



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 AM UTC

PDB ID : 9LMN / pdb_00009lmn
Title : Crystal structure of a polyketide ABM/SchA-like domain-containing protein
WhiE-ORFI from *Streptomyces coelicolor*
Authors : Jiang, K.; Qu, X.D.
Deposited on : 2025-01-19
Resolution : 2.30 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

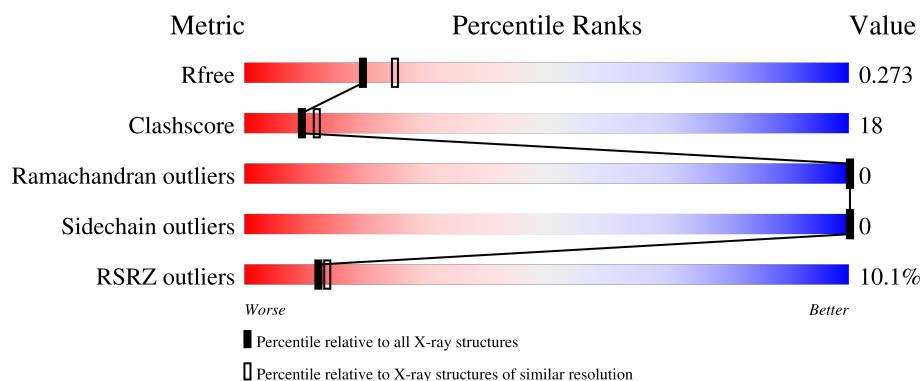
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	397	5% 67% 20% • 9%
1	B	397	13% 63% 26% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5640 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 42.8 kDa protein in whiE locus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2735	1686	513	529	7			
1	B	362	Total	C	N	O	S	0	0	0
			2729	1685	511	526	7			

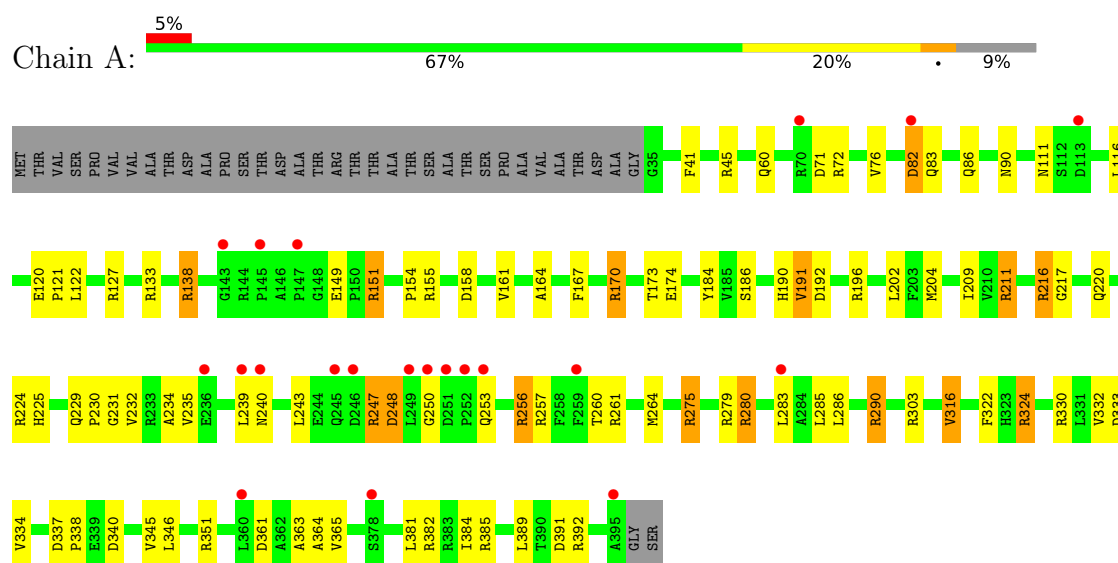
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	66	Total	O	0	0
			66	66		

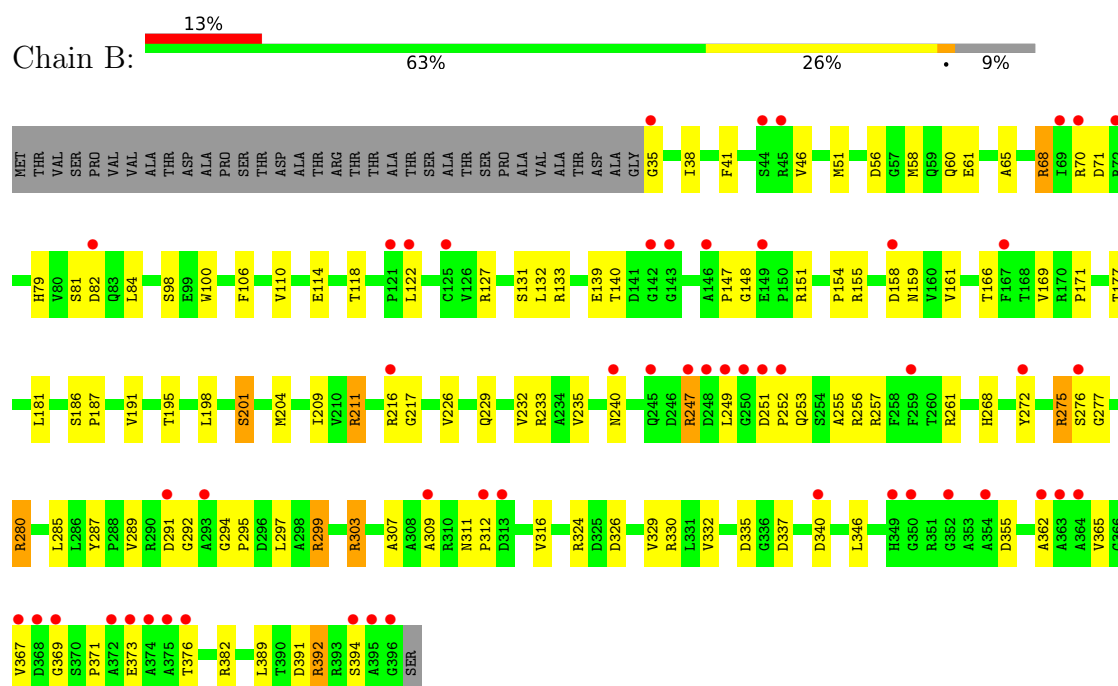
3 Residue-property plots [i](#)

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: 42.8 kDa protein in whiE locus



- Molecule 1: 42.8 kDa protein in whiE locus



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.82Å 75.85Å 142.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.63 – 2.30 36.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.63-2.30) 99.5 (36.63-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.238 , 0.273 0.239 , 0.273	Depositor DCC
R_{free} test set	1830 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5640	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.94	0/2788	1.42	16/3804 (0.4%)
1	B	0.80	2/2782 (0.1%)	1.18	14/3797 (0.4%)
All	All	0.87	2/5570 (0.0%)	1.30	30/7601 (0.4%)

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	21
1	B	0	14
All	All	0	35

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	PRO	N-CD	-15.31	1.26	1.47
1	B	201	SER	CA-CB	-5.28	1.45	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	VAL	N-CA-C	-8.81	103.30	111.67
1	A	167	PHE	CA-CB-CG	8.19	121.99	113.80
1	A	122	LEU	N-CA-C	-8.14	103.37	113.38
1	B	311	ASN	O-C-N	8.13	128.58	121.34
