



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:45 PM UTC

PDB ID : 4JZA / pdb_00004jza
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

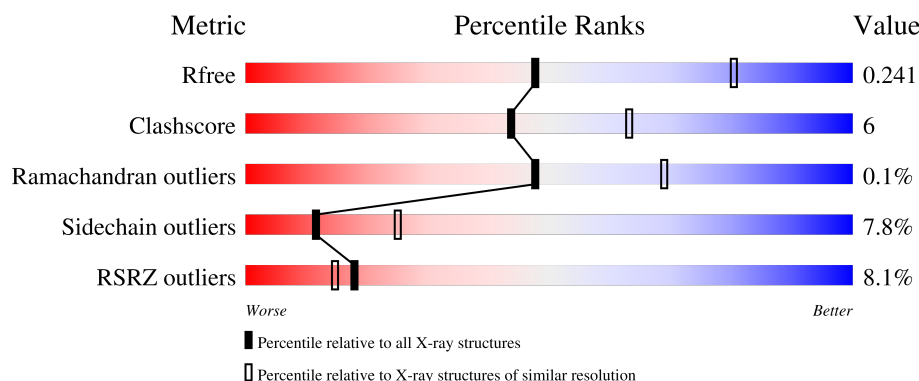
1 Overall quality at a glance

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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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	
1	B	825	

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			

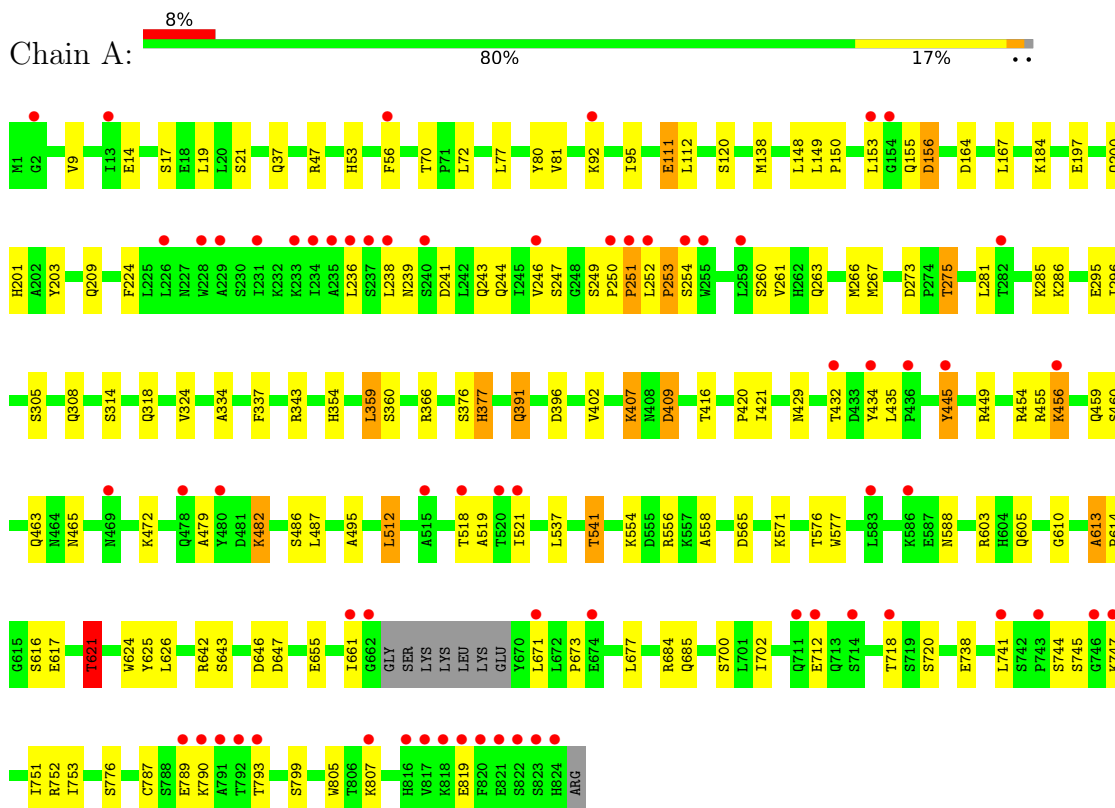
- Molecule 2 is water.

