Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2024 – 10:32 AM EDT

PDB ID	:	4EC6
Title	:	Ntf2-like, potential transfer protein TraM from Gram-positive conjugative plasmid pIP501
Authors	:	Goessweiner-Mohr, N.; Grumet, L.; Pavkov-Keller, T.; Wang, M.; Keller, W.
Deposited on	:	2012-03-26
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

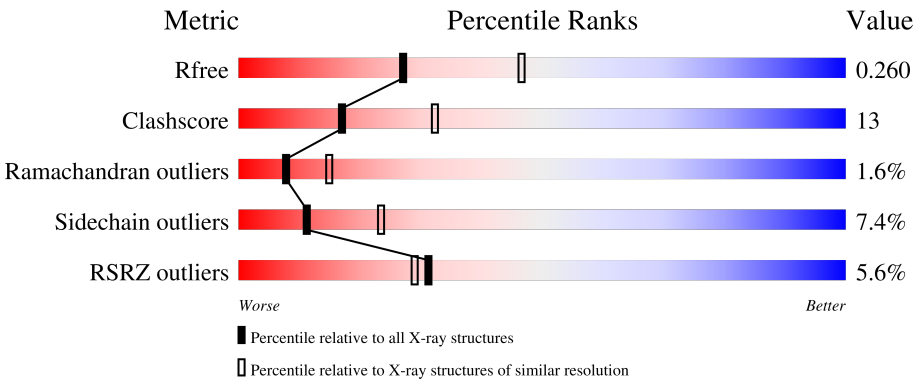
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 <=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	161	4% 55% 10% • • 32%
1	B	161	% 51% 14% • 32%
1	C	161	4% 52% 12% • • 32%
1	D	161	2% 55% 11% • 32%
1	E	161	6% 44% 16% 7% • 32%

