



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:02 PM GMT

PDB ID : 4AT6
Title : Fab fragment of antiporphyrin antibody 14H7
Authors : Golinelli-Pimpaneau, B.; Mahy, J.P.
Deposited on : 2012-05-04
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

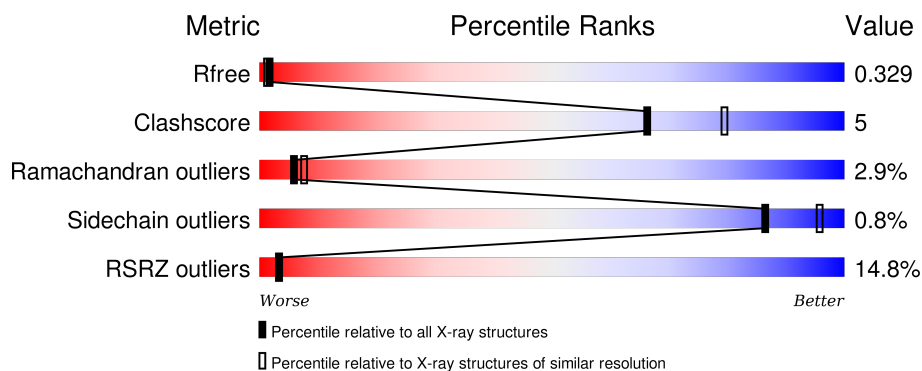
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	217	
1	C	217	
1	E	217	
1	G	217	
1	H	217	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	217	
1	M	217	
1	O	217	
2	B	212	
2	D	212	
2	F	212	
2	I	212	
2	K	212	
2	L	212	
2	N	212	
2	P	212	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25238 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 FAB 14H7 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1551	980	255	309	7			
1	C	209	Total	C	N	O	S	0	0	0
			1534	971	252	305	6			
1	E	209	Total	C	N	O	S	0	0	0
			1528	965	252	305	6			
1	G	205	Total	C	N	O	S	0	0	0
			1489	939	247	297	6			
1	H	211	Total	C	N	O	S	0	0	0
			1550	981	255	307	7			
1	J	207	Total	C	N	O	S	0	0	0
			1503	951	250	295	7			
1	M	203	Total	C	N	O	S	0	0	0
			1483	938	244	295	6			
1	O	204	Total	C	N	O	S	0	0	0
			1480	933	244	297	6			

- Molecule 2 is a protein called FAB 14H7 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	D	212	Total	C	N	O	S	0	0	0
			1594	995	269	324	6			
2	F	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	I	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	K	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	L	212	Total	C	N	O	S	0	0	0
			1591	993	268	324	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			
2	P	212	Total	C	N	O	S	0	0	0
			1596	996	269	325	6			

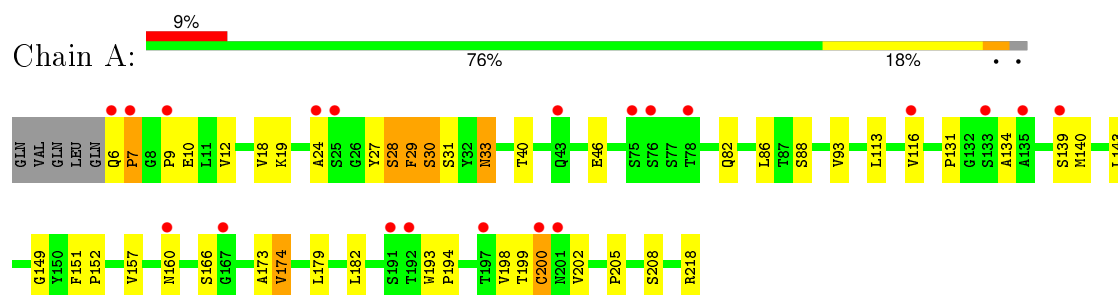
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	31	Total	O	0	0
			31	31		
3	C	25	Total	O	0	0
			25	25		
3	D	26	Total	O	0	0
			26	26		
3	E	24	Total	O	0	0
			24	24		
3	F	23	Total	O	0	0
			23	23		
3	G	16	Total	O	0	0
			16	16		
3	H	15	Total	O	0	0
			15	15		
3	I	23	Total	O	0	0
			23	23		
3	J	22	Total	O	0	0
			22	22		
3	K	27	Total	O	0	0
			27	27		
3	L	21	Total	O	0	0
			21	21		
3	M	12	Total	O	0	0
			12	12		
3	N	24	Total	O	0	0
			24	24		
3	O	16	Total	O	0	0
			16	16		
3	P	35	Total	O	0	0
			35	35		

