Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 08:55 PM EDT

PDB ID	:	7JWP
Title	:	Fab CJ11 in complex IL-18 peptide liberated by Caspase cleavage
Authors	:	Payandeh, J.; Ho, H.
Deposited on	:	2020-08-26
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 ⓘ 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 ⓘ) were used in the production of this report:

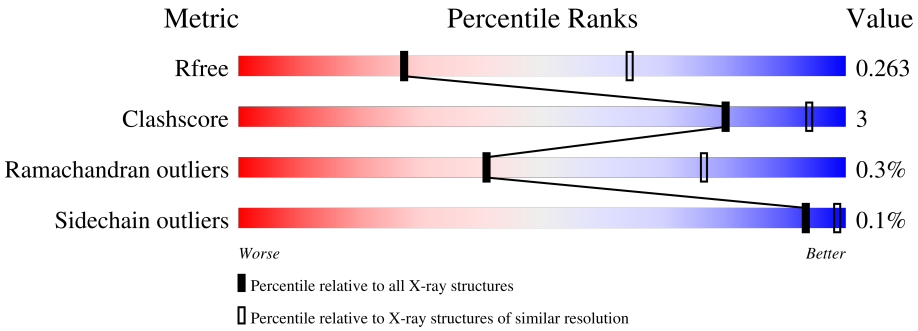
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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)

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%

Mol	Chain	Length	Quality of chain
1	A	219	85% 10% 5%
1	C	219	85% 9% 5%
1	E	219	87% 9% 5%
1	G	219	90% 5% 5%
1	I	219	86% 8% 5%
1	K	219	89% 7% 5%
1	M	219	90% 5% 5%

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Mol	Chain	Length	Quality of chain
1	O	219	92% 5%
2	B	217	91% 8%
2	D	217	91% 9%
2	F	217	94% 6%
2	H	217	94% 6%
2	J	217	89% 10%
2	L	217	90% 9%
2	N	217	90% 9%
2	P	217	93% 6%
3	Q	6	83% 17%
3	R	6	83% 17%
3	S	6	100%
3	T	6	83% 17%
3	U	6	100%
3	V	6	100%
3	W	6	67% 17% 17%
3	X	6	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 50918 atoms, of which 25165 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 CJ11 Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	208	Total	C	H	N	O	S	0	0	0
			3071	985	1528	250	302	6			
1	C	208	Total	C	H	N	O	S	0	0	0
			3071	985	1528	250	302	6			
1	E	209	Total	C	H	N	O	S	0	0	0
			3078	987	1531	251	303	6			
1	G	209	Total	C	H	N	O	S	0	0	0
			3078	987	1531	251	303	6			
1	I	208	Total	C	H	N	O	S	0	0	0
			3071	985	1528	250	302	6			
1	K	209	Total	C	H	N	O	S	0	0	0
			3078	987	1531	251	303	6			
1	M	208	Total	C	H	N	O	S	0	0	0
			3071	985	1528	250	302	6			
1	O	209	Total	C	H	N	O	S	0	0	0
			3078	987	1531	251	303	6			

- Molecule 2 is a protein called Fab CJ11 Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	216	Total	C	H	N	O	S	0	0	0
			3226	1020	1589	276	336	5			
2	D	216	Total	C	H	N	O	S	0	0	0
			3225	1020	1588	276	336	5			
2	F	216	Total	C	H	N	O	S	0	0	0
			3226	1020	1589	276	336	5			
2	H	216	Total	C	H	N	O	S	0	0	0
			3226	1020	1589	276	336	5			
2	J	215	Total	C	H	N	O	S	0	0	0
			3212	1016	1583	275	333	5			
2	L	214	Total	C	H	N	O	S	0	0	0
			3197	1011	1577	274	330	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	N	214	Total	C	H	N	O	S	0	0	0
			3197	1011	1577	274	330	5			
2	P	215	Total	C	H	N	O	S	0	0	0
			3211	1015	1583	275	333	5			

- Molecule 3 is a protein called IL-18 peptide.

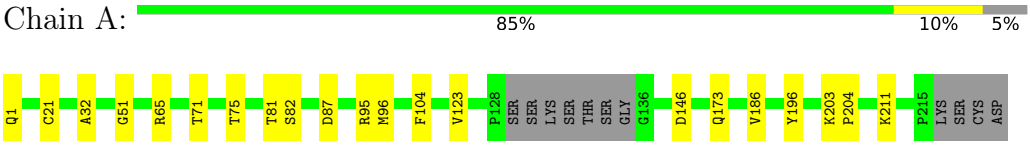
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	R	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	S	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	T	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	U	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	V	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			
3	W	5	Total	C	H	N	O	0	0	0
			70	22	30	5	13			
3	X	6	Total	C	H	N	O	0	0	0
			76	24	32	6	14			

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. 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. 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.