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Mol	Chain	Length	Quality of chain
1	F	161	5% 53% 12% • 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5811 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	109	902	576	145	180	1	0	0	0
1	B	109	902	576	145	180	1	0	0	0
1	C	109	902	576	145	180	1	0	0	0
1	D	109	902	576	145	180	1	0	0	0
1	E	109	902	576	145	180	1	0	0	0
1	F	109	902	576	145	180	1	0	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MSE	-	expression tag	UNP Q8L1C7
A	163	LYS	-	expression tag	UNP Q8L1C7
A	164	HIS	-	expression tag	UNP Q8L1C7
A	165	HIS	-	expression tag	UNP Q8L1C7
A	166	HIS	-	expression tag	UNP Q8L1C7
A	167	HIS	-	expression tag	UNP Q8L1C7
A	168	HIS	-	expression tag	UNP Q8L1C7
A	169	HIS	-	expression tag	UNP Q8L1C7
A	170	HIS	-	expression tag	UNP Q8L1C7
A	171	SER	-	expression tag	UNP Q8L1C7
A	172	ASP	-	expression tag	UNP Q8L1C7
A	173	TYR	-	expression tag	UNP Q8L1C7
A	174	ASP	-	expression tag	UNP Q8L1C7
A	175	ILE	-	expression tag	UNP Q8L1C7
A	176	PRO	-	expression tag	UNP Q8L1C7
A	177	THR	-	expression tag	UNP Q8L1C7
A	178	THR	-	expression tag	UNP Q8L1C7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	179	GLU	-	expression tag	UNP Q8L1C7
A	180	ASN	-	expression tag	UNP Q8L1C7
A	181	LEU	-	expression tag	UNP Q8L1C7
A	182	TYR	-	expression tag	UNP Q8L1C7
A	183	PHE	-	expression tag	UNP Q8L1C7
A	184	GLN	-	expression tag	UNP Q8L1C7
A	185	GLY	-	expression tag	UNP Q8L1C7
A	186	SER	-	expression tag	UNP Q8L1C7
A	187	GLY	-	expression tag	UNP Q8L1C7
A	188	SER	-	expression tag	UNP Q8L1C7
A	189	THR	-	expression tag	UNP Q8L1C7
B	162	MSE	-	expression tag	UNP Q8L1C7
B	163	LYS	-	expression tag	UNP Q8L1C7
B	164	HIS	-	expression tag	UNP Q8L1C7
B	165	HIS	-	expression tag	UNP Q8L1C7
B	166	HIS	-	expression tag	UNP Q8L1C7
B	167	HIS	-	expression tag	UNP Q8L1C7
B	168	HIS	-	expression tag	UNP Q8L1C7
B	169	HIS	-	expression tag	UNP Q8L1C7
B	170	HIS	-	expression tag	UNP Q8L1C7
B	171	SER	-	expression tag	UNP Q8L1C7
B	172	ASP	-	expression tag	UNP Q8L1C7
B	173	TYR	-	expression tag	UNP Q8L1C7
B	174	ASP	-	expression tag	UNP Q8L1C7
B	175	ILE	-	expression tag	UNP Q8L1C7
B	176	PRO	-	expression tag	UNP Q8L1C7
B	177	THR	-	expression tag	UNP Q8L1C7
B	178	THR	-	expression tag	UNP Q8L1C7
B	179	GLU	-	expression tag	UNP Q8L1C7
B	180	ASN	-	expression tag	UNP Q8L1C7
B	181	LEU	-	expression tag	UNP Q8L1C7
B	182	TYR	-	expression tag	UNP Q8L1C7
B	183	PHE	-	expression tag	UNP Q8L1C7
B	184	GLN	-	expression tag	UNP Q8L1C7
B	185	GLY	-	expression tag	UNP Q8L1C7
B	186	SER	-	expression tag	UNP Q8L1C7
B	187	GLY	-	expression tag	UNP Q8L1C7
B	188	SER	-	expression tag	UNP Q8L1C7
B	189	THR	-	expression tag	UNP Q8L1C7
C	162	MSE	-	expression tag	UNP Q8L1C7
C	163	LYS	-	expression tag	UNP Q8L1C7
C	164	HIS	-	expression tag	UNP Q8L1C7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	expression tag	UNP Q8L1C7
C	166	HIS	-	expression tag	UNP Q8L1C7
C	167	HIS	-	expression tag	UNP Q8L1C7
C	168	HIS	-	expression tag	UNP Q8L1C7
C	169	HIS	-	expression tag	UNP Q8L1C7
C	170	HIS	-	expression tag	UNP Q8L1C7
C	171	SER	-	expression tag	UNP Q8L1C7
C	172	ASP	-	expression tag	UNP Q8L1C7
C	173	TYR	-	expression tag	UNP Q8L1C7
C	174	ASP	-	expression tag	UNP Q8L1C7
C	175	ILE	-	expression tag	UNP Q8L1C7
C	176	PRO	-	expression tag	UNP Q8L1C7
C	177	THR	-	expression tag	UNP Q8L1C7
C	178	THR	-	expression tag	UNP Q8L1C7
C	179	GLU	-	expression tag	UNP Q8L1C7
C	180	ASN	-	expression tag	UNP Q8L1C7
C	181	LEU	-	expression tag	UNP Q8L1C7
C	182	TYR	-	expression tag	UNP Q8L1C7
C	183	PHE	-	expression tag	UNP Q8L1C7
