



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:28 PM UTC

PDB ID : 6MHK / pdb_00006mhh
Title : Crystal structure of ketosynthase nine from bacillaene polyketide synthase in *Bacillus amyloliquefaciens*
Authors : Meinke, J.L.; Keatinge-Clay, A.T.
Deposited on : 2018-09-18
Resolution : 1.93 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

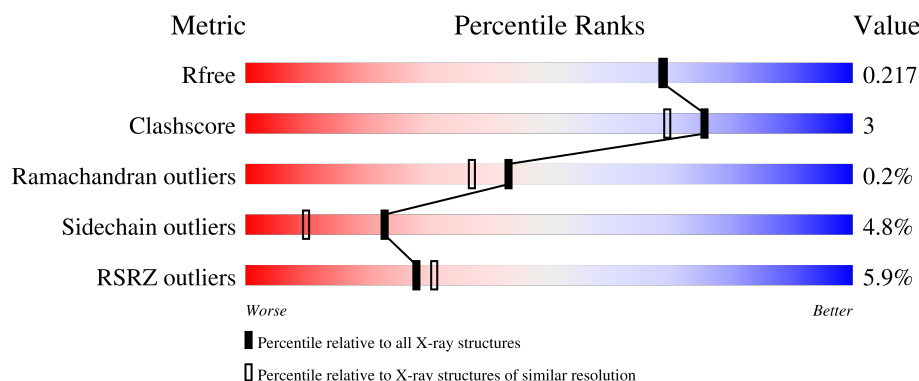
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	614	5% 74% 11% • 13%
1	B	614	5% 75% 10% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8679 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4144	2628	715	787	14			
1	B	534	Total	C	N	O	S	0	0	0
			4134	2620	711	789	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q1RS71
A	-21	GLY	-	expression tag	UNP Q1RS71
A	-20	SER	-	expression tag	UNP Q1RS71
A	-19	SER	-	expression tag	UNP Q1RS71
A	-18	HIS	-	expression tag	UNP Q1RS71
A	-17	HIS	-	expression tag	UNP Q1RS71
A	-16	HIS	-	expression tag	UNP Q1RS71
A	-15	HIS	-	expression tag	UNP Q1RS71
A	-14	HIS	-	expression tag	UNP Q1RS71
A	-13	HIS	-	expression tag	UNP Q1RS71
A	-12	SER	-	expression tag	UNP Q1RS71
A	-11	SER	-	expression tag	UNP Q1RS71
A	-10	GLY	-	expression tag	UNP Q1RS71
A	-9	LEU	-	expression tag	UNP Q1RS71
A	-8	VAL	-	expression tag	UNP Q1RS71
A	-7	PRO	-	expression tag	UNP Q1RS71
A	-6	ARG	-	expression tag	UNP Q1RS71
A	-5	GLY	-	expression tag	UNP Q1RS71
A	-4	SER	-	expression tag	UNP Q1RS71
A	-3	SER	-	expression tag	UNP Q1RS71
B	-22	MET	-	initiating methionine	UNP Q1RS71
B	-21	GLY	-	expression tag	UNP Q1RS71
B	-20	SER	-	expression tag	UNP Q1RS71
B	-19	SER	-	expression tag	UNP Q1RS71
B	-18	HIS	-	expression tag	UNP Q1RS71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	HIS	-	expression tag	UNP Q1RS71
B	-16	HIS	-	expression tag	UNP Q1RS71
B	-15	HIS	-	expression tag	UNP Q1RS71
B	-14	HIS	-	expression tag	UNP Q1RS71
B	-13	HIS	-	expression tag	UNP Q1RS71
B	-12	SER	-	expression tag	UNP Q1RS71
B	-11	SER	-	expression tag	UNP Q1RS71
B	-10	GLY	-	expression tag	UNP Q1RS71
B	-9	LEU	-	expression tag	UNP Q1RS71
B	-8	VAL	-	expression tag	UNP Q1RS71
B	-7	PRO	-	expression tag	UNP Q1RS71
B	-6	ARG	-	expression tag	UNP Q1RS71
B	-5	GLY	-	expression tag	UNP Q1RS71
B	-4	SER	-	expression tag	UNP Q1RS71
B	-3	SER	-	expression tag	UNP Q1RS71