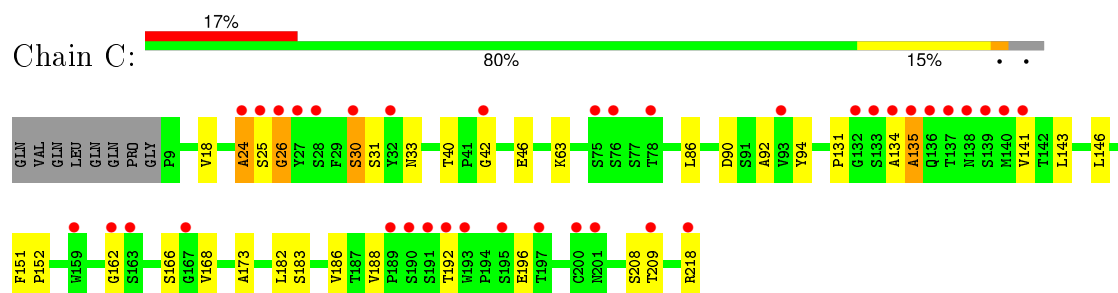
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

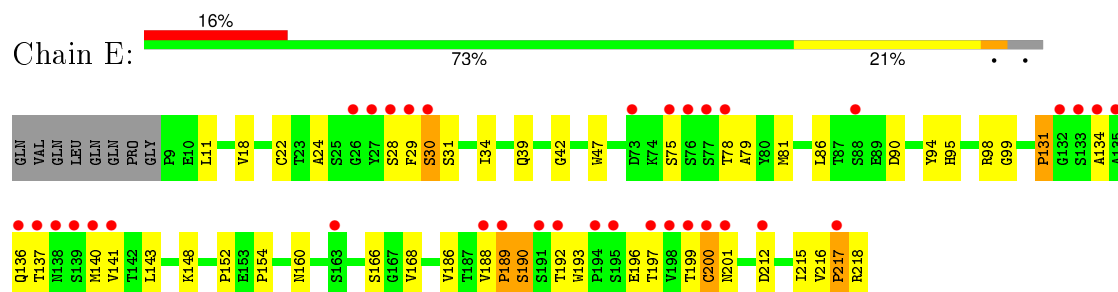
• Molecule 1: FAB 14H7 HEAVY CHAIN



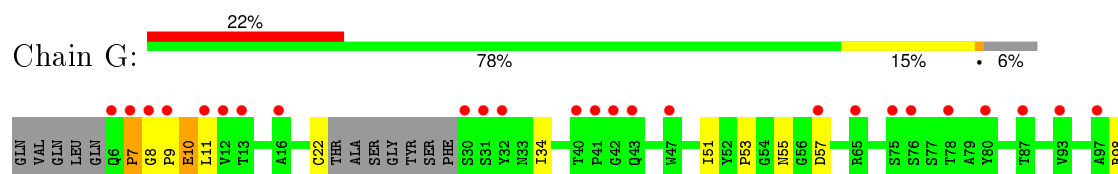
• Molecule 1: FAB 14H7 HEAVY CHAIN

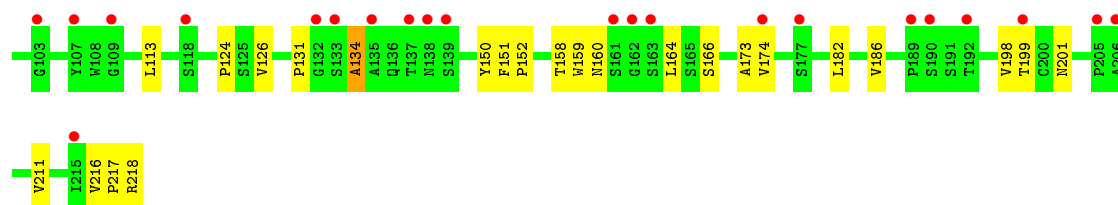


• Molecule 1: FAB 14H7 HEAVY CHAIN

