



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:22 am GMT

PDB ID : 2QMI
Title : Structure of the octameric penicillin-binding protein homologue from *Pyrococcus abyssi*
Authors : Delfosse, V.; Girard, E.; Moulinier, L.; Schultz, P.; Mayer, C.
Deposited on : 2007-07-16
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

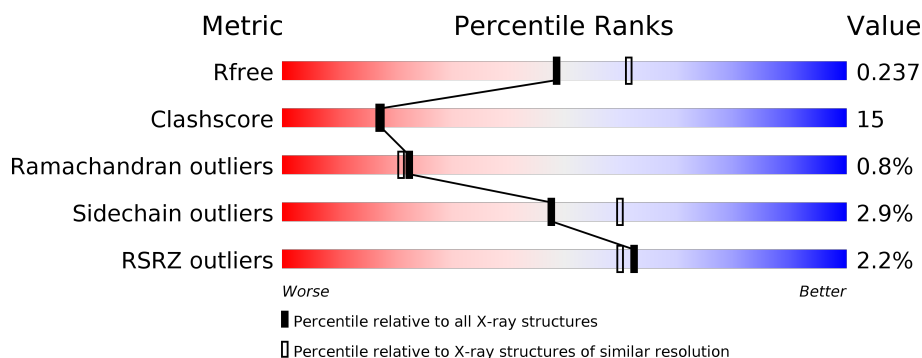
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



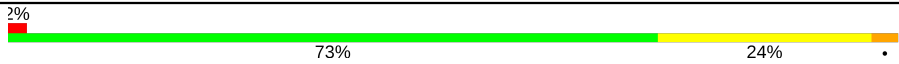

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	447	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
1	B	447	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div>.</div> </div> </div>
1	C	447	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	D	447	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	E	447	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>.</div> </div> </div>
1	F	447	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	447	
1	H	447	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DO3	E	450	-	-	-	X
3	DO3	H	449	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 30882 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 Pbp related beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3551	2325	558	654	14			
1	B	447	Total	C	N	O	S	0	0	0
			3549	2325	555	655	14			
1	C	446	Total	C	N	O	S	0	0	0
			3534	2317	553	650	14			
1	D	446	Total	C	N	O	S	0	0	0
			3545	2323	555	653	14			
1	E	446	Total	C	N	O	S	0	0	0
			3544	2322	556	652	14			
1	F	447	Total	C	N	O	S	0	0	0
			3549	2325	555	655	14			
1	G	447	Total	C	N	O	S	0	0	0
			3559	2331	559	655	14			
1	H	447	Total	C	N	O	S	0	0	0
			3554	2326	558	656	14			

- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

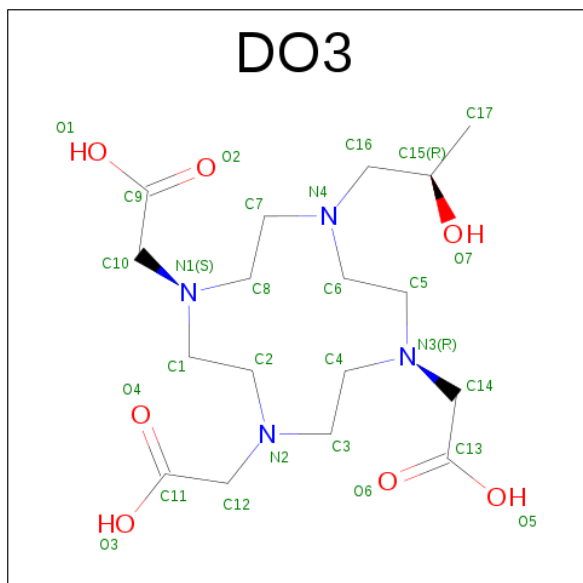
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Lu	0	0
			3	3		
2	D	2	Total	Lu	0	0
			2	2		
2	E	2	Total	Lu	0	0
			2	2		
2	H	1	Total	Lu	0	0
			1	1		
2	B	2	Total	Lu	0	0
			2	2		
2	C	2	Total	Lu	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Lu	0	0
			2	2		
2	F	3	Total	Lu	0	0
			3	3		