C	184	GLN	-	expression tag	UNP Q8L1C7
C	185	GLY	-	expression tag	UNP Q8L1C7
C	186	SER	-	expression tag	UNP Q8L1C7
C	187	GLY	-	expression tag	UNP Q8L1C7
C	188	SER	-	expression tag	UNP Q8L1C7
C	189	THR	-	expression tag	UNP Q8L1C7
D	162	MSE	-	expression tag	UNP Q8L1C7
D	163	LYS	-	expression tag	UNP Q8L1C7
D	164	HIS	-	expression tag	UNP Q8L1C7
D	165	HIS	-	expression tag	UNP Q8L1C7
D	166	HIS	-	expression tag	UNP Q8L1C7
D	167	HIS	-	expression tag	UNP Q8L1C7
D	168	HIS	-	expression tag	UNP Q8L1C7
D	169	HIS	-	expression tag	UNP Q8L1C7
D	170	HIS	-	expression tag	UNP Q8L1C7
D	171	SER	-	expression tag	UNP Q8L1C7
D	172	ASP	-	expression tag	UNP Q8L1C7
D	173	TYR	-	expression tag	UNP Q8L1C7
D	174	ASP	-	expression tag	UNP Q8L1C7
D	175	ILE	-	expression tag	UNP Q8L1C7
D	176	PRO	-	expression tag	UNP Q8L1C7
D	177	THR	-	expression tag	UNP Q8L1C7
D	178	THR	-	expression tag	UNP Q8L1C7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	179	GLU	-	expression tag	UNP Q8L1C7
D	180	ASN	-	expression tag	UNP Q8L1C7
D	181	LEU	-	expression tag	UNP Q8L1C7
D	182	TYR	-	expression tag	UNP Q8L1C7
D	183	PHE	-	expression tag	UNP Q8L1C7
D	184	GLN	-	expression tag	UNP Q8L1C7
D	185	GLY	-	expression tag	UNP Q8L1C7
D	186	SER	-	expression tag	UNP Q8L1C7
D	187	GLY	-	expression tag	UNP Q8L1C7
D	188	SER	-	expression tag	UNP Q8L1C7
D	189	THR	-	expression tag	UNP Q8L1C7
E	162	MSE	-	expression tag	UNP Q8L1C7
E	163	LYS	-	expression tag	UNP Q8L1C7
E	164	HIS	-	expression tag	UNP Q8L1C7
E	165	HIS	-	expression tag	UNP Q8L1C7
E	166	HIS	-	expression tag	UNP Q8L1C7
E	167	HIS	-	expression tag	UNP Q8L1C7
E	168	HIS	-	expression tag	UNP Q8L1C7
E	169	HIS	-	expression tag	UNP Q8L1C7
E	170	HIS	-	expression tag	UNP Q8L1C7
E	171	SER	-	expression tag	UNP Q8L1C7
E	172	ASP	-	expression tag	UNP Q8L1C7
E	173	TYR	-	expression tag	UNP Q8L1C7
E	174	ASP	-	expression tag	UNP Q8L1C7
E	175	ILE	-	expression tag	UNP Q8L1C7
E	176	PRO	-	expression tag	UNP Q8L1C7
E	177	THR	-	expression tag	UNP Q8L1C7
E	178	THR	-	expression tag	UNP Q8L1C7
E	179	GLU	-	expression tag	UNP Q8L1C7
E	180	ASN	-	expression tag	UNP Q8L1C7
E	181	LEU	-	expression tag	UNP Q8L1C7
E	182	TYR	-	expression tag	UNP Q8L1C7
E	183	PHE	-	expression tag	UNP Q8L1C7
E	184	GLN	-	expression tag	UNP Q8L1C7
E	185	GLY	-	expression tag	UNP Q8L1C7
E	186	SER	-	expression tag	UNP Q8L1C7
E	187	GLY	-	expression tag	UNP Q8L1C7
E	188	SER	-	expression tag	UNP Q8L1C7
E	189	THR	-	expression tag	UNP Q8L1C7
F	162	MSE	-	expression tag	UNP Q8L1C7
F	163	LYS	-	expression tag	UNP Q8L1C7
F	164	HIS	-	expression tag	UNP Q8L1C7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	165	HIS	-	expression tag	UNP Q8L1C7
F	166	HIS	-	expression tag	UNP Q8L1C7
F	167	HIS	-	expression tag	UNP Q8L1C7
F	168	HIS	-	expression tag	UNP Q8L1C7
F	169	HIS	-	expression tag	UNP Q8L1C7
F	170	HIS	-	expression tag	UNP Q8L1C7
F	171	SER	-	expression tag	UNP Q8L1C7
F	172	ASP	-	expression tag	UNP Q8L1C7
F	173	TYR	-	expression tag	UNP Q8L1C7
F	174	ASP	-	expression tag	UNP Q8L1C7
F	175	ILE	-	expression tag	UNP Q8L1C7
F	176	PRO	-	expression tag	UNP Q8L1C7
F	177	THR	-	expression tag	UNP Q8L1C7
F	178	THR	-	expression tag	UNP Q8L1C7
F	179	GLU	-	expression tag	UNP Q8L1C7
F	180	ASN	-	expression tag	UNP Q8L1C7
F	181	LEU	-	expression tag	UNP Q8L1C7
F	182	TYR	-	expression tag	UNP Q8L1C7
F	183	PHE	-	expression tag	UNP Q8L1C7
F	184	GLN	-	expression tag	UNP Q8L1C7
F	185	GLY	-	expression tag	UNP Q8L1C7
F	186	SER	-	expression tag	UNP Q8L1C7
F	187	GLY	-	expression tag	UNP Q8L1C7
F	188	SER	-	expression tag	UNP Q8L1C7
F	189	THR	-	expression tag	UNP Q8L1C7

