Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:49 pm BST

PDB ID	:	6IZ8
Title	:	Crystal Structure of TagF from Pseudomonas aeruginosa
Authors	:	Chang, J.H.; Ok, C.K.
Deposited on	:	2018-12-18
Resolution	:	2.70 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

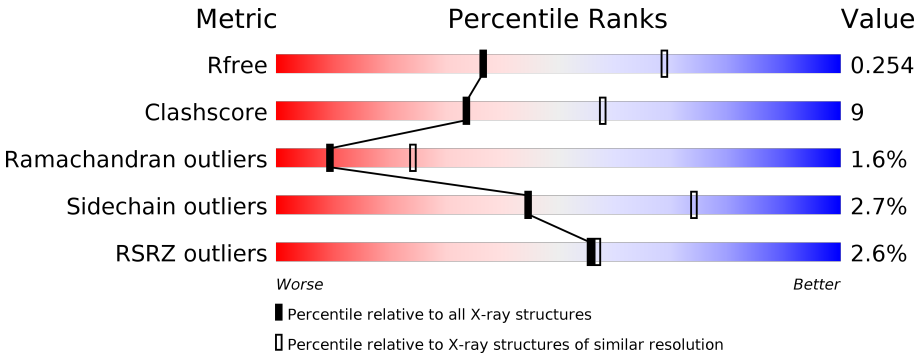
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	247	2% 74% 14% • 10%
1	B	247	% 69% 17% • 13%
1	C	247	5% 76% 16% • • 5%
1	D	247	2% 70% 15% • 14%
1	F	247	• • 95%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6802 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 Type VI secretion-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1657	1058	290	302	7			
1	B	215	Total	C	N	O	S	0	0	0
			1609	1028	278	296	7			
1	C	234	Total	C	N	O	S	0	0	0
			1755	1120	310	318	7			
1	D	212	Total	C	N	O	S	0	0	0
			1585	1013	274	292	6			
1	F	12	Total	C	N	O		0	0	0
			93	56	23	14				

