



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:51 PM UTC

PDB ID : 6KI7 / pdb_00006ki7
Title : Pyrophosphatase mutant K30R from *Acinetobacter baumannii*
Authors : Su, J.
Deposited on : 2019-07-17
Resolution : 2.75 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

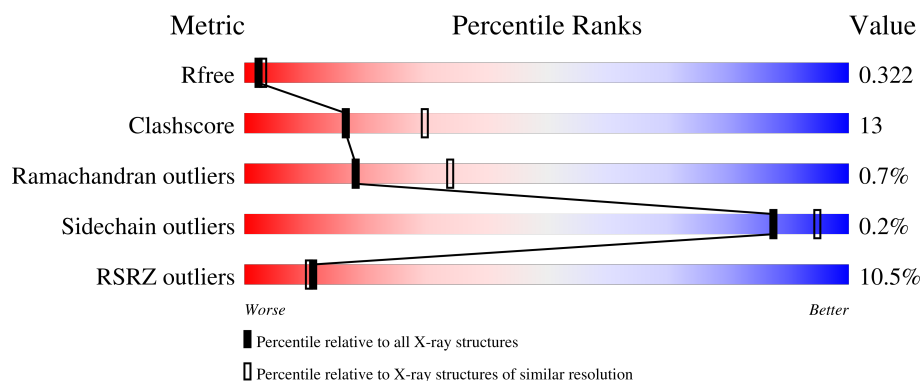
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	177	5% 83% 15% .
1	B	177	2% 74% 23% ..
1	C	177	% 84% 14% .
1	D	177	49% 54% 39% ...
1	E	177	2% 69% 29% .

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Mol	Chain	Length	Quality of chain
1	F	177	3% 71% 27% .
1	G	177	18% 82% 16% .
1	H	177	2% 75% 23% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10804 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 Inorganic pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	B	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	C	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	D	173	Total	C	N	O	S	0	0	0
			1345	868	216	258	3			
1	E	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	F	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	G	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			
1	H	173	Total	C	N	O	S	0	0	0
			1348	870	216	258	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP N9S5K0
A	-2	SER	-	expression tag	UNP N9S5K0
A	-1	HIS	-	expression tag	UNP N9S5K0
A	29	ARG	LYS	engineered mutation	UNP N9S5K0
A	139	SER	ALA	engineered mutation	UNP N9S5K0
B	-3	GLY	-	expression tag	UNP N9S5K0
B	-2	SER	-	expression tag	UNP N9S5K0
B	-1	HIS	-	expression tag	UNP N9S5K0
B	29	ARG	LYS	engineered mutation	UNP N9S5K0
B	139	SER	ALA	engineered mutation	UNP N9S5K0
C	-3	GLY	-	expression tag	UNP N9S5K0
C	-2	SER	-	expression tag	UNP N9S5K0
C	-1	HIS	-	expression tag	UNP N9S5K0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ARG	LYS	engineered mutation	UNP N9S5K0
C	139	SER	ALA	engineered mutation	UNP N9S5K0
D	-3	GLY	-	expression tag	UNP N9S5K0
D	-2	SER	-	expression tag	UNP N9S5K0
D	-1	HIS	-	expression tag	UNP N9S5K0
D	29	ARG	LYS	engineered mutation	UNP N9S5K0
D	139	SER	ALA	engineered mutation	UNP N9S5K0
E	-3	GLY	-	expression tag	UNP N9S5K0
E	-2	SER	-	expression tag	UNP N9S5K0
E	-1	HIS	-	expression tag	UNP N9S5K0
E	29	ARG	LYS	engineered mutation	UNP N9S5K0
E	139	SER	ALA	engineered mutation	UNP N9S5K0
F	-3	GLY	-	expression tag	UNP N9S5K0
F	-2	SER	-	expression tag	UNP N9S5K0
F	-1	HIS	-	expression tag	UNP N9S5K0
F	29	ARG	LYS	engineered mutation	UNP N9S5K0
F	139	SER	ALA	engineered mutation	UNP N9S5K0
G	-3	GLY	-	expression tag	UNP N9S5K0
G	-2	SER	-	expression tag	UNP N9S5K0
G	-1	HIS	-	expression tag	UNP N9S5K0
G	29	ARG	LYS	engineered mutation	UNP N9S5K0
G	139	SER	ALA	engineered mutation	UNP N9S5K0
H	-3	GLY	-	expression tag	UNP N9S5K0
H	-2	SER	-	expression tag	UNP N9S5K0
H	-1	HIS	-	expression tag	UNP N9S5K0
H	29	ARG	LYS	engineered mutation	UNP N9S5K0
H	139	SER	ALA	engineered mutation	UNP N9S5K0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0
2	D	3	Total O 3 3	0	0
2	E	2	Total O 2 2	0	0
2	F	4	Total O 4 4	0	0