- Molecule 2 is water.

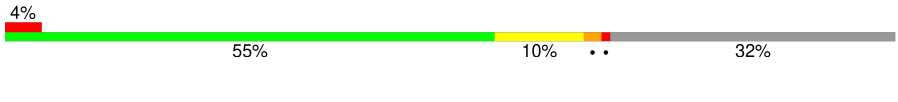
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	75	75	75	0	0
			Total	O		
2	B	66	66	66	0	0
			Total	O		
2	C	65	65	65	0	0
			Total	O		
2	D	63	63	63	0	0
			Total	O		
2	E	57	57	57	0	0
			Total	O		
2	F	73	73	73	0	0

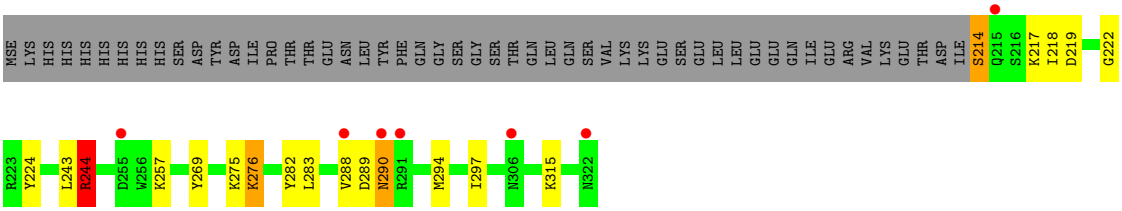
3 Residue-property plots (i)

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: Putative uncharacterized protein

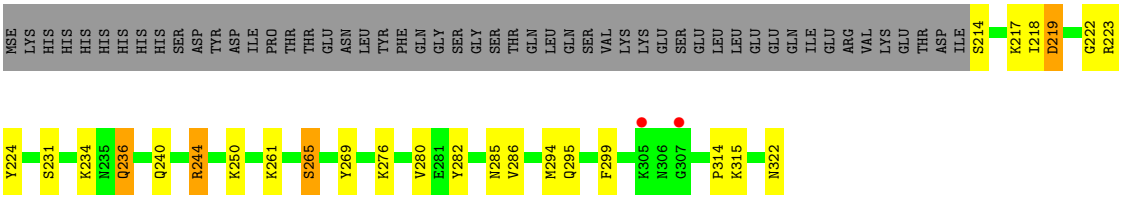
Chain A:





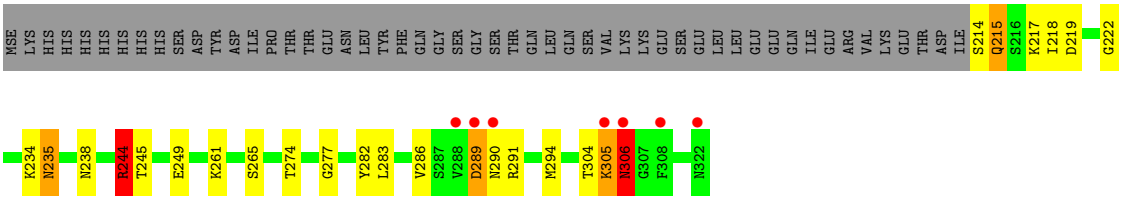
• Molecule 1: Putative uncharacterized protein

Chain B:



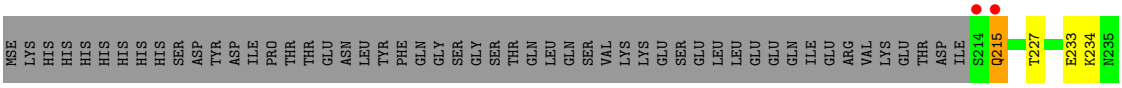
• Molecule 1: Putative uncharacterized protein

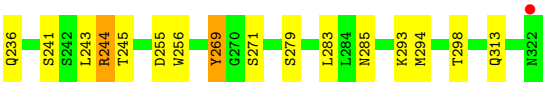
Chain C:



• Molecule 1: Putative uncharacterized protein

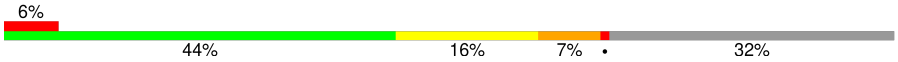
Chain D:

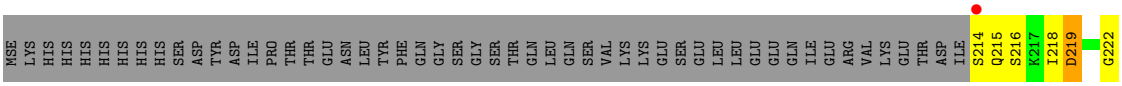


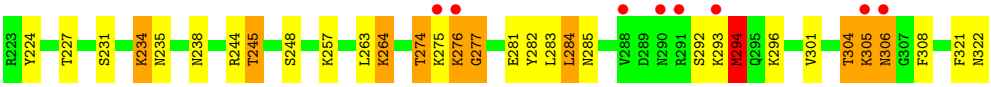


• Molecule 1: Putative uncharacterized protein

Chain E:

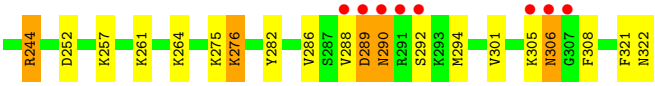






• Molecule 1: Putative uncharacterized protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.21Å 54.98Å 93.47Å 89.91° 86.44° 78.63°	Depositor
Resolution (Å)	46.89 – 2.50 46.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.89-2.50) 97.9 (46.89-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.261 0.210 , 0.260	Depositor DCC
R_{free} test set	1295 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5811	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.83	0/920	0.99	4/1236 (0.3%)
1	B	0.78	0/920	0.89	1/1236 (0.1%)
1	C	0.77	0/920	0.93	2/1236 (0.2%)
1	D	0.75	0/920	0.84	0/1236
1	E	0.78	0/920	0.92	2/1236 (0.2%)
1	F	0.77	0/920	0.90	2/1236 (0.2%)
All	All	0.78	0/5520	0.91	11/7416 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	244	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	C	244	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	244	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	244	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	219	ASP	CB-CG-OD1	6.61	124.25	118.30
1	E	219	ASP	CB-CG-OD1	6.14	123.83	118.30
1	E	294	MSE	CA-CB-CG	-5.79	103.45	113.30
1	F	252	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	219	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	219	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	219	ASP	CB-CG-OD2	-5.53	113.32	118.30

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	902	0	879	17	0
1	B	902	0	879	19	0
1	C	902	0	879	25	0
1	D	902	0	879	15	0
1	E	902	0	879	43	0
1	F	902	0	879	25	0
2	A	75	0	0	3	0
2	B	66	0	0	3	0
2	C	65	0	0	4	0
2	D	63	0	0	8	0
2	E	57	0	0	10	0
2	F	73	0	0	4	0
All	All	5811	0	5274	134	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.

