



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 5OX7 / pdb_00005ox7
Title : Structure of P110 from Mycoplasma genitalium at 2.4Å with potassium ion
Authors : Aparicio, D.; Fita, I.
Deposited on : 2017-09-06
Resolution : 2.40 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
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

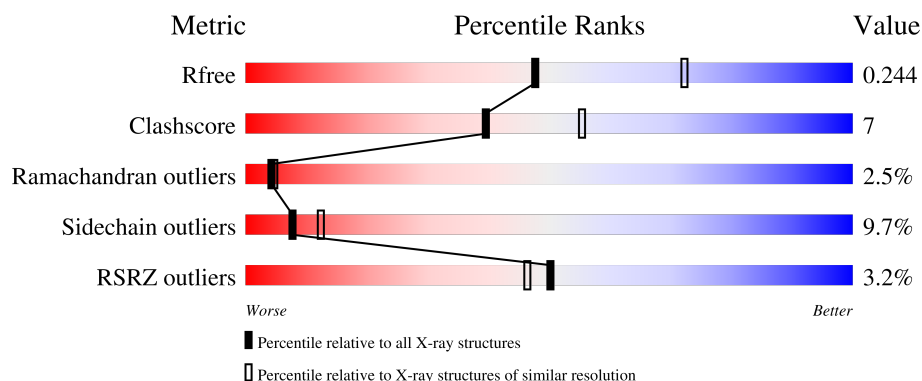
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

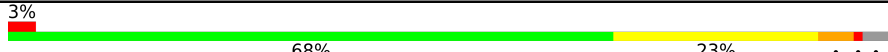
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	916	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6940 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	887	Total	C	N	O	S	0	1	0
			6826	4277	1140	1403	6			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

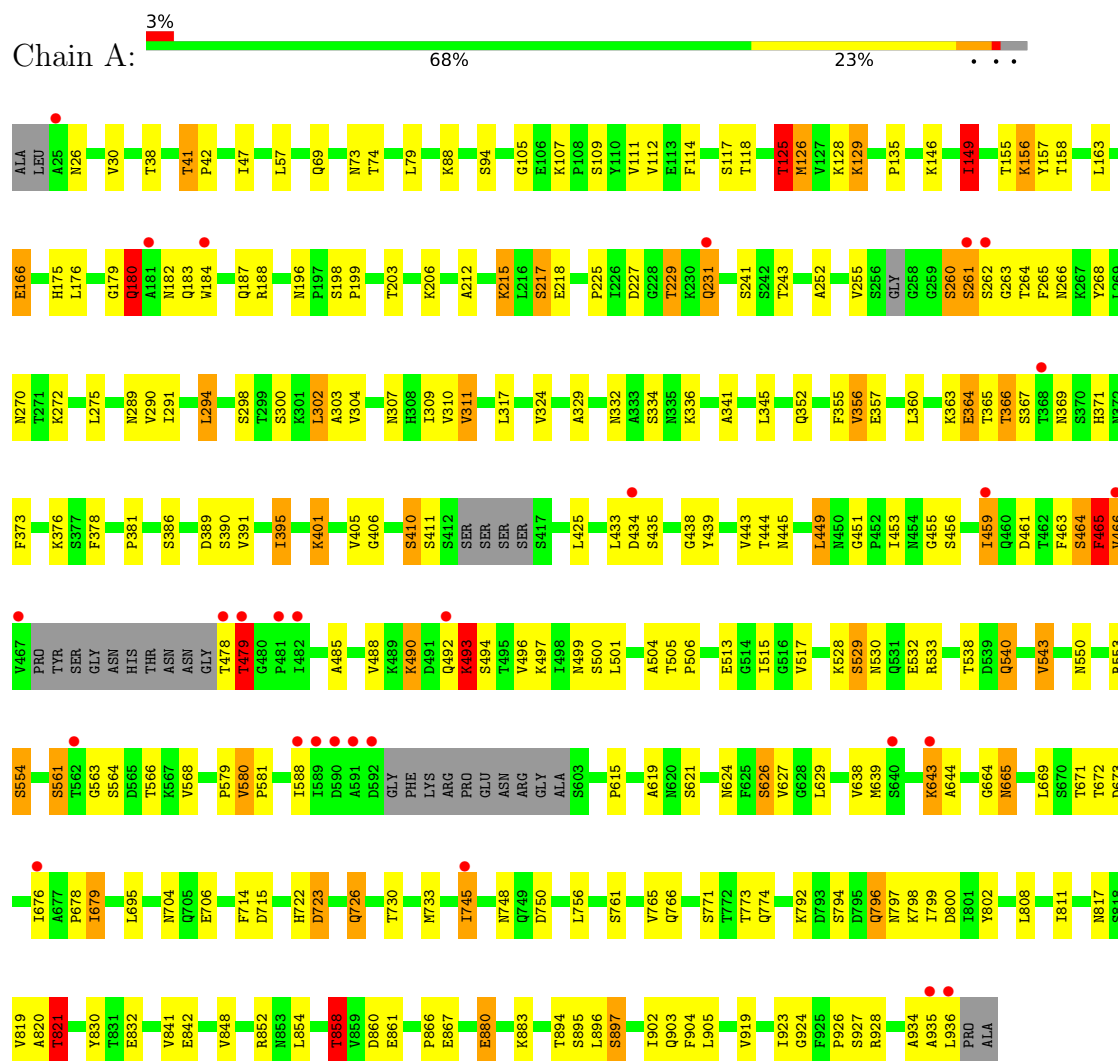
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		