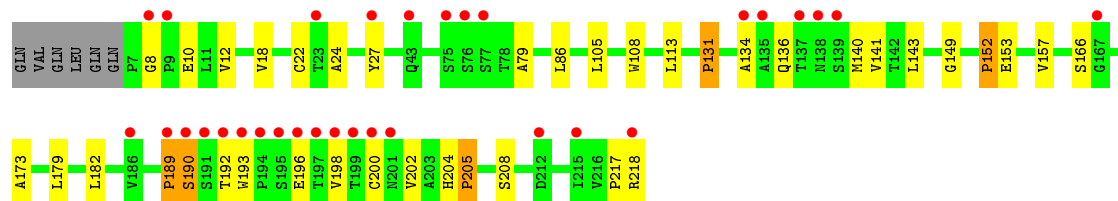
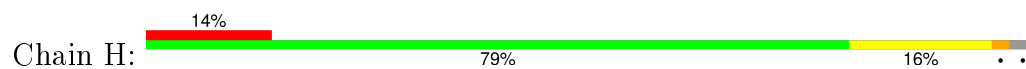


• Molecule 1: FAB 14H7 HEAVY CHAIN

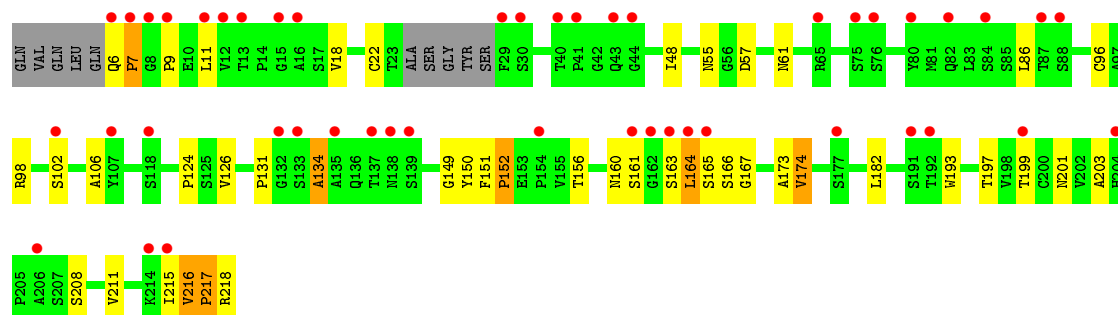
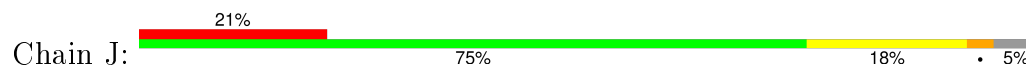




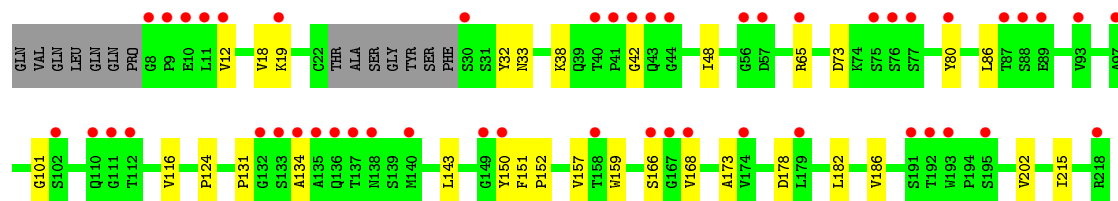
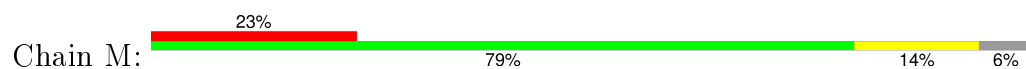
• Molecule 1: FAB 14H7 HEAVY CHAIN



