

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3UJ4
Title	:	Crystal structure of the apo-inositol 1,4,5-trisphosphate receptor
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Deposited on	:	2011-11-07
Resolution	:	3.00 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 (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
CCP4	:	$7.0.044 \ (Gargrove)$
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	$1990 \ (3.00-3.00)$

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	А	604	% 67%	12%	•	20%		
1	В	604	^{2%} 65%	15%	•	19%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7454 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	196	Total	С	Ν	Ο	S	0	0	0
	400	3721	2372	656	688	5	0	0	0	
1	р	400	Total	С	Ν	Ο	S	0	0	0
	490	3700	2351	646	698	5	0		0	

• Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	CYS	engineered mutation	UNP P29994
A	37	ALA	CYS	engineered mutation	UNP P29994
A	56	ALA	CYS	engineered mutation	UNP P29994
A	61	ALA	CYS	engineered mutation	UNP P29994
A	206	ALA	CYS	engineered mutation	UNP P29994
A	214	ALA	CYS	engineered mutation	UNP P29994
A	253	ALA	CYS	engineered mutation	UNP P29994
A	292	ALA	CYS	engineered mutation	UNP P29994
A	326	ALA	CYS	engineered mutation	UNP P29994
A	394	ALA	CYS	engineered mutation	UNP P29994
A	530	ALA	CYS	engineered mutation	UNP P29994
A	553	ALA	CYS	engineered mutation	UNP P29994
A	556	ALA	CYS	engineered mutation	UNP P29994
В	15	ALA	CYS	engineered mutation	UNP P29994
В	37	ALA	CYS	engineered mutation	UNP P29994
В	56	ALA	CYS	engineered mutation	UNP P29994
В	61	ALA	CYS	engineered mutation	UNP P29994
В	206	ALA	CYS	engineered mutation	UNP P29994
В	214	ALA	CYS	engineered mutation	UNP P29994
В	253	ALA	CYS	engineered mutation	UNP P29994
В	292	ALA	CYS	engineered mutation	UNP P29994
В	326	ALA	CYS	engineered mutation	UNP P29994
В	394	ALA	CYS	engineered mutation	UNP P29994
В	530	ALA	CYS	engineered mutation	UNP P29994
В	553	ALA	CYS	engineered mutation	UNP P29994

There are 26 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	556	ALA	CYS	engineered mutation	UNP P29994

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 5	0 4	${ m S}$ 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	14	Total O 14 14	0	0
3	В	14	Total O 14 14	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: Inositol 1,4,5-trisphosphate receptor type 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	63.11Å 77.19Å 101.51Å	Depositor
a, b, c, α , β , γ	105.36° 99.98° 101.04°	Depositor
Bosolution (Å)	50.00 - 3.00	Depositor
	46.79 - 3.00	EDS
% Data completeness	98.5(50.00-3.00)	Depositor
(in resolution range)	98.6(46.79-3.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.87 (at 3.01 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
B B.	0.208 , 0.256	Depositor
n, n_{free}	0.208 , 0.255	DCC
R_{free} test set	1746 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	76.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29 , 54.4	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms $(Å^2)$	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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).

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	2/3794~(0.1%)	0.59	0/5153	
1	В	0.49	3/3771~(0.1%)	0.57	0/5129	
All	All	0.49	5/7565~(0.1%)	0.58	0/10282	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	73	TRP	CD2-CE2	5.19	1.47	1.41
1	В	226	TRP	CD2-CE2	5.17	1.47	1.41
1	В	299	TRP	CD2-CE2	5.08	1.47	1.41
1	В	73	TRP	CD2-CE2	5.04	1.47	1.41
1	А	160	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	3721	0	3629	39	0
1	В	3700	0	3531	53	0
2	В	5	0	0	0	0
3	А	14	0	0	1	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	14	0	0	2	0
All	All	7454	0	7160	90	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 (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:251:LEU:HD12	1:A:418:ILE:HD13	1.59	0.83
1:B:204:PRO:HA	3:B:611:HOH:O	1.80	0.82
1:A:251:LEU:HD12	1:A:418:ILE:CD1	2.12	0.79
1:B:64:ASN:H	1:B:122:GLN:NE2	1.86	0.72
1:B:293:ARG:CG	1:B:293:ARG:HH11	2.02	0.72
1:A:64:ASN:H	1:A:122:GLN:NE2	1.88	0.71
1:B:389:ARG:HG3	1:B:427:LYS:HD2	1.73	0.69
1:B:391:ARG:HH11	1:B:396:ASN:HD21	1.41	0.69
1:B:64:ASN:HB2	1:B:122:GLN:HE22	1.58	0.68
1:B:385:ASN:HB3	1:B:434:PRO:HD3	1.77	0.67
1:A:456:ILE:HD13	1:A:473:VAL:HB	1.79	0.65
1:A:300:ASN:HD22	1:A:300:ASN:H	1.44	0.64
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.63	0.63
1:A:114:VAL:HG23	1:B:106:GLU:OE1	2.00	0.62
1:B:288:GLN:HG2	1:B:293:ARG:HB3	1.83	0.61
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.36	0.59
1:A:391:ARG:HH11	1:A:396:ASN:ND2	2.01	0.59
1:A:407:ASP:HB2	1:A:410:GLU:HB2	1.86	0.58
1:B:55:ASP:O	1:B:125:HIS:HE1	1.86	0.57
1:B:121:ILE:HD12	1:B:163:ILE:HB	1.85	0.57
1:B:147:MET:HB2	1:B:211:SER:HB3	1.85	0.57
1:B:398:TRP:O	1:B:420:THR:HA	2.05	0.57
1:A:29:THR:HG23	1:A:125:HIS:CE1	2.40	0.57
1:B:293:ARG:CG	1:B:293:ARG:NH1	2.66	0.57
1:A:251:LEU:CD1	1:A:418:ILE:CD1	2.83	0.56
1:A:288:GLN:HG2	1:A:293:ARG:HB3	1.87	0.56
1:B:364:ILE:HG22	1:B:394:ALA:HB2	1.87	0.56
1:B:557:TYR:HA	1:B:560:LEU:HD12	1.88	0.54
1:A:38:VAL:HB	1:A:206:ALA:HB1	1.90	0.54
1:B:125:HIS:HD2	1:B:128:SER:OG	1.91	0.53
1:A:125:HIS:HD2	1:A:128:SER:H	1.56	0.53
1:B:388:VAL:HG21	1:B:432:ILE:HD11	1.91	0.53



