Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 11:39 pm GMT

PDB ID	:	4UXG
Title	:	Crystal structure of the carboxy-terminal region of the bacteriophage T4 proximal long tail fibre protein gp34, R32 native crystal
Authors	:	Granell, M.; Alvira, S.; Garcia-Doval, C.; Singh, A.K.; van Raaij, M.J.
Deposited on	:	2014-08-22
Resolution	:	3.00 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 (1)) were used in the production of this report:

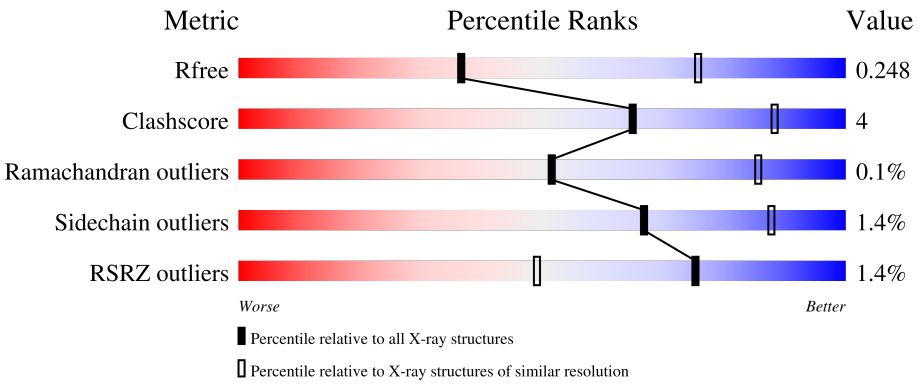
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	410	89% 7% •
1	B	410	90% 6% •
1	C	410	90% 7% •
1	D	410	81% 14% •
1	E	410	2% 85% 11% • •

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Mol	Chain	Length	Quality of chain
1	F	410	86% 10%
1	G	410	3% 85% 11%
1	H	410	2% 89% 7%
1	I	410	85% 11%
1	J	410	3% 83% 13%
1	K	410	2% 82% 13% 5%
1	L	410	3% 82% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 36241 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 LARGE TAIL FIBER PROTEIN P34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3020	1886	532	597	5	0	0	0
1	B	395	3020	1886	532	597	5	0	0	0
1	C	398	3043	1898	536	604	5	0	0	0
1	D	395	3020	1886	532	597	5	0	0	0
1	E	398	3043	1898	536	604	5	0	0	0
1	F	396	3027	1891	533	598	5	0	0	0
1	G	395	3020	1886	532	597	5	0	0	0
1	H	394	3013	1881	531	596	5	0	0	0
1	I	394	3014	1883	531	595	5	0	0	0
1	J	394	3014	1883	531	595	5	0	0	0
1	K	391	2987	1864	527	591	5	0	0	0
1	L	395	3020	1886	532	597	5	0	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	MET	-	expression tag	UNP P18771
A	881	GLY	-	expression tag	UNP P18771
A	882	SER	-	expression tag	UNP P18771
A	883	SER	-	expression tag	UNP P18771
A	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
A	885	HIS	-	expression tag	UNP P18771
A	886	HIS	-	expression tag	UNP P18771
A	887	HIS	-	expression tag	UNP P18771
A	888	HIS	-	expression tag	UNP P18771
A	889	HIS	-	expression tag	UNP P18771
A	890	SER	-	expression tag	UNP P18771
A	891	GLN	-	expression tag	UNP P18771
A	892	ASP	-	expression tag	UNP P18771
A	893	PRO	-	expression tag	UNP P18771
B	880	MET	-	expression tag	UNP P18771
B	881	GLY	-	expression tag	UNP P18771
B	882	SER	-	expression tag	UNP P18771
B	883	SER	-	expression tag	UNP P18771
B	884	HIS	-	expression tag	UNP P18771
B	885	HIS	-	expression tag	UNP P18771
B	886	HIS	-	expression tag	UNP P18771
B	887	HIS	-	expression tag	UNP P18771
B	888	HIS	-	expression tag	UNP P18771
B	889	HIS	-	expression tag	UNP P18771
B	890	SER	-	expression tag	UNP P18771
B	891	GLN	-	expression tag	UNP P18771
B	892	ASP	-	expression tag	UNP P18771
B	893	PRO	-	expression tag	UNP P18771
C	880	MET	-	expression tag	UNP P18771
C	881	GLY	-	expression tag	UNP P18771
C	882	SER	-	expression tag	UNP P18771
C	883	SER	-	expression tag	UNP P18771
C	884	HIS	-	expression tag	UNP P18771
C	885	HIS	-	expression tag	UNP P18771
C	886	HIS	-	expression tag	UNP P18771
C	887	HIS	-	expression tag	UNP P18771
C	888	HIS	-	expression tag	UNP P18771
C	889	HIS	-	expression tag	UNP P18771
C	890	SER	-	expression tag	UNP P18771
C	891	GLN	-	expression tag	UNP P18771
C	892	ASP	-	expression tag	UNP P18771
C	893	PRO	-	expression tag	UNP P18771
D	880	MET	-	expression tag	UNP P18771
D	881	GLY	-	expression tag	UNP P18771
D	882	SER	-	expression tag	UNP P18771
D	883	SER	-	expression tag	UNP P18771
D	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
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D	886	HIS	-	expression tag	UNP P18771
D	887	HIS	-	expression tag	UNP P18771
D	888	HIS	-	expression tag	UNP P18771
D	889	HIS	-	expression tag	UNP P18771
D	890	SER	-	expression tag	UNP P18771
D	891	GLN	-	expression tag	UNP P18771
D	892	ASP	-	expression tag	UNP P18771
D	893	PRO	-	expression tag	UNP P18771
E	880	MET	-	expression tag	UNP P18771
E	881	GLY	-	expression tag	UNP P18771
E	882	SER	-	expression tag	UNP P18771
E	883	SER	-	expression tag	UNP P18771
E	884	HIS	-	expression tag	UNP P18771
E	885	HIS	-	expression tag	UNP P18771
E	886	HIS	-	expression tag	UNP P18771
E	887	HIS	-	expression tag	UNP P18771
E	888	HIS	-	expression tag	UNP P18771
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E	891	GLN	-	expression tag	UNP P18771
E	892	ASP	-	expression tag	UNP P18771
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F	881	GLY	-	expression tag	UNP P18771
F	882	SER	-	expression tag	UNP P18771
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F	886	HIS	-	expression tag	UNP P18771
F	887	HIS	-	expression tag	UNP P18771
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F	890	SER	-	expression tag	UNP P18771
F	891	GLN	-	expression tag	UNP P18771
F	892	ASP	-	expression tag	UNP P18771
F	893	PRO	-	expression tag	UNP P18771
G	880	MET	-	expression tag	UNP P18771
G	881	GLY	-	expression tag	UNP P18771
G	882	SER	-	expression tag	UNP P18771
G	883	SER	-	expression tag	UNP P18771
G	884	HIS	-	expression tag	UNP P18771

