS
1	A	174	ASN
1	A	184	ASP
1	A	185	SER
1	A	198	ILE
1	B	85	GLU
1	B	87	LEU
1	B	90	GLU
1	B	104	ARG
1	B	115	ILE
1	B	119	LEU
1	B	130	SER
1	B	133	ARG
1	B	198	ILE
1	B	222	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	B	218	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	B	501	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	A	301	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	503	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	302	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.11	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	SO4	1	0
2	B	504	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	214/275 (77%)	0.82	26 (12%)	8 7	67, 101, 148, 175	0
1	B	213/275 (77%)	1.33	55 (25%)	1 1	62, 88, 136, 167	0
All	All	427/550 (77%)	1.07	81 (18%)	3 3	62, 95, 143, 175	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	LEU	5.6
1	B	175	SER	5.5
1	A	42	ILE	5.5
1	A	70	THR	5.1
1	B	230	SER	4.9
1	B	42	ILE	4.7
1	B	156	ARG	4.5
1	B	183	PRO	4.4
1	A	81	MET	4.3
1	B	144	GLU	4.2
1	B	81	MET	4.2
1	A	230	SER	4.1
1	B	147	PHE	4.0
1	A	183	PRO	3.9
1	A	140	TYR	3.9
1	A	157	GLY	3.8
1	B	187	PHE	3.8
1	B	103	SER	3.7
1	A	185	SER	3.6
1	B	158	LEU	3.6
1	A	121	LYS	3.6
1	B	148	TRP	3.5
1	B	70	THR	3.4
1	A	85	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	140	TYR	3.4
1	B	90	GLU	3.3
1	A	83	VAL	3.2
1	A	68	HIS	3.2
1	B	151	GLU	3.2
1	A	186	ALA	3.1
1	B	41	GLU	3.1
1	B	100	LYS	3.1
1	B	150	PRO	3.0
1	B	102	GLY	2.9
1	A	84	LEU	2.9
1	B	143	LYS	2.9
1	B	109	ASP	2.9
1	B	155	LEU	2.9
1	B	146	SER	2.8
1	B	131	GLY	2.8
1	B	108	PRO	2.8
1	B	254	GLY	2.7
1	A	146	SER	2.7
1	B	172	SER	2.7
1	B	139	VAL	2.7
1	A	58	GLU	2.7
1	A	69	GLY	2.7
1	B	137	PHE	2.6
1	B	93	LYS	2.6
1	B	121	LYS	2.5
1	B	153	LYS	2.5
1	B	228	ASN	2.5
1	B	154	LEU	2.4
1	A	148	TRP	2.4
1	A	156	ARG	2.4
1	B	152	ARG	2.4
1	B	120	LYS	2.4
1	B	174	ASN	2.4
1	B	45	LYS	2.4
1	B	184	ASP	2.4
1	B	135	SER	2.4
1	B	119	LEU	2.4
1	A	238	ASP	2.3
1	B	157	GLY	2.3
1	A	41	GLU	2.3
1	B	113	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	44	VAL	2.3
1	A	54	THR	2.3
1	B	186	ALA	2.2
1	B	149	LYS	2.2
1	B	106	TRP	2.2
1	B	253	ASP	2.2
1	B	142	HIS	2.1
1	A	90	GLU	2.1
1	B	82	MET	2.1
1	B	250	HIS	2.1
1	A	87	LEU	2.1
1	B	107	TYR	2.1
1	B	124	GLY	2.0
1	B	166	THR	2.0
1	A	82	MET	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	301	5/5	0.73	0.27	188,189,189,189	0
2	SO4	B	504	5/5	0.73	0.24	142,144,144,144	0
2	SO4	A	302	5/5	0.76	0.26	165,166,166,167	0
2	SO4	B	503	5/5	0.77	0.12	151,152,153,153	0
2	SO4	B	502	5/5	0.88	0.14	150,150,151,152	0
2	SO4	B	501	5/5	0.89	0.19	120,120,120,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.