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: Mgp-operon protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	109.60Å 151.29Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.54 – 2.40 62.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (62.54-2.40) 94.1 (62.54-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.240 0.196 , 0.244	Depositor DCC
R_{free} test set	2770 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
K

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	1.59	73/6963 (1.0%)	1.44	53/9469 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	927	SER	C-O	-11.78	1.09	1.23
1	A	363	LYS	N-CA	10.55	1.58	1.45
1	A	464	SER	CA-C	9.97	1.66	1.52
1	A	935	ALA	CA-C	9.89	1.62	1.53
1	A	924	GLY	N-CA	9.45	1.59	1.45
1	A	466	VAL	CA-CB	9.13	1.66	1.54
1	A	897	SER	CA-C	-8.12	1.42	1.52
1	A	615	PRO	CA-C	-8.04	1.44	1.52
1	A	897	SER	C-O	-7.82	1.14	1.23
1	A	363	LYS	CA-C	7.45	1.61	1.52
1	A	923	ILE	C-O	7.42	1.33	1.24
1	A	74	THR	CA-C	-7.38	1.43	1.52
1	A	300	SER	N-CA	7.30	1.55	1.46
1	A	129	LYS	C-O	-7.14	1.15	1.23
1	A	811	ILE	C-O	-6.90	1.15	1.24
1	A	830	TYR	C-O	-6.67	1.16	1.24
1	A	766	GLN	C-O	-6.67	1.16	1.24
1	A	336	LYS	C-O	6.57	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	PRO	N-CA	-6.46	1.39	1.46
1	A	842	GLU	C-O	-6.43	1.16	1.24
1	A	464	SER	N-CA	6.41	1.54	1.46
1	A	465	PHE	N-CA	6.41	1.54	1.46
1	A	317	LEU	C-O	6.37	1.31	1.24
1	A	175	HIS	CA-C	6.35	1.61	1.52
1	A	643	LYS	CA-C	6.31	1.60	1.52
1	A	166	GLU	N-CA	6.31	1.53	1.46
1	A	109	SER	CA-C	6.23	1.60	1.52
1	A	94	SER	CA-C	6.19	1.58	1.52
1	A	157	TYR	C-O	-6.14	1.15	1.24
1	A	466	VAL	CA-C	6.10	1.60	1.52
1	A	639	MET	N-CA	6.01	1.53	1.46
1	A	819	VAL	CA-CB	-5.87	1.46	1.54
1	A	665	ASN	CA-C	5.85	1.60	1.52
1	A	490	LYS	CA-C	5.77	1.60	1.52
1	A	695	LEU	C-O	-5.76	1.16	1.24
1	A	704	ASN	C-O	5.75	1.30	1.24
1	A	926	PRO	N-CA	-5.72	1.40	1.47
1	A	30	VAL	C-O	-5.67	1.18	1.24
1	A	903	GLN	CA-CB	-5.65	1.45	1.53
1	A	799	ILE	C-O	-5.64	1.18	1.24
1	A	714	PHE	CA-CB	-5.63	1.43	1.53
1	A	820	ALA	CA-C	-5.59	1.44	1.52
1	A	723	ASP	CB-CG	-5.57	1.38	1.52
1	A	626	SER	CB-OG	5.55	1.53	1.42
1	A	356	VAL	C-O	-5.54	1.18	1.24
1	A	722	HIS	CA-C	5.53	1.59	1.52
1	A	644	ALA	N-CA	5.46	1.53	1.46
1	A	180	GLN	CA-C	5.46	1.60	1.52
1	A	38	THR	C-O	-5.45	1.17	1.23
1	A	212	ALA	C-O	5.41	1.30	1.23
1	A	550	ASN	N-CA	5.41	1.53	1.46
1	A	802	TYR	N-CA	-5.38	1.39	1.46
1	A	733	MET	N-CA	-5.38	1.39	1.46
1	A	821	THR	CB-OG1	-5.32	1.35	1.43
1	A	485	ALA	C-O	5.32	1.30	1.23
1	A	304	VAL	N-CA	-5.29	1.40	1.46
1	A	135	PRO	CA-C	5.28	1.59	1.52
1	A	261	SER	N-CA	5.25	1.52	1.46
1	A	624	ASN	CA-C	-5.24	1.45	1.53