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Chain	Residue	Modelled	Actual	Comment	Reference
G	885	HIS	-	expression tag	UNP P18771
G	886	HIS	-	expression tag	UNP P18771
G	887	HIS	-	expression tag	UNP P18771
G	888	HIS	-	expression tag	UNP P18771
G	889	HIS	-	expression tag	UNP P18771
G	890	SER	-	expression tag	UNP P18771
G	891	GLN	-	expression tag	UNP P18771
G	892	ASP	-	expression tag	UNP P18771
G	893	PRO	-	expression tag	UNP P18771
H	880	MET	-	expression tag	UNP P18771
H	881	GLY	-	expression tag	UNP P18771
H	882	SER	-	expression tag	UNP P18771
H	883	SER	-	expression tag	UNP P18771
H	884	HIS	-	expression tag	UNP P18771
H	885	HIS	-	expression tag	UNP P18771
H	886	HIS	-	expression tag	UNP P18771
H	887	HIS	-	expression tag	UNP P18771
H	888	HIS	-	expression tag	UNP P18771
H	889	HIS	-	expression tag	UNP P18771
H	890	SER	-	expression tag	UNP P18771
H	891	GLN	-	expression tag	UNP P18771
H	892	ASP	-	expression tag	UNP P18771
H	893	PRO	-	expression tag	UNP P18771
I	880	MET	-	expression tag	UNP P18771
I	881	GLY	-	expression tag	UNP P18771
I	882	SER	-	expression tag	UNP P18771
I	883	SER	-	expression tag	UNP P18771
I	884	HIS	-	expression tag	UNP P18771
I	885	HIS	-	expression tag	UNP P18771
I	886	HIS	-	expression tag	UNP P18771
I	887	HIS	-	expression tag	UNP P18771
I	888	HIS	-	expression tag	UNP P18771
I	889	HIS	-	expression tag	UNP P18771
I	890	SER	-	expression tag	UNP P18771
I	891	GLN	-	expression tag	UNP P18771
I	892	ASP	-	expression tag	UNP P18771
I	893	PRO	-	expression tag	UNP P18771
J	880	MET	-	expression tag	UNP P18771
J	881	GLY	-	expression tag	UNP P18771
J	882	SER	-	expression tag	UNP P18771
J	883	SER	-	expression tag	UNP P18771
J	884	HIS	-	expression tag	UNP P18771

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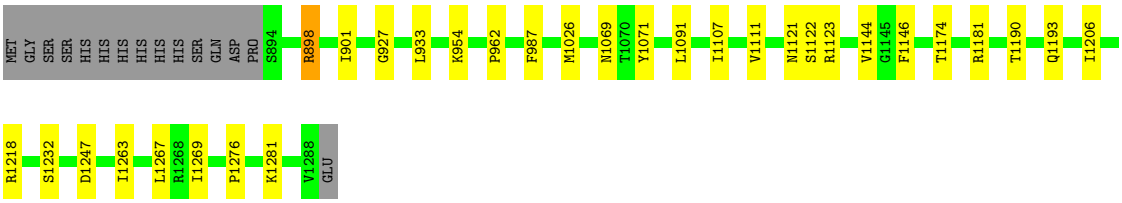
Chain	Residue	Modelled	Actual	Comment	Reference
J	885	HIS	-	expression tag	UNP P18771
J	886	HIS	-	expression tag	UNP P18771
J	887	HIS	-	expression tag	UNP P18771
J	888	HIS	-	expression tag	UNP P18771
J	889	HIS	-	expression tag	UNP P18771
J	890	SER	-	expression tag	UNP P18771
J	891	GLN	-	expression tag	UNP P18771
J	892	ASP	-	expression tag	UNP P18771
J	893	PRO	-	expression tag	UNP P18771
K	880	MET	-	expression tag	UNP P18771
K	881	GLY	-	expression tag	UNP P18771
K	882	SER	-	expression tag	UNP P18771
K	883	SER	-	expression tag	UNP P18771
K	884	HIS	-	expression tag	UNP P18771
K	885	HIS	-	expression tag	UNP P18771
K	886	HIS	-	expression tag	UNP P18771
K	887	HIS	-	expression tag	UNP P18771
K	888	HIS	-	expression tag	UNP P18771
K	889	HIS	-	expression tag	UNP P18771
K	890	SER	-	expression tag	UNP P18771
K	891	GLN	-	expression tag	UNP P18771
K	892	ASP	-	expression tag	UNP P18771
K	893	PRO	-	expression tag	UNP P18771
L	880	MET	-	expression tag	UNP P18771
L	881	GLY	-	expression tag	UNP P18771
L	882	SER	-	expression tag	UNP P18771
L	883	SER	-	expression tag	UNP P18771
L	884	HIS	-	expression tag	UNP P18771
L	885	HIS	-	expression tag	UNP P18771
L	886	HIS	-	expression tag	UNP P18771
L	887	HIS	-	expression tag	UNP P18771
L	888	HIS	-	expression tag	UNP P18771
L	889	HIS	-	expression tag	UNP P18771
L	890	SER	-	expression tag	UNP P18771
L	891	GLN	-	expression tag	UNP P18771
L	892	ASP	-	expression tag	UNP P18771
L	893	PRO	-	expression tag	UNP P18771

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.

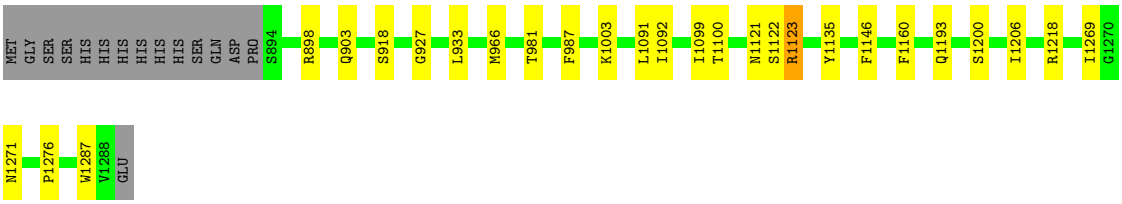
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain A:



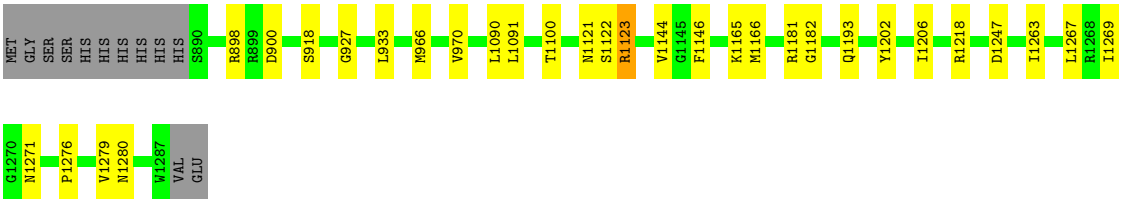
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain B:



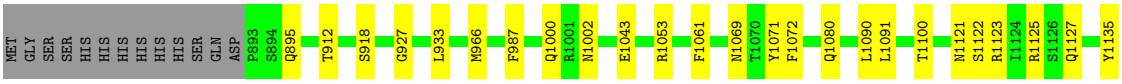
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