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

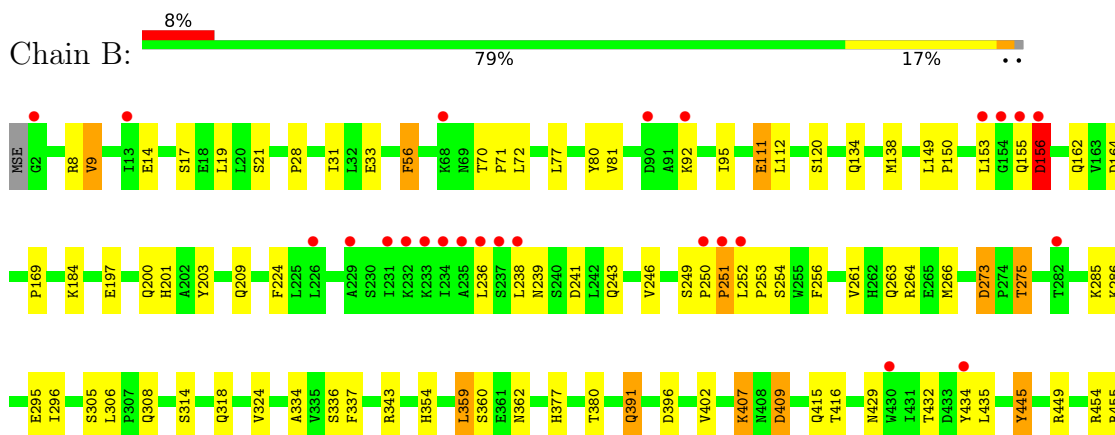
3 Residue-property plots [i](#)