1	A	324	VAL	C-O	-5.23	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ASN	C-N	5.20	1.37	1.33
1	A	356	VAL	CA-C	-5.18	1.46	1.52
1	A	389	ASP	CA-C	5.13	1.59	1.52
1	A	465	PHE	CA-C	5.12	1.59	1.52
1	A	261	SER	CA-C	5.11	1.59	1.52
1	A	456	SER	N-CA	5.11	1.51	1.45
1	A	504	ALA	C-O	5.09	1.31	1.24
1	A	858	THR	N-CA	-5.09	1.40	1.45
1	A	730	THR	N-CA	5.05	1.52	1.45
1	A	41	THR	N-CA	-5.04	1.38	1.45
1	A	902	ILE	CA-C	-5.03	1.46	1.52
1	A	493	LYS	N-CA	5.02	1.52	1.46
1	A	706	GLU	CA-C	5.01	1.59	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	SER	N-CA-C	10.84	128.40	114.75
1	A	363	LYS	N-CA-C	9.36	124.65	110.14
1	A	880	GLU	CA-C-N	-8.86	108.28	123.25
1	A	880	GLU	C-N-CA	-8.86	108.28	123.25
1	A	455	GLY	N-CA-C	-8.58	99.40	110.38
1	A	307	ASN	N-CA-C	7.96	123.17	113.38
1	A	410	SER	N-CA-C	7.28	118.86	111.07
1	A	671	THR	N-CA-C	-7.02	99.58	109.69
1	A	149	ILE	CB-CA-C	6.85	121.05	110.50
1	A	919	VAL	CA-C-O	6.73	123.12	119.15
1	A	923	ILE	N-CA-C	-6.65	101.00	109.58
1	A	766	GLN	N-CA-C	-6.60	99.64	109.15
1	A	722	HIS	CA-C-N	6.58	132.66	120.95
1	A	722	HIS	C-N-CA	6.58	132.66	120.95
1	A	723	ASP	N-CA-CB	-6.47	101.49	110.29
1	A	109	SER	CB-CA-C	6.45	120.44	109.53
1	A	386	SER	N-CA-C	6.38	118.23	111.28
1	A	580	VAL	N-CA-C	-6.35	103.12	109.02
1	A	451	GLY	CA-C-N	6.28	126.29	119.89
1	A	451	GLY	C-N-CA	6.28	126.29	119.89
1	A	126	MET	CG-SD-CE	-6.18	87.30	100.90
1	A	231	GLN	N-CA-C	6.07	120.82	113.17
1	A	366	THR	N-CA-C	-6.05	103.84	111.11
1	A	217	SER	CA-CB-OG	-6.04	99.03	111.10
1	A	894	THR	N-CA-CB	-5.94	102.68	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	PHE	N-CA-C	5.87	123.30	110.80
1	A	311	VAL	CB-CA-C	5.78	118.77	110.33
1	A	880	GLU	N-CA-C	5.64	117.88	111.11
1	A	726	GLN	N-CA-C	5.63	119.45	112.47
1	A	820	ALA	CA-C-N	-5.62	114.15	122.41
1	A	820	ALA	C-N-CA	-5.62	114.15	122.41
1	A	496	VAL	N-CA-C	5.55	116.48	110.21
1	A	266	ASN	N-CA-C	-5.51	105.68	112.90
1	A	156	LYS	CB-CA-C	-5.51	101.31	110.68
1	A	125	THR	CB-CA-C	5.44	120.42	109.38
1	A	135	PRO	N-CA-C	5.42	119.69	111.19
1	A	841	VAL	CA-C-O	-5.42	114.76	120.39
1	A	723	ASP	CB-CA-C	-5.39	97.61	110.02
1	A	543	VAL	N-CA-CB	-5.36	102.66	111.45
1	A	517	VAL	CB-CA-C	-5.35	105.03	112.04
1	A	553	ARG	N-CA-C	5.33	116.77	111.07
1	A	566	THR	N-CA-C	-5.33	102.58	110.46
1	A	334	SER	CB-CA-C	5.33	119.54	109.37
1	A	880	GLU	O-C-N	-5.29	116.58	122.09
1	A	796	GLN	N-CA-C	5.19	120.09	113.55
1	A	832	GLU	N-CA-C	5.18	116.93	111.28
1	A	334	SER	N-CA-C	-5.16	100.99	109.40
1	A	218	GLU	N-CA-C	-5.14	101.86	109.94
1	A	264	THR	N-CA-C	5.12	120.18	113.88
1	A	895	SER	N-CA-C	5.10	117.00	108.99
1	A	364	GLU	N-CA-CB	5.05	119.02	110.49
1	A	73	ASN	CA-C-N	-5.02	114.11	122.08
1	A	73	ASN	C-N-CA	-5.02	114.11	122.08