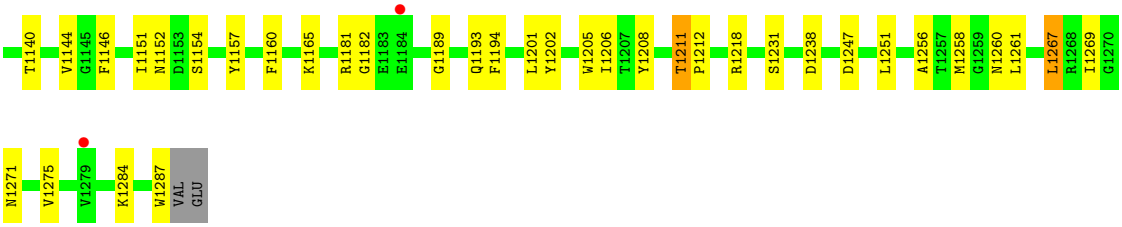
Chain C:



• Molecule 1: LARGE TAIL FIBER PROTEIN P34

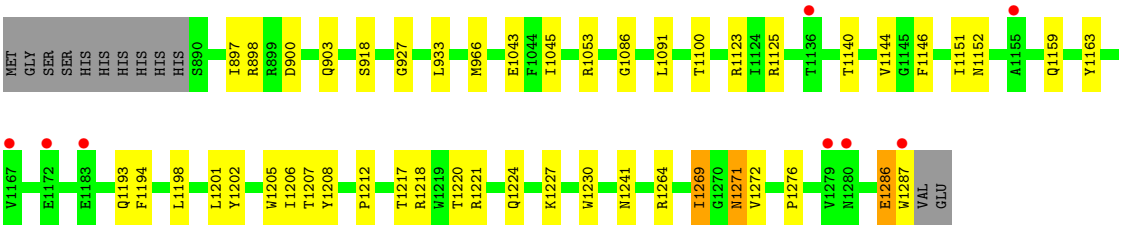
Chain D:





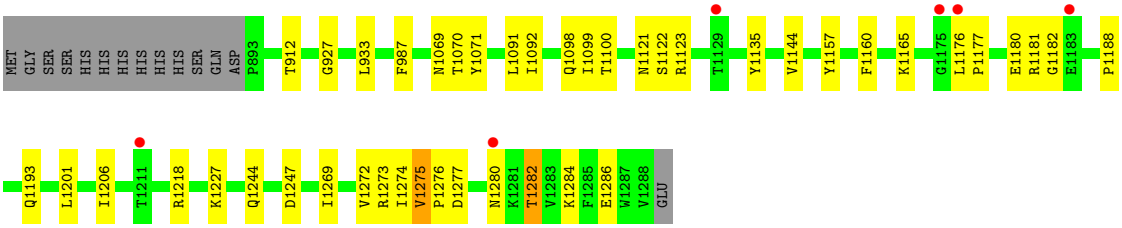
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain E:



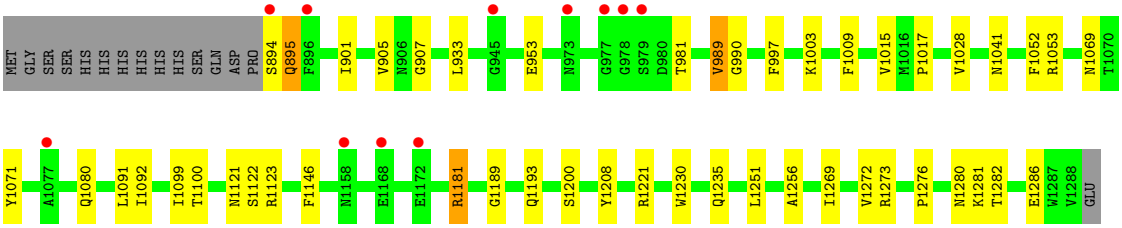
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain F:



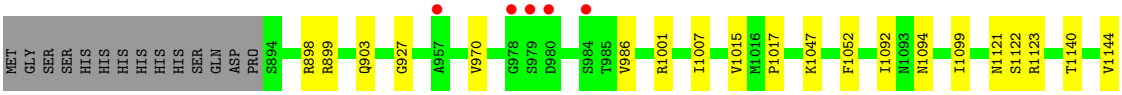
• Molecule 1: LARGE TAIL FIBER PROTEIN P34

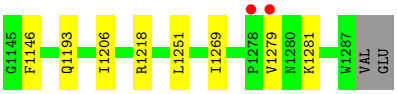
Chain G:



• Molecule 1: LARGE TAIL FIBER PROTEIN P34

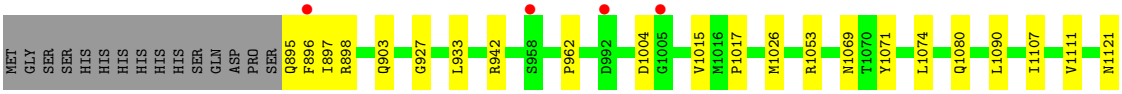
Chain H:

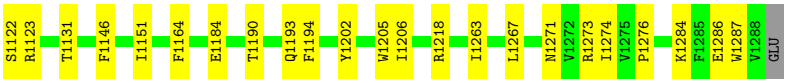




• Molecule 1: LARGE TAIL FIBER PROTEIN P34

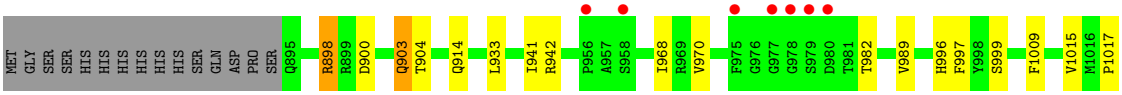
Chain I:

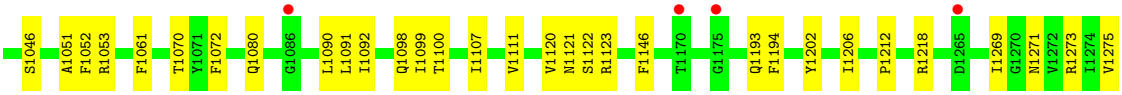




• Molecule 1: LARGE TAIL FIBER PROTEIN P34

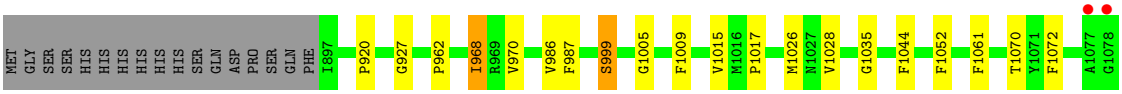
Chain J:

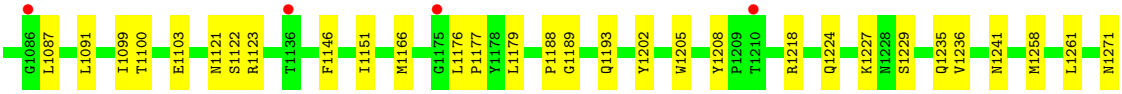


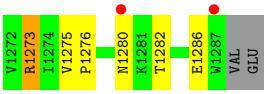


• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain K:

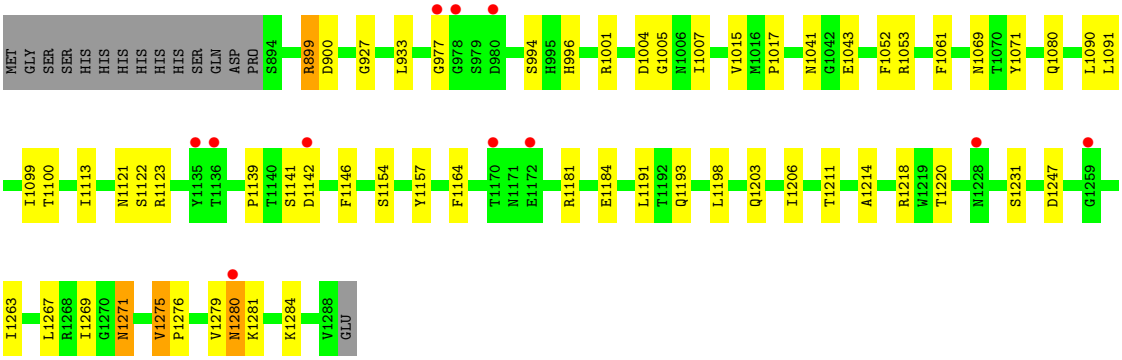






• Molecule 1: LARGE TAIL FIBER PROTEIN P34

Chain L:


MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
GLN
ASP
PRO
S894
R899
D900
G927
L933
G977
G978
S979
D980
S994
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P1017
N1041
G1042
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R1053
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L1091
I1099
T1100
I1113
N1121
S1122
R1123
Y1135
T1136
P1139
T1140
S1141
D1142
F1146
S1154
Y1157
F1164
T1170
N1171
E1172
R1181
E1184
L1191
T1192
Q1193
L1198
Q1203
I1206
T1211
A1214
R1218
W1219
T1220
N1228
S1231
D1247
G1259
I1263
L1267
R1268
I1269
G1270
N1271
V1275
P1276
V1279
N1280
K1281
K1284
V1288
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	228.49Å 228.49Å 1069.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.99-3.00) 99.9 (29.99-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.226 , 0.249 0.225 , 0.248	Depositor DCC
R_{free} test set	3005 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	1.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	36241	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.51% 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	0.32	0/3085	0.52	0/4197
1	B	0.32	0/3085	0.51	0/4197
1	C	0.32	0/3109	0.51	0/4230
1	D	0.29	0/3086	0.52	1/4198 (0.0%)
1	E	0.30	0/3109	0.52	0/4230
1	F	0.29	0/3093	0.49	0/4208
1	G	0.25	0/3085	0.49	0/4197
1	H	0.25	0/3078	0.48	0/4187
1	I	0.26	0/3079	0.47	0/4189
1	J	0.26	0/3079	0.48	0/4189
1	K	0.25	0/3051	0.49	0/4151
1	L	0.26	0/3085	0.48	0/4197
All	All	0.28	0/37024	0.50	1/50370 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1267	LEU	CA-CB-CG	6.75	130.81	115.30

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	3020	0	2921	19	0
1	B	3020	0	2921	19	0
1	C	3043	0	2936	22	0
1	D	3020	0	2920	42	0
1	E	3043	0	2936	38	0
1	F	3027	0	2929	29	0
1	G	3020	0	2921	29	0
1	H	3013	0	2912	20	0
1	I	3014	0	2916	29	0
1	J	3014	0	2916	38	0
1	K	2987	0	2890	43	0
1	L	3020	0	2921	40	0
All	All	36241	0	35039	290	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 4.

