wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 03:37 am BST

PDB ID	:	3WPR
Title	:	Acinetobacter sp. Tol 5 AtaA N-terminal half of C-terminal stalk fused to GCN4 adaptors (CstalkN)
Authors	:	Koiwai, K.; Hartmann, M.D.; Yoshimoto, S.; Nur 'Izzah, N.; Suzuki, A.; Linke, D.; Lupas, A.N.; Hori, K.
Deposited on	:	2014-01-15
Resolution	:	1.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.6%
RSRZ outliers		7.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
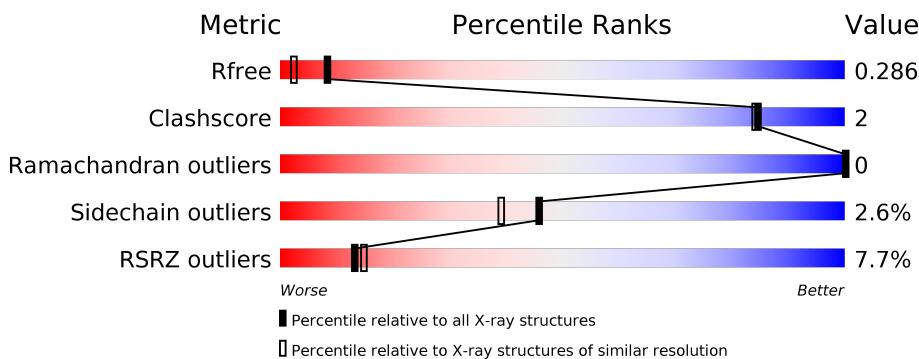
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 <=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	229	4% — 90% — 8% ·
1	B	229	5% — 85% — 5% 10%
1	C	229	13% — 88% — 7% 5%
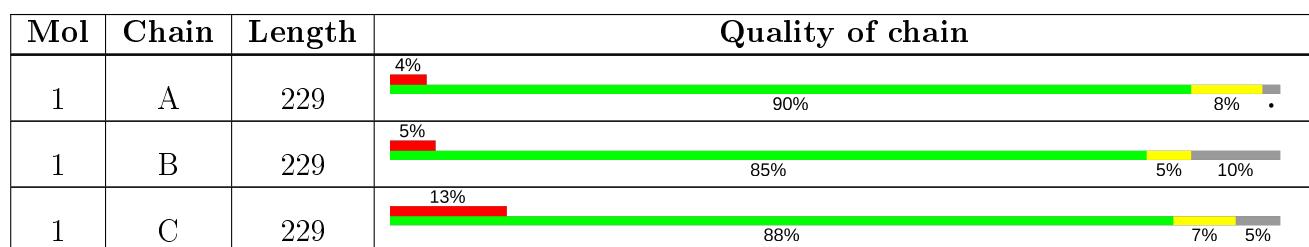
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4869 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 Trimeric autotransporter adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1599	980	278	340	1			
1	B	207	Total	C	N	O	S	0	0	0
			1450	885	252	312	1			
1	C	218	Total	C	N	O	S	0	0	0
			1557	952	270	334	1			