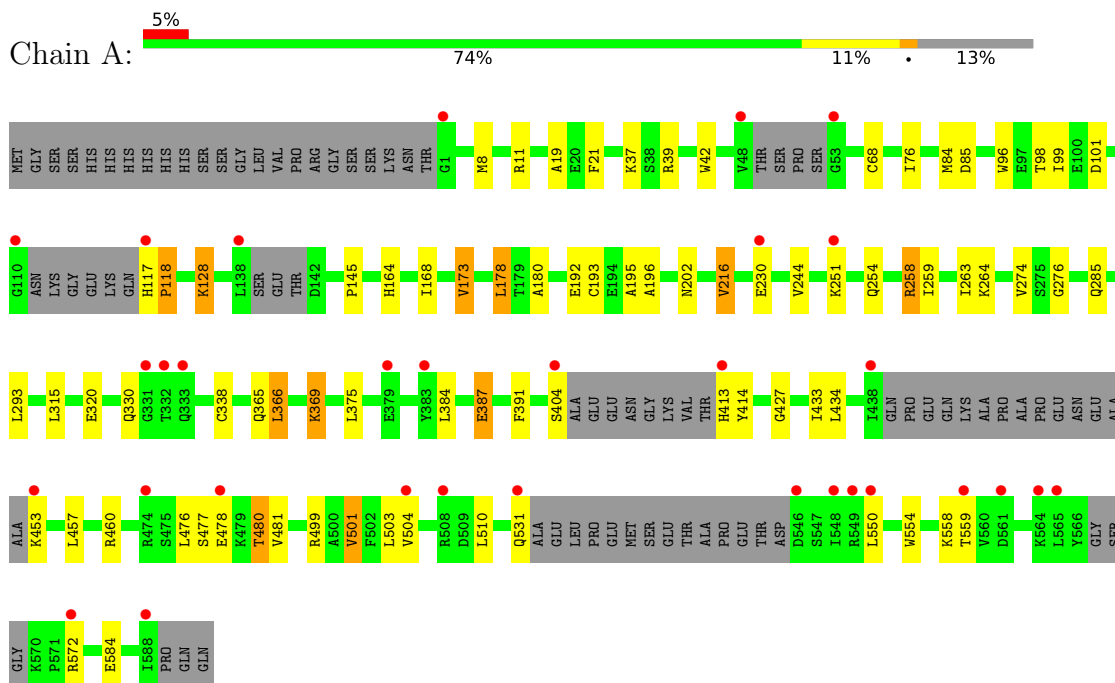
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	187	Total O 187 187	0	0
2	B	214	Total O 214 214	0	0

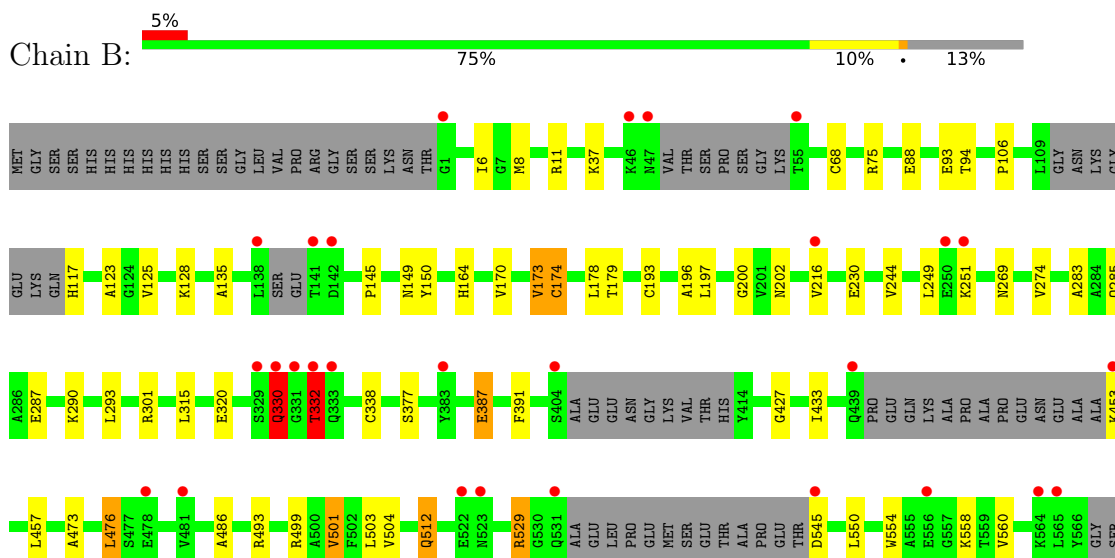
3 Residue-property plots [i](#)