- Molecule 3 is 10-((2R)-2-HYDROXYPROPYL)-1,4,7,10-TETRAAZACYCLODODECANE 1,4,7-TRIACETIC ACID (three-letter code: DO3) (formula: C₁₇H₃₂N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			28	17	4	7		
3	F	1	Total	C	N	O	0	0
			28	17	4	7		
3	G	1	Total	C	N	O	0	0
			28	17	4	7		
3	H	1	Total	C	N	O	0	0
			28	17	4	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total	O	0	0
			285	285		
4	B	279	Total	O	0	0
			279	279		
4	C	237	Total	O	0	0
			237	237		

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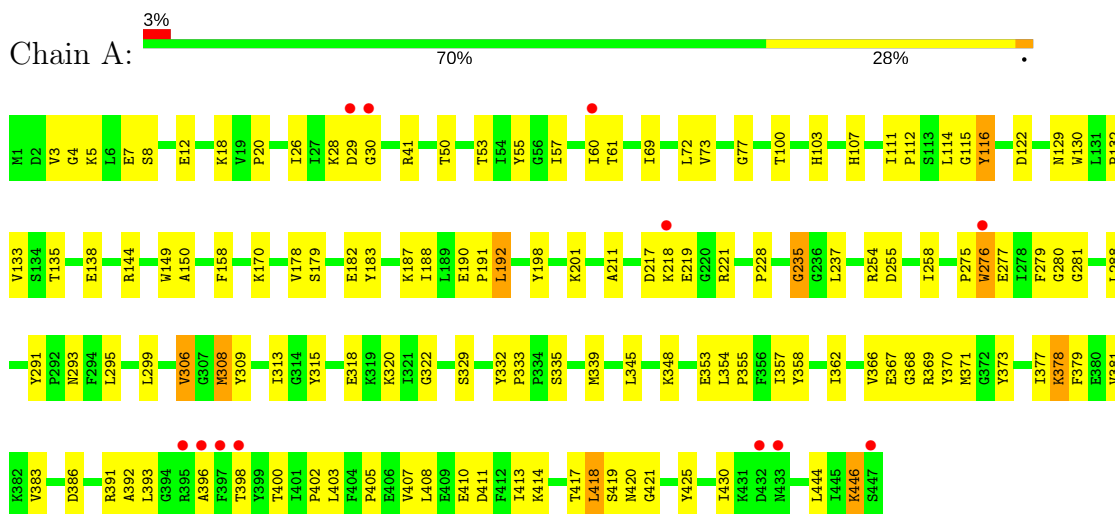
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	259	Total 259	O 259	0	0
4	E	337	Total 337	O 337	0	0
4	F	311	Total 311	O 311	0	0
4	G	351	Total 351	O 351	0	0
4	H	309	Total 309	O 309	0	0

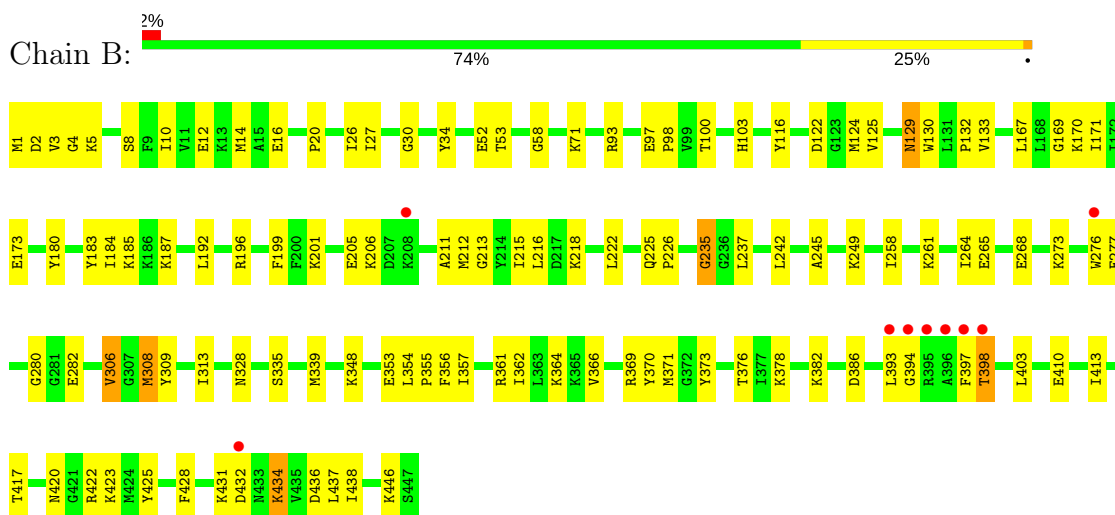
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Pbp related beta-lactamase