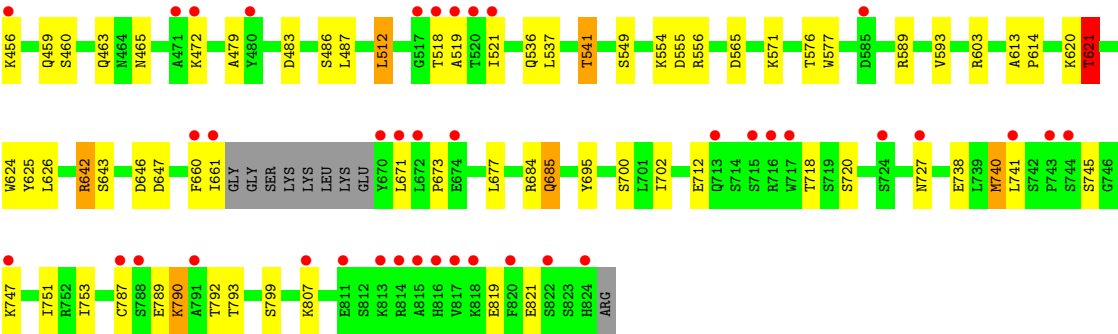
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (4.88%)	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 , 35.5	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	1.03	13/6737 (0.2%)	1.10	24/9116 (0.3%)
1	B	1.07	15/6725 (0.2%)	1.10	27/9101 (0.3%)
All	All	1.05	28/13462 (0.2%)	1.10	51/18217 (0.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	621	THR	C-O	-9.09	1.19	1.23
1	A	249	SER	C-N	8.53	1.41	1.33
1	A	621	THR	C-O	-7.40	1.20	1.23
1	B	249	SER	C-N	6.54	1.41	1.33
1	A	149	LEU	C-N	6.51	1.41	1.33
1	B	149	LEU	C-N	6.31	1.41	1.33
1	B	252	LEU	C-N	6.12	1.41	1.33
1	B	685	GLN	CD-NE2	-5.95	1.20	1.33
1	A	377	HIS	C-O	-5.64	1.17	1.23
1	B	251	PRO	N-CD	5.60	1.55	1.47
1	A	613	ALA	C-N	5.53	1.40	1.33
1	A	252	LEU	C-N	5.44	1.41	1.33
1	B	162	GLN	CD-NE2	-5.34	1.22	1.33
1	B	134	GLN	CD-NE2	-5.33	1.22	1.33
1	B	613	ALA	C-N	5.30	1.40	1.33
1	A	150	PRO	N-CD	5.25	1.55	1.47
1	B	253	PRO	N-CD	5.20	1.55	1.47
1	B	150	PRO	N-CD	5.19	1.55	1.47
1	A	251	PRO	N-CD	5.17	1.55	1.47
1	B	28	PRO	C-O	-5.17	1.17	1.23
1	A	614	PRO	N-CD	5.16	1.54	1.47
1	B	250	PRO	N-CD	5.15	1.54	1.47
1	B	614	PRO	N-CD	5.14	1.54	1.47
1	A	621	THR	CB-CG2	-5.12	1.35	1.52
1	A	250	PRO	N-CD	5.11	1.54	1.47
1	A	253	PRO	N-CD	5.09	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	LEU	C-O	-5.08	1.19	1.24
1	A	655	GLU	CA-C	5.08	1.59	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	LYS	N-CA-C	-10.55	99.94	113.12
1	A	249	SER	CA-C-N	-9.12	113.00	119.66
1	A	249	SER	C-N-CA	-9.12	113.00	119.66
1	A	250	PRO	C-N-CD	8.76	139.88	120.60
1	B	250	PRO	C-N-CD	8.23	138.70	120.60
1	A	472	LYS	N-CA-C	-8.12	101.17	112.45
1	B	249	SER	CA-C-N	-7.13	113.03	120.38
1	B	249	SER	C-N-CA	-7.13	113.03	120.38
1	B	296	ILE	N-CA-C	6.67	118.50	112.17
1	B	613	ALA	CA-C-N	-6.61	112.95	119.76
1	B	613	ALA	C-N-CA	-6.61	112.95	119.76
1	B	149	LEU	CA-C-N	-6.58	112.99	119.90
1	B	149	LEU	C-N-CA	-6.58	112.99	119.90
1	A	252	LEU	CA-C-N	-6.52	113.07	119.78
1	A	252	LEU	C-N-CA	-6.52	113.07	119.78
1	A	613	ALA	CA-C-N	-6.36	113.21	119.76
1	A	613	ALA	C-N-CA	-6.36	113.21	119.76
1	B	252	LEU	CA-C-N	-6.35	113.00	120.11
1	B	252	LEU	C-N-CA	-6.35	113.00	120.11
1	B	519	ALA	N-CA-C	-6.35	101.06	110.46
1	A	588	ASN	N-CA-C	6.18	118.01	111.28
1	A	296	ILE	N-CA-C	6.15	118.92	112.83
1	A	149	LEU	CA-C-N	-6.14	113.19	120.13
1	A	149	LEU	C-N-CA	-6.14	113.19	120.13
1	B	621	THR	CB-CA-C	6.12	116.46	110.71
1	A	621	THR	CB-CA-C	6.07	116.41	110.71
1	A	519	ALA	N-CA-C	-5.89	101.74	110.46
1	A	250	PRO	CA-C-O	-5.80	116.72	120.90
1	B	273	ASP	CA-C-N	5.76	125.43	119.56
1	B	273	ASP	C-N-CA	5.76	125.43	119.56
1	B	9	VAL	N-CA-CB	-5.70	103.23	111.21
1	A	167	LEU	CA-C-N	-5.52	114.70	120.38
1	A	167	LEU	C-N-CA	-5.52	114.70	120.38
1	B	642	ARG	CB-CA-C	-5.51	98.98	109.95
1	B	155	GLN	N-CA-C	-5.51	105.27	111.28
1	A	239	ASN	N-CA-C	5.50	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASP	N-CA-C	5.49	117.26	111.28
1	A	495	ALA	N-CA-C	5.43	117.20	111.28
1	B	740	MSE	CA-CB-CG	-5.38	103.35	114.10
1	B	660	PHE	N-CA-C	5.30	119.39	113.02
1	B	626	LEU	CA-C-N	5.30	125.23	119.78
1	B	626	LEU	C-N-CA	5.30	125.23	119.78
1	B	31	ILE	CB-CA-C	-5.29	102.78	110.81
1	A	626	LEU	CA-C-N	5.19	125.13	119.78
1	A	626	LEU	C-N-CA	5.19	125.13	119.78
1	A	250	PRO	CA-C-N	-5.13	114.68	127.00
1	A	250	PRO	C-N-CA	-5.13	114.68	127.00
1	A	53	HIS	N-CA-C	-5.12	105.39	110.97
1	B	239	ASN	N-CA-C	5.01	117.39	111.33
1	B	250	PRO	CA-C-N	-5.00	115.00	127.00
1	B	250	PRO	C-N-CA	-5.00	115.00	127.00