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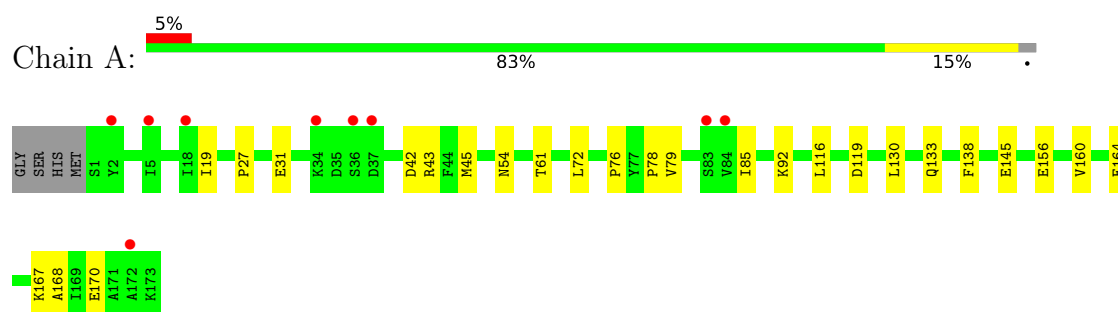
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	4	Total	O	0	0
			4	4		

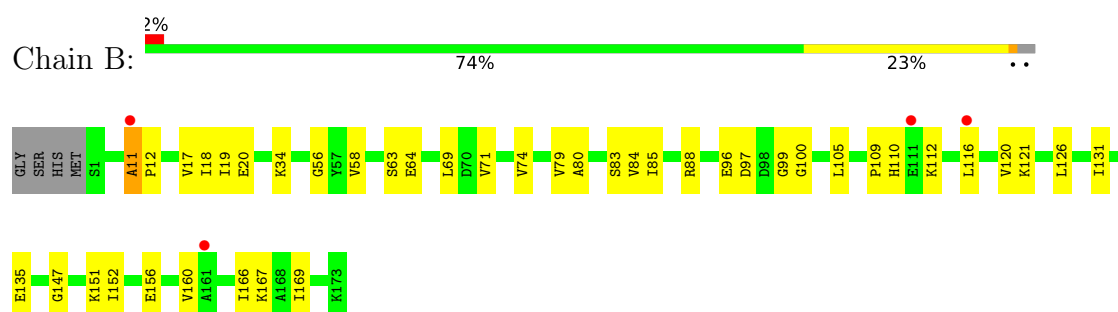
3 Residue-property plots [i](#)

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.