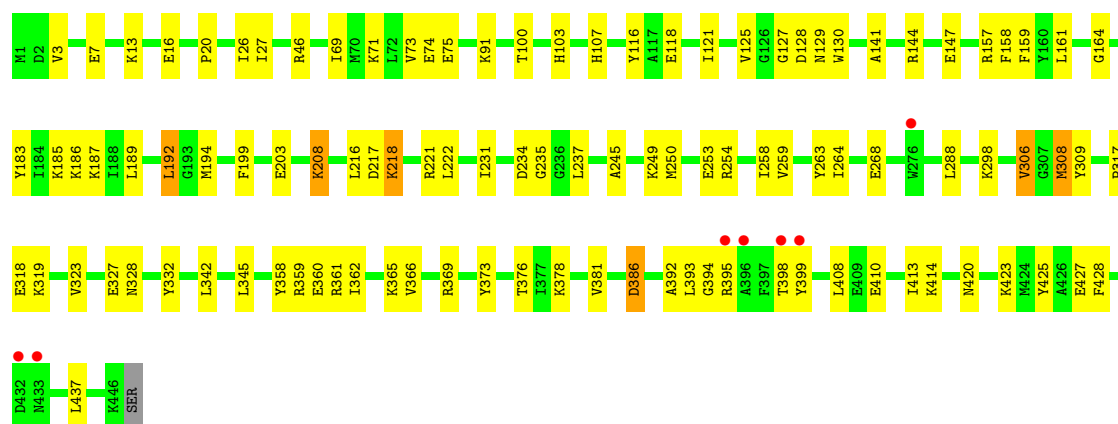


• Molecule 1: Pbp related beta-lactamase

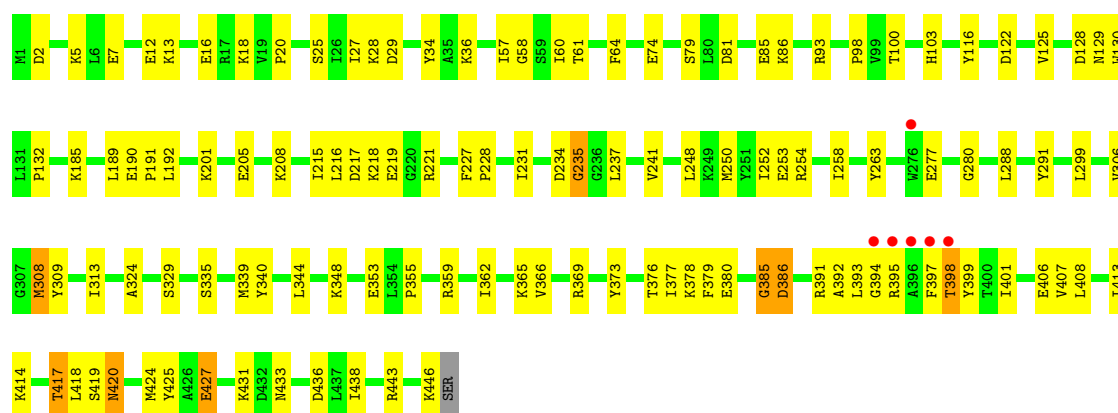
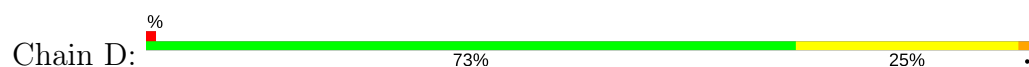