All (290) 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:A:1190:THR:HG1	1:B:1200:SER:HG	1.16	0.86
1:G:989:VAL:HG12	1:G:990:GLY:H	1.46	0.79
1:E:1207:THR:HG22	1:E:1217:THR:H	1.50	0.76
1:F:1275:VAL:HG13	1:F:1284:LYS:HB2	1.66	0.76
1:J:904:THR:O	1:L:899:ARG:NH2	2.21	0.73
1:B:898:ARG:N	1:B:903:GLN:OE1	2.16	0.73
1:A:1269:ILE:HG22	1:C:1276:PRO:HG3	1.71	0.71
1:K:1123:ARG:NH1	1:L:1141:SER:O	2.24	0.71
1:C:1181:ARG:NH2	1:C:1247:ASP:OD2	2.20	0.69
1:F:1273:ARG:HB2	1:F:1286:GLU:HB2	1.73	0.69
1:D:1211:THR:HG22	1:D:1212:PRO:HD2	1.73	0.69
1:D:1269:ILE:HG22	1:F:1276:PRO:HG3	1.75	0.69
1:F:1193:GLN:HE21	1:F:1201:LEU:HD11	1.59	0.67
1:A:1069:ASN:HD22	1:A:1091:LEU:HD13	1.59	0.67
1:D:1218:ARG:HD2	1:E:1220:THR:HG21	1.77	0.67
1:E:1152:ASN:OD1	1:E:1208:TYR:OH	2.13	0.66
1:D:1152:ASN:OD1	1:D:1208:TYR:OH	2.12	0.66
1:I:1273:ARG:HB3	1:I:1286:GLU:HB3	1.79	0.65
1:J:1206:ILE:HG13	1:J:1218:ARG:HG2	1.79	0.65
1:J:914:GLN:HE22	1:K:920:PRO:HB2	1.60	0.64
1:K:1276:PRO:HG3	1:L:1269:ILE:HG22	1.78	0.64
1:E:897:ILE:HG23	1:E:903:GLN:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1015:VAL:HG22	1:H:1017:PRO:HD3	1.80	0.64
1:I:898:ARG:N	1:I:903:GLN:OE1	2.23	0.63
1:D:1125:ARG:NH2	1:D:1127:GLN:OE1	2.31	0.63
1:E:1206:ILE:HG13	1:E:1218:ARG:HG2	1.82	0.62
1:G:1269:ILE:HG22	1:I:1276:PRO:HG3	1.80	0.62
1:K:1151:ILE:HD12	1:K:1205:TRP:HZ3	1.66	0.61
1:B:1276:PRO:HG3	1:C:1269:ILE:HG22	1.84	0.60
1:E:1264:ARG:HG3	1:E:1264:ARG:HH11	1.67	0.60
1:I:1015:VAL:HG22	1:I:1017:PRO:HD3	1.83	0.59
1:A:1276:PRO:HG3	1:B:1269:ILE:HG22	1.84	0.58
1:E:1286:GLU:OE1	1:E:1287:TRP:N	2.36	0.58
1:G:1276:PRO:HG3	1:H:1269:ILE:HG22	1.84	0.58
1:G:1052:PHE:CE2	1:H:1052:PHE:HB3	2.39	0.58
1:A:1206:ILE:HG13	1:A:1218:ARG:HG2	1.85	0.58
1:D:1123:ARG:HD2	1:E:1144:VAL:O	2.04	0.58
1:G:1092:ILE:HG12	1:G:1099:ILE:HG12	1.85	0.58
1:J:898:ARG:NH1	1:J:900:ASP:OD1	2.38	0.57
1:D:1193:GLN:HE21	1:D:1201:LEU:HD11	1.70	0.56
1:D:1275:VAL:HG13	1:D:1284:LYS:HB2	1.87	0.56
1:E:1193:GLN:HE21	1:E:1201:LEU:HD11	1.71	0.56
1:L:1001:ARG:NH1	1:L:1005:GLY:O	2.39	0.56
1:E:1091:LEU:HG	1:E:1100:THR:HB	1.87	0.56
1:H:898:ARG:H	1:H:903:GLN:HG3	1.71	0.56
1:J:1271:ASN:HB3	1:J:1287:TRP:CZ3	2.40	0.55
1:E:1269:ILE:HG23	1:E:1272:VAL:HG13	1.88	0.55
1:A:927:GLY:O	1:B:933:LEU:HD12	2.07	0.55
1:G:1280:ASN:O	1:G:1282:THR:HG23	2.06	0.55
1:J:1273:ARG:HB3	1:J:1286:GLU:HB2	1.87	0.55
1:L:1280:ASN:OD1	1:L:1281:LYS:N	2.37	0.55
1:A:1181:ARG:NH2	1:A:1247:ASP:OD2	2.40	0.55
1:G:1273:ARG:HB2	1:G:1286:GLU:HB2	1.89	0.55
1:J:1053:ARG:NE	1:L:1043:GLU:OE2	2.40	0.54
1:L:1271:ASN:O	1:L:1271:ASN:ND2	2.39	0.54
1:C:898:ARG:HG2	1:C:900:ASP:OD1	2.08	0.54
1:G:981:THR:O	1:G:1003:LYS:HD2	2.08	0.54
1:J:1194:PHE:HB2	1:J:1202:TYR:CE1	2.43	0.53
1:J:1015:VAL:HG22	1:J:1017:PRO:HD3	1.90	0.53
1:E:1224:GLN:OE1	1:E:1227:LYS:HD2	2.08	0.53
1:J:1053:ARG:NH1	1:J:1080:GLN:O	2.39	0.53
1:D:1193:GLN:NE2	1:D:1201:LEU:HD11	2.24	0.53
1:G:1015:VAL:HG22	1:G:1017:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:ARG:HG2	1:A:901:ILE:HG12	1.91	0.53
1:D:1165:LYS:O	1:D:1182:GLY:N	2.40	0.52
1:G:894:SER:OG	1:G:895:GLN:N	2.42	0.52
1:J:996:HIS:HA	1:L:1007:ILE:HD13	1.90	0.52
1:D:1206:ILE:HG13	1:D:1218:ARG:HG2	1.91	0.52
1:J:1280:ASN:OD1	1:J:1282:THR:OG1	2.27	0.52
1:I:1206:ILE:HG13	1:I:1218:ARG:HG2	1.91	0.51
1:J:1271:ASN:HB3	1:J:1287:TRP:HZ3	1.74	0.51
1:J:1091:LEU:HG	1:J:1100:THR:HB	1.93	0.51
1:K:999:SER:OG	1:L:996:HIS:ND1	2.36	0.51
1:D:1258:MET:HE1	1:D:1261:LEU:HD22	1.93	0.50
1:E:1151:ILE:HD12	1:E:1205:TRP:HZ3	1.76	0.50
1:C:1206:ILE:HG13	1:C:1218:ARG:HG2	1.94	0.50
1:D:1271:ASN:HB2	1:D:1287:TRP:CD1	2.46	0.50
1:L:1053:ARG:NH1	1:L:1080:GLN:O	2.43	0.49
1:F:1069:ASN:HB2	1:F:1071:TYR:CE1	2.47	0.49
1:F:1181:ARG:NH2	1:F:1247:ASP:OD2	2.44	0.49
1:H:1092:ILE:HG12	1:H:1099:ILE:HG12	1.94	0.49
1:I:1053:ARG:NH1	1:I:1080:GLN:O	2.44	0.49
1:A:1069:ASN:HB2	1:A:1071:TYR:CE1	2.47	0.49
1:E:1043:GLU:HB3	1:E:1045:ILE:HD11	1.94	0.49
1:E:1151:ILE:HD12	1:E:1205:TRP:CZ3	2.47	0.49
1:F:1206:ILE:HG13	1:F:1218:ARG:HG2	1.94	0.49
1:A:1144:VAL:O	1:C:1123:ARG:HD3	2.12	0.49
1:E:898:ARG:NH2	1:E:900:ASP:OD2	2.46	0.49
1:B:981:THR:O	1:B:1003:LYS:HD2	2.13	0.49
1:J:1052:PHE:CE2	1:K:1052:PHE:HB3	2.48	0.49
1:K:1273:ARG:HD2	1:K:1286:GLU:HB3	1.95	0.49
1:E:1086:GLY:HA3	1:K:1005:GLY:HA3	1.95	0.48
1:E:1123:ARG:NH1	1:E:1125:ARG:HG3	2.27	0.48
1:K:1070:THR:HG21	1:L:1061:PHE:CD2	2.48	0.48
1:D:933:LEU:HD12	1:F:927:GLY:O	2.12	0.48
1:G:989:VAL:HG12	1:G:990:GLY:N	2.23	0.48
1:K:927:GLY:O	1:L:933:LEU:HD12	2.14	0.48
1:H:1206:ILE:HG13	1:H:1218:ARG:HG2	1.95	0.48
1:I:1194:PHE:HB2	1:I:1202:TYR:CE1	2.48	0.48
1:K:1258:MET:SD	1:K:1261:LEU:HB2	2.53	0.48
1:L:1263:ILE:HD13	1:L:1267:LEU:HB2	1.96	0.48
1:K:1123:ARG:HD3	1:L:1142:ASP:O	2.13	0.48
1:L:1139:PRO:HG2	1:L:1198:LEU:HD21	1.96	0.48
1:J:1269:ILE:HG22	1:L:1276:PRO:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1091:LEU:HG	1:K:1100:THR:HB	1.95	0.48
1:E:1212:PRO:HA	1:F:1227:LYS:HE2	1.95	0.47
1:E:1217:THR:HG22	1:E:1241:ASN:ND2	2.28	0.47
1:F:1180:GLU:HA	1:F:1244:GLN:HE22	1.79	0.47
1:G:1069:ASN:HB2	1:G:1071:TYR:CE1	2.49	0.47
1:L:900:ASP:OD1	1:L:900:ASP:N	2.46	0.47
1:A:1146:PHE:HA	1:A:1193:GLN:O	2.13	0.47
1:E:1140:THR:O	1:E:1144:VAL:HG23	2.14	0.47
1:F:1092:ILE:HG12	1:F:1099:ILE:HG12	1.96	0.47
1:B:927:GLY:O	1:C:933:LEU:HD12	2.14	0.47
1:G:1146:PHE:HA	1:G:1193:GLN:O	2.15	0.47
1:I:1164:PHE:HE1	1:I:1184:GLU:HB2	1.79	0.47
1:G:1181:ARG:NH2	1:G:1235:GLN:OE1	2.47	0.47
1:J:1121:ASN:HA	1:J:1122:SER:HA	1.55	0.47
1:K:1146:PHE:HA	1:K:1193:GLN:O	2.14	0.47
1:L:1206:ILE:HG13	1:L:1218:ARG:HG2	1.95	0.47
1:D:1135:TYR:HB2	1:D:1160:PHE:CE1	2.49	0.47
1:E:1194:PHE:HB2	1:E:1202:TYR:CE1	2.49	0.47
1:F:1091:LEU:HG	1:F:1100:THR:HB	1.96	0.47
1:C:1271:ASN:OD1	1:C:1271:ASN:N	2.47	0.47
1:D:1043:GLU:OE2	1:E:1053:ARG:NE	2.43	0.47
1:C:1121:ASN:HA	1:C:1122:SER:HA	1.55	0.46
1:C:1091:LEU:HG	1:C:1100:THR:HB	1.97	0.46
1:C:1263:ILE:HD13	1:C:1267:LEU:HB2	1.97	0.46
1:G:1121:ASN:HA	1:G:1122:SER:HA	1.54	0.46
1:K:1099:ILE:HD11	1:L:1090:LEU:HB2	1.98	0.46
1:G:1251:LEU:HD11	1:G:1256:ALA:HB1	1.97	0.46
1:I:895:GLN:HA	1:I:896:PHE:HA	1.54	0.46
1:J:1098:GLN:HG2	1:K:1103:GLU:O	2.16	0.46
1:C:1279:VAL:HG13	1:C:1280:ASN:OD1	2.16	0.46
1:H:1099:ILE:HD11	1:I:1090:LEU:HB2	1.98	0.46
1:B:1099:ILE:HD11	1:C:1090:LEU:HB2	1.98	0.46
1:B:987:PHE:HB2	1:C:966:MET:SD	2.56	0.46
1:G:1272:VAL:HA	1:G:1286:GLU:O	2.16	0.46
1:D:1061:PHE:CD2	1:F:1070:THR:HG21	2.51	0.46
1:B:1092:ILE:HG12	1:B:1099:ILE:HG12	1.98	0.45
1:D:927:GLY:O	1:E:933:LEU:HD12	2.16	0.45
1:I:1121:ASN:HA	1:I:1122:SER:HA	1.49	0.45
1:J:914:GLN:NE2	1:K:920:PRO:HB2	2.28	0.45
1:J:1092:ILE:HG12	1:J:1099:ILE:HG12	1.97	0.45
1:K:1035:GLY:HA2	1:L:1041:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1235:GLN:NE2	1:K:1241:ASN:HB3	2.31	0.45
1:D:1121:ASN:HA	1:D:1122:SER:HA	1.67	0.45
1:E:1123:ARG:HD2	1:F:1144:VAL:O	2.16	0.45
1:F:1121:ASN:HA	1:F:1122:SER:HA	1.59	0.45
1:F:1272:VAL:HA	1:F:1286:GLU:O	2.17	0.45
1:I:1069:ASN:HB2	1:I:1071:TYR:CE1	2.51	0.45
1:K:1280:ASN:ND2	1:K:1282:THR:OG1	2.50	0.45
1:H:927:GLY:O	1:I:933:LEU:HD12	2.15	0.45