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	83	0
1	B	6585	0	6520	78	0
2	A	73	0	0	5	0
2	B	88	0	0	3	0
All	All	13343	0	13055	160	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 (160) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:PHE:C	1:B:56:PHE:HD1	1.95	0.75
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:B:56:PHE:C	1:B:56:PHE:CD1	2.65	0.71
1:A:72:LEU:HA	1:A:685:GLN:HE22	1.54	0.71
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:776:SER:HG	1:A:805:TRP:CD1	2.24	0.56
1:A:56:PHE:CD1	1:A:56:PHE:C	2.78	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: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:A:445:TYR:C	1:A:445:TYR:CD1	2.86	0.54
1:B:72:LEU:HA	1:B:685:GLN:HE22	1.71	0.54
1:A:445:TYR:C	1:A:445:TYR:HD1	2.16	0.53
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:B:445:TYR:C	1:B:445:TYR:CD1	2.87	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
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:359:LEU:C	1:A:359:LEU:HD12	2.36	0.50
1:A:429:ASN:C	1:A:434:TYR:HE1	2.20	0.50
1:A:244:GLN:OE1	1:A:251:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:445:TYR:C	1:B:445:TYR:HD1	2.20	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: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:B:359:LEU:HD12	1:B:359:LEU:C	2.40	0.47
1:A:359:LEU:HD12	1:A:360:SER:N	2.29	0.47
1:A:429:ASN:C	1:A:434:TYR:CE1	2.92	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:148:LEU:HD23	1:A:148:LEU:C	2.41	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:621:THR:CG2	1:A:624:TRP:HB3	2.46	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:TYR:O	1:B:435:LEU:C	2.61	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: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:A:376:SER:O	1:A:377:HIS:C	2.60	0.43
1:B:111:GLU:HG2	1:B:677:LEU:HD22	2.00	0.43
1:A:434:TYR:O	1:A:435:LEU:C	2.61	0.43
1:B:555:ASP:CG	1:B:620:LYS:HB2	2.44	0.43
1:A:111:GLU:HB2	1:A:671:LEU:HD22	2.00	0.42
1:A:260:SER:O	1:A:261:VAL:C	2.62	0.42
1:B:111:GLU:HB2	1:B:671:LEU:HD22	2.00	0.42
1:B:449:ARG:HA	1:B:463:GLN:HE22	1.83	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:B:429:ASN:C	1:B:434:TYR:HE1	2.28	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: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
1:B:70:THR:HG23	1:B:71:PRO:HD2	2.01	0.40