• Molecule 1: Pbp related beta-lactamase

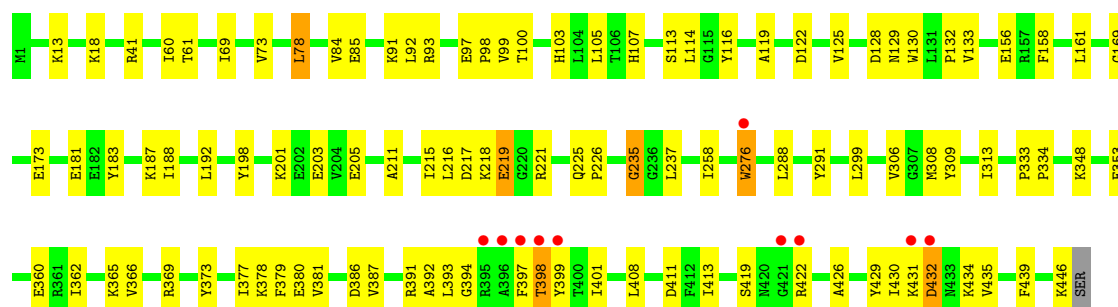
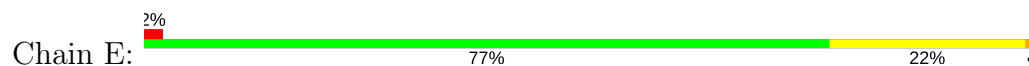




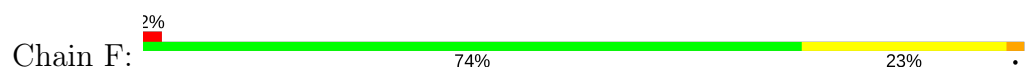
• Molecule 1: Pbp related beta-lactamase

