



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:42 PM UTC

PDB ID : 5X47 / pdb_00005x47
Title : Crystal structure of dehydroquinase dehydratase from *Acinetobacter baumannii* at 2.5 Angstrom resolution
Authors : Iqbal, N.; Singh, P.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2017-02-10
Resolution : 2.54 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

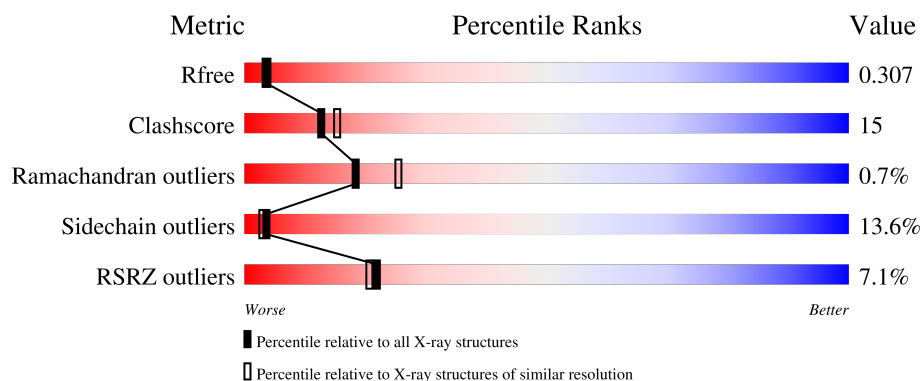
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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.



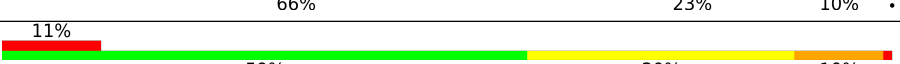
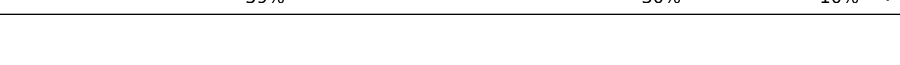
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	145	
1	B	145	
1	C	145	
1	D	145	
1	E	145	

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Mol	Chain	Length	Quality of chain
1	F	145	
1	G	145	
1	H	145	
1	I	145	
1	J	145	
1	K	145	
1	L	145	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13478 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 3-dehydroquinase dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	B	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	C	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	D	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	E	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	F	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	G	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	H	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	I	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	J	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	K	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	L	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	8	Total	O	0	0
			8	8		

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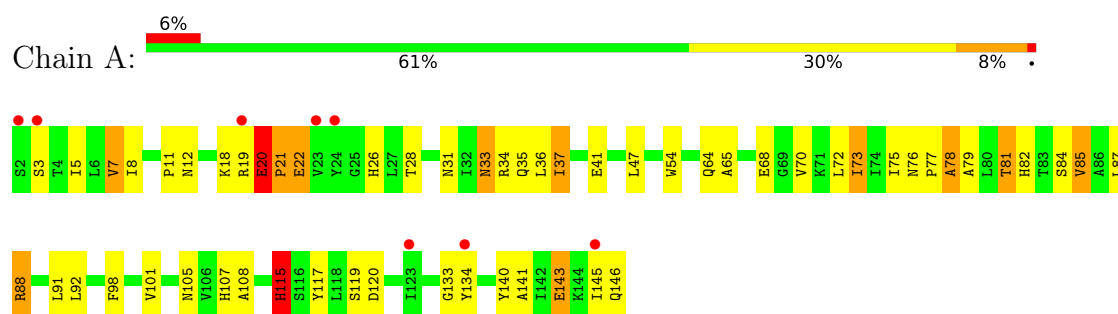
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	5	Total 5	O 5	0	0
2	D	2	Total 2	O 2	0	0
2	E	3	Total 3	O 3	0	0
2	F	2	Total 2	O 2	0	0
2	G	3	Total 3	O 3	0	0
2	H	4	Total 4	O 4	0	0
2	J	1	Total 1	O 1	0	0
2	L	2	Total 2	O 2	0	0