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: Polyketide synthase



• Molecule 1: Polyketide synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.86Å 116.49Å 141.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 50.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.93) 99.0 (50.00-1.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.182 , 0.210 0.191 , 0.217	Depositor DCC
R_{free} test set	5231 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.9	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	0.95	EDS
Total number of atoms	8679	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.06% 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	1.37	23/4235 (0.5%)	1.12	11/5726 (0.2%)
1	B	1.39	24/4224 (0.6%)	1.11	9/5713 (0.2%)
All	All	1.38	47/8459 (0.6%)	1.12	20/11439 (0.2%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ASN	C-O	-7.59	1.15	1.23
1	A	192	GLU	C-O	-7.10	1.15	1.24
1	B	200	GLY	C-O	-6.91	1.17	1.23
1	A	39	ARG	C-O	-6.82	1.18	1.23
1	A	19	ALA	C-O	-6.81	1.16	1.24
1	A	193	CYS	C-O	-6.77	1.15	1.23
1	B	560	VAL	C-O	-6.51	1.17	1.24
1	B	179	THR	C-O	-6.31	1.16	1.24
1	B	377	SER	N-CA	-6.28	1.39	1.46
1	A	99	ILE	C-O	-6.27	1.17	1.24
1	A	21	PHE	C-O	-6.23	1.17	1.24
1	A	180	ALA	C-O	-6.20	1.17	1.24
1	B	93	GLU	C-O	-6.20	1.17	1.24
1	A	145	PRO	CA-C	6.14	1.58	1.52
1	B	178	LEU	C-O	-6.09	1.16	1.24
1	B	123	ALA	C-O	-5.96	1.16	1.24
1	B	94	THR	C-O	-5.92	1.17	1.24
1	B	6	ILE	N-CA	5.87	1.52	1.46
1	B	11	ARG	CA-C	-5.79	1.45	1.52
1	B	504	VAL	C-O	-5.62	1.18	1.24
1	A	11	ARG	CA-C	-5.61	1.45	1.52
1	B	145	PRO	CA-C	5.59	1.57	1.52
1	A	366	LEU	C-O	-5.57	1.17	1.24
1	A	202	ASN	C-O	-5.57	1.17	1.23
1	A	196	ALA	C-O	-5.56	1.16	1.23
1	A	414	TYR	N-CA	5.53	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	PRO	C-O	-5.52	1.17	1.24
1	A	264	LYS	C-O	-5.46	1.16	1.24
1	A	501	VAL	C-O	-5.43	1.18	1.24
1	A	42	TRP	N-CA	-5.42	1.39	1.46
1	A	195	ALA	N-CA	5.41	1.52	1.46
1	B	135	ALA	C-O	-5.41	1.17	1.24
1	B	174	CYS	C-O	-5.41	1.17	1.24
1	B	249	LEU	C-O	-5.40	1.17	1.24
1	A	178	LEU	C-O	-5.37	1.17	1.24
1	A	98	THR	C-O	-5.37	1.17	1.24
1	A	96	TRP	N-CA	5.36	1.52	1.46
1	B	196	ALA	CA-C	-5.23	1.45	1.52
1	B	75	ARG	CA-C	-5.16	1.46	1.53
1	B	88	GLU	C-O	-5.16	1.18	1.24
1	A	365	GLN	C-O	-5.14	1.18	1.24
1	B	493	ARG	C-O	5.14	1.30	1.23
1	A	173	VAL	C-O	-5.10	1.18	1.24
1	B	251	LYS	C-O	-5.05	1.18	1.24
1	A	164	HIS	C-O	-5.03	1.17	1.24
1	B	173	VAL	C-O	-5.03	1.18	1.24
1	B	486	ALA	C-O	-5.03	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	LEU	N-CA-C	8.44	120.56	111.36
1	A	427	GLY	N-CA-C	7.54	125.19	114.64
1	A	501	VAL	CB-CA-C	-7.13	100.21	110.83
1	B	332	THR	CB-CA-C	-6.99	98.68	110.43
1	B	427	GLY	N-CA-C	6.47	123.70	114.64
1	B	330	GLN	N-CA-C	-6.38	96.36	108.17
1	A	274	VAL	N-CA-C	-6.17	101.29	108.82
1	B	274	VAL	N-CA-C	-5.89	101.64	108.82
1	B	529	ARG	NE-CZ-NH2	-5.76	114.02	119.20
1	A	193	CYS	CB-CA-C	-5.71	98.08	109.33
1	B	501	VAL	CB-CA-C	-5.70	102.34	110.83
1	B	315	LEU	CA-C-N	5.66	126.23	119.94
1	B	315	LEU	C-N-CA	5.66	126.23	119.94
1	A	118	PRO	CA-N-CD	-5.64	104.10	112.00
1	B	125	VAL	CB-CA-C	-5.57	100.84	110.65
1	A	330	GLN	N-CA-C	-5.56	104.44	111.11
1	A	375	LEU	N-CA-C	5.32	117.73	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	LEU	CA-C-N	5.22	125.78	119.98
1	A	315	LEU	C-N-CA	5.22	125.78	119.98
1	A	276	GLY	N-CA-C	-5.11	103.00	110.87

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	4144	0	4083	27	0
1	B	4134	0	4067	25	0
2	A	187	0	0	0	0
2	B	214	0	0	2	0
All	All	8679	0	8150	49	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 3.