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP A0A1Y3KGX5
A	-19	GLY	-	expression tag	UNP A0A1Y3KGX5
A	-18	SER	-	expression tag	UNP A0A1Y3KGX5
A	-17	SER	-	expression tag	UNP A0A1Y3KGX5
A	-16	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-15	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-14	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-13	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-12	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-11	HIS	-	expression tag	UNP A0A1Y3KGX5
A	-10	SER	-	expression tag	UNP A0A1Y3KGX5
A	-9	SER	-	expression tag	UNP A0A1Y3KGX5
A	-8	GLY	-	expression tag	UNP A0A1Y3KGX5
A	-7	LEU	-	expression tag	UNP A0A1Y3KGX5
A	-6	VAL	-	expression tag	UNP A0A1Y3KGX5
A	-5	PRO	-	expression tag	UNP A0A1Y3KGX5
A	-4	ARG	-	expression tag	UNP A0A1Y3KGX5
A	-3	GLY	-	expression tag	UNP A0A1Y3KGX5
A	-2	SER	-	expression tag	UNP A0A1Y3KGX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP A0A1Y3KGX5
A	0	MET	-	expression tag	UNP A0A1Y3KGX5
A	1	LEU	-	expression tag	UNP A0A1Y3KGX5
B	-20	MET	-	expression tag	UNP A0A1Y3KGX5
B	-19	GLY	-	expression tag	UNP A0A1Y3KGX5
B	-18	SER	-	expression tag	UNP A0A1Y3KGX5
B	-17	SER	-	expression tag	UNP A0A1Y3KGX5
B	-16	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-15	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-14	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-13	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-12	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-11	HIS	-	expression tag	UNP A0A1Y3KGX5
B	-10	SER	-	expression tag	UNP A0A1Y3KGX5
B	-9	SER	-	expression tag	UNP A0A1Y3KGX5
B	-8	GLY	-	expression tag	UNP A0A1Y3KGX5
B	-7	LEU	-	expression tag	UNP A0A1Y3KGX5
B	-6	VAL	-	expression tag	UNP A0A1Y3KGX5
B	-5	PRO	-	expression tag	UNP A0A1Y3KGX5
B	-4	ARG	-	expression tag	UNP A0A1Y3KGX5
B	-3	GLY	-	expression tag	UNP A0A1Y3KGX5
B	-2	SER	-	expression tag	UNP A0A1Y3KGX5
B	-1	HIS	-	expression tag	UNP A0A1Y3KGX5
B	0	MET	-	expression tag	UNP A0A1Y3KGX5
B	1	LEU	-	expression tag	UNP A0A1Y3KGX5
C	-20	MET	-	expression tag	UNP A0A1Y3KGX5
C	-19	GLY	-	expression tag	UNP A0A1Y3KGX5
C	-18	SER	-	expression tag	UNP A0A1Y3KGX5
C	-17	SER	-	expression tag	UNP A0A1Y3KGX5
C	-16	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-15	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-14	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-13	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-12	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-11	HIS	-	expression tag	UNP A0A1Y3KGX5
C	-10	SER	-	expression tag	UNP A0A1Y3KGX5
C	-9	SER	-	expression tag	UNP A0A1Y3KGX5
C	-8	GLY	-	expression tag	UNP A0A1Y3KGX5
C	-7	LEU	-	expression tag	UNP A0A1Y3KGX5
C	-6	VAL	-	expression tag	UNP A0A1Y3KGX5
C	-5	PRO	-	expression tag	UNP A0A1Y3KGX5
C	-4	ARG	-	expression tag	UNP A0A1Y3KGX5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP A0A1Y3KGX5
C	-2	SER	-	expression tag	UNP A0A1Y3KGX5
C	-1	HIS	-	expression tag	UNP A0A1Y3KGX5
C	0	MET	-	expression tag	UNP A0A1Y3KGX5
C	1	LEU	-	expression tag	UNP A0A1Y3KGX5
D	-20	MET	-	expression tag	UNP A0A1Y3KGX5
D	-19	GLY	-	expression tag	UNP A0A1Y3KGX5
D	-18	SER	-	expression tag	UNP A0A1Y3KGX5
D	-17	SER	-	expression tag	UNP A0A1Y3KGX5
D	-16	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-15	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-14	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-13	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-12	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-11	HIS	-	expression tag	UNP A0A1Y3KGX5
D	-10	SER	-	expression tag	UNP A0A1Y3KGX5
D	-9	SER	-	expression tag	UNP A0A1Y3KGX5
D	-8	GLY	-	expression tag	UNP A0A1Y3KGX5
D	-7	LEU	-	expression tag	UNP A0A1Y3KGX5
D	-6	VAL	-	expression tag	UNP A0A1Y3KGX5
D	-5	PRO	-	expression tag	UNP A0A1Y3KGX5
D	-4	ARG	-	expression tag	UNP A0A1Y3KGX5
D	-3	GLY	-	expression tag	UNP A0A1Y3KGX5
D	-2	SER	-	expression tag	UNP A0A1Y3KGX5
D	-1	HIS	-	expression tag	UNP A0A1Y3KGX5
D	0	MET	-	expression tag	UNP A0A1Y3KGX5
D	1	LEU	-	expression tag	UNP A0A1Y3KGX5
F	-5	MET	-	expression tag	UNP A0A1Y3KGX5
F	-4	GLY	-	expression tag	UNP A0A1Y3KGX5
F	-3	SER	-	expression tag	UNP A0A1Y3KGX5
F	-2	SER	-	expression tag	UNP A0A1Y3KGX5
F	-1	HIS	-	expression tag	UNP A0A1Y3KGX5
F	0	HIS	-	expression tag	UNP A0A1Y3KGX5
F	1	HIS	-	expression tag	UNP A0A1Y3KGX5
F	2	HIS	-	expression tag	UNP A0A1Y3KGX5
F	3	HIS	-	expression tag	UNP A0A1Y3KGX5
F	4	HIS	-	expression tag	UNP A0A1Y3KGX5
F	5	SER	-	expression tag	UNP A0A1Y3KGX5
F	6	SER	-	expression tag	UNP A0A1Y3KGX5
F	7	GLY	-	expression tag	UNP A0A1Y3KGX5
F	8	LEU	-	expression tag	UNP A0A1Y3KGX5
F	9	VAL	-	expression tag	UNP A0A1Y3KGX5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	10	PRO	-	expression tag	UNP A0A1Y3KGX5
F	11	ARG	-	expression tag	UNP A0A1Y3KGX5
F	12	GLY	-	expression tag	UNP A0A1Y3KGX5
F	13	SER	-	expression tag	UNP A0A1Y3KGX5
F	14	HIS	-	expression tag	UNP A0A1Y3KGX5
F	15	MET	-	expression tag	UNP A0A1Y3KGX5
F	16	LEU	-	expression tag	UNP A0A1Y3KGX5

- Molecule 2 is water.