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3141	MET	-	expression tag	UNP K7ZP88
A	3142	LYS	-	expression tag	UNP K7ZP88
A	3143	GLN	-	expression tag	UNP K7ZP88
A	3144	ILE	-	expression tag	UNP K7ZP88
A	3145	GLU	-	expression tag	UNP K7ZP88
A	3146	ASP	-	expression tag	UNP K7ZP88
A	3147	LYS	-	expression tag	UNP K7ZP88
A	3148	ILE	-	expression tag	UNP K7ZP88
A	3149	GLU	-	expression tag	UNP K7ZP88
A	3150	GLU	-	expression tag	UNP K7ZP88
A	3151	ILE	-	expression tag	UNP K7ZP88
A	3152	LEU	-	expression tag	UNP K7ZP88
A	3153	SER	-	expression tag	UNP K7ZP88
A	3154	LYS	-	expression tag	UNP K7ZP88
A	3155	ILE	-	expression tag	UNP K7ZP88
A	3156	TYR	-	expression tag	UNP K7ZP88
A	3157	HIS	-	expression tag	UNP K7ZP88
A	3158	ILE	-	expression tag	UNP K7ZP88
A	3159	GLU	-	expression tag	UNP K7ZP88
A	3160	ASN	-	expression tag	UNP K7ZP88
A	3161	GLU	-	expression tag	UNP K7ZP88
A	3162	ILE	-	expression tag	UNP K7ZP88
A	3163	ALA	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3164	ARG	-	expression tag	UNP K7ZP88
A	3165	ILE	-	expression tag	UNP K7ZP88
A	3166	LYS	-	expression tag	UNP K7ZP88
A	3167	LYS	-	expression tag	UNP K7ZP88
A	3168	LEU	-	expression tag	UNP K7ZP88
A	3169	ILE	-	expression tag	UNP K7ZP88
A	3333	MET	-	expression tag	UNP K7ZP88
A	3334	LYS	-	expression tag	UNP K7ZP88
A	3335	GLN	-	expression tag	UNP K7ZP88
A	3336	ILE	-	expression tag	UNP K7ZP88
A	3337	GLU	-	expression tag	UNP K7ZP88
A	3338	ASP	-	expression tag	UNP K7ZP88
A	3339	LYS	-	expression tag	UNP K7ZP88
A	3340	ILE	-	expression tag	UNP K7ZP88
A	3341	GLU	-	expression tag	UNP K7ZP88
A	3342	GLU	-	expression tag	UNP K7ZP88
A	3343	ILE	-	expression tag	UNP K7ZP88
A	3344	LEU	-	expression tag	UNP K7ZP88
A	3345	SER	-	expression tag	UNP K7ZP88
A	3346	LYS	-	expression tag	UNP K7ZP88
A	3347	ILE	-	expression tag	UNP K7ZP88
A	3348	TYR	-	expression tag	UNP K7ZP88
A	3349	HIS	-	expression tag	UNP K7ZP88
A	3350	ILE	-	expression tag	UNP K7ZP88
A	3351	GLU	-	expression tag	UNP K7ZP88
A	3352	ASN	-	expression tag	UNP K7ZP88
A	3353	GLU	-	expression tag	UNP K7ZP88
A	3354	ILE	-	expression tag	UNP K7ZP88
A	3355	ALA	-	expression tag	UNP K7ZP88
A	3356	ARG	-	expression tag	UNP K7ZP88
A	3357	ILE	-	expression tag	UNP K7ZP88
A	3358	LYS	-	expression tag	UNP K7ZP88
A	3359	LYS	-	expression tag	UNP K7ZP88
A	3360	LEU	-	expression tag	UNP K7ZP88
A	3361	ILE	-	expression tag	UNP K7ZP88
A	3362	LYS	-	expression tag	UNP K7ZP88
A	3363	LEU	-	expression tag	UNP K7ZP88
A	3364	HIS	-	expression tag	UNP K7ZP88
A	3365	HIS	-	expression tag	UNP K7ZP88
A	3366	HIS	-	expression tag	UNP K7ZP88
A	3367	HIS	-	expression tag	UNP K7ZP88
A	3368	HIS	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3369	HIS	-	expression tag	UNP K7ZP88
B	3141	MET	-	expression tag	UNP K7ZP88
B	3142	LYS	-	expression tag	UNP K7ZP88
B	3143	GLN	-	expression tag	UNP K7ZP88
B	3144	ILE	-	expression tag	UNP K7ZP88
B	3145	GLU	-	expression tag	UNP K7ZP88
B	3146	ASP	-	expression tag	UNP K7ZP88
B	3147	LYS	-	expression tag	UNP K7ZP88
B	3148	ILE	-	expression tag	UNP K7ZP88
B	3149	GLU	-	expression tag	UNP K7ZP88
B	3150	GLU	-	expression tag	UNP K7ZP88
B	3151	ILE	-	expression tag	UNP K7ZP88
B	3152	LEU	-	expression tag	UNP K7ZP88
B	3153	SER	-	expression tag	UNP K7ZP88
B	3154	LYS	-	expression tag	UNP K7ZP88
B	3155	ILE	-	expression tag	UNP K7ZP88
B	3156	TYR	-	expression tag	UNP K7ZP88
B	3157	HIS	-	expression tag	UNP K7ZP88
B	3158	ILE	-	expression tag	UNP K7ZP88
B	3159	GLU	-	expression tag	UNP K7ZP88
B	3160	ASN	-	expression tag	UNP K7ZP88
B	3161	GLU	-	expression tag	UNP K7ZP88
B	3162	ILE	-	expression tag	UNP K7ZP88
B	3163	ALA	-	expression tag	UNP K7ZP88
B	3164	ARG	-	expression tag	UNP K7ZP88
B	3165	ILE	-	expression tag	UNP K7ZP88
B	3166	LYS	-	expression tag	UNP K7ZP88
B	3167	LYS	-	expression tag	UNP K7ZP88
B	3168	LEU	-	expression tag	UNP K7ZP88
B	3169	ILE	-	expression tag	UNP K7ZP88
B	3333	MET	-	expression tag	UNP K7ZP88
B	3334	LYS	-	expression tag	UNP K7ZP88
B	3335	GLN	-	expression tag	UNP K7ZP88
B	3336	ILE	-	expression tag	UNP K7ZP88
