

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 10:45 am BST

PDB ID : 5LT2

Title : nucleotide-free kinesin-1 motor domain, P1 crystal form

Authors : Cao, L.; Gigant, B.

Deposited on : 2016-09-06

Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

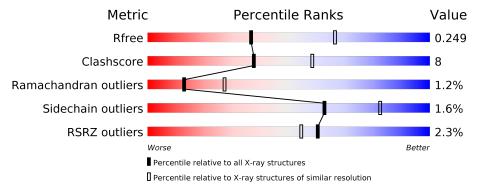
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.60 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	$\begin{array}{c} \textbf{Whole archive} \\ (\# \textbf{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60 - 2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	325	83%	13%	
1	В	325	81%	13%	• 6%
1	С	325	80%	14%	• 5%
1	D	325	76%	20%	
1	Е	325	81%	12%	• 6%
1	K	325	76%	17%	• 6%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14214 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 Kinesin-like protein.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	314	Total	С	N	О	S	0	0	0
1	A	314	2362	1473	405	475	9	0	U	U
1	В	307	Total	С	N	О	S	0	0	0
1	Ъ	307	2260	1418	387	446	9	0	0	0
1	С	308	Total	С	N	О	S	0	0	0
1		300	2335	1460	402	464	9	0	0	
1	D	313	Total	С	N	О	S	0	0	0
1	D	313	2339	1463	403	464	9	0	0	
1	Е	307	Total	С	N	О	S	0	0	0
1		507	2256	1411	384	452	9	0	0	0
1	K	307	Total	С	N	О	S	0	0	0
1	17	307	2288	1435	392	452	9		0	U

There are 30 discrepancies between the modelled and reference sequences:

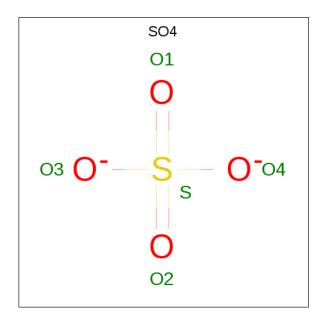
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	CYS	engineered mutation	UNP Q6P164
A	65	ALA	CYS	engineered mutation	UNP Q6P164
A	168	ALA	CYS	engineered mutation	UNP Q6P164
A	174	SER	CYS	engineered mutation	UNP Q6P164
A	294	ALA	CYS	engineered mutation	UNP Q6P164
В	7	SER	CYS	engineered mutation	UNP Q6P164
В	65	ALA	CYS	engineered mutation	UNP Q6P164
В	168	ALA	CYS	engineered mutation	UNP Q6P164
В	174	SER	CYS	engineered mutation	UNP Q6P164
В	294	ALA	CYS	engineered mutation	UNP Q6P164
С	7	SER	CYS	engineered mutation	UNP Q6P164
С	65	ALA	CYS	engineered mutation	UNP Q6P164
С	168	ALA	CYS	engineered mutation	UNP Q6P164
С	174	SER	CYS	engineered mutation	UNP Q6P164
С	294	ALA	CYS	engineered mutation	UNP Q6P164
D	7	SER	CYS	engineered mutation	UNP Q6P164
D	65	ALA	CYS	engineered mutation	UNP Q6P164



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Chain	Residue	Modelled	Actual	Comment	Reference
D	168	ALA	CYS	engineered mutation	UNP Q6P164
D	174	SER	CYS	engineered mutation	UNP Q6P164
D	294	ALA	CYS	engineered mutation	UNP Q6P164
E	7	SER	CYS	engineered mutation	UNP Q6P164
Е	65	ALA	CYS	engineered mutation	UNP Q6P164
E	168	ALA	CYS	engineered mutation	UNP Q6P164
E	174	SER	CYS	engineered mutation	UNP Q6P164
Е	294	ALA	CYS	engineered mutation	UNP Q6P164
K	7	SER	CYS	engineered mutation	UNP Q6P164
K	65	ALA	CYS	engineered mutation	UNP Q6P164
K	168	ALA	CYS	engineered mutation	UNP Q6P164
K	174	SER	CYS	engineered mutation	UNP Q6P164
K	294	ALA	CYS	engineered mutation	UNP Q6P164

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	Δ	1	Total O S	0	0	
	7.1	1	5 4 1	O	U	
$\frac{1}{2}$	В	1	Total O S	0	0	
	Ъ	1	5 4 1	0	U	
2	С	1	Total O S	0	0	
			5 4 1	0		
2	С	1	Total O S	0	0	
		1	5 4 1	0	0	
2	C	1	Total O S	0	0	
		1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0	



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	Е	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