1	B	312	PRO	CA-C-N	-7.91	109.98	122.08
1	B	312	PRO	C-N-CA	-7.91	109.98	122.08
1	A	82	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	191	VAL	N-CA-C	-7.02	105.52	111.56
1	B	326	ASP	N-CA-C	-6.36	104.68	112.88
1	A	151	ARG	N-CA-C	-6.29	104.23	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	VAL	N-CA-CB	6.25	118.00	110.31
1	B	211	ARG	CA-CB-CG	6.19	126.49	114.10
1	A	340	ASP	N-CA-C	-6.17	105.75	113.28
1	B	365	VAL	N-CA-C	-6.06	107.59	113.53
1	B	276	SER	N-CA-C	-6.05	102.12	110.35
1	B	326	ASP	CB-CA-C	5.84	120.59	110.72
1	B	211	ARG	CG-CD-NE	5.82	124.80	112.00
1	B	41	PHE	N-CA-CB	-5.68	101.60	110.98
1	A	322	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	151	ARG	N-CA-C	-5.54	106.11	112.92
1	A	41	PHE	N-CA-CB	-5.31	102.22	110.98
1	A	351	ARG	N-CA-CB	-5.30	102.14	110.46
1	A	192	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	365	VAL	N-CA-C	-5.26	107.17	112.17
1	A	76	VAL	N-CA-CB	5.24	115.98	110.17
1	A	192	ASP	N-CA-C	5.20	114.70	107.73
1	B	253	GLN	CB-CA-C	-5.15	102.10	110.85
1	A	333	ASP	CB-CA-C	5.14	118.23	109.75
1	B	166	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	248	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	133	ARG	Sidechain
1	A	138	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	196	ARG	Sidechain
1	A	211	ARG	Sidechain
1	A	216	ARG	Sidechain
1	A	247	ARG	Sidechain
1	A	256	ARG	Sidechain
1	A	257	ARG	Sidechain
1	A	261	ARG	Sidechain
1	A	275	ARG	Sidechain
1	A	279	ARG	Sidechain
1	A	280	ARG	Sidechain
1	A	290	ARG	Sidechain
1	A	303	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	324	ARG	Sidechain
1	A	330	ARG	Sidechain
1	A	382	ARG	Sidechain
1	A	385	ARG	Sidechain
1	B	211	ARG	Sidechain
1	B	233	ARG	Sidechain
1	B	247	ARG	Sidechain
1	B	256	ARG	Sidechain
1	B	275	ARG	Sidechain
1	B	280	ARG	Sidechain
1	B	299	ARG	Sidechain
1	B	303	ARG	Sidechain
1	B	324	ARG	Sidechain
1	B	330	ARG	Sidechain
1	B	382	ARG	Sidechain
1	B	392	ARG	Sidechain
1	B	68	ARG	Sidechain
1	B	70	ARG	Sidechain

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	2735	0	2650	102	0
1	B	2729	0	2645	99	0
2	A	110	0	0	34	0