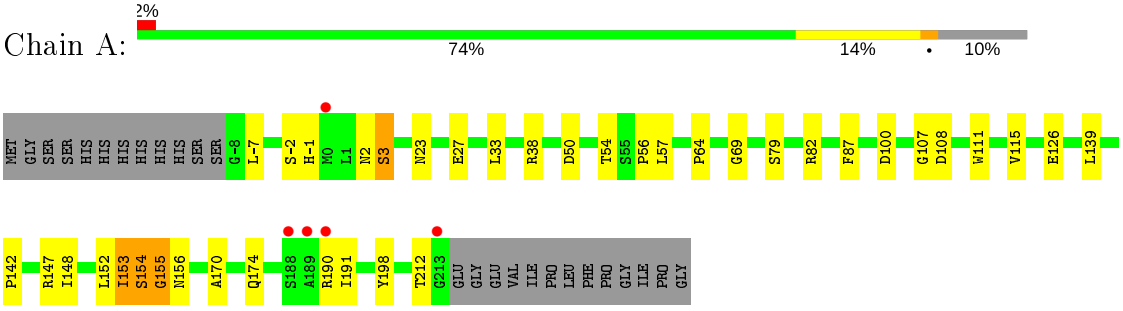
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	37	Total O 37 37	0	0
2	C	21	Total O 21 21	0	0
2	D	23	Total O 23 23	0	0
2	F	2	Total O 2 2	0	0

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.

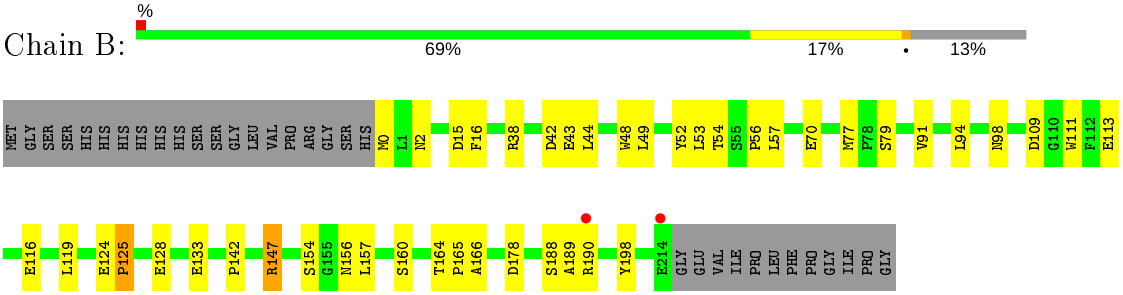
- Molecule 1: Type VI secretion-associated protein

Chain A:



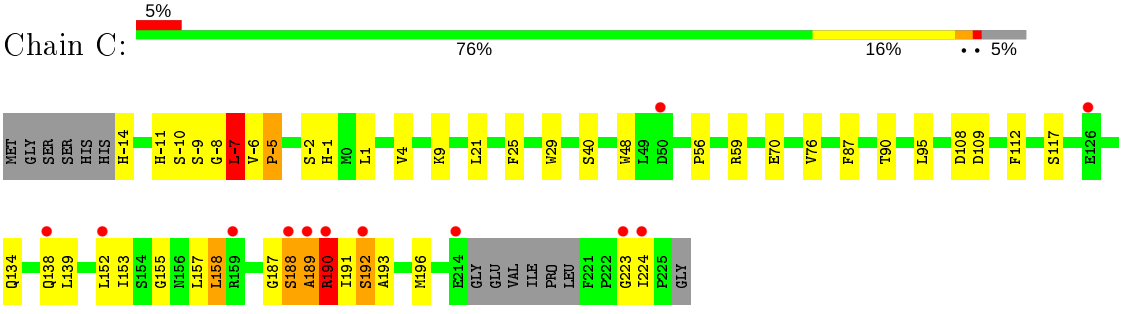
- Molecule 1: Type VI secretion-associated protein

