Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:00 am BST

PDB ID	:	4JZA
Title	:	Crystal structure of a Legionella phosphoinositide phosphatase: insights into lipid metabolism in pathogen host interaction
Authors	:	Toulabi, L.; Wu, X.; Cheng, Y.; Mao, Y.
Deposited on	:	2013-04-02
Resolution	:	2.58 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 following versions of software and data (see references ⓘ) were used in the production of this report:

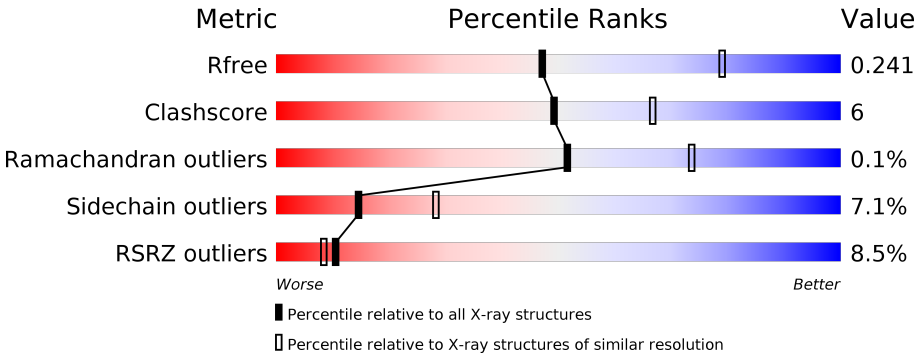
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.58 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	825	8% 82% 15%
1	B	825	8% 81% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13343 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	817	Total	C	N	O	S	Se	0	0	0
			6597	4203	1116	1259	8	11			
1	B	815	Total	C	N	O	S	Se	0	0	0
			6585	4196	1114	1257	8	10			

- Molecule 2 is water.

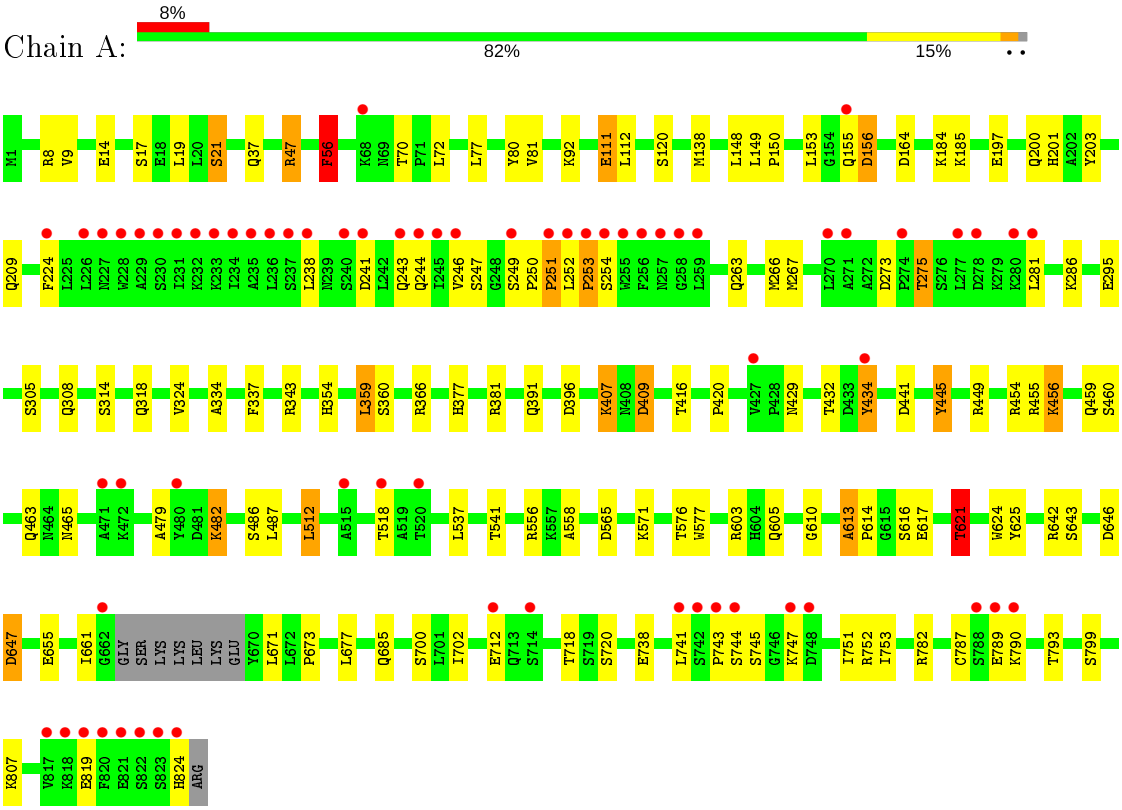
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	88	Total	O	0	0
			88	88		