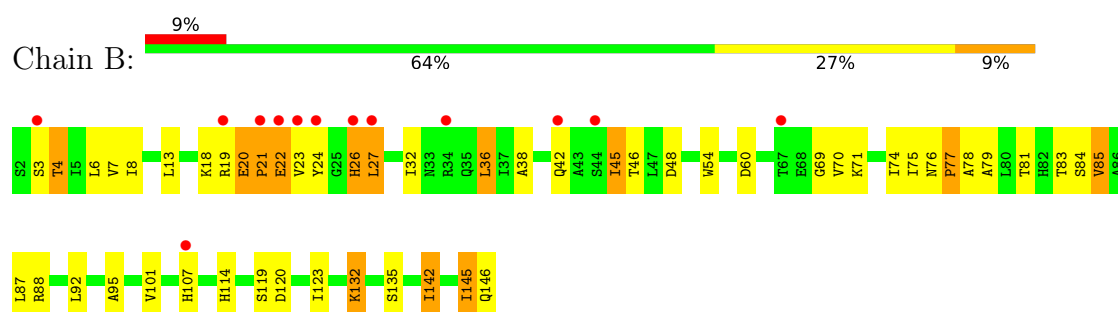
3 Residue-property plots

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.

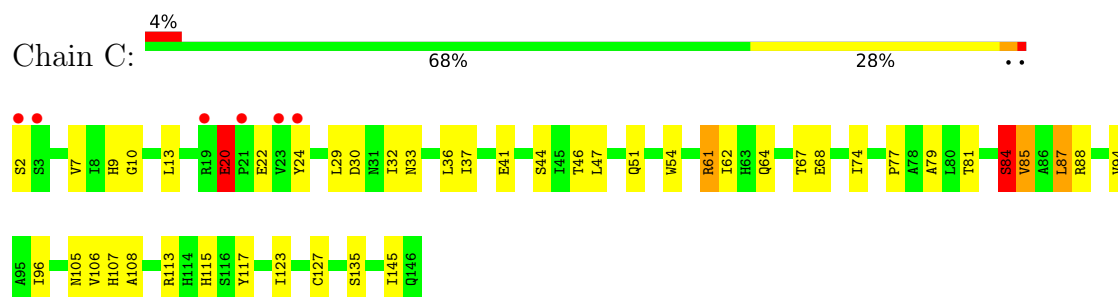
• Molecule 1: 3-dehydroquinase dehydratase