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	
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

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%)	672 (92%)	57 (8%)	11	25
1	B	728/725 (100%)	671 (92%)	57 (8%)	11	25
All	All	1457/1450 (100%)	1343 (92%)	114 (8%)	11	25

All (114) 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	92	LYS

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Mol	Chain	Res	Type
1	A	95	ILE
1	A	111	GLU
1	A	120	SER
1	A	153	LEU
1	A	155	GLN
1	A	156	ASP
1	A	209	GLN
1	A	236	LEU
1	A	254	SER
1	A	275	THR
1	A	285	LYS
1	A	286	LYS
1	A	295	GLU
1	A	359	LEU
1	A	391	GLN
1	A	402	VAL
1	A	407	LYS
1	A	409	ASP
1	A	421	ILE
1	A	432	THR
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	521	ILE
1	A	541	THR
1	A	554	LYS
1	A	576	THR
1	A	621	THR
1	A	643	SER
1	A	661	ILE
1	A	684	ARG
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

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Mol	Chain	Res	Type
1	A	745	SER
1	A	747	LYS
1	A	751	ILE
1	A	753	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	B	9	VAL
1	B	14	GLU
1	B	19	LEU
1	B	56	PHE
1	B	92	LYS
1	B	95	ILE
1	B	111	GLU
1	B	120	SER
1	B	153	LEU
1	B	156	ASP
1	B	209	GLN
1	B	236	LEU
1	B	251	PRO
1	B	254	SER
1	B	275	THR
1	B	285	LYS
1	B	286	LYS
1	B	295	GLU
1	B	359	LEU
1	B	380	THR
1	B	391	GLN
1	B	402	VAL
1	B	407	LYS
1	B	409	ASP
1	B	432	THR
1	B	445	TYR
1	B	456	LYS
1	B	460	SER
1	B	486	SER
1	B	512	LEU
1	B	518	THR

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Mol	Chain	Res	Type
1	B	521	ILE
1	B	541	THR
1	B	554	LYS
1	B	576	THR
1	B	621	THR
1	B	643	SER
1	B	661	ILE
1	B	684	ARG
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	745	SER
1	B	747	LYS
1	B	751	ILE
1	B	753	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	116	ASN
1	A	155	GLN
1	A	200	GLN
1	A	201	HIS
1	A	308	GLN
1	A	354	HIS
1	A	391	GLN
1	A	392	GLN
1	A	410	GLN
1	A	463	GLN
1	A	465	ASN