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.

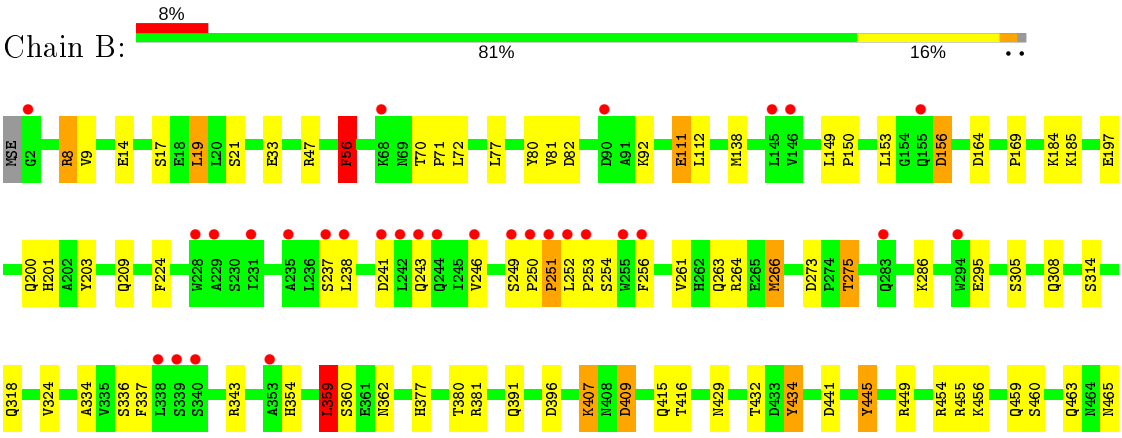
- Molecule 1: Uncharacterized protein

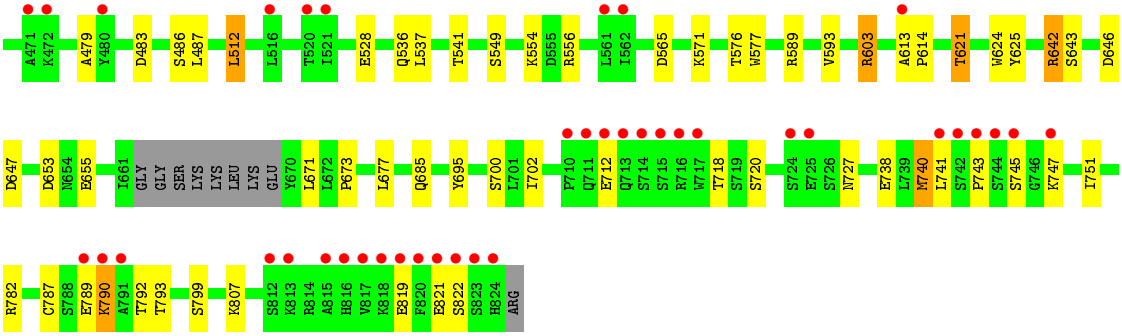
Chain A:



- Molecule 1: Uncharacterized protein

Chain B:




