Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:56 PM GMT

PDB ID	:	3WZZ
Title	:	Crystal structure of PIP4KIIBETA
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Deposited on	:	2014-10-08
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/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:

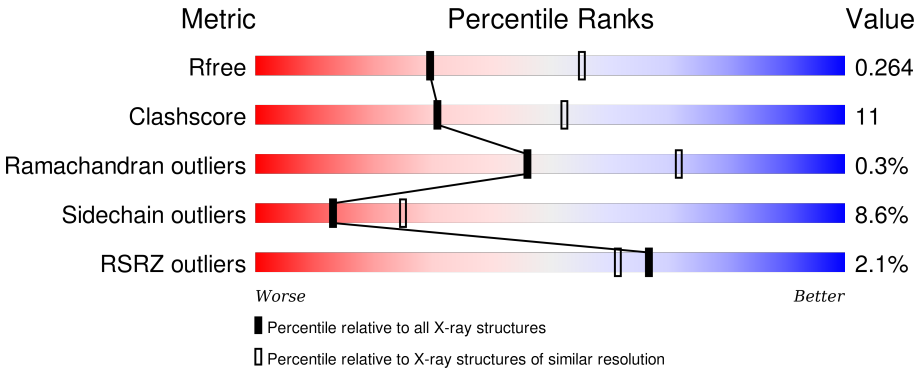
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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	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)

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 <=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	393	2% 62% 17% • 18%
1	B	393	2% 59% 16% • 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5213 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 Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2645	1681	450	500	14			
1	B	306	Total	C	N	O	S	0	0	0
			2517	1611	429	464	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P78356
A	25	PRO	-	EXPRESSION TAG	UNP P78356
A	26	ASN	-	EXPRESSION TAG	UNP P78356
A	27	CYS	-	EXPRESSION TAG	UNP P78356
A	28	ALA	-	EXPRESSION TAG	UNP P78356
A	29	PRO	-	EXPRESSION TAG	UNP P78356
A	30	GLY	-	EXPRESSION TAG	UNP P78356
B	24	GLY	-	EXPRESSION TAG	UNP P78356
B	25	PRO	-	EXPRESSION TAG	UNP P78356
B	26	ASN	-	EXPRESSION TAG	UNP P78356
B	27	CYS	-	EXPRESSION TAG	UNP P78356
B	28	ALA	-	EXPRESSION TAG	UNP P78356
B	29	PRO	-	EXPRESSION TAG	UNP P78356
B	30	GLY	-	EXPRESSION TAG	UNP P78356

- Molecule 2 is water.

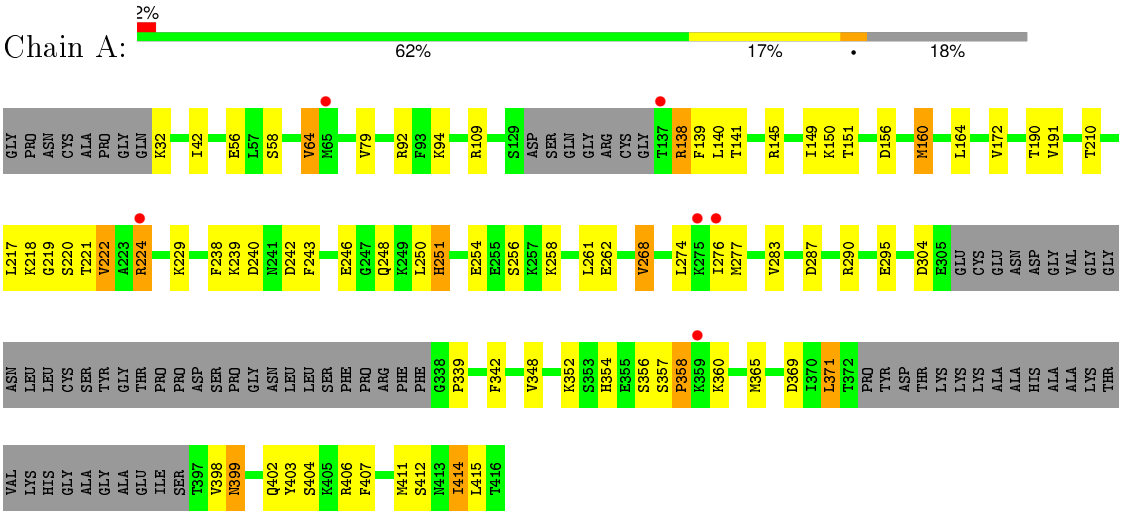
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	31	Total	O	0	0
			31	31		

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 (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.