1:I:1274:ILE:HA	1:I:1284:LYS:O	2.17	0.45
1:C:1146:PHE:HA	1:C:1193:GLN:O	2.17	0.45
1:K:1166:MET:HG3	1:K:1179:LEU:HB3	1.99	0.45
1:E:1159:GLN:OE1	1:E:1159:GLN:N	2.50	0.45
1:L:1275:VAL:HG13	1:L:1284:LYS:HG3	1.98	0.45
1:B:1091:LEU:HG	1:B:1100:THR:HB	1.99	0.45
1:H:970:VAL:HG12	1:I:962:PRO:HG3	1.99	0.45
1:I:1273:ARG:NH2	1:I:1286:GLU:HG2	2.32	0.45
1:G:1091:LEU:HG	1:G:1100:THR:HB	1.99	0.44
1:K:1044:PHE:HB2	1:L:1052:PHE:HD1	1.81	0.44
1:K:1235:GLN:HE21	1:K:1241:ASN:HB3	1.82	0.44
1:E:1193:GLN:NE2	1:E:1201:LEU:HD11	2.31	0.44
1:F:1277:ASP:OD2	1:F:1280:ASN:ND2	2.48	0.44
1:J:970:VAL:HG12	1:K:962:PRO:HG3	1.99	0.44
1:F:1135:TYR:HB2	1:F:1160:PHE:CE1	2.53	0.44
1:F:1277:ASP:HB3	1:F:1282:THR:HG23	1.98	0.44
1:K:1189:GLY:HA2	1:K:1208:TYR:CD2	2.53	0.44
1:D:1053:ARG:NH1	1:D:1080:GLN:O	2.47	0.44
1:H:1140:THR:O	1:H:1144:VAL:HG13	2.17	0.44
1:H:1146:PHE:HA	1:H:1193:GLN:O	2.17	0.44
1:I:1271:ASN:O	1:I:1287:TRP:HA	2.17	0.44
1:C:1165:LYS:O	1:C:1166:MET:HE2	2.18	0.44
1:D:987:PHE:HB2	1:E:966:MET:SD	2.58	0.44
1:J:1206:ILE:HD13	1:K:1202:TYR:CE2	2.53	0.44
1:K:1218:ARG:HH21	1:L:1220:THR:HB	1.81	0.44
1:A:954:LYS:HA	1:A:962:PRO:HG2	2.00	0.44
1:E:1146:PHE:HA	1:E:1193:GLN:O	2.18	0.44
1:E:1221:ARG:HD2	1:E:1230:TRP:HB3	2.00	0.44
1:E:1271:ASN:O	1:E:1271:ASN:ND2	2.37	0.44
1:L:1069:ASN:HB2	1:L:1071:TYR:CE1	2.52	0.44
1:D:1251:LEU:HD11	1:D:1256:ALA:HB1	1.99	0.44
1:C:900:ASP:OD1	1:C:900:ASP:N	2.51	0.44
1:D:1146:PHE:HA	1:D:1193:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:903:GLN:HG2	1:L:899:ARG:HH12	1.83	0.44
1:J:1146:PHE:HA	1:J:1193:GLN:O	2.18	0.44
1:B:1135:TYR:HB2	1:B:1160:PHE:CE1	2.53	0.43
1:D:1181:ARG:NH2	1:D:1247:ASP:OD2	2.51	0.43
1:H:1121:ASN:HA	1:H:1122:SER:HA	1.59	0.43
1:H:1206:ILE:HD13	1:I:1202:TYR:CE2	2.53	0.43
1:K:1061:PHE:CE1	1:K:1072:PHE:HB3	2.52	0.43
1:K:1273:ARG:HD3	1:K:1275:VAL:HG23	1.99	0.43
1:A:933:LEU:HD12	1:C:927:GLY:O	2.18	0.43
1:F:1165:LYS:O	1:F:1182:GLY:N	2.51	0.43
1:G:1189:GLY:HA2	1:G:1208:TYR:CD2	2.53	0.43
1:K:1166:MET:CG	1:K:1179:LEU:HB3	2.49	0.43
1:L:1091:LEU:HG	1:L:1100:THR:HB	2.00	0.43
1:G:1200:SER:OG	1:I:1190:THR:OG1	2.24	0.43
1:J:1202:TYR:CE2	1:L:1206:ILE:HD13	2.53	0.43
1:A:1281:LYS:HA	1:B:1271:ASN:HD21	1.84	0.43
1:D:966:MET:SD	1:F:987:PHE:HB2	2.58	0.43
1:E:1276:PRO:CG	1:F:1269:ILE:HG22	2.49	0.43
1:H:1094:ASN:HA	1:I:1074:LEU:HD13	1.99	0.43
1:J:1212:PRO:HA	1:K:1227:LYS:HE2	1.99	0.43
1:L:1121:ASN:HA	1:L:1122:SER:HA	1.57	0.43
1:J:914:GLN:NE2	1:K:920:PRO:O	2.52	0.43
1:L:1164:PHE:HE1	1:L:1184:GLU:HB2	1.84	0.43
1:B:1206:ILE:HG13	1:B:1218:ARG:HG2	2.01	0.43
1:E:1264:ARG:HH11	1:E:1264:ARG:CG	2.30	0.43
1:G:1028:VAL:HG21	1:I:1026:MET:SD	2.58	0.43
1:L:1154:SER:HA	1:L:1157:TYR:CE2	2.54	0.43
1:F:1176:LEU:HA	1:F:1177:PRO:HD3	1.84	0.43
1:J:933:LEU:HD12	1:L:927:GLY:O	2.18	0.43
1:D:1123:ARG:HH21	1:D:1125:ARG:HD3	1.83	0.42
1:K:1026:MET:HE3	1:K:1028:VAL:HG23	1.99	0.42
1:D:1000:GLN:NE2	1:D:1002:ASN:OD1	2.47	0.42
1:D:1260:ASN:OD1	1:D:1260:ASN:N	2.52	0.42
1:K:1121:ASN:HA	1:K:1122:SER:HA	1.59	0.42
1:L:1191:LEU:HD11	1:L:1203:GLN:NE2	2.33	0.42
1:D:912:THR:HA	1:E:918:SER:OG	2.19	0.42
1:G:933:LEU:HD12	1:I:927:GLY:O	2.19	0.42
1:H:1281:LYS:HB3	1:I:1287:TRP:CZ3	2.54	0.42
1:I:1107:ILE:HG21	1:I:1111:VAL:HG22	2.01	0.42
1:L:1146:PHE:HA	1:L:1193:GLN:O	2.19	0.42
1:G:901:ILE:HD12	1:G:901:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1120:VAL:HG22	1:L:1113:ILE:HD12	2.01	0.42
1:I:1146:PHE:HA	1:I:1193:GLN:O	2.20	0.42
1:I:1263:ILE:HD13	1:I:1267:LEU:HB2	2.01	0.42
1:J:1273:ARG:HG2	1:J:1275:VAL:HG23	2.01	0.42
1:A:1107:ILE:HG21	1:A:1111:VAL:HG22	2.01	0.42
1:D:918:SER:OG	1:F:912:THR:HA	2.20	0.42
1:B:1123:ARG:HD3	1:C:1144:VAL:O	2.19	0.42
1:C:1165:LYS:O	1:C:1182:GLY:N	2.48	0.42
1:D:1140:THR:O	1:D:1144:VAL:HG13	2.20	0.42
1:K:1188:PRO:HB2	1:K:1208:TYR:CZ	2.54	0.42
1:A:962:PRO:HG3	1:C:970:VAL:HG12	2.01	0.42
1:A:987:PHE:HB2	1:B:966:MET:SD	2.60	0.42
1:G:1053:ARG:NH1	1:G:1080:GLN:O	2.48	0.42
1:D:1154:SER:HA	1:D:1157:TYR:CE2	2.55	0.42
1:E:1144:VAL:HG13	1:E:1201:LEU:HD13	2.00	0.42
1:J:903:GLN:CG	1:L:899:ARG:HH12	2.33	0.42
1:H:970:VAL:HA	1:H:986:VAL:O	2.19	0.41
1:L:1001:ARG:NH2	1:L:1007:ILE:HD11	2.35	0.41
1:B:1146:PHE:HA	1:B:1193:GLN:O	2.19	0.41
1:K:1176:LEU:HA	1:K:1177:PRO:HD3	1.81	0.41
1:B:1206:ILE:HD13	1:C:1202:TYR:CE2	2.56	0.41
1:F:1274:ILE:HA	1:F:1284:LYS:O	2.20	0.41
1:I:1151:ILE:HD12	1:I:1205:TRP:CZ3	2.55	0.41
1:J:1061:PHE:CE1	1:J:1072:PHE:HB3	2.56	0.41
1:A:1121:ASN:HA	1:A:1122:SER:HA	1.57	0.41
1:H:899:ARG:HB2	1:I:897:ILE:HG13	2.02	0.41
1:J:1090:LEU:HB2	1:L:1099:ILE:HD11	2.01	0.41
1:K:968:ILE:O	1:K:968:ILE:HG13	2.19	0.41
1:D:1061:PHE:CE1	1:D:1072:PHE:HB3	2.55	0.41
1:G:953:GLU:OE2	1:I:942:ARG:HD3	2.21	0.41
1:G:1041:ASN:HA	1:H:1047:LYS:HB2	2.02	0.41
1:J:1107:ILE:HG21	1:J:1111:VAL:HG22	2.02	0.41
1:D:1194:PHE:HB2	1:D:1202:TYR:CE1	2.56	0.41
1:J:1070:THR:HG21	1:K:1061:PHE:CD2	2.55	0.41
1:D:1069:ASN:HB2	1:D:1071:TYR:CE1	2.56	0.41
1:D:1151:ILE:HD12	1:D:1205:TRP:CZ3	2.56	0.41
1:E:1163:TYR:HB3	1:E:1207:THR:HG21	2.03	0.41
1:B:1121:ASN:HA	1:B:1122:SER:HA	1.60	0.41
1:D:1090:LEU:HB2	1:F:1099:ILE:HD11	2.03	0.41
1:E:1276:PRO:HG3	1:F:1269:ILE:HG22	2.03	0.41
1:G:905:VAL:HG12	1:G:907:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1046:SER:HB3	1:J:1051:ALA:HB1	2.03	0.41
1:K:968:ILE:HD13	1:K:987:PHE:CZ	2.56	0.41
1:K:970:VAL:HA	1:K:986:VAL:O	2.20	0.41
1:K:1218:ARG:HB2	1:K:1236:VAL:HB	2.03	0.41
1:L:1211:THR:OG1	1:L:1214:ALA:HB2	2.21	0.41
1:D:1189:GLY:HA2	1:D:1208:TYR:CD1	2.56	0.41
1:D:1238:ASP:OD1	1:D:1238:ASP:N	2.54	0.41
1:G:1221:ARG:HD2	1:G:1230:TRP:HB3	2.02	0.41
1:J:968:ILE:HG12	1:J:989:VAL:HG22	2.03	0.40
1:G:1251:LEU:HD23	1:H:1251:LEU:HD22	2.03	0.40
1:K:1015:VAL:HG22	1:K:1017:PRO:HD3	2.04	0.40
1:L:1015:VAL:HG22	1:L:1017:PRO:HD3	2.02	0.40
1:L:1181:ARG:NH2	1:L:1247:ASP:OD2	2.51	0.40
1:A:1263:ILE:HD13	1:A:1267:LEU:HB2	2.02	0.40
1:D:1271:ASN:OD1	1:D:1271:ASN:N	2.50	0.40
1:F:1157:TYR:CZ	1:F:1188:PRO:HD3	2.57	0.40
1:D:1061:PHE:HE1	1:D:1072:PHE:HB3	1.86	0.40
1:D:1091:LEU:HG	1:D:1100:THR:HB	2.03	0.40
1:E:927:GLY:O	1:F:933:LEU:HD12	2.22	0.40
1:H:1001:ARG:NH2	1:H:1007:ILE:HD11	2.37	0.40
1:J:1275:VAL:HB	1:J:1284:LYS:HB2	2.04	0.40
1:K:1224:GLN:NE2	1:K:1227:LYS:HD2	2.36	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	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	B	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	C	396/410 (97%)	379 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	393/410 (96%)	379 (96%)	14 (4%)	0	100	100
1	E	396/410 (97%)	382 (96%)	14 (4%)	0	100	100
1	F	394/410 (96%)	379 (96%)	15 (4%)	0	100	100
1	G	393/410 (96%)	377 (96%)	13 (3%)	3 (1%)	19	57
1	H	392/410 (96%)	378 (96%)	14 (4%)	0	100	100
1	I	392/410 (96%)	376 (96%)	16 (4%)	0	100	100
1	J	392/410 (96%)	377 (96%)	14 (4%)	1 (0%)	41	76
1	K	389/410 (95%)	375 (96%)	14 (4%)	0	100	100
1	L	393/410 (96%)	376 (96%)	14 (4%)	3 (1%)	19	57
All	All	4716/4920 (96%)	4536 (96%)	173 (4%)	7 (0%)	51	85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1279	VAL
1	J	1281	LYS
1	L	1280	ASN
1	G	1281	LYS
1	L	977	GLY
1	G	895	GLN
1	G	989	VAL

