



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 06:04 AM EDT

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

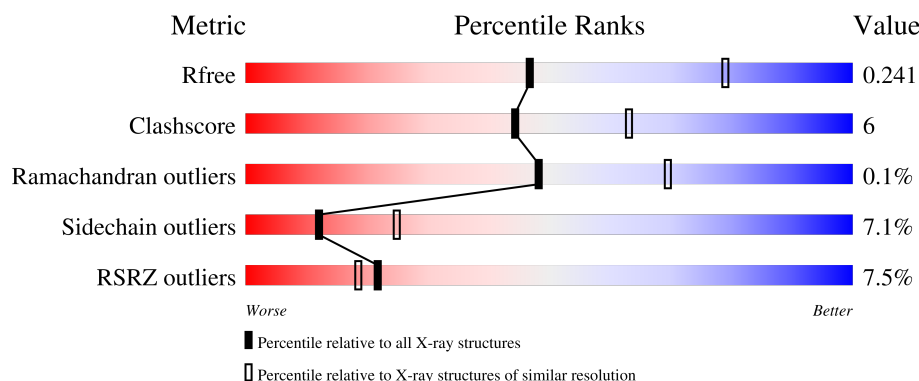
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (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 of 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 $\leq 5\%$. 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	A	825	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	825	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>

2 Entry composition

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		

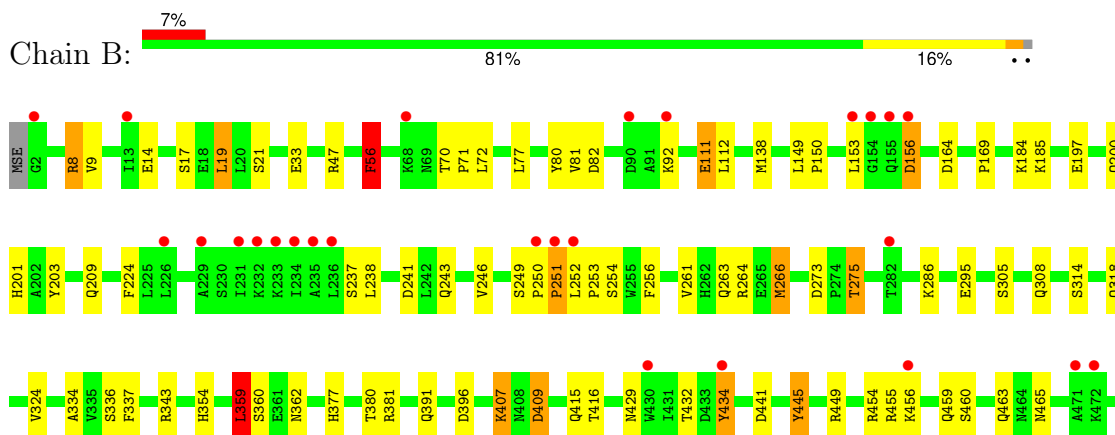
3 Residue-property plots

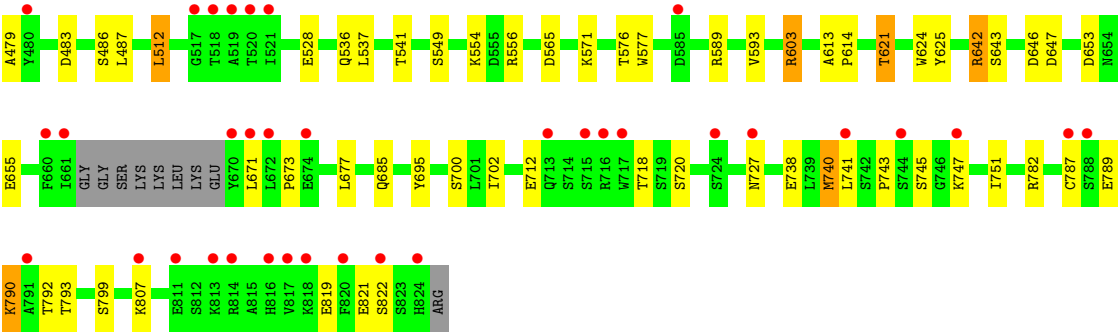
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Uncharacterized protein





4 Data and refinement statistics

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 49.44 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.44-2.58) 97.1 (49.44-2.58)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	4206 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)	0.36 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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.

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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:OD1	1:A:156:ASP:N	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:C	1:B:56:PHE:HD1	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:CD1	1:B:56:PHE:O	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:O	1:A:621:THR:CG2	2.54	0.56
1:B:70:THR:HG22	1:B:72:LEU:N	2.17	0.55
1:B:415:GLN:NE2	1:B:536:GLN:HE21	2.04	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:CD1	1:A:56:PHE:C	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:N	1:B:409:ASP:OD1	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:HD23	1:B:487:LEU:O	2.13	0.49
1:A:445:TYR:C	1:A:445:TYR:CD1	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:O	1:A:487:LEU:HD23	2.13	0.49
1:A:80:TYR:HD2	1:A:112:LEU:HD22	1.78	0.49
1:A:445:TYR:C	1:A:445:TYR:HD1	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:HD12	1:A:359:LEU:C	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:N	1:B:407:LYS:CD	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:N	1:A:407:LYS:CD	2.81	0.44
1:A:455:ARG:NH1	1:A:459:GLN:OE1	2.49	0.44
1:A:37:GLN:HG3	1:B:727:ASN:HD21	1.82	0.44
1:A:482:LYS:HB3	1:A:482:LYS:HE3	1.84	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:A:391:GLN:CG	2:A:924:HOH:O	2.61	0.41
1:B:8:ARG:HA	1:B:33:GLU:O	2.21	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:OE2	1:B:821:GLU:HA	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%)	48	69
1	B	811/825 (98%)	787 (97%)	23 (3%)	1 (0%)	48	69
All	All	1624/1650 (98%)	1576 (97%)	46 (3%)	2 (0%)	48	69