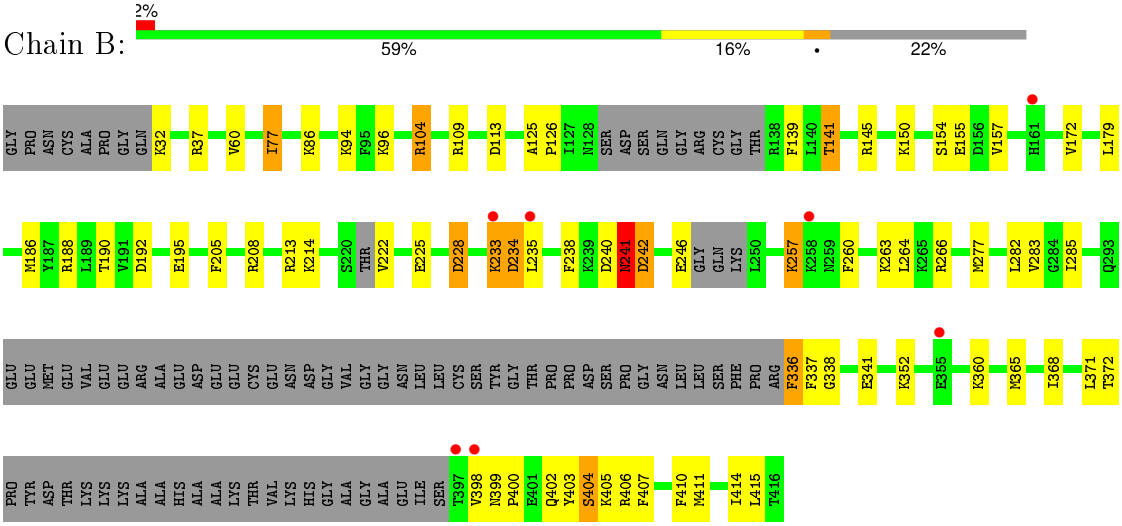
- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta

Chain A:



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.14Å 182.40Å 105.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 2.60 69.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.70-2.60) 99.6 (69.47-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.211 , 0.260 0.216 , 0.264	Depositor DCC
R_{free} test set	1601 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.2	EDS
Estimated twinning fraction	0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 32022 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5213	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.45	0/2698	0.59	1/3630 (0.0%)
1	B	0.48	2/2569 (0.1%)	0.58	0/3455
All	All	0.46	2/5267 (0.0%)	0.59	1/7085 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	ASN	C-N	5.86	1.47	1.34
1	B	240	ASP	C-O	-5.82	1.12	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	VAL	CB-CA-C	-5.46	101.03	111.40

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	A	2645	0	2614	54	0
1	B	2517	0	2498	59	0
2	A	20	0	0	0	0
2	B	31	0	0	0	0
All	All	5213	0	5112	112	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 11.