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	329/343 (96%)	324 (98%)	5 (2%)	65	87
1	B	329/343 (96%)	326 (99%)	3 (1%)	78	92
1	C	332/343 (97%)	330 (99%)	2 (1%)	86	95
1	D	329/343 (96%)	325 (99%)	4 (1%)	71	90
1	E	332/343 (97%)	328 (99%)	4 (1%)	71	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	330/343 (96%)	326 (99%)	4 (1%)	71	90
1	G	329/343 (96%)	325 (99%)	4 (1%)	71	90
1	H	328/343 (96%)	326 (99%)	2 (1%)	86	95
1	I	328/343 (96%)	325 (99%)	3 (1%)	78	92
1	J	328/343 (96%)	318 (97%)	10 (3%)	41	75
1	K	325/343 (95%)	318 (98%)	7 (2%)	52	81
1	L	329/343 (96%)	322 (98%)	7 (2%)	53	82
All	All	3948/4116 (96%)	3893 (99%)	55 (1%)	67	88

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	898	ARG
1	A	1026	MET
1	A	1123	ARG
1	A	1174	THR
1	A	1232	SER
1	B	918	SER
1	B	1123	ARG
1	B	1287	TRP
1	C	918	SER
1	C	1123	ARG
1	D	895	GLN
1	D	1211	THR
1	D	1231	SER
1	D	1267	LEU
1	E	1198	LEU
1	E	1269	ILE
1	E	1271	ASN
1	E	1286	GLU
1	F	1098	GLN
1	F	1123	ARG
1	F	1275	VAL
1	F	1282	THR
1	G	997	PHE
1	G	1009	PHE
1	G	1123	ARG
1	G	1181	ARG
1	H	1123	ARG
1	H	1279	VAL