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	THR	Peptide
1	A	263	GLY	Peptide
1	A	664	GLY	Peptide
1	A	796	GLN	Peptide
1	A	934	ALA	Peptide

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	6826	0	6602	90	0
2	A	1	0	0	0	0
3	A	113	0	0	1	1
All	All	6940	0	6602	90	1

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 7.

All (90) 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:183:GLN:HB3	1:A:187:GLN:HE21	1.37	0.90
1:A:848:VAL:HG22	1:A:852:ARG:HD3	1.67	0.76
1:A:289:ASN:HD22	1:A:291:ILE:HG22	1.50	0.76
1:A:464:SER:C	1:A:465:PHE:CD1	2.65	0.75
1:A:817:ASN:O	1:A:821:THR:HG23	1.90	0.72
1:A:464:SER:O	1:A:465:PHE:CG	2.45	0.69
1:A:255:VAL:HG23	1:A:726:GLN:HB3	1.75	0.68
1:A:183:GLN:HB3	1:A:187:GLN:NE2	2.06	0.67
1:A:231:GLN:O	1:A:268:TYR:OH	2.09	0.67
1:A:540:GLN:HG2	1:A:579:PRO:HA	1.77	0.67
1:A:126:MET:HE1	1:A:129:LYS:HD2	1.77	0.67
1:A:302:LEU:HD12	1:A:303:ALA:N	2.10	0.67
1:A:289:ASN:ND2	1:A:291:ILE:HG22	2.12	0.64
1:A:149:ILE:HG22	1:A:501:LEU:HB3	1.79	0.64
1:A:227:ASP:OD1	1:A:229:THR:HB	1.99	0.63
1:A:745:ILE:HD13	1:A:756:LEU:HD22	1.79	0.63
1:A:513:GLU:HG3	1:A:515:ILE:HG22	1.81	0.62
1:A:180:GLN:HE21	1:A:182:ASN:HB2	1.64	0.62
1:A:126:MET:HE2	1:A:129:LYS:HB2	1.82	0.62
1:A:463:PHE:CB	1:A:515:ILE:HD13	2.31	0.61
1:A:128:LYS:NZ	1:A:329:ALA:O	2.30	0.61
1:A:464:SER:O	1:A:465:PHE:CD1	2.54	0.60
1:A:310:VAL:HG21	1:A:395:ILE:CD1	2.31	0.60
1:A:183:GLN:CB	1:A:187:GLN:HE21	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:C	1:A:465:PHE:CG	2.81	0.59
1:A:439:TYR:CD2	1:A:678:PRO:HD3	2.38	0.58
1:A:341:ALA:HB1	1:A:378:PHE:HB3	1.87	0.57
1:A:112:VAL:HG13	1:A:126:MET:HE3	1.87	0.56
1:A:858:THR:HG22	1:A:861:GLU:H	1.69	0.56
1:A:501:LEU:C	1:A:501:LEU:HD12	2.31	0.55
1:A:126:MET:CE	1:A:129:LYS:HB2	2.37	0.55
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.86	0.55
1:A:669:LEU:HD23	1:A:679:ILE:HG23	1.90	0.54
1:A:310:VAL:HG21	1:A:395:ILE:HD13	1.88	0.54
1:A:203:THR:O	1:A:425:LEU:HA	2.08	0.54
1:A:463:PHE:HB3	1:A:515:ILE:HD13	1.90	0.53
1:A:290:VAL:HG12	1:A:294:LEU:HD22	1.91	0.52
1:A:356:VAL:O	1:A:360:LEU:HD13	2.11	0.51
1:A:406:GLY:HA2	1:A:499:ASN:O	2.11	0.50
1:A:528:LYS:O	1:A:529:SER:O	2.30	0.50
1:A:117:SER:HB3	1:A:125:THR:CG2	2.41	0.50