All (134) 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:E:274:THR:HG22	1:E:277:GLY:CA	1.41	1.47
1:E:274:THR:CG2	1:E:277:GLY:HA2	1.76	1.12
1:E:274:THR:HG22	1:E:277:GLY:HA2	1.12	1.05
1:E:274:THR:HG22	1:E:277:GLY:HA3	1.32	1.05
1:E:274:THR:CG2	1:E:277:GLY:CA	2.34	1.04
1:F:218:ILE:HD11	1:F:301:VAL:HG21	1.41	0.99
1:E:283:LEU:HD13	1:E:294:MSE:HE2	1.45	0.98
1:D:283:LEU:HD23	1:D:294:MSE:HE1	1.51	0.92
1:E:283:LEU:HD13	1:E:294:MSE:CE	2.00	0.92
1:F:276:LYS:HE3	2:F:470:HOH:O	1.72	0.90
1:D:227:THR:HG22	2:D:462:HOH:O	1.73	0.88
1:F:276:LYS:H	1:F:276:LYS:HD2	1.40	0.87
1:A:244:ARG:O	1:A:244:ARG:HD3	1.76	0.85
1:E:245:THR:HB	2:E:420:HOH:O	1.77	0.83
1:C:235:ASN:ND2	1:C:238:ASN:OD1	2.14	0.81
1:E:274:THR:HG21	2:E:436:HOH:O	1.79	0.80
1:D:283:LEU:HD23	1:D:294:MSE:CE	2.13	0.78
1:F:218:ILE:CD1	1:F:301:VAL:HG21	2.15	0.76
1:E:308:PHE:HD2	2:E:435:HOH:O	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ARG:O	1:F:244:ARG:HD3	1.86	0.74
1:E:293:LYS:HG2	2:E:404:HOH:O	1.88	0.74
1:D:298:THR:HG22	2:D:451:HOH:O	1.90	0.72
1:A:288:VAL:HG21	2:A:471:HOH:O	1.89	0.71
1:F:276:LYS:H	1:F:276:LYS:CD	2.03	0.71
1:E:294:MSE:HE3	1:F:224:TYR:CZ	2.25	0.71
1:E:308:PHE:CD2	2:E:435:HOH:O	2.43	0.70
1:A:276:LYS:HG2	2:A:467:HOH:O	1.91	0.69
1:C:244:ARG:O	1:C:244:ARG:HD3	1.92	0.68
1:C:283:LEU:HD13	1:C:294:MSE:CE	2.24	0.67
1:F:289:ASP:O	1:F:290:ASN:HB2	1.96	0.66
1:C:274:THR:HG22	1:C:277:GLY:C	2.17	0.65
1:E:294:MSE:HE3	1:F:224:TYR:CE2	2.33	0.64
1:E:215:GLN:HB2	2:E:453:HOH:O	1.97	0.63
2:D:408:HOH:O	1:E:304:THR:HG21	1.98	0.63
1:E:274:THR:HG21	1:E:277:GLY:HA2	1.79	0.62
1:E:214:SER:HB3	1:E:216:SER:HB2	1.81	0.62
1:E:274:THR:HG22	1:E:277:GLY:C	2.17	0.62
1:A:224:TYR:CZ	1:C:294:MSE:HE3	2.34	0.61
1:F:321:PHE:O	1:F:322:ASN:HB2	2.00	0.61
1:A:214:SER:HB3	1:A:217:LYS:HG3	1.83	0.61
1:A:283:LEU:HD13	1:A:294:MSE:CE	2.31	0.59
1:B:244:ARG:O	1:B:244:ARG:HD3	2.02	0.59
1:A:289:ASP:O	1:A:290:ASN:HB2	2.02	0.59
1:E:235:ASN:ND2	1:E:238:ASN:OD1	2.36	0.59
1:C:283:LEU:HD13	1:C:294:MSE:HE1	1.85	0.59
1:F:276:LYS:CD	1:F:276:LYS:N	2.62	0.59
1:C:274:THR:HG21	2:C:426:HOH:O	2.03	0.58
1:A:244:ARG:HD3	1:A:244:ARG:C	2.17	0.58
1:C:245:THR:HG22	2:C:419:HOH:O	2.04	0.58
1:D:245:THR:HG22	2:D:459:HOH:O	2.04	0.58
1:E:227:THR:HG22	2:E:443:HOH:O	2.04	0.57
1:C:214:SER:O	1:C:215:GLN:HB2	2.05	0.57
1:C:214:SER:O	1:C:215:GLN:CB	2.52	0.57
1:B:222:GLY:HA3	1:B:282:TYR:OH	2.05	0.56
1:A:283:LEU:HD13	1:A:294:MSE:HE2	1.88	0.55
1:A:294:MSE:HE3	1:B:224:TYR:CZ	2.41	0.55
1:F:218:ILE:HD13	1:F:308:PHE:CE1	2.42	0.55
1:E:263:LEU:HD11	1:E:284:LEU:HG	1.89	0.54
1:E:304:THR:O	1:E:306:ASN:N	2.40	0.54
1:F:288:VAL:HG23	1:F:289:ASP:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:LYS:N	1:E:277:GLY:HA3	2.22	0.54
1:E:294:MSE:HE1	1:E:321:PHE:CE2	2.42	0.54
1:D:255:ASP:HB2	2:D:419:HOH:O	2.07	0.53
1:E:301:VAL:HG23	1:E:301:VAL:O	2.06	0.53
1:C:215:GLN:O	1:C:218:ILE:HG22	2.08	0.53
1:C:261:LYS:HD3	1:C:286:VAL:HG11	1.91	0.53