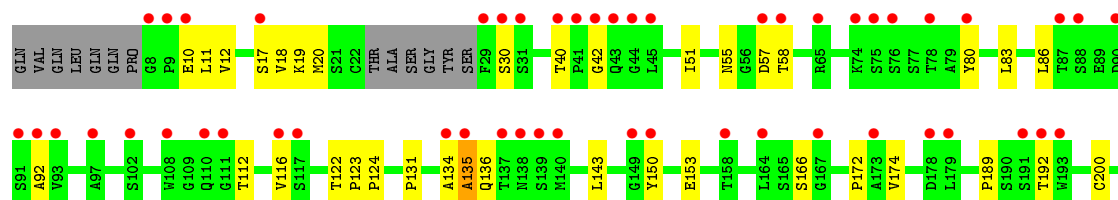
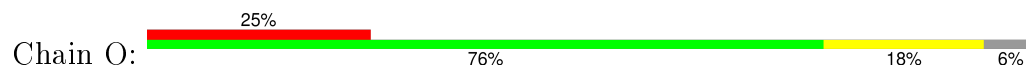
• Molecule 1: FAB 14H7 HEAVY CHAIN

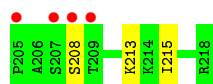


• Molecule 1: FAB 14H7 HEAVY CHAIN

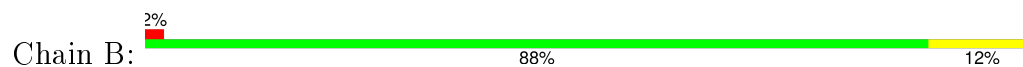


• Molecule 1: FAB 14H7 HEAVY CHAIN

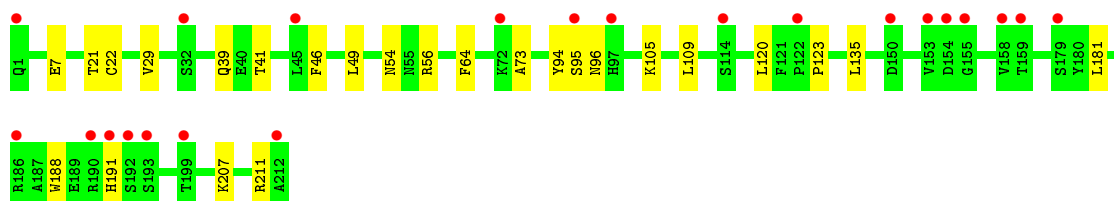
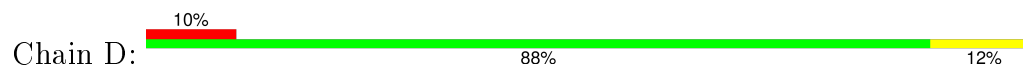




• Molecule 2: FAB 14H7 LIGHT CHAIN



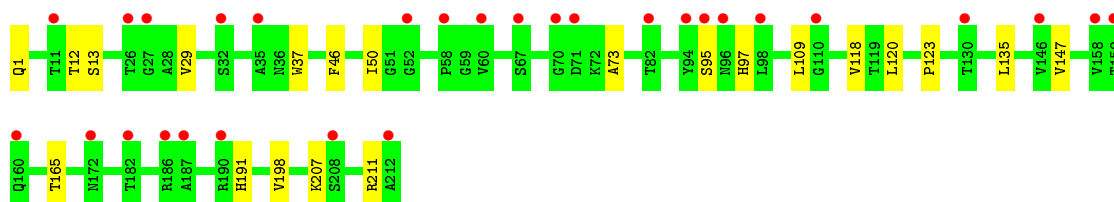
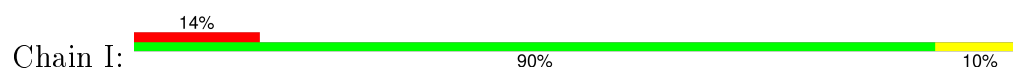
• Molecule 2: FAB 14H7 LIGHT CHAIN