1:A:745:ILE:HD13	1:A:756:LEU:CD2	2.43	0.49
1:A:817:ASN:O	1:A:821:THR:CG2	2.59	0.49
1:A:158:THR:O	1:A:619:ALA:HB3	2.13	0.49
1:A:41:THR:HB	1:A:42:PRO:CD	2.43	0.48
1:A:231:GLN:O	1:A:268:TYR:CZ	2.67	0.48
1:A:492:GLN:O	1:A:494:SER:N	2.46	0.48
1:A:26[B]:ASN:O	1:A:26[B]:ASN:ND2	2.46	0.48
1:A:445:ASN:OD1	1:A:445:ASN:C	2.57	0.48
1:A:435:SER:HB2	1:A:445:ASN:HD22	1.77	0.47
1:A:252:ALA:HA	1:A:265:PHE:CE1	2.50	0.47
1:A:357:GLU:HA	1:A:360:LEU:HD13	1.96	0.46
1:A:126:MET:HE1	1:A:129:LYS:CD	2.45	0.46
1:A:528:LYS:C	1:A:529:SER:O	2.56	0.46
1:A:513:GLU:CG	1:A:515:ILE:HG22	2.46	0.45
1:A:554:SER:HB2	1:A:568:VAL:HG13	1.98	0.45
1:A:771:SER:OG	1:A:774:GLN:HG3	2.16	0.45
1:A:501:LEU:HD12	1:A:501:LEU:O	2.17	0.44
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.00	0.44
1:A:270:ASN:OD1	1:A:270:ASN:C	2.60	0.44
1:A:463:PHE:HB2	1:A:515:ILE:HD13	2.00	0.44
1:A:715:ASP:OD1	1:A:715:ASP:C	2.60	0.44
1:A:26[B]:ASN:C	1:A:26[B]:ASN:HD22	2.25	0.43
1:A:302:LEU:HD12	1:A:302:LEU:C	2.42	0.43
1:A:896:LEU:HD12	1:A:896:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PHE:CE1	1:A:449:LEU:HA	2.53	0.43
1:A:904:PHE:CG	1:A:905:LEU:N	2.86	0.43
1:A:444:THR:O	1:A:445:ASN:C	2.62	0.43
1:A:580:VAL:HG13	1:A:581:PRO:HD2	2.01	0.43
1:A:352:GLN:CD	1:A:443:VAL:HG11	2.44	0.43
1:A:401:LYS:NZ	1:A:538:THR:O	2.34	0.43
1:A:638:VAL:CG2	1:A:748:ASN:HB3	2.49	0.42
1:A:438:GLY:O	1:A:439:TYR:C	2.62	0.42
1:A:184:TRP:CD2	1:A:199:PRO:HB3	2.55	0.42
1:A:798:LYS:NZ	1:A:800:ASP:OD1	2.50	0.42
1:A:57:LEU:HD23	1:A:114:PHE:CE1	2.55	0.42
1:A:371:HIS:ND1	1:A:376:LYS:HE3	2.35	0.42
1:A:126:MET:HE1	1:A:129:LYS:CG	2.50	0.41
1:A:310:VAL:CG2	1:A:395:ILE:CD1	2.97	0.41
1:A:459:ILE:HG23	1:A:459:ILE:O	2.20	0.41
1:A:369:ASN:HD22	1:A:497:LYS:NZ	2.19	0.41
1:A:373:PHE:CD2	1:A:381:PRO:HG3	2.56	0.41
1:A:621:SER:HB2	3:A:1114:HOH:O	2.21	0.41
1:A:149:ILE:HD11	1:A:215:LYS:HG2	2.02	0.40
1:A:294:LEU:O	1:A:298:SER:HB3	2.21	0.40
1:A:561:SER:OG	1:A:564:SER:O	2.34	0.40
1:A:505:THR:HB	1:A:506:PRO:CD	2.51	0.40
1:A:897:SER:HA	1:A:928:ARG:O	2.22	0.40
1:A:166:GLU:HG3	1:A:206:LYS:HB2	2.03	0.40
1:A:478:THR:O	1:A:479:THR:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:HOH:O	3:A:1208:HOH:O[4_576]	0.58	1.62

