



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:05 AM GMT

PDB ID : 1ZHO
Title : The structure of a ribosomal protein L1 in complex with mRNA
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Nikonov, O.; Nikulin, A.; Kohrer, C.; Piendl, W.; Zimmermann, R.; Stockley,
P.; Garber, M.; Nikonov, S.
Deposited on : 2005-04-26
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

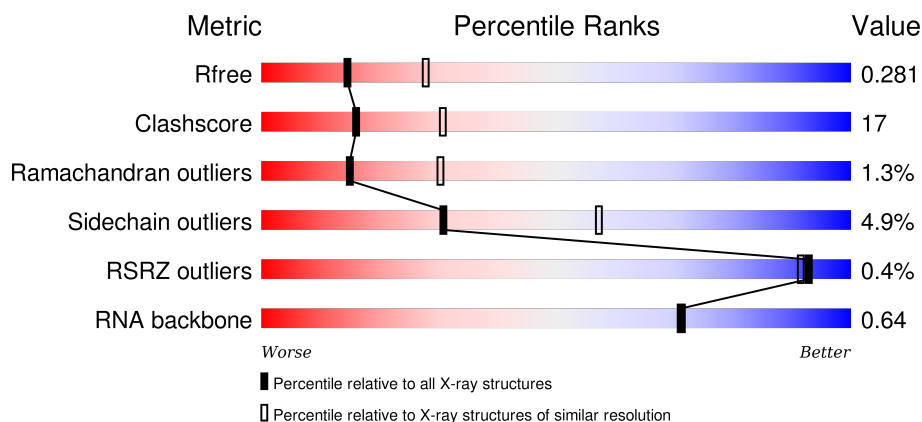
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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. 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	B	38	<div> <div>55%</div> <div>39%</div> <div>5%</div> </div>
1	D	38	<div> <div>61%</div> <div>32%</div> <div>8%</div> </div>
1	F	38	<div> <div>47%</div> <div>37%</div> <div>13%</div> <div>•</div> </div>
1	H	38	<div> <div>39%</div> <div>39%</div> <div>18%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	A	228	<div><div></div><div>66%</div><div>32%</div><div></div></div>
2	C	228	<div><div></div><div>54%</div><div>44%</div><div></div></div>
2	E	228	<div><div>%</div><div></div><div>56%</div><div>40%</div><div></div></div>
2	G	228	<div><div></div><div>66%</div><div>31%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10515 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 RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	D	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	F	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	H	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			

- Molecule 2 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	C	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	E	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	G	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	MSE	MET	MODIFIED RESIDUE	UNP P27150
A	120	MSE	MET	MODIFIED RESIDUE	UNP P27150
A	218	MSE	MET	MODIFIED RESIDUE	UNP P27150
C	108	MSE	MET	MODIFIED RESIDUE	UNP P27150
C	120	MSE	MET	MODIFIED RESIDUE	UNP P27150
C	218	MSE	MET	MODIFIED RESIDUE	UNP P27150
E	108	MSE	MET	MODIFIED RESIDUE	UNP P27150
E	120	MSE	MET	MODIFIED RESIDUE	UNP P27150
E	218	MSE	MET	MODIFIED RESIDUE	UNP P27150

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Chain	Residue	Modelled	Actual	Comment	Reference
G	108	MSE	MET	MODIFIED RESIDUE	UNP P27150
G	120	MSE	MET	MODIFIED RESIDUE	UNP P27150
G	218	MSE	MET	MODIFIED RESIDUE	UNP P27150

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

- Molecule 4 is water.

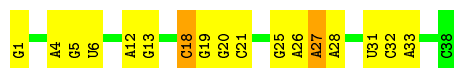
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	B	43	Total O 43 43	0	0
4	C	26	Total O 26 26	0	0
4	D	44	Total O 44 44	0	0
4	E	33	Total O 33 33	0	0
4	F	24	Total O 24 24	0	0
4	G	26	Total O 26 26	0	0
4	H	32	Total O 32 32	0	0

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 errors 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 ($\text{RSRZ} > 2$). 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: mRNA

Chain B: 



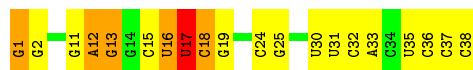
- Molecule 1: mRNA

Chain D: 



- Molecule 1: mRNA

Chain F: 



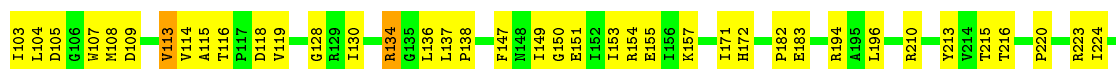
- Molecule 1: mRNA

Chain H: 