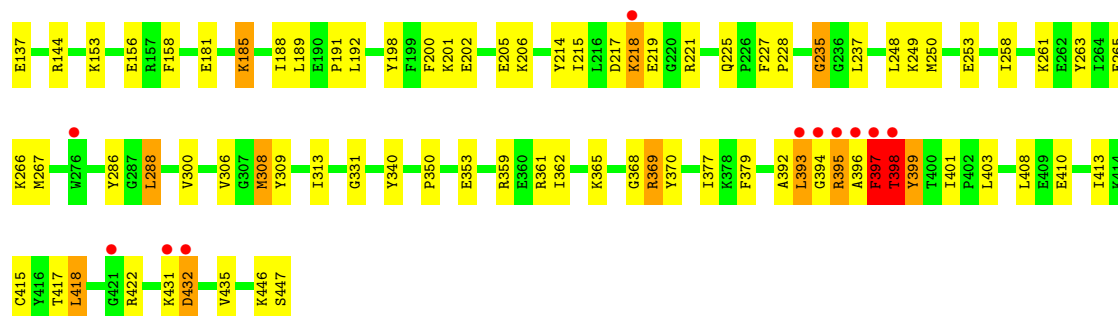


• Molecule 1: Pbp related beta-lactamase

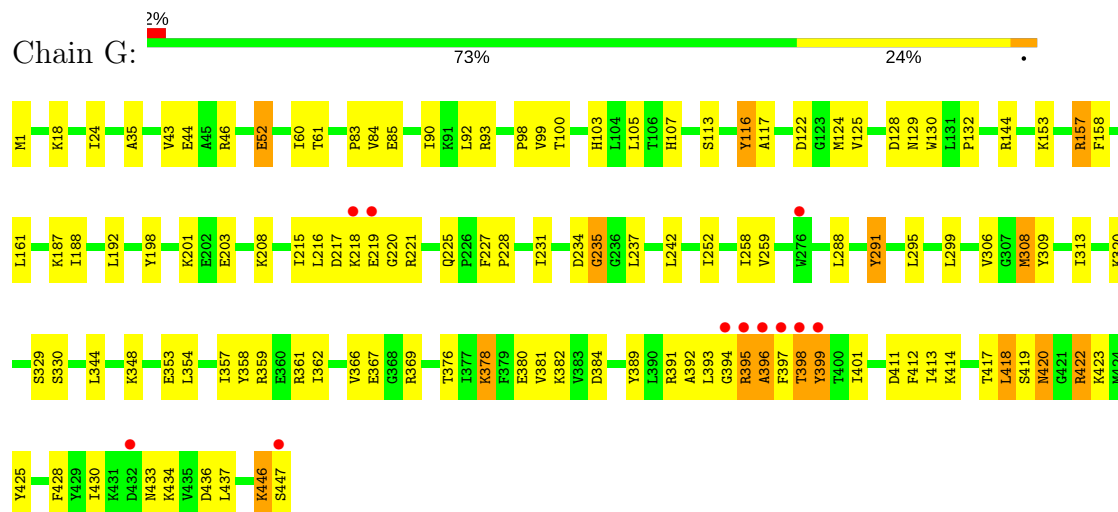


• Molecule 1: Pbp related beta-lactamase

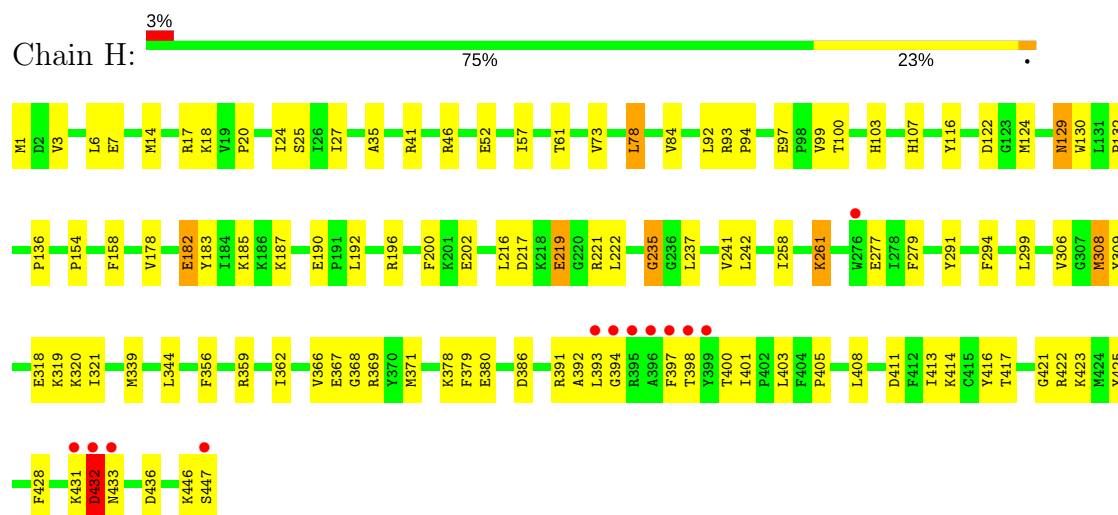




- Molecule 1: Pbp related beta-lactamase



- Molecule 1: Pbp related beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.94Å 105.63Å 112.92Å 72.17° 66.51° 81.39°	Depositor
Resolution (Å)	30.00 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.20) 88.3 (29.75-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.77 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.241 0.193 , 0.237	Depositor DCC
R_{free} test set	9931 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30882	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DO3, LU