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	878/916 (96%)	793 (90%)	63 (7%)	22 (2%)	4 5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	260	SER
1	A	261	SER
1	A	367	SER
1	A	493	LYS
1	A	529	SER
1	A	797	ASN
1	A	179	GLY
1	A	262	SER
1	A	411	SER
1	A	453	ILE
1	A	461	ASP
1	A	465	PHE
1	A	530	ASN
1	A	532	GLU
1	A	673	ASP
1	A	364	GLU
1	A	866	PRO
1	A	459	ILE
1	A	479	THR
1	A	563	GLY
1	A	105	GLY

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	775/795 (98%)	700 (90%)	75 (10%)	8 12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	69	GLN
1	A	79	LEU
1	A	88	LYS
1	A	107	LYS
1	A	118	THR
1	A	125	THR
1	A	146	LYS
1	A	149	ILE
1	A	155	THR
1	A	156	LYS
1	A	163	LEU
1	A	176	LEU
1	A	180	GLN
1	A	188	ARG
1	A	198	SER
1	A	215	LYS
1	A	217	SER
1	A	229	THR
1	A	241	SER
1	A	260	SER
1	A	272	LYS
1	A	275	LEU
1	A	294	LEU
1	A	302	LEU
1	A	311	VAL
1	A	332	ASN
1	A	345	LEU
1	A	365	THR
1	A	366	THR
1	A	390	SER
1	A	391	VAL
1	A	395	ILE
1	A	401	LYS
1	A	410	SER
1	A	433	LEU
1	A	434	ASP
1	A	449	LEU
1	A	466	VAL
1	A	479	THR
1	A	488	VAL
1	A	490	LYS

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Mol	Chain	Res	Type
1	A	493	LYS
1	A	500	SER
1	A	533	ARG
1	A	540	GLN
1	A	543	VAL
1	A	554	SER
1	A	561	SER
1	A	588	ILE
1	A	626	SER
1	A	627	VAL
1	A	629	LEU
1	A	643	LYS
1	A	665	ASN
1	A	672	THR
1	A	676	ILE
1	A	679	ILE
1	A	723	ASP
1	A	745	ILE
1	A	750	ASP
1	A	761	SER
1	A	765	VAL
1	A	773	THR
1	A	792	LYS
1	A	794	SER
1	A	808	LEU
1	A	821	THR
1	A	854	LEU
1	A	858	THR
1	A	860	ASP
1	A	867	GLU
1	A	880	GLU
1	A	883	LYS
1	A	936	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	96	ASN
1	A	104	GLN
1	A	175	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	189	ASN
1	A	194	ASN
1	A	195	ASN
1	A	266	ASN
1	A	332	ASN
1	A	344	ASN
1	A	369	ASN
1	A	380	GLN
1	A	450	ASN
1	A	454	ASN
1	A	492	GLN
1	A	531	GLN
1	A	569	ASN
1	A	662	ASN
1	A	665	ASN
1	A	806	ASN
1	A	833	ASN

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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	887/916 (96%)	0.02	28 (3%)	50 46	34, 71, 135, 185	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	936	LEU	5.7
1	A	588	ILE	5.2
1	A	467	VAL	4.6
1	A	459	ILE	4.3
1	A	466	VAL	4.1
1	A	434	ASP	4.0
1	A	643	LYS	3.7
1	A	591	ALA	3.6
1	A	479	THR	3.4
1	A	181	ALA	3.4
1	A	745	ILE	3.2
1	A	935	ALA	3.0
1	A	478	THR	2.9
1	A	589	ILE	2.6
1	A	492	GLN	2.6
1	A	590	ASP	2.5
1	A	592	ASP	2.5
1	A	262	SER	2.5
1	A	25	ALA	2.4
1	A	184	TRP	2.3
1	A	481	PRO	2.2
1	A	231	GLN	2.2
1	A	676	ILE	2.2
1	A	562	THR	2.2
1	A	482	ILE	2.1
1	A	368	THR	2.1
1	A	640	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	261	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](#)

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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	K	A	1001	1/1	0.99	0.03	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.