• Molecule 1: 3-dehydroquinase dehydratase

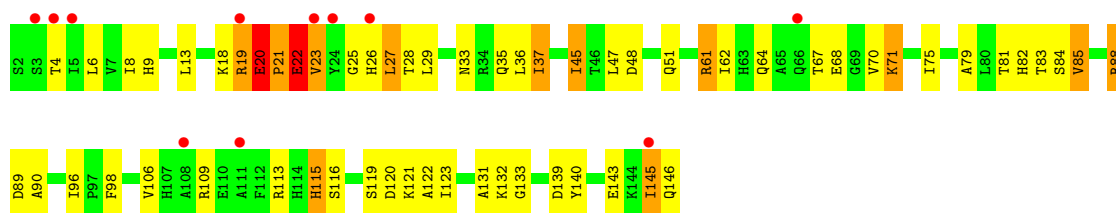


• Molecule 1: 3-dehydroquinase dehydratase

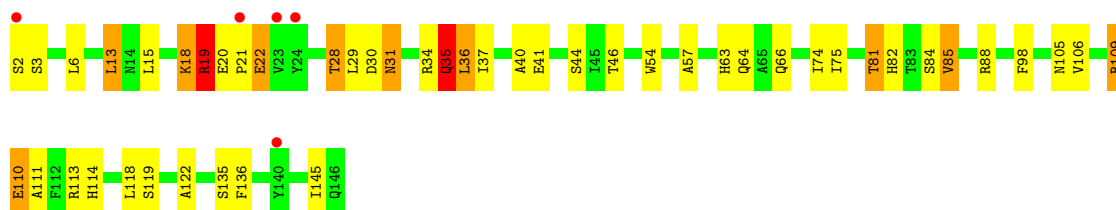


• Molecule 1: 3-dehydroquinase dehydratase

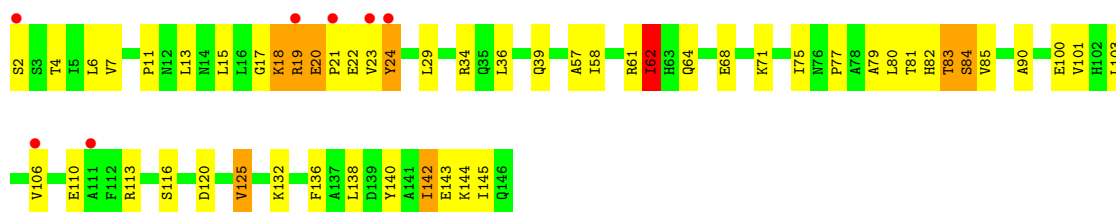




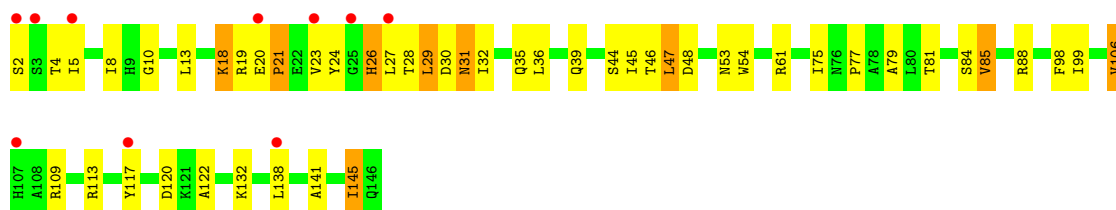
• Molecule 1: 3-dehydroquinatase dehydratase



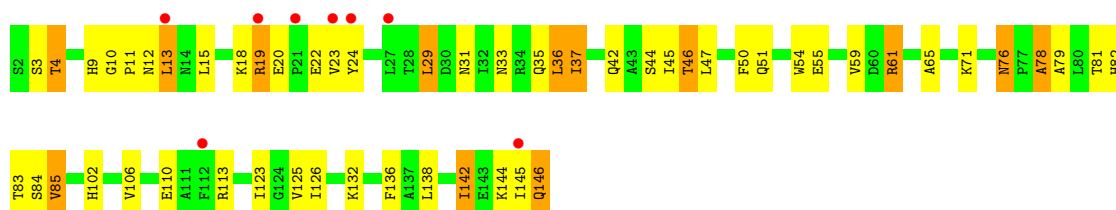
• Molecule 1: 3-dehydroquinatase dehydratase



• Molecule 1: 3-dehydroquinatase dehydratase



• Molecule 1: 3-dehydroquinatase dehydratase



Chain I:

Category	Percentage
Red	11%
Green	52%
Yellow	40%
Orange	6%

Chain J:

Category	Percentage
S2	9%
S3	54%
T4	54%
I5	54%
I8	54%
L13	54%
N14	54%
L15	54%
L16	54%
G17	54%
K18	54%
E19	54%
E20	54%
P21	54%
E22	54%
V23	54%
Y24	54%
G25	54%
H26	54%
L29	54%
D30	54%
N31	54%
I32	54%
N33	54%
R34	54%
Q35	54%
L36	54%
I37	54%
Q39	54%
A40	54%
E41	54%
Q42	54%
A43	54%
S44	54%
I45	54%
D48	35%
T49	35%
W54	35%
R61	35%
E68	35%
G69	35%
V70	35%
I74	35%
I75	35%
A79	35%
L80	35%
T81	35%
H82	35%
T83	35%
S84	35%
V85	10%
A86	10%
L87	10%
R88	10%
D89	10%
A90	10%
V101	10%
H107	10%
A108	10%
R109	10%
E110	10%
F111	10%
R113	10%
H114	10%
H115	10%
S116	10%
Y117	10%
L118	10%
S119	10%
D120	10%
I123	10%
K132	10%
F136	10%
A137	10%
D138	10%
D139	10%
Y140	10%
A141	10%
E142	10%
E143	10%
K144	10%
I145	10%
Q146	10%