Chain B:



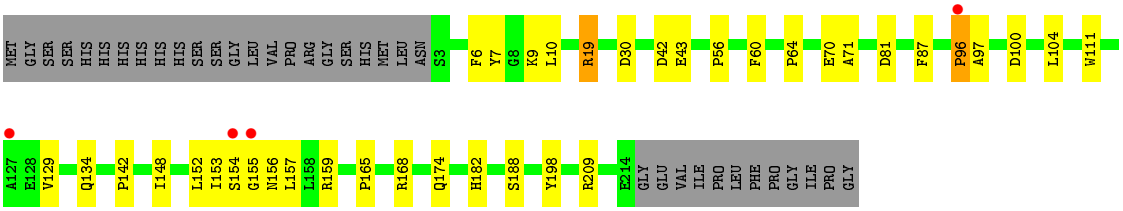
- Molecule 1: Type VI secretion-associated protein

Chain C:



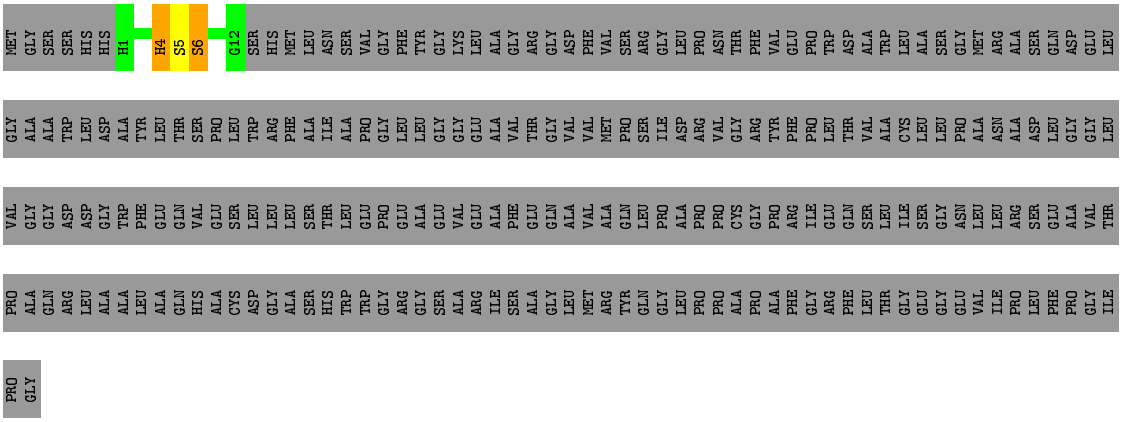
- Molecule 1: Type VI secretion-associated protein

Chain D:



• Molecule 1: Type VI secretion-associated protein

Chain F: 95%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.72Å 92.39Å 151.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.57 – 2.70 49.62 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.57-2.70) 94.4 (49.62-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.58 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.201 , 0.254 0.201 , 0.254	Depositor DCC
R_{free} test set	1972 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6802	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

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	0.44	0/1703	0.62	0/2324
1	B	0.44	0/1653	0.63	0/2256
1	C	0.44	1/1807 (0.1%)	0.63	1/2465 (0.0%)
1	D	0.42	0/1629	0.60	1/2224 (0.0%)
1	F	0.35	0/97	0.56	0/130
All	All	0.43	1/6889 (0.0%)	0.62	2/9399 (0.0%)

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	C	0	2
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-5	PRO	N-CD	-5.25	1.40	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	-7	LEU	CA-CB-CG	5.77	128.56	115.30
1	D	42	ASP	CB-CG-OD2	5.53	123.27	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	190	ARG	Peptide
1	C	192	SER	Peptide
1	D	96	PRO	Peptide

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	1657	0	1624	26	0
1	B	1609	0	1572	33	0
1	C	1755	0	1704	37	0
1	D	1585	0	1543	24	0
1	F	93	0	86	2	0
2	A	20	0	0	1	0
2	B	37	0	0	5	0
2	C	21	0	0	3	0
2	D	23	0	0	1	0
2	F	2	0	0	0	0
All	All	6802	0	6529	113	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 9.