B	3337	GLU	-	expression tag	UNP K7ZP88
B	3338	ASP	-	expression tag	UNP K7ZP88
B	3339	LYS	-	expression tag	UNP K7ZP88
B	3340	ILE	-	expression tag	UNP K7ZP88
B	3341	GLU	-	expression tag	UNP K7ZP88
B	3342	GLU	-	expression tag	UNP K7ZP88
B	3343	ILE	-	expression tag	UNP K7ZP88
B	3344	LEU	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3345	SER	-	expression tag	UNP K7ZP88
B	3346	LYS	-	expression tag	UNP K7ZP88
B	3347	ILE	-	expression tag	UNP K7ZP88
B	3348	TYR	-	expression tag	UNP K7ZP88
B	3349	HIS	-	expression tag	UNP K7ZP88
B	3350	ILE	-	expression tag	UNP K7ZP88
B	3351	GLU	-	expression tag	UNP K7ZP88
B	3352	ASN	-	expression tag	UNP K7ZP88
B	3353	GLU	-	expression tag	UNP K7ZP88
B	3354	ILE	-	expression tag	UNP K7ZP88
B	3355	ALA	-	expression tag	UNP K7ZP88
B	3356	ARG	-	expression tag	UNP K7ZP88
B	3357	ILE	-	expression tag	UNP K7ZP88
B	3358	LYS	-	expression tag	UNP K7ZP88
B	3359	LYS	-	expression tag	UNP K7ZP88
B	3360	LEU	-	expression tag	UNP K7ZP88
B	3361	ILE	-	expression tag	UNP K7ZP88
B	3362	LYS	-	expression tag	UNP K7ZP88
B	3363	LEU	-	expression tag	UNP K7ZP88
B	3364	HIS	-	expression tag	UNP K7ZP88
B	3365	HIS	-	expression tag	UNP K7ZP88
B	3366	HIS	-	expression tag	UNP K7ZP88
B	3367	HIS	-	expression tag	UNP K7ZP88
B	3368	HIS	-	expression tag	UNP K7ZP88
B	3369	HIS	-	expression tag	UNP K7ZP88
C	3141	MET	-	expression tag	UNP K7ZP88
C	3142	LYS	-	expression tag	UNP K7ZP88
C	3143	GLN	-	expression tag	UNP K7ZP88
C	3144	ILE	-	expression tag	UNP K7ZP88
C	3145	GLU	-	expression tag	UNP K7ZP88
C	3146	ASP	-	expression tag	UNP K7ZP88
C	3147	LYS	-	expression tag	UNP K7ZP88
C	3148	ILE	-	expression tag	UNP K7ZP88
C	3149	GLU	-	expression tag	UNP K7ZP88
C	3150	GLU	-	expression tag	UNP K7ZP88
C	3151	ILE	-	expression tag	UNP K7ZP88
C	3152	LEU	-	expression tag	UNP K7ZP88
C	3153	SER	-	expression tag	UNP K7ZP88
C	3154	LYS	-	expression tag	UNP K7ZP88
C	3155	ILE	-	expression tag	UNP K7ZP88
C	3156	TYR	-	expression tag	UNP K7ZP88
C	3157	HIS	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3158	ILE	-	expression tag	UNP K7ZP88
C	3159	GLU	-	expression tag	UNP K7ZP88
C	3160	ASN	-	expression tag	UNP K7ZP88
C	3161	GLU	-	expression tag	UNP K7ZP88
C	3162	ILE	-	expression tag	UNP K7ZP88
C	3163	ALA	-	expression tag	UNP K7ZP88
C	3164	ARG	-	expression tag	UNP K7ZP88
C	3165	ILE	-	expression tag	UNP K7ZP88
C	3166	LYS	-	expression tag	UNP K7ZP88
C	3167	LYS	-	expression tag	UNP K7ZP88
C	3168	LEU	-	expression tag	UNP K7ZP88
C	3169	ILE	-	expression tag	UNP K7ZP88
C	3333	MET	-	expression tag	UNP K7ZP88
C	3334	LYS	-	expression tag	UNP K7ZP88
C	3335	GLN	-	expression tag	UNP K7ZP88
C	3336	ILE	-	expression tag	UNP K7ZP88
C	3337	GLU	-	expression tag	UNP K7ZP88
C	3338	ASP	-	expression tag	UNP K7ZP88
C	3339	LYS	-	expression tag	UNP K7ZP88
C	3340	ILE	-	expression tag	UNP K7ZP88
C	3341	GLU	-	expression tag	UNP K7ZP88
C	3342	GLU	-	expression tag	UNP K7ZP88
C	3343	ILE	-	expression tag	UNP K7ZP88
C	3344	LEU	-	expression tag	UNP K7ZP88
C	3345	SER	-	expression tag	UNP K7ZP88
C	3346	LYS	-	expression tag	UNP K7ZP88
C	3347	ILE	-	expression tag	UNP K7ZP88
C	3348	TYR	-	expression tag	UNP K7ZP88
C	3349	HIS	-	expression tag	UNP K7ZP88
C	3350	ILE	-	expression tag	UNP K7ZP88
C	3351	GLU	-	expression tag	UNP K7ZP88
C	3352	ASN	-	expression tag	UNP K7ZP88
C	3353	GLU	-	expression tag	UNP K7ZP88
C	3354	ILE	-	expression tag	UNP K7ZP88
C	3355	ALA	-	expression tag	UNP K7ZP88
C	3356	ARG	-	expression tag	UNP K7ZP88
C	3357	ILE	-	expression tag	UNP K7ZP88
C	3358	LYS	-	expression tag	UNP K7ZP88
C	3359	LYS	-	expression tag	UNP K7ZP88
C	3360	LEU	-	expression tag	UNP K7ZP88
C	3361	ILE	-	expression tag	UNP K7ZP88
C	3362	LYS	-	expression tag	UNP K7ZP88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3363	LEU	-	expression tag	UNP K7ZP88
C	3364	HIS	-	expression tag	UNP K7ZP88
C	3365	HIS	-	expression tag	UNP K7ZP88
C	3366	HIS	-	expression tag	UNP K7ZP88
C	3367	HIS	-	expression tag	UNP K7ZP88
C	3368	HIS	-	expression tag	UNP K7ZP88
C	3369	HIS	-	expression tag	UNP K7ZP88