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	0.38	0/3637	0.61	1/4909 (0.0%)
1	B	0.37	0/3635	0.60	0/4906
1	C	0.37	0/3620	0.60	0/4889
1	D	0.38	0/3631	0.60	0/4902
1	E	0.38	0/3630	0.61	0/4901
1	F	0.38	0/3635	0.62	0/4906
1	G	0.38	0/3645	0.61	0/4917
1	H	0.39	0/3640	0.62	0/4913
All	All	0.38	0/29073	0.61	1/39243 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	N-CA-C	-5.32	96.63	111.00

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	3551	0	3588	123	0
1	B	3549	0	3586	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3534	0	3566	98	0
1	D	3545	0	3585	119	0
1	E	3544	0	3581	101	0
1	F	3549	0	3586	120	0
1	G	3559	0	3608	133	0
1	H	3554	0	3590	115	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
3	E	28	0	28	0	0
3	F	28	0	28	1	0
3	G	28	0	28	0	0
3	H	28	0	28	0	0
4	A	285	0	0	11	0
4	B	279	0	0	9	0
4	C	237	0	0	14	0
4	D	259	0	0	12	0
4	E	337	0	0	14	0
4	F	311	0	0	15	0
4	G	351	0	0	21	0
4	H	309	0	0	14	0
All	All	30882	0	28802	884	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 884 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:433:ASN:HD22	1:G:434:LYS:HD2	1.03	1.17
1:F:392:ALA:HB3	1:F:398:THR:HG21	1.14	1.12
1:D:369:ARG:HG3	1:D:378:LYS:HE3	1.36	1.08
1:H:431:LYS:HG3	1:H:432:ASP:H	1.22	1.00
1:H:84:VAL:HG21	1:H:92:LEU:HD12	1.44	0.98

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	445/447 (100%)	409 (92%)	32 (7%)	4 (1%)	20	18
1	B	445/447 (100%)	415 (93%)	26 (6%)	4 (1%)	20	18
1	C	444/447 (99%)	410 (92%)	33 (7%)	1 (0%)	51	58
1	D	444/447 (99%)	413 (93%)	27 (6%)	4 (1%)	20	18
1	E	444/447 (99%)	419 (94%)	23 (5%)	2 (0%)	32	34
1	F	445/447 (100%)	417 (94%)	23 (5%)	5 (1%)	17	13
1	G	445/447 (100%)	407 (92%)	33 (7%)	5 (1%)	17	13
1	H	445/447 (100%)	415 (93%)	26 (6%)	4 (1%)	20	18
All	All	3557/3576 (100%)	3305 (93%)	223 (6%)	29 (1%)	22	21

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	TRP
1	A	420	ASN
1	D	398	THR
1	E	398	THR
1	F	393	LEU

5.3.2 Protein sidechains [i](#)

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	378/381 (99%)	369 (98%)	9 (2%)	54	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	378/381 (99%)	371 (98%)	7 (2%)	62	76
1	C	375/381 (98%)	364 (97%)	11 (3%)	48	60
1	D	378/381 (99%)	366 (97%)	12 (3%)	44	56
1	E	377/381 (99%)	368 (98%)	9 (2%)	54	67
1	F	378/381 (99%)	362 (96%)	16 (4%)	34	43
1	G	380/381 (100%)	367 (97%)	13 (3%)	42	53
1	H	379/381 (100%)	369 (97%)	10 (3%)	51	64
All	All	3023/3048 (99%)	2936 (97%)	87 (3%)	48	60