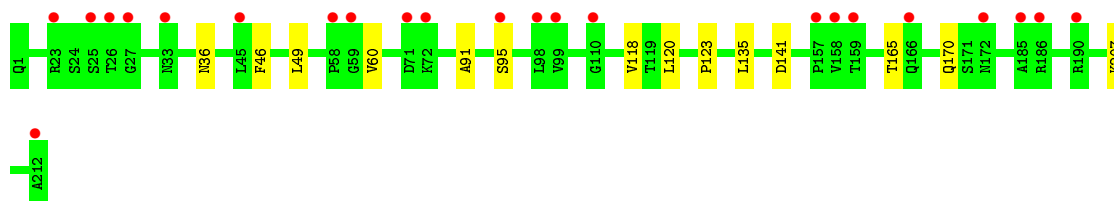
• Molecule 2: FAB 14H7 LIGHT CHAIN



• Molecule 2: FAB 14H7 LIGHT CHAIN

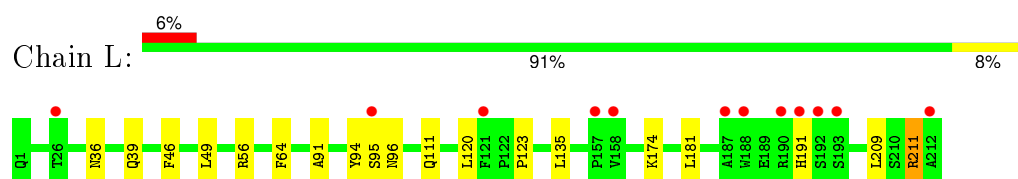


• Molecule 2: FAB 14H7 LIGHT CHAIN

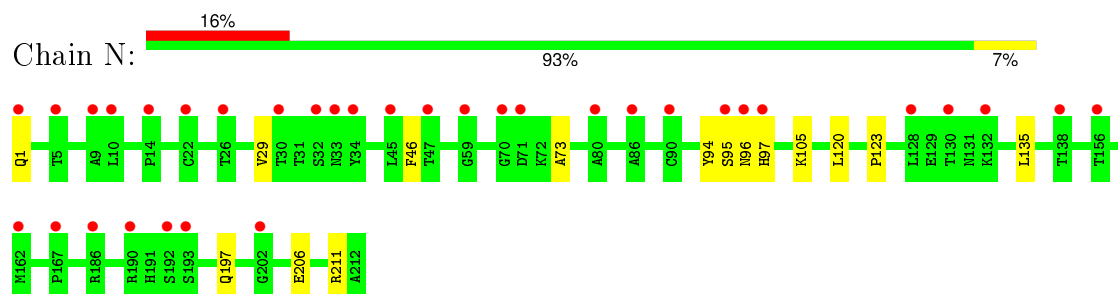


• Molecule 2: FAB 14H7 LIGHT CHAIN

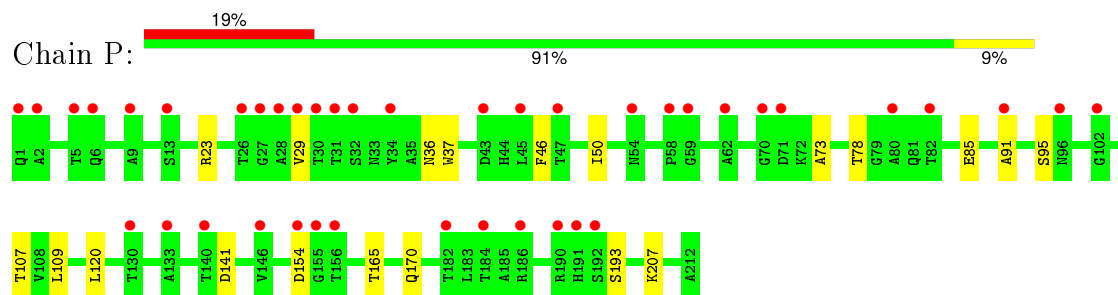




- Molecule 2: FAB 14H7 LIGHT CHAIN



- Molecule 2: FAB 14H7 LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.20 Å 228.16 Å 146.59 Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	16.65 – 2.55 16.65 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.5 (16.65-2.55) 93.0 (16.65-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.55 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.279 , 0.328 0.283 , 0.329	Depositor DCC
R_{free} test set	5009 reflections (4.49%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 75.0	EDS
Estimated twinning fraction	0.499 for H,-K,-L 0.459 for h,-k,-l	Xtriage
Reported twinning fraction	0.499 for H,-K,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 111576 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25238	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5837e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	0/1594	0.50	0/2189
1	C	0.23	0/1576	0.48	1/2163 (0.0%)
1	E	0.23	0/1569	0.50	0/2153
1	G	0.22	0/1529	0.46	0/2100
1	H	0.23	0/1593	0.46	0/2186
1	J	0.24	0/1543	0.49	0/2117
1	M	0.21	0/1522	0.44	0/2090
1	O	0.21	0/1519	0.44	0/2086
2	B	0.23	0/1632	0.42	0/2232
2	D	0.21	0/1630	0.40	0/2229
2	F	0.21	0/1632	0.41	0/2232
2	I	0.21	0/1632	0.41	0/2232
2	K	0.21	0/1632	0.41	0/2232
2	L	0.21	0/1627	0.41	0/2227
2	N	0.21	0/1632	0.40	0/2232
2	P	0.21	0/1632	0.41	0/2232
All	All	0.22	0/25494	0.44	1/34932 (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	J	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLY	N-CA-C	-6.36	97.19	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	ALA	Peptide
1	C	26	GLY	Peptide
1	J	215	ILE	Peptide
1	J	216	VAL	Peptide

5.2 Too-close contacts ⓘ