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Mol	Chain	Res	Type
1	I	1004	ASP
1	I	1123	ARG
1	I	1131	THR
1	J	898	ARG
1	J	903	GLN
1	J	941	ILE
1	J	942	ARG
1	J	982	THR
1	J	997	PHE
1	J	999	SER
1	J	1009	PHE
1	J	1123	ARG
1	J	1282	THR
1	K	968	ILE
1	K	999	SER
1	K	1009	PHE
1	K	1087	LEU
1	K	1229	SER
1	K	1271	ASN
1	K	1273	ARG
1	L	899	ARG
1	L	994	SER
1	L	1004	ASP
1	L	1123	ARG
1	L	1231	SER
1	L	1271	ASN
1	L	1275	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1193	GLN
1	J	914	GLN
1	J	1255	ASN
1	L	1012	ASN
1	L	1193	GLN
1	L	1203	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 monosaccharides 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	395/410 (96%)	-0.56	0	100	100	4, 19, 62, 121	0
1	B	395/410 (96%)	-0.53	0	100	100	5, 21, 56, 130	0
1	C	398/410 (97%)	-0.55	0	100	100	4, 19, 62, 124	0
1	D	395/410 (96%)	-0.21	2 (0%)	91	75	5, 42, 92, 135	0
1	E	398/410 (97%)	-0.12	8 (2%)	65	36	5, 42, 94, 129	0
1	F	396/410 (96%)	-0.20	6 (1%)	73	46	4, 43, 93, 125	0
1	G	395/410 (96%)	0.09	11 (2%)	53	25	36, 69, 103, 125	0
1	H	394/410 (96%)	-0.00	7 (1%)	68	40	31, 64, 100, 137	0
1	I	394/410 (96%)	-0.06	4 (1%)	82	59	26, 65, 100, 134	0
1	J	394/410 (96%)	0.02	11 (2%)	53	25	28, 62, 99, 134	0
1	K	391/410 (95%)	0.07	8 (2%)	65	36	27, 64, 105, 143	0
1	L	395/410 (96%)	0.07	11 (2%)	53	25	28, 64, 104, 152	0
All	All	4740/4920 (96%)	-0.17	68 (1%)	75	49	4, 52, 97, 152	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1183	GLU	4.4
1	J	978	GLY	4.3
1	G	979	SER	4.1
1	E	1279	VAL	3.8
1	D	1184	GLU	3.5
1	E	1172	GLU	3.5
1	I	896	PHE	3.5
1	J	979	SER	3.4
1	H	978	GLY	3.3
1	E	1167	VAL	3.3
1	H	1279	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	1280	ASN	3.0
1	I	1005	GLY	3.0
1	G	973	ASN	3.0
1	K	1280	ASN	3.0
1	L	980	ASP	3.0
1	J	980	ASP	2.9
1	E	1155	ALA	2.8
1	L	978	GLY	2.8
1	K	1287	TRP	2.8
1	F	1129	THR	2.8
1	J	977	GLY	2.8
1	H	979	SER	2.7
1	G	978	GLY	2.7
1	K	1078	GLY	2.7
1	L	1259	GLY	2.7
1	E	1280	ASN	2.6
1	H	957	ALA	2.6
1	H	984	SER	2.6
1	G	1168	GLU	2.5
1	K	1077	ALA	2.5
1	L	1142	ASP	2.5
1	J	1086	GLY	2.5
1	L	1136	THR	2.5
1	F	1211	THR	2.5
1	G	1158	ASN	2.4
1	J	1265	ASP	2.4
1	G	945	GLY	2.4
1	G	896	PHE	2.4
1	G	977	GLY	2.4
1	J	958	SER	2.4
1	K	1136	THR	2.3
1	E	1136	THR	2.3
1	L	977	GLY	2.3
1	F	1175	GLY	2.3
1	H	980	ASP	2.3
1	I	958	SER	2.3
1	G	1172	GLU	2.2
1	L	1172	GLU	2.2
1	L	1228	ASN	2.2
1	G	1077	ALA	2.2
1	L	1135	TYR	2.2
1	G	894	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	1175	GLY	2.2
1	E	1287	TRP	2.1
1	J	1170	THR	2.1
1	K	1175	GLY	2.1
1	L	1170	THR	2.1
1	F	1280	ASN	2.1
1	F	1176	LEU	2.1
1	J	975	PHE	2.0
1	K	1210	THR	2.0
1	J	956	PRO	2.0
1	E	1183	GLU	2.0
1	H	1278	PRO	2.0
1	K	1086	GLY	2.0
1	I	992	ASP	2.0
1	D	1279	VAL	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.