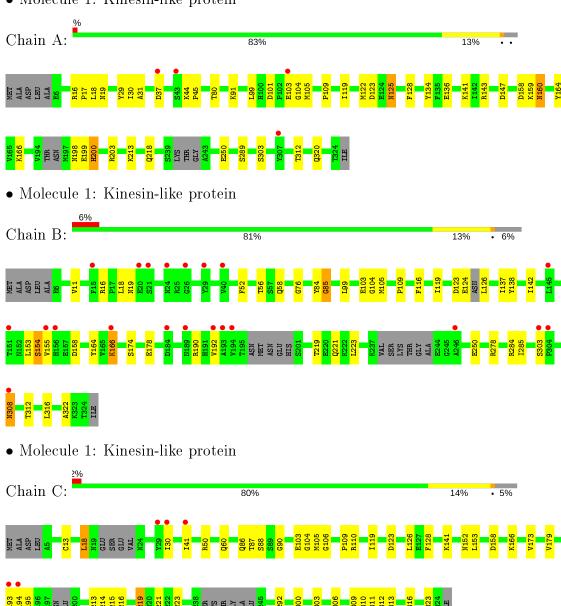
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	В	21	Total O 21 21	0	0
3	С	74	Total O 74 74	0	0
3	D	57	Total O 57 57	0	0
3	E	47	Total O 47 47	0	0
3	K	43	Total O 43 43	0	0



3 Residue-property plots (i)

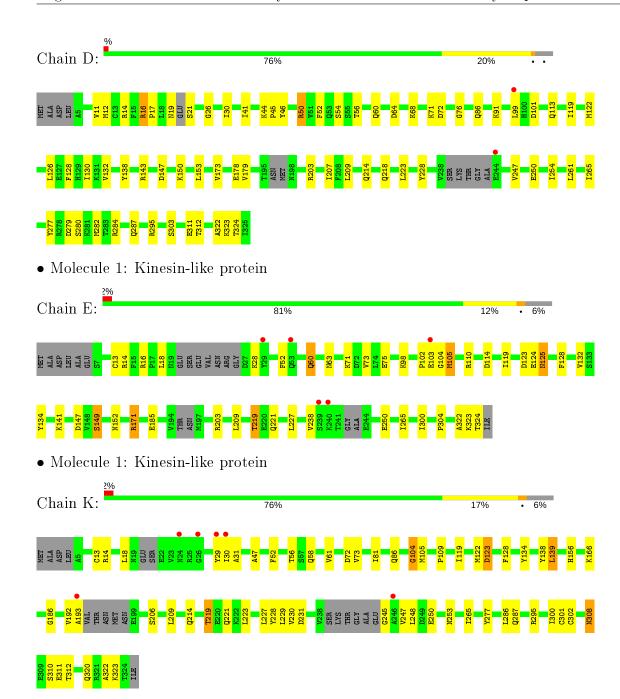
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Kinesin-like protein



• Molecule 1: Kinesin-like protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	56.74\AA 101.45\AA 101.59\AA	Danasitan
a, b, c, α , β , γ	119.24° 91.96° 91.93°	Depositor
Resolution (Å)	38.40 - 2.60	Depositor
Resolution (A)	49.00 - 2.60	EDS
% Data completeness	98.0 (38.40-2.60)	Depositor
(in resolution range)	92.4 (49.00-2.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.80 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692, BUSTER	Depositor
D D	0.193 , 0.249	Depositor
R, R_{free}	0.195 , 0.249	DCC
R_{free} test set	2016 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34,60.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14214	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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

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	
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.49	0/2398	0.71	1/3247~(0.0%)
1	В	0.49	1/2295~(0.0%)	0.63	0/3114
1	С	0.50	0/2370	0.69	2/3204 (0.1%)
1	D	0.49	0/2373	0.68	1/3212 (0.0%)
1	Ε	0.47	0/2289	0.67	1/3107~(0.0%)
1	K	0.48	0/2322	0.70	1/3144 (0.0%)
All	All	0.49	1/14047~(0.0%)	0.68	6/19028 (0.0%)

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	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	154	SER	CB-OG	7.64	1.52	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	50	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	С	18	LEU	N-CA-C	-6.22	94.20	111.00
1	E	104	GLY	N-CA-C	-5.43	99.53	113.10
1	A	158	ASP	CB-CG-OD1	5.24	123.02	118.30
1	С	158	ASP	CB-CG-OD1	5.18	122.96	118.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	308	ASN	Peptide

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	2362	0	2229	29	0
1	В	2260	0	2080	27	0
1	С	2335	0	2225	34	0
1	D	2339	0	2215	51	0
1	Е	2256	0	2065	31	0
1	K	2288	0	2156	40	0
2	A	5	0	0	1	0
2	В	5	0	0	0	0
2	С	15	0	0	0	0
2	D	15	0	0	1	0
2	Е	5	0	0	0	0
2	K	10	0	0	0	0
3	A	77	0	0	4	0
3	В	21	0	0	0	0
3	С	74	0	0	5	2
3	D	57	0	0	6	0
3	E	47	0	0	3	1
3	K	43	0	0	5	1
All	All	14214	0	12970	208	2