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	1551	0	1483	25	0
1	C	1534	0	1474	15	0
1	E	1528	0	1470	28	0
1	G	1489	0	1413	21	0
1	H	1550	0	1492	22	0
1	J	1503	0	1427	23	0
1	M	1483	0	1422	14	0
1	O	1480	0	1406	19	0
2	B	1596	0	1545	13	0
2	D	1594	0	1540	18	0
2	F	1596	0	1545	13	0
2	I	1596	0	1545	11	0
2	K	1596	0	1545	7	0
2	L	1591	0	1531	12	0
2	N	1596	0	1545	8	0
2	P	1596	0	1545	11	0
3	A	19	0	0	0	0
3	B	31	0	0	1	0
3	C	25	0	0	0	0
3	D	26	0	0	2	0
3	E	24	0	0	0	0
3	F	23	0	0	0	0
3	G	16	0	0	1	0
3	H	15	0	0	1	0
3	I	23	0	0	1	0
3	J	22	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	27	0	0	0	0
3	L	21	0	0	0	0
3	M	12	0	0	0	0
3	N	24	0	0	1	0
3	O	16	0	0	1	0
3	P	35	0	0	1	0
All	All	25238	0	23928	238	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 5.

The worst 5 of 238 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:J:160:ASN:ND2	1:J:197:THR:O	2.23	0.70
1:J:18:VAL:HG13	1:J:86:LEU:HD11	1.74	0.69
1:C:135:ALA:HB3	2:D:207:LYS:HD2	1.74	0.69
1:E:160:ASN:N	1:E:199:THR:O	2.18	0.68
1:H:192:THR:O	1:H:196:GLU:N	2.27	0.68

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	210/217 (97%)	173 (82%)	26 (12%)	11 (5%)	2	2
1	C	207/217 (95%)	169 (82%)	28 (14%)	10 (5%)	3	3
1	E	207/217 (95%)	174 (84%)	18 (9%)	15 (7%)	1	1
1	G	201/217 (93%)	167 (83%)	27 (13%)	7 (4%)	4	5
1	H	209/217 (96%)	174 (83%)	27 (13%)	8 (4%)	4	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	203/217 (94%)	164 (81%)	29 (14%)	10 (5%)	3	2
1	M	199/217 (92%)	173 (87%)	23 (12%)	3 (2%)	13	22
1	O	200/217 (92%)	166 (83%)	26 (13%)	8 (4%)	4	4
2	B	210/212 (99%)	194 (92%)	12 (6%)	4 (2%)	10	15
2	D	210/212 (99%)	198 (94%)	9 (4%)	3 (1%)	14	23
2	F	210/212 (99%)	196 (93%)	11 (5%)	3 (1%)	14	23
2	I	210/212 (99%)	194 (92%)	13 (6%)	3 (1%)	14	23
2	K	210/212 (99%)	194 (92%)	14 (7%)	2 (1%)	19	33
2	L	210/212 (99%)	192 (91%)	15 (7%)	3 (1%)	14	23
2	N	210/212 (99%)	194 (92%)	13 (6%)	3 (1%)	14	23
2	P	210/212 (99%)	194 (92%)	13 (6%)	3 (1%)	14	23
All	All	3316/3432 (97%)	2916 (88%)	304 (9%)	96 (3%)	6	7