2	B	66	0	0	33	0
All	All	5640	0	5295	192	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 18.

All (192) 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:264:MET:SD	2:A:457:HOH:O	1.91	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:OE1	1:A:253:GLN:NE2	1.68	1.25
1:A:82:ASP:OD1	1:B:140:THR:HB	1.37	1.25
1:B:147:PRO:HG2	2:B:405:HOH:O	1.40	1.17
1:A:45:ARG:NE	2:A:401:HOH:O	1.81	1.13
1:A:170:ARG:O	1:A:173:THR:HG22	1.49	1.13
1:A:364:ALA:N	2:A:402:HOH:O	1.81	1.11
1:A:280:ARG:CD	2:A:404:HOH:O	2.00	1.10
1:A:216:ARG:NE	2:A:405:HOH:O	1.88	1.06
1:A:239:LEU:HD21	1:A:243:LEU:HD21	1.34	1.05
1:A:283:LEU:CD1	1:A:285:LEU:HG	1.88	1.03
1:B:35:GLY:HA3	2:B:408:HOH:O	1.56	1.02
1:B:35:GLY:CA	2:B:408:HOH:O	2.08	1.02
1:A:45:ARG:NH2	2:A:401:HOH:O	1.91	1.01
1:A:280:ARG:CG	2:A:404:HOH:O	2.10	0.99
1:B:275:ARG:HG2	2:B:406:HOH:O	1.63	0.98
1:B:275:ARG:CD	2:B:406:HOH:O	2.11	0.98
1:A:234:ALA:CB	2:A:403:HOH:O	2.10	0.97
1:A:82:ASP:OD1	1:B:140:THR:CB	2.12	0.97
1:A:216:ARG:CD	2:A:405:HOH:O	2.13	0.96
1:A:230:PRO:O	2:A:403:HOH:O	1.82	0.96
1:A:280:ARG:HD2	2:A:404:HOH:O	1.63	0.95
1:A:234:ALA:HB3	2:A:403:HOH:O	1.67	0.94
1:A:216:ARG:HD2	2:A:405:HOH:O	1.69	0.92
1:B:275:ARG:NH2	2:B:406:HOH:O	2.01	0.92
1:B:217:GLY:O	2:B:402:HOH:O	1.89	0.90
1:A:239:LEU:CD2	1:A:243:LEU:HD21	2.03	0.89
1:A:217:GLY:O	2:A:406:HOH:O	1.89	0.88
1:B:35:GLY:N	2:B:408:HOH:O	2.06	0.87
1:A:280:ARG:HG3	2:A:404:HOH:O	1.70	0.87
1:A:280:ARG:NH2	2:A:404:HOH:O	1.85	0.87
1:B:275:ARG:CG	2:B:406:HOH:O	2.18	0.86
1:B:71:ASP:OD1	2:B:404:HOH:O	1.93	0.85
1:A:45:ARG:CZ	2:A:401:HOH:O	2.12	0.83
1:A:264:MET:CG	2:A:457:HOH:O	2.14	0.82
1:A:234:ALA:N	2:A:403:HOH:O	1.83	0.81
1:A:202:LEU:CD2	1:A:211:ARG:HB2	2.10	0.81
1:A:71:ASP:OD1	2:A:407:HOH:O	1.98	0.80
1:B:252:PRO:N	2:B:410:HOH:O	2.14	0.80
1:A:264:MET:HG2	2:A:457:HOH:O	1.78	0.80
1:B:252:PRO:CA	2:B:410:HOH:O	2.31	0.79
1:B:147:PRO:CG	2:B:405:HOH:O	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD21	1:A:243:LEU:CD2	2.14	0.78
2:A:410:HOH:O	1:B:38:ILE:HD11	1.83	0.78
1:A:120:GLU:CD	1:A:253:GLN:NE2	2.43	0.76
1:B:252:PRO:HA	2:B:410:HOH:O	1.86	0.76