1:E:274:THR:CG2	1:E:277:GLY:HA3	2.22	0.53
1:C:289:ASP:CG	1:C:290:ASN:H	2.13	0.52
1:E:219:ASP:OD2	2:E:457:HOH:O	2.18	0.52
1:A:269:TYR:CZ	1:B:217:LYS:HG2	2.45	0.52
1:F:322:ASN:ND2	2:F:413:HOH:O	2.42	0.52
1:C:222:GLY:HA3	1:C:282:TYR:OH	2.11	0.51
1:D:215:GLN:HB3	2:D:435:HOH:O	2.09	0.51
1:E:222:GLY:HA3	1:E:282:TYR:OH	2.11	0.51
1:D:256:TRP:CZ2	1:D:313:GLN:HG3	2.45	0.51
1:A:222:GLY:HA3	1:A:282:TYR:OH	2.11	0.50
1:B:218:ILE:CG2	1:B:280:VAL:HG11	2.41	0.50
1:E:274:THR:HG23	1:E:276:LYS:H	1.76	0.50
1:F:222:GLY:HA3	1:F:282:TYR:OH	2.12	0.50
1:F:276:LYS:HD2	1:F:276:LYS:N	2.07	0.49
1:C:218:ILE:CG2	1:C:219:ASP:N	2.76	0.48
1:C:218:ILE:HG23	1:C:219:ASP:N	2.27	0.48
1:C:244:ARG:HD3	1:C:244:ARG:C	2.31	0.48
1:E:215:GLN:O	1:E:218:ILE:HG22	2.14	0.48
1:D:283:LEU:CD2	1:D:294:MSE:HE1	2.33	0.47
1:B:269:TYR:CZ	1:C:217:LYS:HG2	2.49	0.47
1:C:289:ASP:CG	1:C:290:ASN:N	2.67	0.47
1:A:224:TYR:CE2	1:C:294:MSE:HE3	2.50	0.47
1:F:261:LYS:HB3	1:F:286:VAL:HG13	1.97	0.47
1:C:235:ASN:HD21	1:C:238:ASN:CG	2.17	0.47
1:E:264:LYS:HB2	1:E:285:ASN:HB3	1.97	0.47
1:F:261:LYS:HD3	1:F:286:VAL:HG11	1.96	0.47
1:F:244:ARG:HD3	1:F:244:ARG:C	2.32	0.46
1:C:304:THR:O	1:C:306:ASN:N	2.49	0.46
1:F:275:LYS:HG2	2:F:462:HOH:O	2.16	0.46
1:D:269:TYR:CG	1:D:283:LEU:HD13	2.52	0.45
1:E:283:LEU:HD13	1:E:294:MSE:HE1	1.93	0.45
1:E:264:LYS:HE2	2:E:454:HOH:O	2.15	0.45
1:C:283:LEU:HD13	1:C:294:MSE:HE2	1.99	0.45
1:B:322:ASN:HA	2:C:404:HOH:O	2.16	0.45
1:B:214:SER:OG	2:B:402:HOH:O	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:HG2	2:B:465:HOH:O	2.15	0.45
1:E:275:LYS:HD3	1:E:275:LYS:HA	1.78	0.45
2:B:410:HOH:O	1:D:293:LYS:HD3	2.17	0.44
1:E:281:GLU:OE1	1:E:296:LYS:HD2	2.17	0.44
1:B:265:SER:HB3	1:B:285:ASN:HB2	2.00	0.44
1:B:315:LYS:HA	1:B:315:LYS:HD3	1.25	0.44
1:A:275:LYS:HB2	1:A:276:LYS:HE3	2.00	0.44
1:D:243:LEU:C	1:D:243:LEU:HD12	2.38	0.44
1:E:234:LYS:H	1:E:234:LYS:HG2	1.64	0.44
1:E:274:THR:CG2	1:E:276:LYS:H	2.30	0.44
1:F:289:ASP:O	1:F:290:ASN:CB	2.64	0.43
1:B:244:ARG:HD3	1:B:244:ARG:C	2.30	0.43
1:B:250:LYS:HD3	2:D:448:HOH:O	2.18	0.43
1:B:236:GLN:O	1:B:240:GLN:HG3	2.19	0.42
1:F:275:LYS:HB2	1:F:276:LYS:HE2	2.00	0.42
1:C:249:GLU:HG2	2:C:409:HOH:O	2.18	0.42
1:A:243:LEU:C	1:A:243:LEU:HD12	2.39	0.42
1:B:261:LYS:HB3	1:B:286:VAL:HG13	2.00	0.42
1:E:301:VAL:O	1:E:301:VAL:CG2	2.68	0.42
1:A:257:LYS:HD2	2:A:462:HOH:O	2.19	0.42
1:E:304:THR:CG2	1:E:305:LYS:N	2.82	0.42
1:B:294:MSE:HB2	1:B:294:MSE:HE2	1.73	0.42
1:D:294:MSE:HE3	1:E:224:TYR:CZ	2.54	0.41
2:D:417:HOH:O	1:F:322:ASN:HB2	2.20	0.41
1:E:322:ASN:HA	1:F:306:ASN:HD22	1.85	0.41
1:D:271:SER:HA	1:D:279:SER:O	2.21	0.41
1:D:244:ARG:O	1:D:244:ARG:HD3	2.21	0.41
1:B:219:ASP:O	1:B:223:ARG:HG3	2.21	0.41
1:B:299:PHE:HB3	1:B:314:PRO:HA	2.03	0.41
1:E:234:LYS:HG2	2:E:414:HOH:O	2.20	0.41
1:F:264:LYS:HD3	2:F:448:HOH:O	2.21	0.41
1:B:269:TYR:CE1	1:C:217:LYS:HA	2.56	0.40
1:A:297:ILE:HA	1:A:315:LYS:O	2.22	0.40