All (113) 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:108:ASP:OD1	2:C:301:HOH:O	1.99	0.80
1:B:70:GLU:HG3	1:B:94:LEU:HD13	1.65	0.75
1:C:56:PRO:HB3	1:C:188:SER:HB2	1.69	0.74
1:C:-6:VAL:HG11	1:C:-1:HIS:ND1	2.06	0.71
1:C:-14:HIS:HB3	1:C:-11:HIS:HD2	1.54	0.70
1:C:70:GLU:OE2	2:C:302:HOH:O	2.10	0.69
1:A:170:ALA:O	1:A:174:GLN:HG3	1.93	0.69
1:B:57:LEU:HD22	1:B:77:MET:HB2	1.74	0.68
1:C:-14:HIS:HB3	1:C:-11:HIS:CD2	2.29	0.67
1:C:-6:VAL:HG11	1:C:-1:HIS:CE1	2.30	0.66
1:D:209:ARG:HH11	1:D:209:ARG:HG2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:HG3	1:C:191:ILE:N	2.12	0.65
1:D:152:LEU:HD21	1:D:155:GLY:HA2	1.79	0.64
1:B:38:ARG:NH1	1:B:42:ASP:OD2	2.31	0.63
1:A:2:ASN:N	1:A:3:SER:HA	2.12	0.63
1:B:198:TYR:CE1	1:C:157:LEU:HB2	2.35	0.61
1:D:70:GLU:HG2	1:D:96:PRO:HG3	1.81	0.61
1:C:192:SER:HB3	1:C:193:ALA:O	2.02	0.59
1:C:76:VAL:HG23	1:C:90:THR:HG22	1.85	0.59
1:B:164:THR:HG22	1:B:166:ALA:H	1.68	0.59
1:B:54:THR:HG21	1:B:190:ARG:CZ	2.33	0.59
1:A:153:ILE:O	1:A:155:GLY:N	2.36	0.58
1:A:56:PRO:HD3	1:A:191:ILE:HD13	1.85	0.58
1:D:56:PRO:HG3	1:D:188:SER:HB3	1.85	0.58
1:C:29:TRP:CZ2	1:C:90:THR:HG21	2.38	0.58
1:C:29:TRP:HZ2	1:C:90:THR:HG21	1.69	0.57
1:C:40:SER:HG	1:C:48:TRP:HE1	1.53	0.56
1:B:164:THR:HG22	1:B:166:ALA:N	2.21	0.56
1:A:148:ILE:H	1:A:174:GLN:HE22	1.54	0.55
1:B:15:ASP:CG	1:B:16:PHE:H	2.11	0.55
1:D:154:SER:OG	1:D:154:SER:O	2.25	0.54
1:B:91:VAL:HG23	1:B:119:LEU:HD21	1.90	0.54
1:D:209:ARG:HG2	1:D:209:ARG:NH1	2.22	0.53
1:B:128:GLU:OE1	2:B:301:HOH:O	2.19	0.53
1:B:57:LEU:HD22	1:B:77:MET:CB	2.37	0.53
1:B:57:LEU:HD12	1:B:116:GLU:HG2	1.90	0.53
1:C:-6:VAL:HG22	1:F:4:HIS:CE1	2.44	0.53
1:D:43:GLU:OE1	1:D:209:ARG:NH2	2.37	0.52
1:A:111:TRP:CD2	1:A:142:PRO:HB3	2.45	0.52
1:D:6:PHE:CZ	1:D:19:ARG:HG3	2.45	0.52
1:A:-2:SER:O	1:A:2:ASN:ND2	2.43	0.51
1:A:23:ASN:HB3	1:A:27:GLU:OE1	2.12	0.50
1:B:157:LEU:HD11	1:C:196:MET:HB3	1.93	0.49
1:B:43:GLU:HG2	1:B:44:LEU:HD23	1.94	0.49
1:D:168:ARG:HD3	2:D:311:HOH:O	2.12	0.49
1:C:-2:SER:HA	1:C:1:LEU:HD12	1.93	0.49
1:A:174:GLN:HB3	2:A:319:HOH:O	2.12	0.49
1:C:109:ASP:OD2	2:C:303:HOH:O	2.20	0.49
1:B:147:ARG:NH2	1:B:178:ASP:OD1	2.46	0.49
1:D:9:LYS:HD2	1:D:87:PHE:HB2	1.95	0.48
1:D:9:LYS:HD2	1:D:87:PHE:CB	2.44	0.48
1:A:-7:LEU:HD21	1:B:79:SER:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASN:O	1:B:147:ARG:HG2	2.14	0.47
1:B:178:ASP:O	2:B:302:HOH:O	2.20	0.47
1:A:126:GLU:OE1	1:A:126:GLU:N	2.42	0.47
1:C:59:ARG:HD3	1:C:112:PHE:HB3	1.97	0.47
1:C:191:ILE:O	1:C:192:SER:OG	2.20	0.46
1:D:111:TRP:CD2	1:D:142:PRO:HB3	2.51	0.46
1:B:109:ASP:O	1:B:113:GLU:HG3	2.16	0.46
1:A:64:PRO:HB3	1:A:69:GLY:O	2.16	0.46
1:C:56:PRO:CB	1:C:188:SER:HB2	2.42	0.45
1:C:9:LYS:HG3	1:C:87:PHE:HB3	1.98	0.45
1:D:153:ILE:HB	1:D:157:LEU:HD23	1.97	0.45
1:A:100:ASP:OD1	1:A:174:GLN:HG2	2.17	0.45
1:A:190:ARG:NH1	1:A:212:THR:HG22	2.31	0.45
1:C:4:VAL:HG21	1:C:139:LEU:HD23	1.98	0.45
1:A:156:ASN:CG	1:D:198:TYR:HE1	2.19	0.45
2:B:311:HOH:O	1:C:158:LEU:HD23	2.17	0.45
1:B:54:THR:HG21	1:B:190:ARG:NH2	2.32	0.45