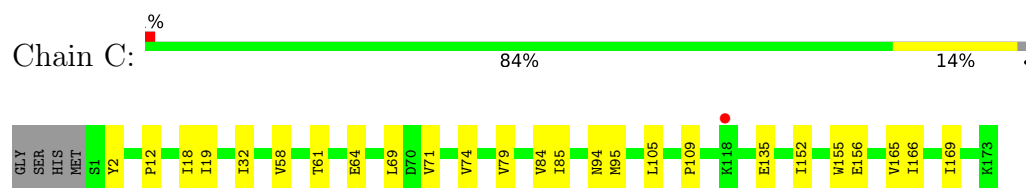
- Molecule 1: Inorganic pyrophosphatase



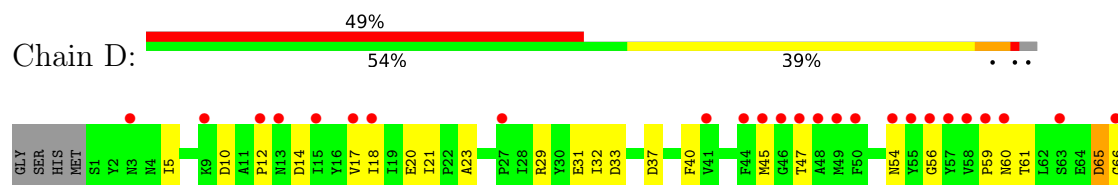
- Molecule 1: Inorganic pyrophosphatase

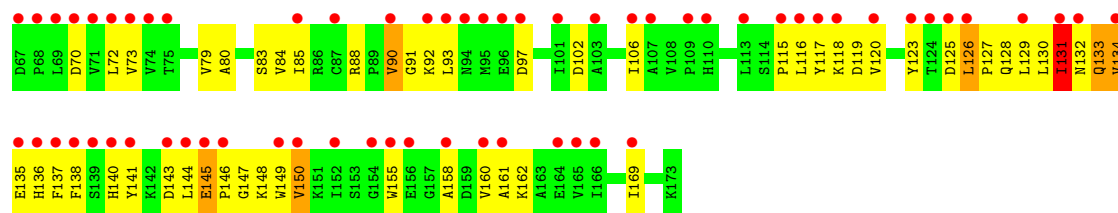


- Molecule 1: Inorganic pyrophosphatase

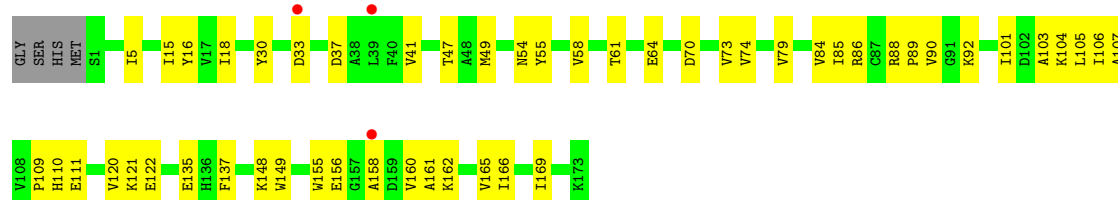


- Molecule 1: Inorganic pyrophosphatase

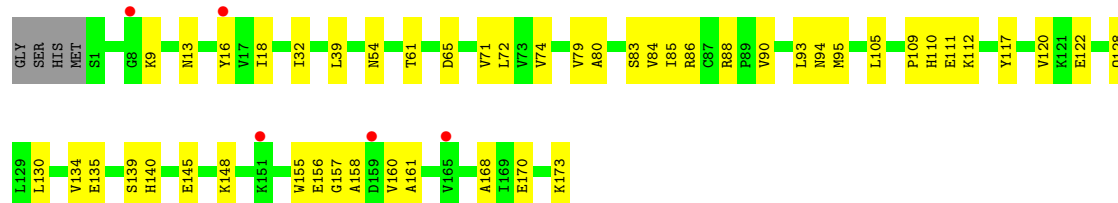




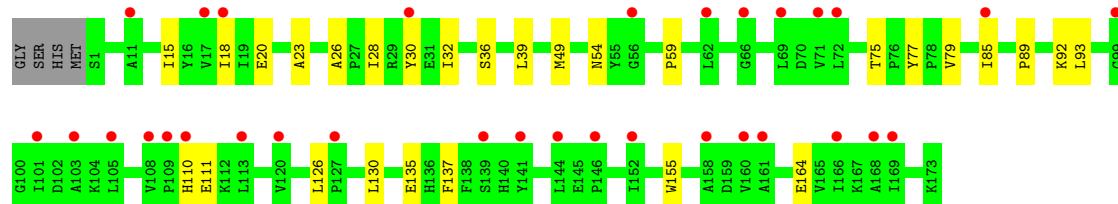
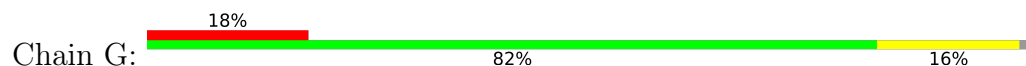
• Molecule 1: Inorganic pyrophosphatase



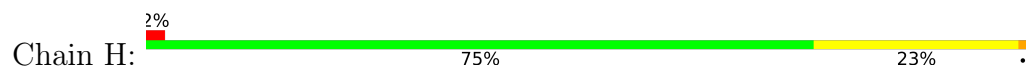
• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