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	100	Total O 100 100	0	0
2	B	85	Total O 85 85	0	0
2	C	78	Total O 78 78	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: Trimeric autotransporter adhesin
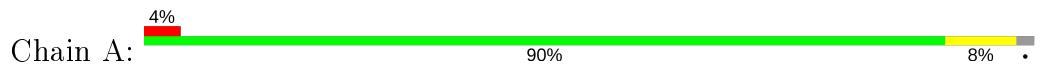
- Molecule 1: Trimeric autotransporter adhesin
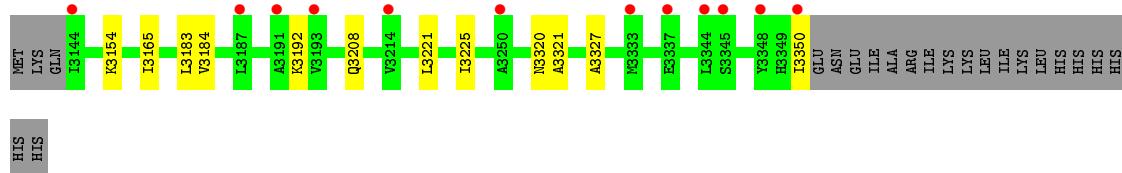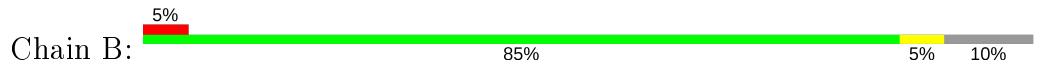
- Molecule 1: Trimeric autotransporter adhesin
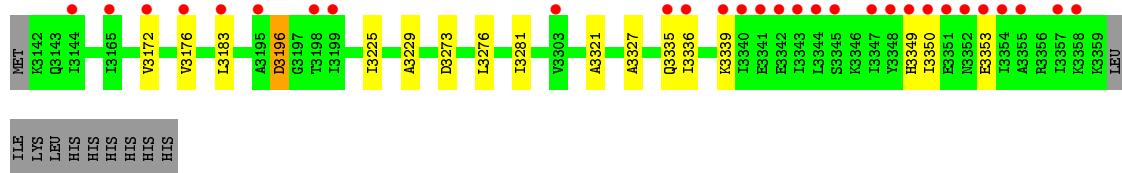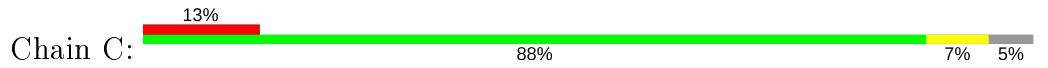
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.39Å 42.98Å 118.07Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	38.63 – 1.90 38.63 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.63-1.90) 99.3 (38.63-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.236 , 0.279 0.240 , 0.286	Depositor DCC
R_{free} test set	2787 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.4	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4869	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/1606	0.44	0/2192
1	B	0.25	0/1455	0.44	0/1989
1	C	0.26	0/1564	0.44	0/2133
All	All	0.26	0/4625	0.44	0/6314