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
1:A:300:ASN:ND2	1:A:300:ASN:H	2.06	0.53	
1:B:28:SER:HB2	1:B:55:ASP:OD1	2.09	0.52	
1:A:279:LYS:O	1:A:307:HIS:HE1	1.91	0.52	
1:B:14:ILE:HG12	1:B:126:LEU:HD11	1.91	0.51	
1:B:247:GLN:HA	1:B:247:GLN:HE21	1.76	0.50	
1:A:134:VAL:HG21	1:A:186:PRO:HG3	1.94	0.50	
1:A:364:ILE:HG22	1:A:394:ALA:HB2	1.94	0.49	
1:B:279:LYS:O	1:B:307:HIS:HE1	1.95	0.48	
1:A:64:ASN:HB2	1:A:122:GLN:HE22	1.77	0.48	
1:B:230:LYS:O	1:B:235:LYS:HE3	2.14	0.48	
1:A:174:ASP:OD1	1:B:67:SER:HB2	2.13	0.48	
1:B:385:ASN:HA	1:B:432:ILE:O	2.14	0.47	
1:A:298:TYR:O	1:A:301:SER:HB2	2.15	0.47	
1:A:24:ASN:O	1:A:41:PRO:HA	2.14	0.47	
1:B:501:LYS:HA	1:B:502:PRO:HD3	1.75	0.47	
1:B:290:ASP:HB2	1:B:293:ARG:HB2	1.97	0.47	
1:B:29:THR:HG23	1:B:125:HIS:CE1	2.51	0.46	
1:B:508:LYS:HE3	1:B:511:ARG:HH22	1.80	0.46	
1:B:181:LYS:HB3	1:B:217:SER:HB2	1.98	0.46	
1:A:202:ASP:OD2	1:A:203:ASN:ND2	2.49	0.46	
1:B:285:GLU:CB	3:B:612:HOH:O	2.63	0.46	
1:B:9:LEU:HD22	1:B:220:ILE:HD13	1.97	0.45	
1:B:178:ILE:HD12	1:B:222:LEU:HG	1.98	0.45	
1:B:263:PHE:CD1	1:B:415:MET:HG2	2.52	0.45	
1:B:520:PHE:HZ	1:B:574:ILE:HG23	1.82	0.45	
1:A:171:SER:O	1:A:174:ASP:HB2	2.18	0.44	
1:A:288:GLN:HG2	1:A:293:ARG:CB	2.47	0.44	
1:A:564:GLN:HB2	1:A:571:GLN:HG3	2.00	0.43	
1:A:504:ARG:HH22	1:A:568:ARG:HH12	1.66	0.43	
1:B:226:TRP:CG	1:B:227:SER:N	2.87	0.43	
1:A:14:ILE:HG12	1:A:126:LEU:HD11	1.99	0.43	
1:A:186:PRO:HB2	1:A:190:GLY:H	1.83	0.43	
1:B:167:TYR:HE1	1:B:181:LYS:HD2	1.83	0.43	
1:B:551:HIS:CG	1:B:552:ILE:H	2.36	0.43	
1:A:125:HIS:CD2	1:A:128:SER:H	2.37	0.42	
1:A:466:THR:H	1:A:466:THR:HG1	1.62	0.42	
1:B:442:ASP:OD1	1:B:506:ARG:NE	2.53	0.42	
1:A:354:SER:HA	1:A:419:GLY:HA2	2.00	0.42	
1:B:564:GLN:HE21	1:B:574:ILE:HD12	1.85	0.42	
1:A:9:LEU:HG	1:A:115:ILE:HD12	2.02	0.42	
1:B:55:ASP:O	1:B:125:HIS:CE1	2.71	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:B:387:TYR:CE1	1:B:431:ALA:HB2	2.55	0.41
1:B:446:ALA:O	1:B:515:ILE:HD11	2.20	0.41
1:B:146:ALA:HB2	1:B:212:VAL:HB	2.01	0.41
1:A:304:ARG:HD3	1:A:366:SER:OG	2.20	0.41
1:B:64:ASN:HB2	1:B:122:GLN:NE2	2.31	0.41
1:B:40:GLN:HG2	1:B:206:ALA:HB2	2.01	0.41
1:B:561:ARG:O	1:B:563:SER:N	2.53	0.41
1:A:194:HIS:CD2	1:A:214:ALA:CB	3.04	0.41
1:A:223:PHE:O	1:A:293:ARG:O	2.39	0.41
1:B:185:ASN:HA	1:B:186:PRO:HD3	1.86	0.41
1:B:514:ASN:O	1:B:518:GLN:HG2	2.21	0.41
1:A:410:GLU:HB3	3:A:612:HOH:O	2.20	0.41
1:A:253:ALA:HB3	1:A:307:HIS:CE1	2.56	0.41
1:B:282:TRP:CZ3	1:B:307:HIS:HB2	2.56	0.41
1:A:510:MET:HE2	1:A:510:MET:HA	2.03	0.40
1:B:298:TYR:O	1:B:301:SER:HB2	2.20	0.40
1:B:50:PRO:O	1:B:53:PHE:HB2	2.22	0.40