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	28	SER
1	A	131	PRO
1	A	200	CYS
1	C	25	SER

5.3.2 Protein sidechains ⓘ

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	172/184 (94%)	167 (97%)	5 (3%)	50	75
1	C	170/184 (92%)	169 (99%)	1 (1%)	90	97
1	E	170/184 (92%)	169 (99%)	1 (1%)	90	97
1	G	163/184 (89%)	163 (100%)	0	100	100
1	H	172/184 (94%)	170 (99%)	2 (1%)	78	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	162/184 (88%)	158 (98%)	4 (2%)	55	80
1	M	164/184 (89%)	161 (98%)	3 (2%)	66	87
1	O	163/184 (89%)	162 (99%)	1 (1%)	90	97
2	B	179/179 (100%)	178 (99%)	1 (1%)	90	97
2	D	178/179 (99%)	177 (99%)	1 (1%)	90	97
2	F	179/179 (100%)	178 (99%)	1 (1%)	90	97
2	I	179/179 (100%)	179 (100%)	0	100	100
2	K	179/179 (100%)	179 (100%)	0	100	100
2	L	177/179 (99%)	177 (100%)	0	100	100
2	N	179/179 (100%)	179 (100%)	0	100	100
2	P	179/179 (100%)	178 (99%)	1 (1%)	90	97
All	All	2765/2904 (95%)	2744 (99%)	21 (1%)	86	96

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	41	THR
1	H	200	CYS
1	M	73	ASP
1	E	81	MET
1	M	178	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	201	ASN
2	L	97	HIS
2	P	1	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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, 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	212/217 (97%)	0.74	20 (9%) 11 12	20, 38, 71, 84	0
1	C	209/217 (96%)	1.10	37 (17%) 2 2	26, 44, 84, 107	0
1	E	209/217 (96%)	0.96	35 (16%) 2 2	22, 39, 83, 116	0
1	G	205/217 (94%)	1.37	47 (22%) 1 1	28, 52, 84, 109	0
1	H	211/217 (97%)	0.97	31 (14%) 3 3	23, 45, 81, 93	0
1	J	207/217 (95%)	1.41	46 (22%) 1 1	32, 52, 89, 102	0
1	M	203/217 (93%)	1.37	49 (24%) 1 1	27, 51, 82, 105	0
1	O	204/217 (94%)	1.51	55 (26%) 1 0	30, 56, 85, 103	0
2	B	212/212 (100%)	0.29	4 (1%) 70 74	20, 31, 58, 76	0
2	D	212/212 (100%)	0.66	22 (10%) 8 9	24, 38, 70, 89	0
2	F	212/212 (100%)	0.37	13 (6%) 25 28	20, 31, 64, 86	0
2	I	212/212 (100%)	0.94	29 (13%) 4 4	28, 48, 72, 92	0
2	K	212/212 (100%)	0.82	23 (10%) 8 8	34, 48, 72, 90	0
2	L	212/212 (100%)	0.51	12 (5%) 27 32	21, 39, 67, 80	0
2	N	212/212 (100%)	0.96	34 (16%) 3 2	29, 50, 71, 80	0
2	P	212/212 (100%)	1.10	41 (19%) 2 1	31, 50, 72, 82	0
All	All	3356/3432 (97%)	0.94	498 (14%) 3 3	20, 45, 78, 116	0

The worst 5 of 498 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	163	SER	14.4
1	G	162	GLY	12.5
1	O	9	PRO	11.5
1	M	9	PRO	11.1
1	H	200	CYS	10.5

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.