A471 K472 A479 Y480 D483 S486 L487 L512 L516 T520 I521 E528 Q536 L537 T541 S549 K554 D555 R556 L561 I562 D565 K571 T576 W577 R589 V593 R603 A613 P614 T621 W624 Y625 R642 S643 D646
D647 D653 N654 E655 I661 GLY GLY SER LYS LYS LEU LYS GLU Y670 L671 L672 P673 L677 Q685 Y695 S700 L701 I702 P710 Q711 E712 Q713 S714 S715 R716 W717 T718 S719 S720 S724 E725 S726 N727 E738 L739 M740 L741 S742 P743 S744 S745 G746 K747 I751
R782 C787 S788 E789 K790 A791 T792 T793 S799 K807 S812 K813 R814 A815 H816 V817 K818 E819 F820 E821 S822 S823 H824 ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.28Å 119.65Å 133.53Å 90.00° 101.33° 90.00°	Depositor
Resolution (Å)	49.44 – 2.58 49.39 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.44-2.58) 97.2 (49.39-2.58)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.237 0.203 , 0.241	Depositor DCC
R_{free} test set	4205 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13343	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.78	8/6737 (0.1%)	0.87	15/9116 (0.2%)
1	B	0.80	7/6725 (0.1%)	0.89	21/9101 (0.2%)
All	All	0.79	15/13462 (0.1%)	0.88	36/18217 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	PRO	N-CD	5.60	1.55	1.47
1	A	434	TYR	CE1-CZ	-5.42	1.31	1.38
1	A	150	PRO	N-CD	5.18	1.55	1.47
1	A	251	PRO	N-CD	5.17	1.55	1.47
1	B	253	PRO	N-CD	5.13	1.55	1.47
1	B	150	PRO	N-CD	5.12	1.55	1.47
1	A	614	PRO	N-CD	5.09	1.54	1.47
1	B	250	PRO	N-CD	5.08	1.54	1.47
1	B	614	PRO	N-CD	5.07	1.54	1.47
1	A	621	THR	CB-CG2	-5.06	1.35	1.52
1	B	434	TYR	CE1-CZ	-5.05	1.31	1.38
1	A	56	PHE	CG-CD2	-5.04	1.31	1.38
1	A	250	PRO	N-CD	5.04	1.54	1.47
1	B	56	PHE	CG-CD1	-5.02	1.31	1.38
1	A	253	PRO	N-CD	5.01	1.54	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	782	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	782	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	782	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	782	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	653	ASP	CB-CG-OD1	7.38	124.95	118.30
1	A	47	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	655	GLU	OE1-CD-OE2	-6.92	115.00	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	47	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	653	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	82	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	655	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	B	603	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	753	ILE	CG1-CB-CG2	-5.87	98.50	111.40
1	B	740	MSE	CA-CB-CG	-5.85	103.35	113.30
1	B	613	ALA	C-N-CD	5.77	140.51	128.40
1	B	249	SER	C-N-CD	5.76	140.50	128.40
1	A	252	LEU	C-N-CD	5.74	140.46	128.40
1	A	249	SER	C-N-CD	5.74	140.45	128.40
1	B	642	ARG	CB-CA-C	-5.71	98.98	110.40