• Molecule 1: Inorganic pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	113.05Å 113.05Å 551.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.75 19.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.96-2.75) 98.1 (19.96-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.75Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.292 , 0.324 0.293 , 0.322	Depositor DCC
R_{free} test set	2000 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10804	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4797e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.13	0/1383	0.33	0/1886
1	B	0.15	0/1383	0.39	0/1886
1	C	0.12	0/1383	0.32	0/1886
1	D	0.26	0/1380	0.67	3/1883 (0.2%)
1	E	0.19	0/1383	0.39	0/1886
1	F	0.19	0/1383	0.41	0/1886
1	G	0.12	0/1383	0.33	0/1886
1	H	0.14	0/1383	0.39	0/1886
All	All	0.17	0/11061	0.42	3/15085 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	GLN	N-CA-C	-7.09	103.48	111.07
1	D	131	ILE	N-CA-C	-5.27	104.46	111.05
1	D	134	VAL	N-CA-C	-5.12	104.99	110.36

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	1348	0	1330	21	0
1	B	1348	0	1330	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1348	0	1330	15	0
1	D	1345	0	1323	83	0
1	E	1348	0	1330	38	0
1	F	1348	0	1330	39	0
1	G	1348	0	1330	16	0
1	H	1348	0	1330	31	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	2	0
2	E	2	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	4	0	0	0	0
All	All	10804	0	10633	274	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 13.

The worst 5 of 274 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:D:126:LEU:CG	1:D:127:PRO:HD3	1.76	1.15
1:D:126:LEU:CG	1:D:127:PRO:CD	2.30	1.09
1:D:126:LEU:HG	1:D:127:PRO:CD	1.85	1.05
1:D:92:LYS:HZ1	1:D:160:VAL:HB	1.26	1.00
1:D:126:LEU:HG	1:D:127:PRO:HD3	1.02	1.00

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	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	B	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	21	38
1	C	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	D	171/177 (97%)	138 (81%)	26 (15%)	7 (4%)	2	3
1	E	171/177 (97%)	159 (93%)	12 (7%)	0	100	100
1	F	171/177 (97%)	161 (94%)	10 (6%)	0	100	100
1	G	171/177 (97%)	153 (90%)	17 (10%)	1 (1%)	21	38
1	H	171/177 (97%)	164 (96%)	6 (4%)	1 (1%)	21	38
All	All	1368/1416 (97%)	1269 (93%)	89 (6%)	10 (1%)	18	34

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	126	LEU
1	D	145	GLU
1	B	11	ALA
1	D	150	VAL
1	H	11	ALA

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	144/147 (98%)	144 (100%)	0	100	100
1	B	144/147 (98%)	144 (100%)	0	100	100
1	C	144/147 (98%)	144 (100%)	0	100	100
1	D	143/147 (97%)	142 (99%)	1 (1%)	76	86
1	E	144/147 (98%)	143 (99%)	1 (1%)	76	86
1	F	144/147 (98%)	144 (100%)	0	100	100
1	G	144/147 (98%)	144 (100%)	0	100	100
1	H	144/147 (98%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1151/1176 (98%)	1149 (100%)	2 (0%)	87 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	131	ILE
1	E	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	60	ASN
1	H	60	ASN
1	F	13	ASN
1	H	128	GLN
1	F	140	HIS

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 ⓘ

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	173/177 (97%)	0.46	9 (5%) 33 32	40, 63, 92, 101	0
1	B	173/177 (97%)	0.38	4 (2%) 61 59	32, 53, 80, 114	0
1	C	173/177 (97%)	-0.12	1 (0%) 85 86	23, 38, 70, 89	0
1	D	173/177 (97%)	2.04	87 (50%) 0 0	40, 97, 129, 163	0
1	E	173/177 (97%)	0.35	3 (1%) 69 67	45, 80, 122, 141	0
1	F	173/177 (97%)	0.42	5 (2%) 53 52	27, 56, 90, 114	0
1	G	173/177 (97%)	1.33	32 (18%) 3 2	99, 139, 181, 228	0
1	H	173/177 (97%)	0.15	4 (2%) 61 59	25, 50, 89, 116	0
All	All	1384/1416 (97%)	0.63	145 (10%) 11 11	23, 64, 145, 228	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	ILE	5.6
1	D	47	THR	5.2
1	D	63	SER	4.8
1	D	116	LEU	4.8
1	D	48	ALA	4.8

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.