There are no bond length outliers.

There are no bond angle outliers.

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	1599	0	1574	10	0
1	B	1450	0	1427	6	0
1	C	1557	0	1535	9	0
2	A	100	0	0	0	0
2	B	85	0	0	1	0
2	C	78	0	0	0	0
All	All	4869	0	4536	21	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 2.

The worst 5 of 21 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:C:3335:GLN:HG2	1:C:3339:LYS:HE3	1.79	0.65
1:C:3196:ASP:OD1	1:C:3196:ASP:N	2.36	0.58
1:B:3320:ASN:ND2	2:B:3427:HOH:O	2.42	0.51
1:A:3270:LYS:NZ	1:A:3272:GLY:O	2.34	0.49
1:A:3225:ILE:HG12	1:C:3225:ILE:HG12	1.94	0.48

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	223/229 (97%)	221 (99%)	2 (1%)	0	100	100
1	B	205/229 (90%)	204 (100%)	1 (0%)	0	100	100
1	C	216/229 (94%)	213 (99%)	3 (1%)	0	100	100
All	All	644/687 (94%)	638 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	170/189 (90%)	165 (97%)	5 (3%)	42	35
1	B	155/189 (82%)	152 (98%)	3 (2%)	57	53
1	C	167/189 (88%)	162 (97%)	5 (3%)	41	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	492/567 (87%)	479 (97%)	13 (3%)	46 39

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3154	LYS
1	B	3208	GLN
1	C	3349	HIS
1	A	3350	ILE
1	C	3273	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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(Å²)	Q<0.9
1	A	225/229 (98%)	0.47	9 (4%)	38	41	38, 57, 107, 136	0
1	B	207/229 (90%)	0.61	12 (5%)	23	25	38, 58, 103, 126	0
1	C	218/229 (95%)	0.87	29 (13%)	3	3	37, 63, 137, 159	0
All	All	650/687 (94%)	0.65	50 (7%)	13	15	37, 59, 116, 159	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3348	TYR	10.3
1	C	3354	ILE	10.2
1	C	3348	TYR	7.9
1	B	3345	SER	6.5
1	C	3347	ILE	6.4

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 carbohydrates 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.