1	B	47	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	252	LEU	C-N-CD	5.65	140.27	128.40
1	B	149	LEU	C-N-CD	5.63	140.22	128.40
1	A	149	LEU	C-N-CD	5.63	140.22	128.40
1	B	381	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	8	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	613	ALA	C-N-CD	5.58	140.12	128.40
1	A	250	PRO	C-N-CD	5.46	139.88	128.40
1	A	647	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	528	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	B	8	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	19	LEU	CA-CB-CG	5.28	127.43	115.30
1	B	359	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	381	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	47	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	647	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	8	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	A	6597	0	6535	80	0
1	B	6585	0	6520	75	0
2	A	73	0	0	5	0
2	B	88	0	0	3	0
All	All	13343	0	13055	154	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 (154) 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:456:LYS:HE3	2:A:952:HOH:O	1.62	0.99
1:A:56:PHE:CD2	1:A:81:VAL:HG21	1.99	0.97
1:A:56:PHE:CE2	1:A:81:VAL:HG21	1.99	0.96
1:A:70:THR:HG22	1:A:72:LEU:H	1.32	0.94
1:B:70:THR:HG22	1:B:72:LEU:H	1.38	0.85
1:A:156:ASP:O	1:A:360:SER:HB3	1.81	0.79
1:A:56:PHE:HD1	1:A:56:PHE:O	1.68	0.76
1:B:537:LEU:O	1:B:541:THR:HG23	1.87	0.75
1:B:164:ASP:OD1	1:B:354:HIS:HD2	1.69	0.74
1:A:156:ASP:N	1:A:156:ASP:OD1	2.20	0.74
1:B:343:ARG:NH2	1:B:377:HIS:O	2.21	0.73
1:A:72:LEU:HA	1:A:685:GLN:HE22	1.54	0.71
1:B:56:PHE:HD1	1:B:56:PHE:C	1.95	0.70
1:A:156:ASP:O	1:A:360:SER:CB	2.39	0.70
1:A:156:ASP:OD2	1:A:366:ARG:NH2	2.24	0.69
1:A:479:ALA:O	1:A:512:LEU:HD23	1.93	0.69
1:B:479:ALA:O	1:B:512:LEU:HD23	1.92	0.68
1:A:241:ASP:HB3	1:A:253:PRO:HG2	1.76	0.68
1:A:610:GLY:HA3	1:A:617:GLU:HG3	1.76	0.67
1:A:621:THR:HG22	1:A:621:THR:O	1.94	0.67
1:B:203:TYR:HD1	1:B:266:MSE:HE2	1.59	0.67
1:A:343:ARG:NH2	1:A:377:HIS:O	2.28	0.67
1:B:56:PHE:CE2	1:B:81:VAL:HG21	2.29	0.67
1:B:56:PHE:CD2	1:B:81:VAL:HG21	2.30	0.66
1:B:56:PHE:C	1:B:56:PHE:CD1	2.65	0.66
1:A:47:ARG:NH1	1:A:617:GLU:OE2	2.26	0.66
1:A:537:LEU:O	1:A:541:THR:HG23	1.95	0.65
1:A:391:GLN:HG2	2:A:924:HOH:O	1.96	0.65
1:B:621:THR:HG22	1:B:621:THR:O	1.96	0.65
1:A:224:PHE:HB2	1:A:263:GLN:HE21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLN:HG2	2:B:973:HOH:O	1.97	0.63
1:B:77:LEU:HD22	1:B:112:LEU:HD11	1.81	0.63
1:A:56:PHE:HE2	1:A:81:VAL:HG21	1.62	0.62
1:A:56:PHE:HD2	1:A:81:VAL:HG21	1.61	0.62
1:B:324:VAL:HG12	1:B:334:ALA:HB1	1.82	0.61
1:A:77:LEU:HD22	1:A:112:LEU:HD11	1.82	0.61
1:A:164:ASP:OD1	1:A:354:HIS:HD2	1.83	0.61
1:B:354:HIS:HE1	1:B:565:ASP:OD2	1.84	0.61