All (112) 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:357:SER:OG	1:A:358:PRO:HD2	1.49	1.09
1:B:398:VAL:HG12	1:B:399:ASN:H	1.24	0.98
1:B:398:VAL:HG12	1:B:399:ASN:N	1.79	0.96
1:B:398:VAL:CG1	1:B:399:ASN:H	1.87	0.88
1:B:398:VAL:HG11	1:B:406:ARG:HH21	1.39	0.88
1:B:398:VAL:HG13	1:B:402:GLN:HB2	1.54	0.87
1:B:336:PHE:N	1:B:337:PHE:HA	1.89	0.87
1:B:336:PHE:CD1	1:B:336:PHE:O	2.30	0.84
1:A:218:LYS:HD2	1:A:224:ARG:NH1	1.93	0.83
1:A:220:SER:HB3	1:A:222:VAL:HG23	1.60	0.82
1:B:400:PRO:O	1:B:404:SER:HB3	1.84	0.77
1:B:338:GLY:HA3	1:B:341:GLU:OE1	1.84	0.77
1:B:399:ASN:HB3	1:B:400:PRO:HD2	1.67	0.76
1:B:336:PHE:N	1:B:337:PHE:CA	2.48	0.76
1:B:398:VAL:HG11	1:B:406:ARG:NH2	1.99	0.75
1:A:243:PHE:CE1	1:A:248:GLN:HG2	2.22	0.75
1:A:268:VAL:HG13	1:A:404:SER:HB2	1.70	0.72
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.72	0.72
1:B:94:LYS:HB2	1:B:190:THR:HB	1.70	0.72
1:A:224:ARG:HD3	1:A:240:ASP:OD1	1.91	0.71
1:B:411:MET:HA	1:B:414:ILE:HD12	1.74	0.69
1:B:398:VAL:CG1	1:B:402:GLN:HB2	2.22	0.69
1:A:224:ARG:HB2	1:A:240:ASP:HB2	1.73	0.69
1:B:225:GLU:HG3	1:B:241:ASN:HB2	1.75	0.68
1:A:342:PHE:HE1	1:A:352:LYS:HG3	1.58	0.68
1:A:94:LYS:HB2	1:A:190:THR:HB	1.76	0.67
1:B:399:ASN:HB3	1:B:400:PRO:CD	2.26	0.65
1:B:400:PRO:O	1:B:404:SER:N	2.23	0.65
1:A:357:SER:OG	1:A:358:PRO:CD	2.39	0.64
1:A:224:ARG:HH21	1:A:239:LYS:HD3	1.60	0.64
1:B:228:ASP:OD1	1:B:228:ASP:N	2.30	0.63
1:A:156:ASP:O	1:A:371:LEU:CD1	2.47	0.62
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.30	0.62
1:A:242:ASP:O	1:A:246:GLU:HG2	1.99	0.61
1:A:160:MET:HG2	1:A:371:LEU:HD11	1.82	0.61
1:A:258:LYS:NZ	1:A:262:GLU:OE2	2.33	0.61
1:B:225:GLU:HG3	1:B:241:ASN:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:O	1:B:104:ARG:NH2	2.35	0.60
1:A:140:LEU:HB2	1:A:149:ILE:HB	1.85	0.59
1:B:399:ASN:O	1:B:403:TYR:N	2.30	0.56
1:A:224:ARG:CD	1:A:240:ASP:OD1	2.53	0.56
1:B:242:ASP:N	1:B:242:ASP:OD1	2.39	0.56
1:A:218:LYS:HD2	1:A:224:ARG:HH11	1.72	0.55
1:B:260:PHE:CD2	1:B:415:LEU:HD11	2.42	0.55
1:A:354:HIS:CE1	1:A:356:SER:H	2.24	0.54
1:B:157:VAL:HA	1:B:186:MET:HE1	1.89	0.54
1:A:274:LEU:HB2	1:A:276:ILE:HG13	1.90	0.53
1:B:141:THR:HG23	1:B:145:ARG:HA	1.92	0.52
1:B:234:ASP:N	1:B:234:ASP:OD1	2.37	0.51
1:A:243:PHE:CE2	1:A:248:GLN:O	2.63	0.51
1:A:243:PHE:CE1	1:A:248:GLN:CG	2.91	0.51
1:A:156:ASP:O	1:A:371:LEU:HD13	2.10	0.51
1:A:42:ILE:HG13	1:A:191:VAL:HG21	1.92	0.51
1:A:160:MET:HE1	1:A:164:LEU:HD13	1.93	0.49
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.95	0.49
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.42	0.49
1:A:357:SER:O	1:A:358:PRO:O	2.30	0.49
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.94	0.49
1:B:205:PHE:HE1	1:B:214:LYS:HE2	1.78	0.49
1:A:79:VAL:HG22	1:B:77:ILE:HD11	1.95	0.48
1:A:141:THR:CG2	1:A:145:ARG:HA	2.43	0.48
1:A:219:GLY:O	1:A:406:ARG:HD3	2.14	0.48
1:A:229:LYS:HB3	1:A:229:LYS:HE2	1.74	0.47
1:B:411:MET:O	1:B:414:ILE:HB	2.14	0.47
1:A:360:LYS:HE2	1:A:360:LYS:HB3	1.68	0.47
1:B:399:ASN:CB	1:B:400:PRO:CD	2.92	0.47
1:A:156:ASP:HB3	1:A:371:LEU:HD12	1.97	0.47
1:A:354:HIS:CE1	1:A:356:SER:HG	2.32	0.47
1:A:357:SER:CB	1:A:358:PRO:HD2	2.36	0.47
1:B:139:PHE:CE1	1:B:150:LYS:HD2	2.50	0.46
1:B:179:LEU:HG	1:B:263:LYS:HD2	1.97	0.46
1:B:336:PHE:N	1:B:337:PHE:O	2.49	0.46
1:A:217:LEU:HD13	1:A:414:ILE:CD1	2.43	0.46
1:B:94:LYS:HB2	1:B:190:THR:CB	2.45	0.45
1:B:398:VAL:HA	1:B:402:GLN:OE1	2.16	0.45
1:A:407:PHE:O	1:A:411:MET:HG2	2.17	0.44
1:A:251:HIS:HB3	1:A:357:SER:HB2	1.98	0.44
1:B:407:PHE:O	1:B:411:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:HH21	1:A:239:LYS:CD	2.27	0.44
1:B:398:VAL:CG1	1:B:399:ASN:N	2.47	0.44
1:A:109:ARG:NH1	1:A:172:VAL:HG22	2.33	0.44
1:B:238:PHE:HB3	1:B:242:ASP:HB2	2.00	0.43
1:B:399:ASN:O	1:B:403:TYR:CB	2.65	0.43
1:B:213:ARG:HB2	1:B:285:ILE:HD12	2.01	0.43
1:B:282:LEU:HB2	1:B:368:ILE:HD13	2.00	0.43
1:A:399:ASN:HB3	1:A:402:GLN:OE1	2.19	0.43
1:B:264:LEU:HA	1:B:264:LEU:HD12	1.61	0.43
1:B:360:LYS:HE2	1:B:360:LYS:HB2	1.70	0.43
1:A:160:MET:HB3	1:A:160:MET:HE2	1.89	0.43
1:A:238:PHE:HB3	1:A:242:ASP:CB	2.49	0.43
1:A:139:PHE:CE1	1:A:150:LYS:HE2	2.54	0.43
1:A:261:LEU:HD21	1:A:412:SER:HA	2.01	0.43
1:B:283:VAL:HG22	1:B:365:MET:HG2	2.00	0.43
1:B:336:PHE:CD1	1:B:336:PHE:C	2.87	0.42
1:A:42:ILE:H	1:A:42:ILE:HD12	1.83	0.42
1:B:263:LYS:HG2	1:B:266:ARG:NH2	2.33	0.42
1:B:277:MET:SD	1:B:399:ASN:HA	2.59	0.42
1:B:336:PHE:HD1	1:B:336:PHE:O	1.97	0.42
1:A:79:VAL:O	1:A:92:ARG:HA	2.18	0.42
1:B:205:PHE:CE1	1:B:214:LYS:HE2	2.54	0.42
1:A:342:PHE:CE1	1:A:352:LYS:HG3	2.48	0.42
1:B:233:LYS:N	1:B:233:LYS:HD2	2.35	0.42
1:A:138:ARG:HB2	1:A:151:THR:HB	2.01	0.42
1:B:410:PHE:CE2	1:B:414:ILE:HD11	2.55	0.41
1:B:96:LYS:HB3	1:B:188:ARG:HB3	2.02	0.41
1:B:336:PHE:O	1:B:336:PHE:CG	2.72	0.40
1:A:277:MET:HG3	1:A:403:TYR:CG	2.56	0.40
1:B:125:ALA:HA	1:B:126:PRO:HD2	1.86	0.40
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.89	0.40
1:B:399:ASN:O	1:B:403:TYR:HB2	2.21	0.40
1:B:257:LYS:HG3	1:B:415:LEU:HB2	2.03	0.40
1:A:224:ARG:HH21	1:A:239:LYS:CE	2.34	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	Percentiles
1	A	314/393 (80%)	304 (97%)	8 (2%)	2 (1%)	30 56
1	B	294/393 (75%)	281 (96%)	13 (4%)	0	100 100
All	All	608/786 (77%)	585 (96%)	21 (4%)	2 (0%)	46 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	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	A	299/352 (85%)	275 (92%)	24 (8%)	15 29
1	B	284/352 (81%)	258 (91%)	26 (9%)	11 21
All	All	583/704 (83%)	533 (91%)	50 (9%)	13 25