2:A:410:HOH:O	1:B:38:ILE:CD1	2.35	0.75
1:B:355:ASP:OD2	2:B:407:HOH:O	2.04	0.75
1:A:111:ASN:O	1:A:324:ARG:NH2	2.18	0.75
1:A:361:ASP:OD1	2:A:402:HOH:O	2.05	0.75
1:A:283:LEU:CD1	1:A:285:LEU:CG	2.66	0.74
1:A:120:GLU:CD	1:A:253:GLN:HE21	1.95	0.74
1:A:202:LEU:HD21	1:A:211:ARG:HG3	1.68	0.73
1:A:138:ARG:NH1	1:A:151:ARG:HA	2.03	0.73
1:A:239:LEU:HD23	1:A:243:LEU:HG	1.71	0.73
1:B:299:ARG:NH2	2:B:403:HOH:O	1.93	0.72
1:A:283:LEU:HD13	1:A:285:LEU:HG	1.70	0.71
1:B:56:ASP:OD1	2:B:409:HOH:O	2.09	0.71
1:B:275:ARG:HD2	2:B:406:HOH:O	1.84	0.70
1:A:83:GLN:HG2	1:B:139:GLU:HG2	1.74	0.70
1:B:133:ARG:NE	2:B:401:HOH:O	1.81	0.70
1:B:303:ARG:CZ	1:B:307:ALA:HB2	2.21	0.70
1:A:260:THR:O	1:A:324:ARG:NH1	2.26	0.69
1:B:275:ARG:CZ	2:B:406:HOH:O	2.36	0.68
1:B:362:ALA:HB1	1:B:367:VAL:HB	1.76	0.67
1:A:391:ASP:OD2	2:A:408:HOH:O	2.13	0.66
1:B:198:LEU:HA	1:B:394:SER:OG	1.97	0.65
1:A:60:GLN:HA	1:B:154:PRO:HG3	1.78	0.65
1:B:147:PRO:CD	2:B:405:HOH:O	2.40	0.65
1:A:239:LEU:CD2	1:A:243:LEU:CD2	2.74	0.64
1:A:283:LEU:HD11	1:A:285:LEU:HG	1.79	0.64
1:B:299:ARG:NH1	2:B:403:HOH:O	2.31	0.62
1:B:371:PRO:C	1:B:373:GLU:N	2.56	0.61
1:A:363:ALA:C	2:A:402:HOH:O	2.33	0.60
1:B:133:ARG:HG3	2:B:401:HOH:O	2.02	0.59
1:B:251:ASP:C	2:B:410:HOH:O	2.42	0.59
1:A:86:GLN:HE22	1:B:155:ARG:H	1.49	0.59
1:A:239:LEU:HD23	1:A:243:LEU:CG	2.32	0.59
1:A:316:VAL:HG13	1:A:332:VAL:HG13	1.85	0.59
1:A:204:MET:HB2	1:A:389:LEU:HD11	1.84	0.58
1:A:332:VAL:HG12	1:A:334:VAL:HG23	1.84	0.58
1:A:283:LEU:C	1:A:283:LEU:HD12	2.29	0.58
1:B:201:SER:OG	1:B:391:ASP:OD1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:CD2	1:A:211:ARG:CB	2.80	0.58
1:A:283:LEU:HD13	1:A:285:LEU:CD2	2.34	0.57
1:B:287:TYR:O	2:B:411:HOH:O	2.17	0.57
1:A:283:LEU:HD21	1:A:345:VAL:CG1	2.35	0.57
1:B:81:SER:O	1:B:82:ASP:OD1	2.22	0.57
1:A:283:LEU:HD13	1:A:285:LEU:CG	2.33	0.57
1:A:158:ASP:OD1	1:B:56:ASP:HB3	2.05	0.57
1:B:177:THR:HG21	1:B:209:ILE:HD11	1.86	0.57
1:B:79:HIS:NE2	1:B:82:ASP:OD2	2.37	0.56
1:B:133:ARG:CG	2:B:401:HOH:O	2.52	0.56
1:B:272:TYR:CE1	1:B:309:ALA:HA	2.40	0.56
1:A:290:ARG:NH1	2:A:415:HOH:O	2.34	0.56