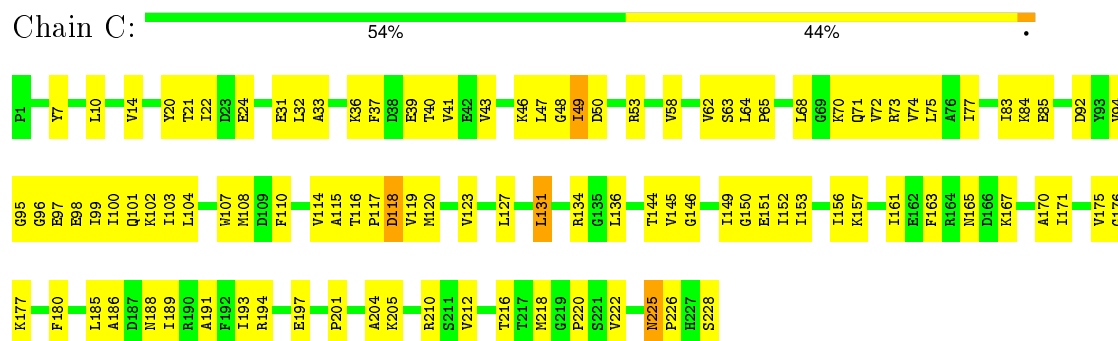


- Molecule 2: 50S ribosomal protein L1

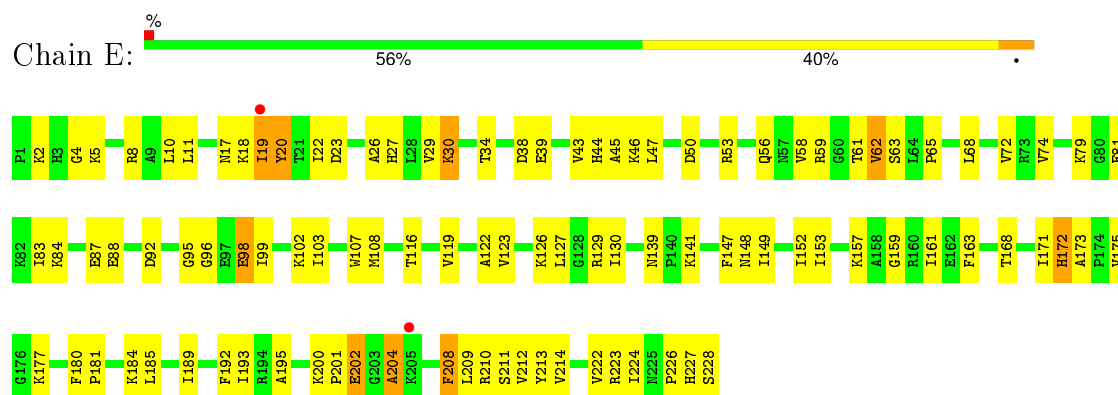
Chain A: 



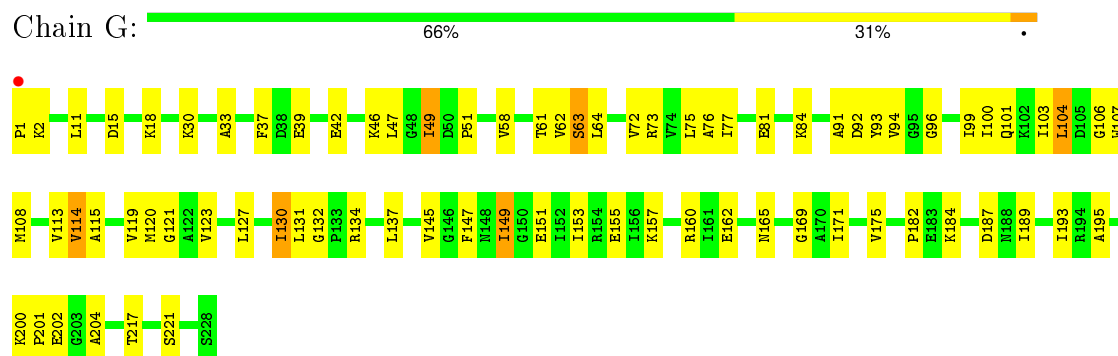
- Molecule 2: 50S ribosomal protein L1



- Molecule 2: 50S ribosomal protein L1



- Molecule 2: 50S ribosomal protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 101.90Å 119.60Å 90.00° 93.66° 90.00°	Depositor
Resolution (Å)	37.06 – 2.60 37.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (37.06-2.60) 96.2 (37.06-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.281 0.219 , 0.281	Depositor DCC
R_{free} test set	2393 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 50908 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 20.65 % 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 8.2984e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
K

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	B	0.67	2/912 (0.2%)	1.07	7/1419 (0.5%)
1	D	0.60	1/912 (0.1%)	0.91	3/1419 (0.2%)
1	F	0.54	1/912 (0.1%)	0.92	3/1419 (0.2%)
1	H	0.61	1/912 (0.1%)	1.17	15/1419 (1.1%)
2	A	0.46	0/1772	0.70	0/2384
2	C	0.48	0/1772	0.78	0/2384
2	E	0.46	0/1772	0.74	1/2384 (0.0%)
2	G	0.44	0/1772	0.73	1/2384 (0.0%)
All	All	0.52	5/10736 (0.0%)	0.86	30/15212 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	G	OP3-P	-7.28	1.52	1.61
1	F	1	G	OP3-P	-7.08	1.52	1.61
1	D	1	G	OP3-P	-6.72	1.53	1.61
1	H	1	G	OP3-P	-6.47	1.53	1.61
1	B	25	G	O3'-P	6.04	1.68	1.61