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	78	LEU
1	F	17	ARG
1	H	182	GLU
1	E	105	LEU
1	E	276	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	433	ASN
1	E	103	HIS
1	G	103	HIS
1	D	103	HIS
1	F	129	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 17 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	DO3	E	450	-	19,28,28	1.63	4 (21%)	27,36,36	1.80	9 (33%)
3	DO3	F	451	-	19,28,28	1.43	3 (15%)	27,36,36	1.53	5 (18%)
3	DO3	G	451	-	19,28,28	1.57	4 (21%)	27,36,36	1.73	7 (25%)
3	DO3	H	449	-	19,28,28	1.45	3 (15%)	27,36,36	1.45	5 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DO3	E	450	-	-	0/30/36/36	0/1/1/1
3	DO3	F	451	-	-	0/30/36/36	0/1/1/1
3	DO3	G	451	-	-	0/30/36/36	0/1/1/1
3	DO3	H	449	-	-	0/30/36/36	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	450	DO3	C4-N3	-2.99	1.40	1.47
3	G	451	DO3	C4-N3	-2.94	1.40	1.47
3	F	451	DO3	C4-N3	-2.72	1.41	1.47
3	H	449	DO3	C4-N3	-2.66	1.41	1.47
3	E	450	DO3	C12-N2	2.08	1.51	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	E	450	DO3	C6-N4-C16	-2.80	105.34	112.01
3	E	450	DO3	C8-N1-C1	-2.70	104.95	111.45
3	H	449	DO3	C7-N4-C6	-2.66	105.04	111.45
3	H	449	DO3	C8-N1-C1	-2.58	105.24	111.45
3	G	451	DO3	C8-N1-C1	-2.57	105.25	111.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	451	DO3	1	0

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	447/447 (100%)	-0.28	12 (2%) 55 52	17, 24, 35, 40	0
1	B	447/447 (100%)	-0.31	9 (2%) 65 63	15, 23, 33, 40	0
1	C	446/447 (99%)	-0.28	7 (1%) 72 70	16, 25, 35, 39	0
1	D	446/447 (99%)	-0.33	6 (1%) 77 75	16, 25, 34, 41	0
1	E	446/447 (99%)	-0.36	10 (2%) 62 60	13, 21, 33, 39	0
1	F	447/447 (100%)	-0.36	11 (2%) 58 55	12, 21, 33, 40	0
1	G	447/447 (100%)	-0.26	11 (2%) 58 55	11, 22, 34, 40	0
1	H	447/447 (100%)	-0.38	12 (2%) 55 52	12, 21, 33, 40	0
All	All	3573/3576 (99%)	-0.32	78 (2%) 62 60	11, 23, 34, 41	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	398	THR	5.9
1	F	396	ALA	5.8
1	B	398	THR	5.5
1	H	398	THR	5.4
1	G	396	ALA	5.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	DO3	H	449	28/28	0.76	0.36	20.24	18,22,26,27	28
3	DO3	E	450	28/28	0.93	0.18	3.33	21,23,25,27	28
3	DO3	G	451	28/28	0.92	0.16	1.07	21,24,29,31	28
2	LU	A	448	1/1	0.98	0.07	-	33,33,33,33	1
2	LU	H	448	1/1	0.99	0.09	-	32,32,32,32	1
2	LU	E	448	1/1	0.99	0.04	-	25,25,25,25	1
2	LU	D	449	1/1	0.98	0.03	-	32,32,32,32	1
2	LU	G	450	1/1	0.98	0.07	-	26,26,26,26	1
2	LU	B	448	1/1	0.99	0.07	-	27,27,27,27	1
2	LU	D	448	1/1	0.96	0.16	-	33,33,33,33	1
2	LU	F	448	1/1	0.99	0.05	-	24,24,24,24	1
2	LU	A	449	1/1	0.96	0.07	-	30,30,30,30	1
2	LU	B	449	1/1	0.99	0.10	-	33,33,33,33	1
2	LU	C	449	1/1	0.96	0.06	-	34,34,34,34	1
2	LU	F	450	1/1	0.99	0.06	-	26,26,26,26	1
2	LU	E	449	1/1	0.99	0.06	-	31,31,31,31	1
2	LU	F	449	1/1	1.00	0.01	-	24,24,24,24	1
2	LU	G	449	1/1	0.97	0.04	-	36,36,36,36	1
2	LU	G	448	1/1	1.00	0.03	-	23,23,23,23	1
3	DO3	F	451	28/28	0.72	0.37	-	18,25,28,29	28
2	LU	C	448	1/1	0.99	0.05	-	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.