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.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:K:86:GLN:NE2	3:K:501:HOH:O	1.94	0.98
1:C:30:ILE:HD11	1:C:306:SER:HA	1.56	0.87



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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:D:86:GLN:HG3	1:D:311:GLU:HG2	1.56	0.85
1:D:323:LYS:HD2	1:D:324:THR:H	1.41	0.85
1:D:323:LYS:HD2	1:D:324:THR:N	1.92	0.85

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
3:C:551:HOH:O	3:K:528:HOH:O[1_665]	2.19	0.01
3:C:573:HOH:O	3:E:512:HOH:O[1_655]	2.19	0.01

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	308/325~(95%)	289 (94%)	12 (4%)	7 (2%)	6 11
1	В	299/325~(92%)	286 (96%)	11 (4%)	2 (1%)	22 43
1	С	$300/325 \; (92\%)$	287 (96%)	10 (3%)	3 (1%)	15 32
1	D	305/325~(94%)	290 (95%)	13 (4%)	2 (1%)	22 43
1	E	299/325~(92%)	288 (96%)	8 (3%)	3 (1%)	15 32
1	K	299/325~(92%)	289 (97%)	6 (2%)	4 (1%)	12 24
All	All	1810/1950 (93%)	1729 (96%)	60 (3%)	21 (1%)	13 27

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	30	ILE
1	A	99	LEU
1	В	85	GLY



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Mol	Chain	Res	Type
1	В	123	ASP

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	250/286~(87%)	245 (98%)	5 (2%)	55 78
1	В	226/286 (79%)	223 (99%)	3 (1%)	69 86
1	С	247/286 (86%)	244 (99%)	3 (1%)	71 87
1	D	245/286~(86%)	243 (99%)	2 (1%)	81 92
1	E	$226/286 \ (79\%)$	220 (97%)	6 (3%)	44 71
1	K	$236/286 \ (82\%)$	232 (98%)	4 (2%)	60 81
All	All	1430/1716 (83%)	1407 (98%)	23 (2%)	62 82

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	219	THR
1	D	218	GLN
1	K	247	VAL
1	D	16	ARG
1	E	60	GLN

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

Mol	Chain	Res	Type
1	A	125	ASN
1	K	320	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

11 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	В	ond leng	gths	Bond angles		
MIGI			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	403	_	4,4,4	0.26	0	6,6,6	0.43	0
2	SO4	С	403	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	С	402	-	4,4,4	0.24	0	6,6,6	0.30	0
2	SO4	K	401	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	E	401	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	С	401	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	A	401	-	4,4,4	0.18	0	6,6,6	0.58	0
2	SO4	В	401	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.40	0
2	SO4	K	402	-	4,4,4	0.33	0	6,6,6	0.24	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	D	403	SO4	1	0
2	A	401	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	#RSF	RZ>	-2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	314/325~(96%)	-0.03	4 (1%)	77	73	23, 44, 84, 103	0
1	В	307/325~(94%)	0.43	21 (6%)	17	12	39, 71, 110, 149	0
1	С	308/325~(94%)	-0.06	5 (1%)	72	68	25, 46, 83, 115	0
1	D	313/325 (96%)	-0.03	2 (0%) 8	89	88	27, 49, 82, 116	0
1	E	307/325~(94%)	0.02	5 (1%)	72	68	27, 51, 86, 113	0
1	K	307/325~(94%)	0.13	6 (1%)	65	60	28, 56, 93, 125	0
All	All	$1856/1950 \; (95\%)$	0.08	43 (2%)	60	54	23, 52, 94, 149	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	26	GLY	4.3
1	В	156	HIS	3.8
1	В	15	PHE	3.8
1	В	193	ALA	3.7
1	В	40	VAL	3.6

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 carbohydrates 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, 95^{th} 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	SO4	K	402	5/5	0.78	0.24	75,76,77,78	0
2	SO4	D	402	5/5	0.81	0.42	76,77,79,81	0
2	SO4	В	401	5/5	0.85	0.17	81,91,92,95	0
2	SO4	D	403	5/5	0.87	0.27	75,76,77,78	0
2	SO4	С	403	5/5	0.88	0.20	76,77,77,79	0
2	SO4	K	401	5/5	0.92	0.11	73,75,78,79	0
2	SO4	С	402	5/5	0.92	0.27	61,66,69,70	0
2	SO4	D	401	5/5	0.93	0.15	54,64,66,68	0
2	SO4	Ε	401	5/5	0.94	0.16	60,69,73,78	0
2	SO4	С	401	5/5	0.95	0.11	54,57,69,76	0
2	SO4	A	401	5/5	0.97	0.10	55,57,62,67	0

6.5 Other polymers (i)

There are no such residues in this entry.