1:B:56:PHE:HD1	1:B:56:PHE:O	1.82	0.61
1:B:621:THR:O	1:B:621:THR:CG2	2.49	0.60
1:B:156:ASP:OD1	1:B:156:ASP:N	2.31	0.60
1:A:603:ARG:NH2	1:A:647:ASP:OD1	2.34	0.60
1:A:243:GLN:HA	1:A:246:VAL:HG12	1.84	0.59
1:A:354:HIS:HE1	1:A:565:ASP:OD2	1.84	0.59
1:B:201:HIS:HD2	1:B:308:GLN:HE21	1.48	0.59
1:B:261:VAL:HG23	2:B:931:HOH:O	2.03	0.58
1:A:201:HIS:HD2	1:A:308:GLN:HE21	1.52	0.57
1:B:56:PHE:O	1:B:56:PHE:CD1	2.56	0.57
1:A:70:THR:HG22	1:A:72:LEU:N	2.12	0.57
1:B:184:LYS:HE3	1:B:305:SER:HB3	1.86	0.57
1:A:17:SER:O	1:A:21:SER:HB2	2.05	0.57
1:A:56:PHE:O	1:A:56:PHE:CD1	2.53	0.56
1:A:184:LYS:HE3	1:A:305:SER:HB3	1.87	0.56
1:B:360:SER:OG	1:B:362:ASN:OD1	2.21	0.56
1:B:243:GLN:HA	1:B:246:VAL:HG12	1.86	0.56
1:B:449:ARG:NH2	1:B:483:ASP:OD2	2.33	0.56
1:A:621:THR:CG2	1:A:621:THR:O	2.54	0.56
1:B:415:GLN:NE2	1:B:536:GLN:HE21	2.04	0.55
1:B:70:THR:HG22	1:B:72:LEU:N	2.17	0.55
1:A:238:LEU:O	1:A:241:ASP:HB2	2.07	0.55
1:A:613:ALA:O	1:A:616:SER:HB2	2.06	0.55
1:A:56:PHE:C	1:A:56:PHE:CD1	2.78	0.55
1:A:324:VAL:HG12	1:A:334:ALA:HB1	1.89	0.54
1:A:396:ASP:OD1	1:A:454:ARG:NH1	2.39	0.54
1:B:72:LEU:HA	1:B:685:GLN:HE22	1.71	0.54
1:B:203:TYR:CD1	1:B:266:MSE:HE2	2.41	0.53
1:B:409:ASP:OD1	1:B:409:ASP:N	2.40	0.53
1:B:256:PHE:CZ	1:B:264:ARG:HG2	2.43	0.52
1:A:354:HIS:CE1	1:A:565:ASP:OD2	2.61	0.52
1:B:354:HIS:CE1	1:B:565:ASP:OD2	2.61	0.52
1:B:169:PRO:CD	1:B:336:SER:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASP:OD1	1:B:454:ARG:NH1	2.42	0.52
1:B:603:ARG:NH2	1:B:647:ASP:OD1	2.42	0.52
1:A:479:ALA:O	1:A:512:LEU:CD2	2.57	0.51
1:B:138:MSE:HG3	1:B:337:PHE:O	2.09	0.51
1:B:479:ALA:O	1:B:512:LEU:CD2	2.59	0.51
1:A:244:GLN:OE1	1:A:251:PRO:HD2	2.11	0.50
1:B:156:ASP:O	1:B:360:SER:CB	2.58	0.50
1:B:621:THR:CG2	1:B:624:TRP:HB3	2.42	0.50
1:A:429:ASN:HA	1:A:434:TYR:CE1	2.47	0.49
1:B:487:LEU:O	1:B:487:LEU:HD23	2.13	0.49
1:A:445:TYR:CD1	1:A:445:TYR:C	2.86	0.49
1:B:273:ASP:OD1	1:B:275:THR:HG23	2.12	0.49
1:A:203:TYR:HD1	1:A:266:MSE:HE2	1.76	0.49
1:B:416:THR:OG1	1:B:465:ASN:ND2	2.37	0.49
1:A:487:LEU:HD23	1:A:487:LEU:O	2.13	0.49
1:A:80:TYR:HD2	1:A:112:LEU:HD22	1.78	0.49
1:A:445:TYR:HD1	1:A:445:TYR:C	2.16	0.49
1:B:314:SER:O	1:B:318:GLN:HG3	2.12	0.49
1:B:224:PHE:HB2	1:B:263:GLN:HE21	1.78	0.48
1:A:244:GLN:HA	1:A:247:SER:OG	2.13	0.48
1:B:343:ARG:NH1	2:B:932:HOH:O	2.47	0.48
1:B:445:TYR:C	1:B:445:TYR:CD1	2.87	0.48
1:B:111:GLU:CG	1:B:677:LEU:HD22	2.44	0.47
1:A:111:GLU:CG	1:A:677:LEU:HD22	2.45	0.47
1:B:169:PRO:HD3	1:B:336:SER:O	2.13	0.47
1:B:17:SER:O	1:B:21:SER:HB2	2.14	0.47
1:A:359:LEU:HD12	1:A:360:SER:N	2.29	0.47
1:A:456:LYS:CE	2:A:952:HOH:O	2.37	0.47
1:A:314:SER:O	1:A:318:GLN:HG3	2.15	0.47
1:A:449:ARG:HA	1:A:463:GLN:HE22	1.80	0.46
1:A:429:ASN:HA	1:A:434:TYR:HE1	1.81	0.46