All (49) 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:B:301:ARG:HD3	1:B:332:THR:HG21	1.56	0.86
1:B:117:HIS:N	1:B:164:HIS:HD1	1.73	0.85
1:A:504:VAL:HG11	1:A:510:LEU:HB2	1.75	0.67
1:A:477:SER:H	1:A:480:THR:CG2	2.07	0.66
1:B:290:LYS:HE2	1:B:330:GLN:NE2	2.14	0.63
1:A:263:ILE:HG12	1:A:434:LEU:CD2	2.30	0.62
1:B:512:GLN:HA	1:B:512:GLN:OE1	2.01	0.60
1:A:366:LEU:O	1:A:369:LYS:HE3	2.04	0.58
1:A:285:GLN:HE22	1:A:320:GLU:HA	1.71	0.56
1:A:101:ASP:O	1:A:258:ARG:NH2	2.39	0.55
1:B:117:HIS:NE2	2:B:601:HOH:O	2.34	0.54
1:B:387:GLU:CD	1:B:387:GLU:H	2.16	0.54
1:B:117:HIS:CE1	2:B:601:HOH:O	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:OD2	1:A:128:LYS:HE3	2.09	0.53
1:B:285:GLN:HE22	1:B:320:GLU:HA	1.74	0.53
1:A:476:LEU:HA	1:A:480:THR:HG21	1.91	0.52
1:A:168:ILE:CG2	1:B:170:VAL:HG23	2.41	0.51
1:B:128:LYS:HG2	1:B:150:TYR:CE1	2.46	0.50
1:A:168:ILE:HG23	1:B:170:VAL:CG2	2.42	0.50
1:B:128:LYS:HG2	1:B:150:TYR:HE1	1.76	0.50
1:A:117:HIS:HB2	1:A:118:PRO:HD3	1.95	0.49
1:A:387:GLU:H	1:A:387:GLU:CD	2.19	0.49
1:A:477:SER:O	1:A:480:THR:HG23	2.12	0.48
1:B:473:ALA:HA	1:B:476:LEU:HD22	1.94	0.48
1:B:68:CYS:HA	1:B:584:GLU:O	2.14	0.47
1:B:216:VAL:HG12	1:B:216:VAL:O	2.13	0.47
1:A:76:ILE:HD13	1:A:84:MET:HE1	1.96	0.47
1:A:68:CYS:HA	1:A:584:GLU:O	2.16	0.45
1:B:8:MET:HG2	1:B:244:VAL:HG12	1.99	0.45
1:B:330:GLN:HE21	1:B:330:GLN:HB2	1.64	0.44
1:A:8:MET:HG2	1:A:244:VAL:HG12	2.00	0.44
1:A:531:GLN:CD	1:A:531:GLN:N	2.76	0.44
1:B:574:THR:O	1:B:576:VAL:HG23	2.18	0.44
1:A:168:ILE:HG23	1:B:170:VAL:HG23	2.00	0.42
1:B:499:ARG:HB3	1:B:554:TRP:CZ3	2.54	0.42
1:A:293:LEU:HD23	1:A:433:ILE:HD13	2.01	0.42
1:A:216:VAL:O	1:A:216:VAL:CG2	2.68	0.42
1:A:293:LEU:HD23	1:A:433:ILE:CD1	2.49	0.42
1:B:290:LYS:HE2	1:B:330:GLN:HE21	1.84	0.41
1:B:338:CYS:O	1:B:391:PHE:HA	2.20	0.41
1:B:293:LEU:HD23	1:B:433:ILE:HD13	2.03	0.41
1:A:263:ILE:HG12	1:A:434:LEU:HD22	2.03	0.41
1:A:258:ARG:HB3	1:A:258:ARG:NH1	2.35	0.41
1:B:269:ASN:OD1	1:B:269:ASN:C	2.63	0.41
1:A:259:ILE:H	1:A:572:ARG:NH2	2.19	0.41
1:A:263:ILE:HG12	1:A:434:LEU:HD21	2.02	0.41
1:A:499:ARG:HB3	1:A:554:TRP:CZ3	2.56	0.40
1:A:338:CYS:O	1:A:391:PHE:HA	2.22	0.40
1:B:283:ALA:O	1:B:287:GLU:HG2	2.21	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	520/614 (85%)	512 (98%)	7 (1%)	1 (0%)	43	37
1	B	518/614 (84%)	511 (99%)	6 (1%)	1 (0%)	43	37
All	All	1038/1228 (84%)	1023 (99%)	13 (1%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	B	173	VAL