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	G	OP2-P-O3'	14.25	136.55	105.20
1	B	25	G	OP1-P-O3'	-13.38	75.77	105.20
1	H	24	C	P-O3'-C3'	-10.54	107.05	119.70
1	H	25	G	OP1-P-O3'	10.09	127.39	105.20
1	F	16	U	OP2-P-O3'	9.16	125.36	105.20

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	B	816	0	413	7	0
1	D	816	0	413	11	0
1	F	816	0	413	17	0
1	H	816	0	412	15	0
2	A	1742	0	1796	54	0
2	C	1742	0	1796	82	0
2	E	1742	0	1796	92	0
2	G	1742	0	1796	59	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
4	A	51	0	0	4	0
4	B	43	0	0	1	0
4	C	26	0	0	2	0
4	D	44	0	0	1	0
4	E	33	0	0	2	0
4	F	24	0	0	0	0
4	G	26	0	0	0	0
4	H	32	0	0	0	0
All	All	10515	0	8835	323	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 17.

The worst 5 of 323 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:H:33:A:H4'	2:G:46:LYS:HD3	1.42	0.99
2:E:8:ARG:HA	2:E:11:LEU:HD12	1.42	0.99
2:E:30:LYS:H	2:E:30:LYS:HD2	1.26	0.98
2:E:99:ILE:HD12	2:E:102:LYS:HD2	1.52	0.92
2:C:115:ALA:HB3	2:C:120:MSE:HE1	1.57	0.87

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	
2	A	226/228 (99%)	212 (94%)	12 (5%)	2 (1%)	21	42
2	C	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	21	42
2	E	226/228 (99%)	191 (84%)	30 (13%)	5 (2%)	8	15
2	G	226/228 (99%)	185 (82%)	38 (17%)	3 (1%)	15	30
All	All	904/912 (99%)	789 (87%)	103 (11%)	12 (1%)	15	30

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	208	PHE
2	E	20	TYR
2	G	202	GLU
2	C	36	LYS
2	E	39	GLU

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	
2	A	180/177 (102%)	171 (95%)	9 (5%)	30	56
2	C	180/177 (102%)	170 (94%)	10 (6%)	26	50
2	E	180/177 (102%)	172 (96%)	8 (4%)	35	63
2	G	180/177 (102%)	172 (96%)	8 (4%)	35	63
All	All	720/708 (102%)	685 (95%)	35 (5%)	31	57

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	98	GLU
2	E	30	LYS
2	G	114	VAL
2	C	131	LEU
2	C	151	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	71	GLN
2	G	57	ASN
2	E	56	GLN
2	C	66	HIS
2	E	27	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	37/38 (97%)	3 (8%)	1 (2%)
1	D	37/38 (97%)	3 (8%)	0
1	F	37/38 (97%)	6 (16%)	3 (8%)
1	H	37/38 (97%)	6 (16%)	2 (5%)
All	All	148/152 (97%)	18 (12%)	6 (4%)

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	12	A
1	B	13	G
1	B	18	C
1	D	12	A
1	D	13	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	F	17	U
1	H	18	C
1	F	18	C

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Mol	Chain	Res	Type
1	F	12	A
1	H	17	U

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 [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, 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	B	38/38 (100%)	-0.51	0	100 100	26, 40, 55, 58	0
1	D	38/38 (100%)	-0.64	0	100 100	29, 39, 52, 60	0
1	F	38/38 (100%)	-0.46	0	100 100	34, 50, 82, 88	0
1	H	38/38 (100%)	-0.42	0	100 100	40, 50, 61, 70	0
2	A	225/228 (98%)	-0.31	1 (0%)	93 91	23, 45, 60, 69	0
2	C	225/228 (98%)	-0.17	0	100 100	34, 51, 69, 80	0
2	E	225/228 (98%)	-0.13	2 (0%)	85 83	30, 54, 73, 78	0
2	G	225/228 (98%)	-0.21	1 (0%)	93 91	31, 50, 81, 92	0
All	All	1052/1064 (98%)	-0.25	4 (0%)	93 91	23, 49, 70, 92	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	PRO	3.7
2	A	1	PRO	2.6
2	E	205	LYS	2.3
2	E	19	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	K	H	39	1/1	0.86	0.20	1.04	61,61,61,61	0
3	K	D	39	1/1	0.94	0.19	0.72	41,41,41,41	0
3	K	E	229	1/1	0.88	0.20	0.01	66,66,66,66	0
3	K	A	229	1/1	0.98	0.13	-1.94	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.