1:A:416:THR:OG1	1:A:465:ASN:ND2	2.39	0.46
1:A:642:ARG:NH1	1:A:646:ASP:OD1	2.48	0.46
1:A:429:ASN:C	1:A:434:TYR:HE1	2.20	0.46
1:A:420:PRO:HG2	1:A:445:TYR:HD2	1.81	0.46
1:B:197:GLU:HB2	1:B:200:GLN:HE21	1.81	0.46
1:B:238:LEU:O	1:B:241:ASP:HB2	2.15	0.45
1:B:224:PHE:HB2	1:B:263:GLN:NE2	2.32	0.45
1:A:273:ASP:OD1	1:A:275:THR:HG23	2.17	0.45
1:A:359:LEU:C	1:A:359:LEU:HD12	2.36	0.45
1:A:621:THR:CG2	1:A:624:TRP:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:CD	1:B:407:LYS:N	2.80	0.45
1:B:56:PHE:HE2	1:B:112:LEU:HD23	1.82	0.45
1:B:571:LYS:HD3	1:B:577:TRP:CE2	2.52	0.45
1:B:790:LYS:O	1:B:792:THR:HG23	2.16	0.45
1:A:70:THR:CG2	1:A:72:LEU:HG	2.47	0.44
1:A:138:MSE:HG3	1:A:337:PHE:O	2.18	0.44
1:B:429:ASN:HA	1:B:434:TYR:CE1	2.51	0.44
1:B:455:ARG:NH1	1:B:459:GLN:OE1	2.51	0.44
1:B:80:TYR:HD2	1:B:112:LEU:HD22	1.82	0.44
1:A:407:LYS:CD	1:A:407:LYS:N	2.81	0.44
1:A:455:ARG:NH1	1:A:459:GLN:OE1	2.49	0.44
1:A:482:LYS:HE3	1:A:482:LYS:HB3	1.84	0.44
1:A:37:GLN:HG3	1:B:727:ASN:HD21	1.82	0.44
1:B:445:TYR:C	1:B:445:TYR:HD1	2.20	0.44
1:A:267:MSE:HE1	1:A:281:LEU:HD21	2.00	0.44
1:B:642:ARG:NH1	1:B:646:ASP:OD1	2.51	0.43
1:B:111:GLU:HG2	1:B:677:LEU:HD22	2.00	0.43
1:A:244:GLN:HA	1:A:247:SER:HG	1.83	0.43
1:A:111:GLU:HB2	1:A:671:LEU:HD22	2.00	0.42
1:B:111:GLU:HB2	1:B:671:LEU:HD22	2.00	0.42
1:B:359:LEU:HD12	1:B:359:LEU:C	2.40	0.42
1:B:449:ARG:HA	1:B:463:GLN:HE22	1.83	0.42
1:A:429:ASN:C	1:A:434:TYR:CE1	2.92	0.42
1:A:571:LYS:HD3	1:A:577:TRP:CE2	2.55	0.42
1:B:156:ASP:O	1:B:360:SER:HB2	2.20	0.42
1:B:256:PHE:CZ	1:B:264:ARG:CG	3.03	0.42
1:B:416:THR:HA	1:B:549:SER:O	2.20	0.41
1:A:409:ASP:OD1	1:A:409:ASP:N	2.53	0.41
1:B:695:TYR:CE2	1:B:740:MSE:HE3	2.55	0.41
1:A:744:SER:HB3	1:A:752:ARG:CZ	2.50	0.41
1:A:558:ALA:HB1	1:A:605:GLN:HB3	2.03	0.41
1:B:8:ARG:HA	1:B:33:GLU:O	2.21	0.41
1:A:391:GLN:CG	2:A:924:HOH:O	2.61	0.41
1:B:589:ARG:O	1:B:593:VAL:HG23	2.21	0.41
1:A:148:LEU:HD23	1:A:148:LEU:C	2.41	0.41
1:B:556:ARG:HD2	1:B:625:TYR:CE1	2.56	0.41
1:A:197:GLU:HB2	1:A:200:GLN:HE21	1.87	0.40
1:A:391:GLN:NE2	2:A:958:HOH:O	2.54	0.40
1:A:556:ARG:HD2	1:A:625:TYR:CE1	2.56	0.40
1:B:821:GLU:HA	1:B:821:GLU:OE2	2.21	0.40
1:A:111:GLU:HG2	1:A:677:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:HG23	1:B:71:PRO:HD2	2.01	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	813/825 (98%)	789 (97%)	23 (3%)	1 (0%)	51 73
1	B	811/825 (98%)	787 (97%)	23 (3%)	1 (0%)	51 73
All	All	1624/1650 (98%)	1576 (97%)	46 (3%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	PRO
1	B	673	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	729/725 (101%)	677 (93%)	52 (7%)	14 28
1	B	728/725 (100%)	677 (93%)	51 (7%)	15 29
All	All	1457/1450 (100%)	1354 (93%)	103 (7%)	14 28