1:B:133:GLU:OE2	2:B:303:HOH:O	2.21	0.45
1:C:70:GLU:H	1:C:70:GLU:CD	2.20	0.45
1:A:147:ARG:HB2	1:A:174:GLN:OE1	2.17	0.44
1:C:152:LEU:HD11	1:C:155:GLY:HA2	1.98	0.44
1:A:-7:LEU:HD13	1:B:53:LEU:HD23	2.00	0.44
1:D:60:PHE:HA	1:D:182:HIS:O	2.16	0.44
1:B:164:THR:HG23	1:B:165:PRO:HD2	2.00	0.44
1:A:198:TYR:CE1	1:D:157:LEU:HB2	2.52	0.44
1:C:134:GLN:O	1:C:138:GLN:HG3	2.17	0.44
1:D:100:ASP:OD2	1:D:174:GLN:HG2	2.18	0.44
1:A:115:VAL:HG22	1:A:139:LEU:HD21	2.00	0.44
1:C:153:ILE:HB	1:C:157:LEU:HD23	2.01	0.43
1:A:154:SER:O	1:A:156:ASN:N	2.44	0.43
1:B:111:TRP:CG	1:B:142:PRO:HB3	2.53	0.43
1:B:124:GLU:HB3	1:B:125:PRO:HD2	1.99	0.43
1:B:48:TRP:CE3	1:B:49:LEU:HA	2.53	0.43
1:B:189:ALA:HB3	1:B:190:ARG:NH1	2.34	0.43
1:D:148:ILE:N	1:D:174:GLN:OE1	2.37	0.43
1:B:52:TYR:C	1:B:54:THR:H	2.21	0.43
1:C:190:ARG:CG	1:C:191:ILE:N	2.81	0.42
1:B:56:PRO:HG3	1:B:188:SER:HB3	2.01	0.42
1:D:9:LYS:HE3	1:D:81:ASP:OD2	2.18	0.42
1:A:79:SER:HB3	1:A:87:PHE:O	2.20	0.42
1:D:7:TYR:OH	1:D:30:ASP:OD1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLY:O	1:C:189:ALA:N	2.53	0.42
1:B:189:ALA:HB3	1:B:190:ARG:HH12	1.85	0.42
1:C:224:ILE:HG23	1:C:224:ILE:O	2.19	0.42
1:C:21:LEU:HD13	1:C:25:PHE:CE2	2.55	0.42
1:D:10:LEU:HD13	1:D:129:VAL:HG23	2.02	0.42
1:B:70:GLU:CG	1:B:94:LEU:HD13	2.41	0.41
1:C:-7:LEU:HA	1:C:-6:VAL:C	2.41	0.41
1:A:57:LEU:HD12	1:A:57:LEU:N	2.35	0.41
1:C:70:GLU:HB3	1:C:95:LEU:O	2.20	0.41
1:D:104:LEU:HA	1:D:104:LEU:HD12	1.80	0.41
1:A:107:GLY:O	1:D:165:PRO:HB3	2.20	0.41
1:A:33:LEU:HA	1:A:33:LEU:HD23	1.87	0.41
1:B:98:ASN:ND2	2:B:306:HOH:O	2.47	0.41
1:C:188:SER:O	1:C:190:ARG:N	2.54	0.41
1:A:50:ASP:O	1:A:54:THR:OG1	2.34	0.41
1:A:152:LEU:HD21	1:A:156:ASN:HA	2.03	0.40
1:D:64:PRO:HD3	1:D:71:ALA:HB2	2.03	0.40
1:B:154:SER:OG	1:B:156:ASN:OD1	2.36	0.40
1:C:188:SER:HB3	1:C:189:ALA:H	1.67	0.40
1:C:-9:SER:HA	1:F:6:SER:O	2.20	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	220/247 (89%)	204 (93%)	13 (6%)	3 (1%)	11 28
1	B	213/247 (86%)	197 (92%)	15 (7%)	1 (0%)	29 54
1	C	230/247 (93%)	210 (91%)	13 (6%)	7 (3%)	4 10
1	D	210/247 (85%)	199 (95%)	9 (4%)	2 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	10/247 (4%)	6 (60%)	3 (30%)	1 (10%)	0 0
All	All	883/1235 (72%)	816 (92%)	53 (6%)	14 (2%)	9 24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	154	SER
1	C	189	ALA
1	C	-5	PRO
1	C	188	SER
1	C	190	ARG
1	D	97	ALA
1	D	156	ASN
1	B	125	PRO
1	F	4	HIS
1	C	-7	LEU
1	C	223	GLY
1	A	155	GLY
1	C	-8	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	165/186 (89%)	160 (97%)	5 (3%)	41 70
1	B	160/186 (86%)	156 (98%)	4 (2%)	47 76
1	C	176/186 (95%)	172 (98%)	4 (2%)	50 78
1	D	157/186 (84%)	154 (98%)	3 (2%)	57 82
1	F	10/186 (5%)	8 (80%)	2 (20%)	1 3
All	All	668/930 (72%)	650 (97%)	18 (3%)	44 74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	3	SER
1	A	38	ARG
1	A	82	ARG
1	A	108	ASP
1	B	0	MET
1	B	2	ASN
1	B	147	ARG
1	B	160	SER
1	C	-10	SER
1	C	-7	LEU
1	C	117	SER
1	C	158	LEU
1	D	19	ARG
1	D	134	GLN
1	D	159	ARG
1	F	5	SER
1	F	6	SER