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	56	GLU
1	A	58	SER
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	138	ARG
1	A	160	MET
1	A	210	THR
1	A	221	THR
1	A	222	VAL
1	A	224	ARG
1	A	250	LEU
1	A	251	HIS
1	A	254	GLU
1	A	256	SER
1	A	268	VAL
1	A	295	GLU
1	A	304	ASP
1	A	348	VAL
1	A	369	ASP
1	A	371	LEU
1	A	398	VAL
1	A	399	ASN
1	A	414	ILE
1	A	415	LEU
1	B	32	LYS
1	B	37	ARG
1	B	77	ILE
1	B	86	LYS
1	B	104	ARG
1	B	113	ASP
1	B	141	THR
1	B	154	SER
1	B	155	GLU
1	B	192	ASP
1	B	195	GLU
1	B	208	ARG
1	B	222	VAL
1	B	228	ASP
1	B	233	LYS
1	B	234	ASP
1	B	235	LEU
1	B	241	ASN
1	B	242	ASP
1	B	246	GLU
1	B	257	LYS
1	B	336	PHE

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Mol	Chain	Res	Type
1	B	352	LYS
1	B	372	THR
1	B	404	SER
1	B	405	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 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			OWAB(Å^2)	Q<0.9
1	A	322/393 (81%)	0.30	6 (1%)	70	64	35, 68, 125, 142	0
1	B	306/393 (77%)	0.34	7 (2%)	64	57	36, 66, 117, 145	0
All	All	628/786 (79%)	0.32	13 (2%)	67	61	35, 66, 120, 145	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	LEU	4.8
1	A	137	THR	3.7
1	B	397	THR	2.8
1	B	355	GLU	2.8
1	B	398	VAL	2.7
1	B	233	LYS	2.5
1	B	161	HIS	2.2
1	B	258	LYS	2.2
1	A	359	LYS	2.1
1	A	224	ARG	2.1
1	A	65	MET	2.1
1	A	275	LYS	2.0
1	A	276	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.