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	14	GLU
1	A	19	LEU
1	A	21	SER
1	A	56	PHE
1	A	92	LYS
1	A	111	GLU
1	A	120	SER
1	A	153	LEU
1	A	155	GLN
1	A	156	ASP
1	A	185	LYS
1	A	209	GLN
1	A	254	SER
1	A	275	THR
1	A	286	LYS
1	A	295	GLU
1	A	359	LEU
1	A	407	LYS
1	A	409	ASP
1	A	432	THR
1	A	441	ASP
1	A	445	TYR
1	A	456	LYS
1	A	460	SER
1	A	482	LYS
1	A	486	SER
1	A	512	LEU
1	A	518	THR
1	A	576	THR
1	A	621	THR
1	A	643	SER
1	A	661	ILE
1	A	700	SER
1	A	702	ILE
1	A	712	GLU
1	A	718	THR
1	A	720	SER
1	A	738	GLU
1	A	741	LEU
1	A	743	PRO
1	A	745	SER

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Mol	Chain	Res	Type
1	A	747	LYS
1	A	751	ILE
1	A	787	CYS
1	A	789	GLU
1	A	790	LYS
1	A	793	THR
1	A	799	SER
1	A	807	LYS
1	A	819	GLU
1	A	824	HIS
1	B	9	VAL
1	B	14	GLU
1	B	19	LEU
1	B	56	PHE
1	B	92	LYS
1	B	111	GLU
1	B	153	LEU
1	B	156	ASP
1	B	185	LYS
1	B	209	GLN
1	B	237	SER
1	B	251	PRO
1	B	254	SER
1	B	266	MSE
1	B	275	THR
1	B	286	LYS
1	B	295	GLU
1	B	359	LEU
1	B	380	THR
1	B	407	LYS
1	B	409	ASP
1	B	432	THR
1	B	441	ASP
1	B	445	TYR
1	B	456	LYS
1	B	460	SER
1	B	486	SER
1	B	512	LEU
1	B	554	LYS
1	B	576	THR
1	B	621	THR
1	B	643	SER