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

Mol	Chain	Res	Type
1	C	-11	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	222/247 (89%)	0.22	5 (2%) 60 62	38, 55, 82, 97	0
1	B	215/247 (87%)	0.10	2 (0%) 84 85	39, 54, 74, 100	0
1	C	234/247 (94%)	0.19	12 (5%) 28 26	43, 61, 82, 99	0
1	D	212/247 (85%)	0.04	4 (1%) 66 69	42, 59, 80, 94	0
1	F	12/247 (4%)	0.49	0 100 100	66, 76, 81, 84	0
All	All	895/1235 (72%)	0.15	23 (2%) 56 57	38, 58, 81, 100	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	4.4
1	A	190	ARG	4.3
1	D	96	PRO	4.3
1	C	189	ALA	3.9
1	D	154	SER	2.9
1	C	188	SER	2.9
1	C	190	ARG	2.7
1	B	214	GLU	2.6
1	C	224	ILE	2.5
1	C	152	LEU	2.5
1	C	126	GLU	2.4
1	A	0	MET	2.3
1	A	188	SER	2.3
1	C	138	GLN	2.3
1	C	223	GLY	2.2
1	D	127	ALA	2.2
1	B	190	ARG	2.2
1	D	155	GLY	2.2
1	C	50	ASP	2.1
1	C	214	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	159	ARG	2.1
1	C	192	SER	2.1
1	A	213	GLY	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 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.