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	438/502 (87%)	415 (95%)	23 (5%)	20	7
1	B	438/502 (87%)	419 (96%)	19 (4%)	26	13
All	All	876/1004 (87%)	834 (95%)	42 (5%)	23	10

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	128	LYS
1	A	178	LEU
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	230	GLU
1	A	251	LYS
1	A	254	GLN
1	A	258	ARG
1	A	369	LYS
1	A	387	GLU
1	A	404	SER
1	A	413	HIS
1	A	453	LYS
1	A	457	LEU
1	A	460	ARG
1	A	478	GLU
1	A	480	THR
1	A	481	VAL
1	A	501	VAL
1	A	503	LEU
1	A	550	LEU
1	A	558	LYS
1	A	559	THR
1	B	37	LYS
1	B	149	ASN
1	B	174	CYS
1	B	193	CYS
1	B	197	LEU
1	B	230	GLU
1	B	330	GLN
1	B	332	THR
1	B	387	GLU
1	B	453	LYS
1	B	457	LEU
1	B	476	LEU
1	B	501	VAL
1	B	503	LEU
1	B	512	GLN
1	B	529	ARG
1	B	545	ASP
1	B	550	LEU
1	B	558	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	155	ASN
1	A	285	GLN
1	A	330	GLN
1	A	335	GLN
1	A	402	GLN
1	A	429	ASN
1	B	117	HIS
1	B	155	ASN
1	B	285	GLN
1	B	330	GLN
1	B	402	GLN
1	B	429	ASN

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	536/614 (87%)	0.13	32 (5%) 27 30	14, 23, 50, 76	0
1	B	534/614 (86%)	0.06	31 (5%) 29 32	13, 22, 44, 78	0
All	All	1070/1228 (87%)	0.10	63 (5%) 28 31	13, 23, 47, 78	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	GLN	7.6
1	A	53	GLY	5.6
1	B	47	ASN	5.1
1	B	588	ILE	5.0
1	A	110	GLY	4.6
1	A	588	ILE	4.4
1	B	332	THR	4.2
1	B	522	GLU	4.2
1	B	142	ASP	4.0
1	B	439	GLN	3.8
1	B	404	SER	3.7
1	A	117	HIS	3.7
1	A	438	ILE	3.7
1	B	141	THR	3.7
1	A	572	ARG	3.6
1	A	48	VAL	3.6
1	B	331	GLY	3.5
1	A	564	LYS	3.5
1	B	478	GLU	3.3
1	B	556	GLU	3.2
1	A	550	LEU	3.2
1	B	1	GLY	3.1
1	B	574	THR	3.1
1	A	561	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	3.0
1	B	55	THR	2.9
1	A	546	ASP	2.9
1	A	413	HIS	2.9
1	A	138	LEU	2.9
1	A	251	LYS	2.8
1	B	453	LYS	2.8
1	A	1	GLY	2.8
1	A	332	THR	2.7
1	B	383	TYR	2.7
1	B	531	GLN	2.6
1	A	478	GLU	2.5
1	B	564	LYS	2.5
1	A	549	ARG	2.4
1	B	565	LEU	2.4
1	B	523	ASN	2.4
1	B	333	GLN	2.3
1	A	548	ILE	2.3
1	B	46	LYS	2.3
1	A	404	SER	2.3
1	B	251	LYS	2.2
1	B	329	SER	2.2
1	B	570	LYS	2.2
1	A	508	ARG	2.2
1	A	504	VAL	2.1
1	B	481	VAL	2.1
1	A	453	LYS	2.1
1	A	474	ARG	2.1
1	B	250	GLU	2.1
1	A	333	GLN	2.1
1	B	216	VAL	2.1
1	A	230	GLU	2.1
1	A	379	GLU	2.1
1	B	545	ASP	2.1
1	A	531	GLN	2.1
1	A	383	TYR	2.0
1	A	559	THR	2.0
1	A	565	LEU	2.0
1	A	331	GLY	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.