1:B:204:MET:HB2	1:B:389:LEU:HD11	1.87	0.56
1:B:127:ARG:NH1	2:B:409:HOH:O	2.35	0.55
1:A:283:LEU:HD11	1:A:285:LEU:CG	2.35	0.55
1:A:283:LEU:HD21	1:A:345:VAL:HG11	1.86	0.55
1:A:290:ARG:NE	2:A:415:HOH:O	2.40	0.55
1:A:202:LEU:CD2	1:A:211:ARG:HG3	2.37	0.55
1:A:161:VAL:HG21	2:A:406:HOH:O	2.07	0.54
1:B:294:GLY:H	1:B:295:PRO:CD	2.20	0.54
1:B:371:PRO:C	1:B:373:GLU:H	2.14	0.54
1:A:184:TYR:H	1:A:392:ARG:HH22	1.53	0.54
1:A:111:ASN:HB3	1:A:324:ARG:HH22	1.73	0.54
1:A:154:PRO:HG3	1:B:60:GLN:HA	1.89	0.54
1:A:290:ARG:HG2	1:A:361:ASP:HB2	1.88	0.54
1:B:169:VAL:HG11	1:B:177:THR:HG21	1.90	0.54
1:A:174:GLU:OE2	2:A:409:HOH:O	2.19	0.53
1:A:240:ASN:HB2	1:A:247:ARG:HH22	1.72	0.53
1:B:294:GLY:H	1:B:295:PRO:HD3	1.73	0.53
1:B:187:PRO:HB2	1:B:229:GLN:HG3	1.90	0.53
1:A:191:VAL:HG22	1:A:225:HIS:HD2	1.73	0.53
1:B:277:GLY:HA3	1:B:335:ASP:OD2	2.08	0.52
1:A:202:LEU:HD23	1:A:211:ARG:CB	2.39	0.52
1:B:82:ASP:OD1	1:B:98:SER:HB3	2.08	0.52
1:A:190:HIS:HD2	2:A:491:HOH:O	1.92	0.52
1:B:289:VAL:HG22	1:B:297:LEU:HD22	1.91	0.52
1:A:164:ALA:HB3	1:A:264:MET:HB3	1.91	0.51
1:B:148:GLY:N	2:B:405:HOH:O	2.01	0.51
1:B:294:GLY:N	1:B:295:PRO:CD	2.73	0.51
1:B:106:PHE:O	1:B:110:VAL:HG12	2.11	0.50
1:B:147:PRO:N	2:B:405:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASN:HD21	1:B:247:ARG:HD2	1.75	0.50
1:B:249:LEU:HD12	1:B:255:ALA:HB2	1.93	0.50
1:B:369:GLY:HA3	1:B:376:THR:CG2	2.41	0.50
1:A:174:GLU:CD	2:A:409:HOH:O	2.54	0.50
1:B:337:ASP:HB3	1:B:340:ASP:OD2	2.12	0.50
1:B:114:GLU:O	1:B:118:THR:HG23	2.12	0.49
1:A:161:VAL:CG2	2:A:406:HOH:O	2.60	0.49
1:A:186:SER:OG	1:A:392:ARG:HD2	2.12	0.49
1:B:114:GLU:HA	1:B:114:GLU:OE1	2.12	0.49
1:A:111:ASN:HB3	1:A:324:ARG:NH2	2.27	0.49
1:B:161:VAL:CG2	2:B:402:HOH:O	2.60	0.49
1:B:187:PRO:HG3	1:B:226:VAL:HG13	1.96	0.47
1:A:231:GLY:C	2:A:403:HOH:O	2.57	0.47
1:B:371:PRO:O	1:B:373:GLU:N	2.48	0.47
1:B:82:ASP:CG	2:B:412:HOH:O	2.57	0.46
1:A:283:LEU:HD11	1:A:285:LEU:HD11	1.98	0.46
1:A:286:LEU:O	1:A:384:ILE:HB	2.16	0.46
1:A:283:LEU:HD11	1:A:285:LEU:CD1	2.45	0.46
1:A:332:VAL:HG12	1:A:334:VAL:CG2	2.45	0.46
1:B:68:ARG:HE	1:B:68:ARG:HB2	1.65	0.46