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Mol	Chain	Res	Type
1	A	685	GLN
1	B	11	HIS
1	B	116	ASN
1	B	134	GLN
1	B	200	GLN
1	B	201	HIS
1	B	244	GLN
1	B	308	GLN
1	B	342	HIS
1	B	354	HIS
1	B	391	GLN
1	B	392	GLN
1	B	410	GLN
1	B	415	GLN
1	B	463	GLN
1	B	465	ASN
1	B	478	GLN
1	B	727	ASN
1	B	735	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 oligosaccharides 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, 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%)	0.36	66 (8%) 17 14	33, 53, 105, 173	0
1	B	805/825 (97%)	0.32	65 (8%) 18 15	29, 51, 110, 161	0
All	All	1611/1650 (97%)	0.34	131 (8%) 18 15	29, 52, 109, 173	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	PHE	7.4
1	B	236	LEU	5.5
1	A	818	LYS	5.3
1	A	824	HIS	5.2
1	B	234	ILE	5.0
1	B	518	THR	4.9
1	A	518	THR	4.8
1	B	741	LEU	4.7
1	B	229	ALA	4.6
1	A	236	LEU	4.6
1	A	662	GLY	4.4
1	A	234	ILE	4.4
1	A	790	LYS	4.4
1	A	251	PRO	4.3
1	A	521	ILE	4.1
1	B	820	PHE	4.1
1	B	251	PRO	4.0
1	B	2	GLY	4.0
1	B	816	HIS	4.0
1	B	480	TYR	3.9
1	B	817	VAL	3.9
1	B	727	ASN	3.9
1	B	13	ILE	3.8
1	A	480	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	817	VAL	3.6
1	B	818	LYS	3.6
1	A	821	GLU	3.6
1	A	741	LEU	3.6
1	A	282	THR	3.5
1	B	717	TRP	3.5
1	A	233	LYS	3.4
1	A	250	PRO	3.4
1	A	92	LYS	3.4
1	B	724	SER	3.4
1	B	226	LEU	3.3
1	B	252	LEU	3.3
1	A	789	GLU	3.3
1	B	822	SER	3.3
1	A	254	SER	3.3
1	A	252	LEU	3.3
1	B	520	THR	3.3
1	A	13	ILE	3.3
1	A	434	TYR	3.2
1	A	2	GLY	3.1
1	B	521	ILE	3.1
1	A	235	ALA	3.1
1	B	92	LYS	3.0
1	B	153	LEU	3.0
1	B	791	ALA	3.0
1	A	743	PRO	3.0
1	A	255	TRP	2.9
1	B	747	LYS	2.9
1	A	226	LEU	2.9
1	B	660	PHE	2.8
1	A	747	LYS	2.8
1	B	661	ILE	2.8
1	B	456	LYS	2.8
1	B	430	TRP	2.8
1	A	520	THR	2.8
1	A	661	ILE	2.7
1	A	515	ALA	2.7
1	B	519	ALA	2.7
1	A	671	LEU	2.7
1	B	713	GLN	2.6
1	A	154	GLY	2.6
1	A	436	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	155	GLN	2.6
1	B	154	GLY	2.6
1	B	814	ARG	2.6
1	A	56	PHE	2.6
1	B	672	LEU	2.6
1	A	246	VAL	2.6
1	B	235	ALA	2.6
1	B	670	TYR	2.6
1	A	674	GLU	2.5
1	A	240	SER	2.5
1	A	791	ALA	2.5
1	A	432	THR	2.5
1	B	715	SER	2.5
1	B	716	ARG	2.5
1	B	250	PRO	2.5
1	B	233	LYS	2.5
1	A	822	SER	2.5
1	B	232	LYS	2.5
1	A	711	GLN	2.5
1	B	811	GLU	2.4
1	B	434	TYR	2.4
1	B	472	LYS	2.4
1	B	787	CYS	2.4
1	A	583	LEU	2.4
1	A	807	LYS	2.4
1	A	238	LEU	2.4
1	B	744	SER	2.3
1	B	517	GLY	2.3
1	A	229	ALA	2.3
1	A	714	SER	2.3
1	B	788	SER	2.3
1	B	807	LYS	2.3
1	A	819	GLU	2.3
1	A	237	SER	2.2
1	B	671	LEU	2.2
1	B	815	ALA	2.2
1	B	282	THR	2.2
1	A	231	ILE	2.2
1	B	231	ILE	2.2
1	A	445	TYR	2.2
1	A	586	LYS	2.2
1	B	90	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	471	ALA	2.2
1	B	585	ASP	2.2
1	B	68	LYS	2.2
1	A	816	HIS	2.1
1	B	824	HIS	2.1
1	A	469	ASN	2.1
1	A	259	LEU	2.1
1	B	743	PRO	2.1
1	B	813	LYS	2.1
1	A	718	THR	2.1
1	A	792	THR	2.1
1	A	228	TRP	2.1
1	A	793	THR	2.1
1	A	456	LYS	2.1
1	A	478	GLN	2.1
1	B	238	LEU	2.1
1	B	674	GLU	2.1
1	A	746	GLY	2.0
1	B	156	ASP	2.0
1	B	237	SER	2.0
1	A	153	LEU	2.0
1	A	712	GLU	2.0
1	A	823	SER	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 oligosaccharides 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.