Chain K:

7% 66% 23% 10%

S2 S3 S4 S5 L13 L16 L17 L18 L19 L20 L21 L22 L23 L24 L25 L26 L27 L28 L29 L30 L31 R34 R35 R36 L45 S52 S53 S54 S61 I75 I76 I77 I78 I79 I80 I81 I82 I83 I84 I85 I86 I87 I88 I89 F98 V106 R109 Y117 Y118 Y119

Chain L:

State	Category
S2	Yellow
S3	Orange
T4	Orange
I5	Yellow
L6	Yellow
V7	Yellow
P11	Green
N12	Green
N13	Orange
N14	Orange
L15	Yellow
L16	Yellow
R19	Green
E20	Yellow
P21	Green
E22	Green
V23	Green
Y24	Green
G25	Green
H26	Green
I27	Yellow
T28	Orange
L29	Red
I32	Orange
N33	Orange
R34	Green
Q35	Green
L36	Orange
I37	Yellow
A40	Yellow
E41	Yellow
T45	Green
T46	Yellow
L47	Yellow
W54	Orange
I58	Orange
V59	Green
D60	Orange
R61	Orange
I62	Orange
H63	Yellow
Q64	Yellow
A65	Green
Q66	Green
V70	Green
K71	Orange
I76	Yellow
A79	Yellow
L80	Orange
T81	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.99Å 136.25Å 143.21Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	47.93 – 2.54 47.93 – 2.54	Depositor EDS
% Data completeness (in resolution range)	70.3 (47.93-2.54) 70.5 (47.93-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.253 , 0.305 0.258 , 0.307	Depositor DCC
R_{free} test set	2142 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13478	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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	1.76	22/1141 (1.9%)	1.35	9/1551 (0.6%)
1	B	1.61	14/1141 (1.2%)	1.30	7/1551 (0.5%)
1	C	1.63	7/1141 (0.6%)	1.30	7/1551 (0.5%)
1	D	1.67	12/1141 (1.1%)	1.38	7/1551 (0.5%)
1	E	1.63	10/1141 (0.9%)	1.29	8/1551 (0.5%)
1	F	1.59	11/1141 (1.0%)	1.33	7/1551 (0.5%)
1	G	1.56	6/1141 (0.5%)	1.30	6/1551 (0.4%)
1	H	1.55	8/1141 (0.7%)	1.45	11/1551 (0.7%)
1	I	1.65	16/1141 (1.4%)	1.38	7/1551 (0.5%)
1	J	1.56	11/1141 (1.0%)	1.44	12/1551 (0.8%)
1	K	1.63	14/1141 (1.2%)	1.36	11/1551 (0.7%)
1	L	1.61	8/1141 (0.7%)	1.49	11/1551 (0.7%)
All	All	1.62	139/13692 (1.0%)	1.36	103/18612 (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	D	0	1
1	H	0	1
All	All	0	2

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ALA	C-O	-10.62	1.14	1.24
1	I	78	ALA	C-O	-10.32	1.14	1.24
1	A	7	VAL	C-O	-9.11	1.14	1.24
1	A	5	ILE	C-O	-8.54	1.15	1.24
1	D	132	LYS	C-O	-8.38	1.14	1.24

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	19	ARG	N-CA-C	-9.08	91.91	107.99
1	J	22	GLU	CA-C-N	-8.99	105.79	121.97
1	J	22	GLU	C-N-CA	-8.99	105.79	121.97
1	H	20	GLU	N-CA-C	8.86	124.80	112.75
1	K	20	GLU	CA-C-N	8.66	128.53	120.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	22	GLU	Peptide
1	H	22	GLU	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	1120	0	1131	35	0
1	B	1120	0	1131	39	0
1	C	1120	0	1131	18	0
1	D	1120	0	1131	37	0
1	E	1120	0	1131	29	0
1	F	1120	0	1131	33	0
1	G	1120	0	1131	28	0
1	H	1120	0	1130	39	0
1	I	1120	0	1130	43	0
1	J	1120	0	1131	47	0
1	K	1120	0	1131	33	0
1	L	1120	0	1131	55	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	5	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	4	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
All	All	13478	0	13570	411	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 15.