1:A:120:GLU:N	1:A:121:PRO:HD2	2.32	0.45
1:B:122:LEU:HD12	1:B:122:LEU:N	2.32	0.45
1:A:116:LEU:CD2	1:A:256:ARG:NH2	2.80	0.45
1:B:158:ASP:OD1	1:B:158:ASP:N	2.49	0.45
1:B:195:THR:HA	1:B:216:ARG:O	2.16	0.45
1:A:72:ARG:HE	1:A:72:ARG:HB3	1.59	0.45
1:B:257:ARG:O	1:B:261:ARG:HG3	2.17	0.44
1:B:61:GLU:H	1:B:61:GLU:CD	2.26	0.44
1:A:346:LEU:HD21	1:A:381:LEU:HA	1.99	0.44
1:B:79:HIS:CE1	1:B:82:ASP:CG	2.96	0.44
1:B:285:LEU:HD13	1:B:346:LEU:HD23	1.98	0.44
1:B:198:LEU:HA	1:B:394:SER:HG	1.83	0.44
1:B:369:GLY:HA3	1:B:376:THR:HG21	2.00	0.44
1:B:51:MET:HE2	1:B:51:MET:HB2	1.93	0.43
1:B:131:SER:O	1:B:132:LEU:HD23	2.18	0.43
1:B:38:ILE:O	1:B:268:HIS:HA	2.18	0.43
1:B:79:HIS:HE2	1:B:82:ASP:CG	2.24	0.43
1:A:239:LEU:CD2	1:A:243:LEU:CG	2.95	0.43
1:B:79:HIS:NE2	1:B:82:ASP:CG	2.77	0.43
1:A:138:ARG:HB2	1:B:84:LEU:HB3	2.01	0.43
1:B:316:VAL:HG13	1:B:332:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLN:HG2	1:A:224:ARG:HD2	2.01	0.42
1:A:283:LEU:HD13	1:A:285:LEU:HD21	2.00	0.42
1:A:90:ASN:OD1	1:B:159:ASN:HA	2.19	0.42
1:B:285:LEU:O	1:B:329:VAL:HA	2.19	0.42
1:A:202:LEU:HD23	1:A:211:ARG:HA	2.02	0.42
1:A:248:ASP:C	1:A:250:GLY:N	2.77	0.42
1:B:232:VAL:HA	1:B:235:VAL:HG12	2.02	0.42
1:B:65:ALA:HA	1:B:68:ARG:CZ	2.50	0.42
1:A:191:VAL:HG22	1:A:225:HIS:CD2	2.53	0.42
1:A:229:GLN:HA	1:A:230:PRO:HD3	1.94	0.42
1:A:275:ARG:O	1:A:280:ARG:NH1	2.52	0.42
1:A:204:MET:HE3	1:A:209:ILE:HD11	2.01	0.42
1:B:272:TYR:CD1	1:B:309:ALA:HA	2.54	0.42
1:B:186:SER:HB3	1:B:392:ARG:HH21	1.84	0.41
1:B:280:ARG:NH1	1:B:335:ASP:OD2	2.53	0.41
1:A:138:ARG:HA	1:A:149:GLU:HG3	2.01	0.41
1:B:161:VAL:HG21	2:B:402:HOH:O	2.20	0.41
1:A:202:LEU:CD2	1:A:211:ARG:CG	2.99	0.41
1:B:181:LEU:HA	1:B:181:LEU:HD23	1.79	0.41
1:B:46:VAL:HB	1:B:100:TRP:HB2	2.03	0.41
1:A:232:VAL:O	1:A:235:VAL:HG12	2.21	0.41
1:A:337:ASP:HA	1:A:338:PRO:HD3	1.95	0.41
1:B:291:ASP:O	1:B:292:GLY:C	2.64	0.41
1:B:58:MET:HA	1:B:61:GLU:OE2	2.21	0.40
1:B:275:ARG:NE	2:B:406:HOH:O	2.36	0.40
1:A:138:ARG:HH12	1:A:151:ARG:HA	1.78	0.40
1:B:275:ARG:HE	1:B:275:ARG:HB3	1.75	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	359/397 (90%)	347 (97%)	12 (3%)	0	100	100