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%)	12	25
1	B	728/725 (100%)	677 (93%)	51 (7%)	12	25
All	All	1457/1450 (100%)	1354 (93%)	103 (7%)	12	25

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

Sometimes 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 [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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

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, 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	A	806/825 (97%)	0.26	60 (7%) 22 19	33, 53, 105, 173	0
1	B	805/825 (97%)	0.22	61 (7%) 21 18	29, 51, 110, 161	0
All	All	1611/1650 (97%)	0.24	121 (7%) 22 18	29, 52, 109, 173	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	PHE	7.2
1	A	818	LYS	5.5
1	B	236	LEU	5.4
1	A	824	HIS	5.1
1	B	234	ILE	5.0
1	B	518	THR	4.8
1	A	518	THR	4.7
1	A	236	LEU	4.6
1	B	741	LEU	4.6
1	B	229	ALA	4.5
1	A	790	LYS	4.4
1	A	662	GLY	4.4
1	A	234	ILE	4.3
1	A	251	PRO	4.2
1	B	251	PRO	4.1
1	B	2	GLY	4.0
1	B	816	HIS	3.9
1	A	521	ILE	3.9
1	B	817	VAL	3.9
1	B	820	PHE	3.9
1	B	480	TYR	3.8
1	B	727	ASN	3.8
1	A	821	GLU	3.7
1	B	818	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	480	TYR	3.7
1	B	13	ILE	3.7
1	A	817	VAL	3.6
1	A	741	LEU	3.5
1	A	282	THR	3.5
1	A	233	LYS	3.4
1	A	789	GLU	3.4
1	A	250	PRO	3.4
1	A	92	LYS	3.4
1	B	724	SER	3.3
1	B	822	SER	3.3
1	A	2	GLY	3.3
1	B	717	TRP	3.3
1	A	254	SER	3.3
1	B	252	LEU	3.2
1	B	520	THR	3.2
1	A	13	ILE	3.2
1	B	226	LEU	3.2
1	A	434	TYR	3.1
1	A	252	LEU	3.1
1	A	235	ALA	3.1
1	A	743	PRO	3.0
1	B	92	LYS	3.0
1	B	521	ILE	2.9
1	B	791	ALA	2.9
1	B	153	LEU	2.9
1	A	747	LYS	2.9
1	B	747	LYS	2.8
1	A	255	TRP	2.8
1	B	661	ILE	2.8
1	B	456	LYS	2.8
1	A	226	LEU	2.8
1	B	660	PHE	2.7
1	B	519	ALA	2.7
1	A	520	THR	2.7
1	B	814	ARG	2.7
1	B	713	GLN	2.7
1	A	661	ILE	2.7
1	B	430	TRP	2.7
1	A	671	LEU	2.6
1	A	515	ALA	2.6
1	A	436	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	2.6
1	A	674	GLU	2.5
1	B	155	GLN	2.5
1	A	240	SER	2.5
1	A	246	VAL	2.5
1	B	250	PRO	2.5
1	A	432	THR	2.5
1	B	232	LYS	2.5
1	B	233	LYS	2.5
1	B	672	LEU	2.5
1	B	235	ALA	2.5
1	B	716	ARG	2.5
1	A	56	PHE	2.5
1	B	715	SER	2.4
1	B	811	GLU	2.4
1	A	711	GLN	2.4
1	B	472	LYS	2.4
1	B	154	GLY	2.4
1	A	791	ALA	2.4
1	B	434	TYR	2.4
1	A	822	SER	2.4
1	B	670	TYR	2.4
1	A	807	LYS	2.4
1	A	583	LEU	2.3
1	B	517	GLY	2.3
1	B	787	CYS	2.3
1	A	238	LEU	2.2
1	A	229	ALA	2.2
1	B	807	LYS	2.2
1	B	90	ASP	2.2
1	A	819	GLU	2.2
1	A	714	SER	2.2
1	B	282	THR	2.2
1	B	788	SER	2.2
1	A	231	ILE	2.2
1	B	68	LYS	2.2
1	B	471	ALA	2.2
1	B	671	LEU	2.1
1	A	237	SER	2.1
1	A	586	LYS	2.1
1	B	585	ASP	2.1
1	B	813	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	2.1
1	A	792	THR	2.1
1	B	744	SER	2.1
1	A	816	HIS	2.1
1	B	231	ILE	2.1
1	A	456	LYS	2.1
1	B	674	GLU	2.1
1	A	469	ASN	2.1
1	B	156	ASP	2.1
1	A	718	THR	2.0
1	A	793	THR	2.0
1	B	824	HIS	2.0
1	A	445	TYR	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 monosaccharides 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.