The worst 5 of 411 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:H:4:THR:HG23	1:H:46:THR:CG2	1.53	1.37
1:L:16:LEU:CD1	1:L:29:LEU:HB2	1.72	1.16
1:H:146:GLN:HE21	1:H:146:GLN:HA	1.14	1.13
1:L:16:LEU:HG	1:L:29:LEU:H	1.06	1.08
1:H:78:ALA:O	1:H:81:THR:HG22	1.54	1.06

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	143/145 (99%)	135 (94%)	6 (4%)	2 (1%)	9	11
1	B	143/145 (99%)	137 (96%)	5 (4%)	1 (1%)	18	25
1	C	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
1	D	143/145 (99%)	136 (95%)	5 (4%)	2 (1%)	9	11
1	E	143/145 (99%)	136 (95%)	5 (4%)	2 (1%)	9	11
1	F	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
1	G	143/145 (99%)	139 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
1	I	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
1	J	143/145 (99%)	135 (94%)	6 (4%)	2 (1%)	9	11
1	K	143/145 (99%)	137 (96%)	3 (2%)	3 (2%)	5	5
1	L	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
All	All	1716/1740 (99%)	1633 (95%)	71 (4%)	12 (1%)	18	25

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLU
1	D	20	GLU
1	D	26	HIS
1	K	24	TYR
1	A	21	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	119/119 (100%)	111 (93%)	8 (7%)	15	21
1	B	119/119 (100%)	108 (91%)	11 (9%)	8	10
1	C	119/119 (100%)	105 (88%)	14 (12%)	5	5
1	D	119/119 (100%)	97 (82%)	22 (18%)	1	1
1	E	119/119 (100%)	103 (87%)	16 (13%)	4	3
1	F	119/119 (100%)	105 (88%)	14 (12%)	5	5
1	G	119/119 (100%)	102 (86%)	17 (14%)	3	3
1	H	119/119 (100%)	103 (87%)	16 (13%)	4	3
1	I	119/119 (100%)	98 (82%)	21 (18%)	2	1
1	J	119/119 (100%)	100 (84%)	19 (16%)	2	2
1	K	119/119 (100%)	103 (87%)	16 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	119/119 (100%)	99 (83%)	20 (17%)	2	2
All	All	1428/1428 (100%)	1234 (86%)	194 (14%)	3	3

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	85	VAL
1	J	20	GLU
1	I	3	SER
1	I	44	SER
1	J	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	146	GLN
1	J	115	HIS
1	L	66	GLN
1	L	35	GLN
1	E	66	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	145/145 (100%)	0.50	8 (5%)	30 30	25, 35, 76, 110	0
1	B	145/145 (100%)	0.58	13 (8%)	15 14	25, 35, 72, 115	0
1	C	145/145 (100%)	0.40	6 (4%)	41 42	25, 34, 72, 145	0
1	D	145/145 (100%)	0.70	11 (7%)	20 19	28, 46, 90, 124	0
1	E	145/145 (100%)	0.52	5 (3%)	48 49	27, 40, 82, 118	0
1	F	145/145 (100%)	0.41	7 (4%)	35 35	25, 34, 75, 122	0
1	G	145/145 (100%)	0.70	10 (6%)	23 22	29, 50, 91, 144	0
1	H	145/145 (100%)	0.75	8 (5%)	30 30	31, 51, 93, 144	0
1	I	145/145 (100%)	0.99	16 (11%)	10 10	34, 64, 104, 148	0
1	J	145/145 (100%)	0.80	13 (8%)	15 14	36, 53, 100, 144	0
1	K	145/145 (100%)	0.73	10 (6%)	23 22	30, 44, 85, 156	0
1	L	145/145 (100%)	0.98	16 (11%)	10 10	32, 57, 100, 127	0
All	All	1740/1740 (100%)	0.67	123 (7%)	22 21	25, 45, 95, 156	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	VAL	5.5
1	A	2	SER	4.6
1	I	75	ILE	4.6
1	A	23	VAL	4.5
1	K	106	VAL	4.4

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.