1	B	360/397 (91%)	344 (96%)	16 (4%)	0	100	100
All	All	719/794 (91%)	691 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	282/316 (89%)	282 (100%)	0	100	100
1	B	280/316 (89%)	280 (100%)	0	100	100
All	All	562/632 (89%)	562 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	86	GLN
1	A	190	HIS
1	A	220	GLN
1	A	225	HIS
1	A	229	GLN
1	A	268	HIS
1	B	190	HIS
1	B	220	GLN
1	B	240	ASN
1	B	268	HIS
1	B	304	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	361/397 (90%)	0.73	21 (5%) 29 31	29, 43, 70, 110	0
1	B	362/397 (91%)	1.07	52 (14%) 6 7	33, 51, 80, 119	0
All	All	723/794 (91%)	0.90	73 (10%) 12 14	29, 46, 75, 119	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	ARG	5.3
1	A	70	ARG	5.3
1	B	372	ALA	4.9
1	B	249	LEU	4.8
1	B	142	GLY	4.3
1	B	248	ASP	4.2
1	B	259	PHE	4.1
1	B	368	ASP	3.8
1	A	259	PHE	3.7
1	B	158	ASP	3.6
1	B	395	ALA	3.6
1	B	374	ALA	3.4
1	B	276	SER	3.4
1	B	82	ASP	3.4
1	B	309	ALA	3.4
1	A	249	LEU	3.4
1	A	395	ALA	3.3
1	B	364	ALA	3.3
1	B	313	ASP	3.2
1	B	394	SER	3.2
1	A	246	ASP	3.1
1	B	250	GLY	3.1
1	B	396	GLY	3.0
1	A	145	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	293	ALA	3.0
1	B	149	GLU	3.0
1	B	354	ALA	2.9
1	A	283	LEU	2.9
1	B	122	LEU	2.9
1	B	143	GLY	2.9
1	B	367	VAL	2.9
1	B	45	ARG	2.9
1	B	352	GLY	2.9
1	B	363	ALA	2.9
1	B	291	ASP	2.9
1	A	143	GLY	2.8
1	A	252	PRO	2.7
1	B	44	SER	2.7
1	A	360	LEU	2.7
1	A	250	GLY	2.6
1	B	376	THR	2.6
1	A	147	PRO	2.6
1	B	240	ASN	2.5
1	B	373	GLU	2.5
1	B	69	ILE	2.5
1	A	239	LEU	2.5
1	A	82	ASP	2.5
1	B	121	PRO	2.5
1	B	216	ARG	2.5
1	A	251	ASP	2.4
1	B	72	ARG	2.4
1	B	245	GLN	2.4
1	B	146	ALA	2.3
1	B	251	ASP	2.3
1	B	35	GLY	2.3
1	A	378	SER	2.3
1	B	167	PHE	2.3
1	B	375	ALA	2.3
1	B	247	ARG	2.2
1	B	349	HIS	2.2
1	A	253	GLN	2.2
1	A	113	ASP	2.2
1	B	340	ASP	2.2
1	A	245	GLN	2.2
1	B	312	PRO	2.1
1	B	252	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	350	GLY	2.1
1	B	362	ALA	2.1
1	A	236	GLU	2.1
1	A	240	ASN	2.1
1	B	369	GLY	2.1
1	B	125	CYS	2.0
1	B	272	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 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.