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Mol	Chain	Res	Type
1	B	700	SER
1	B	702	ILE
1	B	712	GLU
1	B	718	THR
1	B	720	SER
1	B	738	GLU
1	B	741	LEU
1	B	743	PRO
1	B	745	SER
1	B	747	LYS
1	B	751	ILE
1	B	787	CYS
1	B	789	GLU
1	B	790	LYS
1	B	793	THR
1	B	799	SER
1	B	807	LYS
1	B	819	GLU
1	B	822	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	201	HIS
1	A	354	HIS
1	A	391	GLN
1	A	392	GLN
1	A	463	GLN
1	A	465	ASN
1	A	685	GLN
1	A	758	GLN
1	B	134	GLN
1	B	162	GLN
1	B	200	GLN
1	B	201	HIS
1	B	244	GLN
1	B	342	HIS
1	B	354	HIS
1	B	392	GLN
1	B	415	GLN
1	B	463	GLN

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Mol	Chain	Res	Type
1	B	465	ASN
1	B	727	ASN
1	B	758	GLN

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	806/825 (97%)	0.55	67 (8%)	11	9	33, 53, 105, 173	0
1	B	805/825 (97%)	0.66	70 (8%)	10	8	29, 51, 110, 161	0
All	All	1611/1650 (97%)	0.60	137 (8%)	10	8	29, 52, 109, 173	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	824	HIS	9.4
1	B	823	SER	8.3
1	B	822	SER	8.0
1	B	820	PHE	7.7
1	A	236	LEU	7.3
1	A	821	GLU	7.3
1	A	235	ALA	6.9
1	A	237	SER	6.8
1	B	824	HIS	6.6
1	B	480	TYR	6.3
1	A	823	SER	6.3
1	A	234	ILE	6.3
1	A	231	ILE	6.0
1	A	255	TRP	5.9
1	A	822	SER	5.6
1	A	251	PRO	5.6
1	A	743	PRO	5.3
1	B	816	HIS	5.3
1	A	820	PHE	5.2
1	A	244	GLN	5.1
1	B	155	GLN	5.0
1	A	789	GLU	4.9
1	B	255	TRP	4.7
1	A	252	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	712	GLU	4.6
1	B	229	ALA	4.6
1	B	819	GLU	4.6
1	B	724	SER	4.5
1	A	228	TRP	4.5
1	B	251	PRO	4.4
1	B	744	SER	4.4
1	A	271	ALA	4.4
1	B	821	GLU	4.3
1	A	480	TYR	4.2
1	B	818	LYS	4.2
1	B	741	LEU	4.1
1	A	240	SER	4.1
1	A	741	LEU	4.1
1	B	742	SER	4.1
1	A	238	LEU	4.0
1	B	815	ALA	4.0
1	B	243	GLN	4.0
1	A	230	SER	3.9
1	B	717	TRP	3.9
1	B	713	GLN	3.9
1	B	715	SER	3.8
1	B	246	VAL	3.8
1	B	252	LEU	3.7
1	A	744	SER	3.7
1	A	817	VAL	3.7
1	B	711	GLN	3.6
1	A	747	LYS	3.6
1	B	714	SER	3.6
1	A	254	SER	3.6
1	B	743	PRO	3.5
1	A	742	SER	3.5
1	A	241	ASP	3.4
1	A	274	PRO	3.4
1	B	817	VAL	3.4
1	B	813	LYS	3.4
1	A	515	ALA	3.3
1	A	427	VAL	3.3
1	B	745	SER	3.3
1	A	277	LEU	3.2
1	B	520	THR	3.2
1	A	245	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	249	SER	3.2
1	A	249	SER	3.2
1	A	243	GLN	3.2
1	B	68	LYS	3.2
1	B	242	LEU	3.1
1	A	518	THR	3.1
1	B	789	GLU	3.0
1	A	281	LEU	3.0
1	A	224	PHE	3.0
1	B	716	ARG	3.0
1	A	471	ALA	3.0
1	A	819	GLU	3.0
1	B	294	TRP	3.0
1	B	244	GLN	3.0
1	A	233	LYS	2.9
1	A	520	THR	2.9
1	A	278	ASP	2.9
1	A	229	ALA	2.9
1	A	270	LEU	2.9
1	A	790	LYS	2.9
1	B	725	GLU	2.8
1	B	791	ALA	2.8
1	B	250	PRO	2.8
1	B	256	PHE	2.7
1	A	259	LEU	2.7
1	A	258	GLY	2.7
1	A	256	PHE	2.6
1	A	226	LEU	2.6
1	A	712	GLU	2.6
1	A	714	SER	2.6
1	B	253	PRO	2.5
1	B	472	LYS	2.5
1	B	283	GLN	2.5
1	A	68	LYS	2.5
1	B	145	LEU	2.5
1	B	228	TRP	2.5
1	A	434	TYR	2.4
1	A	253	PRO	2.4
1	A	257	ASN	2.4
1	B	339	SER	2.4
1	B	2	GLY	2.3
1	B	521	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	155	GLN	2.3
1	A	246	VAL	2.3
1	B	747	LYS	2.3
1	B	146	VAL	2.3
1	B	238	LEU	2.3
1	B	562	ILE	2.3
1	B	90	ASP	2.3
1	B	710	PRO	2.2
1	A	232	LYS	2.2
1	B	237	SER	2.2
1	A	788	SER	2.2
1	A	280	LYS	2.2
1	B	338	LEU	2.2
1	B	340	SER	2.2
1	A	472	LYS	2.1
1	B	790	LYS	2.1
1	B	231	ILE	2.1
1	A	227	ASN	2.1
1	B	235	ALA	2.1
1	B	516	LEU	2.1
1	B	353	ALA	2.1
1	A	748	ASP	2.1
1	B	241	ASP	2.1
1	B	561	LEU	2.1
1	A	818	LYS	2.1
1	B	812	SER	2.1
1	A	662	GLY	2.0
1	B	471	ALA	2.0
1	B	613	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.