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	107/161 (66%)	103 (96%)	4 (4%)	0	100	100
1	B	107/161 (66%)	103 (96%)	4 (4%)	0	100	100
1	C	107/161 (66%)	99 (92%)	5 (5%)	3 (3%)	4	6
1	D	107/161 (66%)	103 (96%)	3 (3%)	1 (1%)	14	28
1	E	107/161 (66%)	102 (95%)	2 (2%)	3 (3%)	4	6
1	F	107/161 (66%)	100 (94%)	4 (4%)	3 (3%)	4	6
All	All	642/966 (66%)	610 (95%)	22 (3%)	10 (2%)	8	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	215	GLN
1	C	305	LYS
1	E	305	LYS
1	F	290	ASN
1	F	289	ASP
1	C	306	ASN
1	D	233	GLU
1	E	306	ASN
1	F	306	ASN
1	E	277	GLY

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	103/151 (68%)	98 (95%)	5 (5%)	21	42
1	B	103/151 (68%)	96 (93%)	7 (7%)	13	27
1	C	103/151 (68%)	95 (92%)	8 (8%)	10	21
1	D	103/151 (68%)	96 (93%)	7 (7%)	13	27
1	E	103/151 (68%)	90 (87%)	13 (13%)	3	7
1	F	103/151 (68%)	97 (94%)	6 (6%)	17	34
All	All	618/906 (68%)	572 (93%)	46 (7%)	11	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	SER
1	A	218	ILE
1	A	244	ARG
1	A	276	LYS
1	A	290	ASN
1	B	231	SER
1	B	234	LYS
1	B	236	GLN
1	B	244	ARG
1	B	265	SER
1	B	276	LYS
1	B	295	GLN
1	C	234	LYS
1	C	235	ASN
1	C	244	ARG
1	C	265	SER
1	C	289	ASP
1	C	291	ARG
1	C	305	LYS
1	C	306	ASN
1	D	215	GLN
1	D	234	LYS
1	D	236	GLN
1	D	241	SER
1	D	244	ARG
1	D	269	TYR
1	D	285	ASN
1	E	231	SER
1	E	234	LYS
1	E	244	ARG

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Mol	Chain	Res	Type
1	E	245	THR
1	E	248	SER
1	E	257	LYS
1	E	264	LYS
1	E	274	THR
1	E	276	LYS
1	E	284	LEU
1	E	292	SER
1	E	294	MSE
1	E	304	THR
1	F	244	ARG
1	F	257	LYS
1	F	276	LYS
1	F	292	SER
1	F	294	MSE
1	F	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	215	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	108/161 (67%)	0.06	7 (6%)	26	24	9, 20, 62, 88	0
1	B	108/161 (67%)	0.13	2 (1%)	66	63	11, 22, 58, 80	0
1	C	108/161 (67%)	0.16	7 (6%)	26	24	12, 23, 66, 115	0
1	D	108/161 (67%)	0.20	3 (2%)	55	51	11, 26, 52, 72	0
1	E	108/161 (67%)	0.36	9 (8%)	19	18	13, 25, 62, 90	0
1	F	108/161 (67%)	0.20	8 (7%)	22	20	11, 23, 65, 98	0
All	All	648/966 (67%)	0.18	36 (5%)	31	29	9, 24, 63, 115	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	ASN	4.4
1	A	288	VAL	3.8
1	F	288	VAL	3.6
1	F	291	ARG	3.2
1	C	305	LYS	3.0
1	C	289	ASP	3.0
1	F	306	ASN	2.8
1	F	290	ASN	2.7
1	D	214	SER	2.7
1	A	255	ASP	2.7
1	E	288	VAL	2.7
1	B	305	LYS	2.7
1	A	290	ASN	2.7
1	E	275	LYS	2.6
1	E	291	ARG	2.6
1	F	305	LYS	2.6
1	E	293	LYS	2.5
1	C	308	PHE	2.5
1	E	276	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	ARG	2.5
1	F	289	ASP	2.4
1	E	306	ASN	2.4
1	D	215	GLN	2.3
1	E	214	SER	2.3
1	A	322	ASN	2.3
1	D	322	ASN	2.3
1	B	307	GLY	2.2
1	C	322	ASN	2.2
1	A	215	GLN	2.2
1	F	307	GLY	2.2
1	E	290	ASN	2.2
1	C	288	VAL	2.2
1	F	292	SER	2.1
1	E	305	LYS	2.1
1	A	306	ASN	2.1
1	C	290	ASN	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 monosaccharides 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.