There are no symmetry-related clashes.

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	Perce	\mathbf{ntiles}
1	А	472/604~(78%)	447 (95%)	25~(5%)	0	100	100
1	В	472/604~(78%)	443 (94%)	28~(6%)	1 (0%)	47	82
All	All	944/1208~(78%)	890 (94%)	53~(6%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	204	PRO



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	А	384/520~(74%)	354~(92%)	30 (8%)	12 42
1	В	377/520~(72%)	352~(93%)	25~(7%)	16 49
All	All	761/1040 (73%)	706 (93%)	55(7%)	14 45

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	42	GLU
1	А	67	SER
1	А	98	LEU
1	А	169	LEU
1	А	185	ASN
1	А	200	LEU
1	А	201	VAL
1	А	210	ASN
1	А	251	LEU
1	А	252	THR
1	А	277	SER
1	А	286	VAL
1	А	293	ARG
1	А	300	ASN
1	А	302	LEU
1	А	319	ASP
1	А	384	ARG
1	А	389	ARG
1	А	390	LEU
1	А	396	ASN
1	А	407	ASP
1	A	408	LYS
1	А	418	ILE
1	А	465	ILE
1	А	505	GLU
1	А	509	LEU
1	А	522	LEU



Mol	Chain	Res	Type
1	А	523	LEU
1	А	567	TYR
1	А	568	ARG
1	В	22	SER
1	В	46	LEU
1	В	74	LYS
1	В	121	ILE
1	В	129	ASN
1	В	210	ASN
1	В	215	ASN
1	В	222	LEU
1	В	228	ASP
1	В	233	ILE
1	В	252	THR
1	В	286	VAL
1	В	293	ARG
1	В	301	SER
1	В	302	LEU
1	В	318	VAL
1	В	355	LEU
1	В	374	THR
1	В	389	ARG
1	В	396	ASN
1	В	432	ILE
1	В	460	LEU
1	В	475	LYS
1	В	477	LEU
1	В	509	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	122	GLN
1	А	125	HIS
1	А	129	ASN
1	А	185	ASN
1	А	210	ASN
1	А	300	ASN
1	А	307	HIS
1	А	396	ASN
1	А	507	GLN
1	А	514	ASN



\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	А	564	GLN
1	В	122	GLN
1	В	125	HIS
1	В	129	ASN
1	В	185	ASN
1	В	247	GLN
1	В	261	HIS
1	В	307	HIS
1	В	312	HIS
1	В	396	ASN
1	В	564	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)

1 ligand is 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	В	605	-	4,4,4	0.27	0	$6,\!6,\!6$	0.16	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 (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	<RSRZ $>$	#RSRZ >2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	486/604~(80%)	-0.33	5 (1%) 82 59	47, 71, 149, 226	0
1	В	490/604~(81%)	-0.22	12 (2%) 59 30	51, 88, 154, 189	0
All	All	976/1208~(80%)	-0.27	17 (1%) 70 41	47, 78, 153, 226	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	464	THR	4.6
1	В	88	LEU	4.3
1	В	463	GLY	3.8
1	А	91	LYS	3.4
1	А	87	VAL	3.3
1	В	76	ALA	3.3
1	В	462	LYS	2.9
1	В	86	ALA	2.9
1	А	268	GLY	2.7
1	В	460	LEU	2.6
1	В	502	PRO	2.5
1	А	377	GLY	2.3
1	В	522	LEU	2.3
1	А	88	LEU	2.3
1	В	414	VAL	2.1
1	В	91	LYS	2.1
1	В	189	ALA	2.1

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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	SO4	В	605	5/5	0.97	0.11	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.