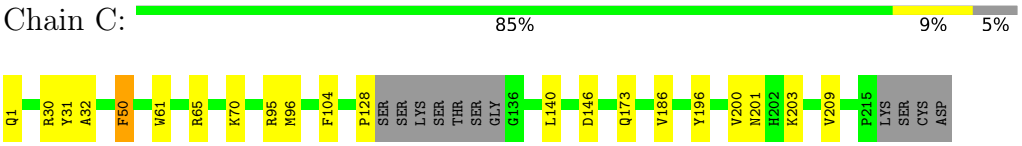
• Molecule 1: Fab CJ11 Heavy chain

Chain A:



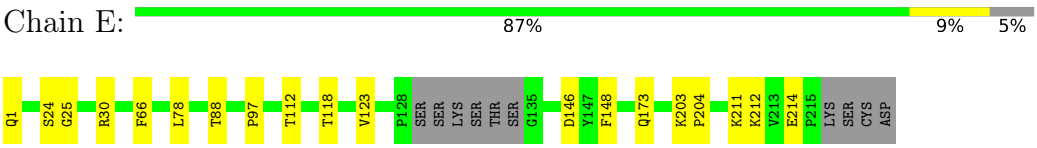
• Molecule 1: Fab CJ11 Heavy chain

Chain C:



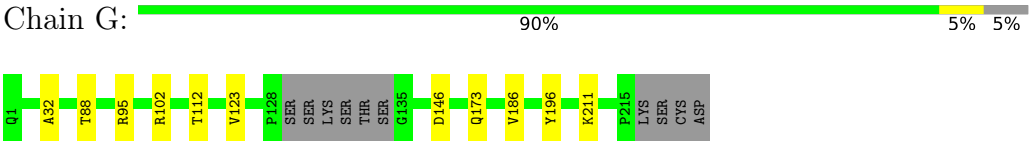
• Molecule 1: Fab CJ11 Heavy chain

Chain E:



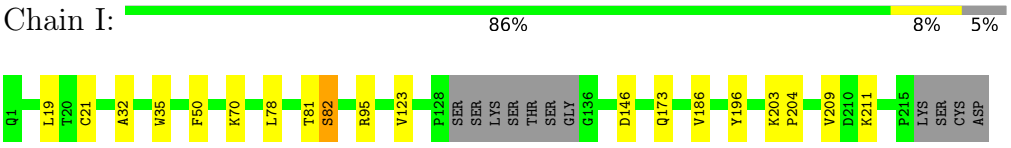
• Molecule 1: Fab CJ11 Heavy chain

Chain G:



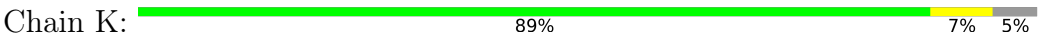
• Molecule 1: Fab CJ11 Heavy chain

Chain I:



• Molecule 1: Fab CJ11 Heavy chain

Chain K:



• Molecule 1: Fab CJ11 Heavy chain

Chain M:

• Molecule 1: Fab CJ11 Heavy chain

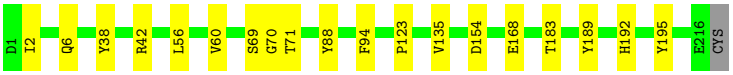
Chain O:

• Molecule 2: Fab CJ11 Light chain

Chain B:

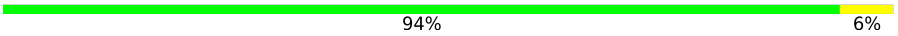
• Molecule 2: Fab CJ11 Light chain

Chain D:



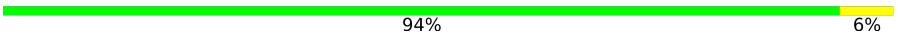
• Molecule 2: Fab CJ11 Light chain

Chain F:



• Molecule 2: Fab CJ11 Light chain

Chain H:

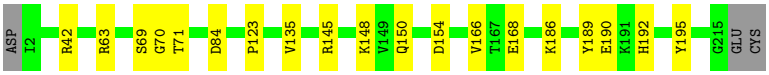


• Molecule 2: Fab CJ11 Light chain

Chain J:

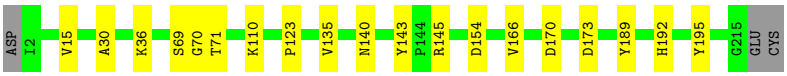
• Molecule 2: Fab CJ11 Light chain

Chain L:



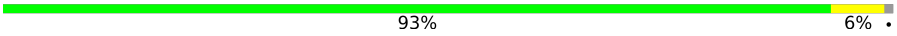
• Molecule 2: Fab CJ11 Light chain

Chain N:



• Molecule 2: Fab CJ11 Light chain

Chain P:



• Molecule 3: IL-18 peptide

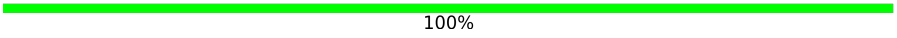
Chain Q:

• Molecule 3: IL-18 peptide

Chain R:

• Molecule 3: IL-18 peptide

Chain S:



There are no outlier residues recorded for this chain.

• Molecule 3: IL-18 peptide

Chain T:

• Molecule 3: IL-18 peptide

Chain U:

There are no outlier residues recorded for this chain.

• Molecule 3: IL-18 peptide

Chain V:

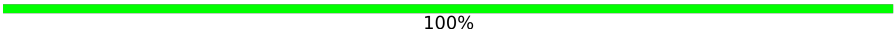
There are no outlier residues recorded for this chain.

• Molecule 3: IL-18 peptide

Chain W:

• Molecule 3: IL-18 peptide

Chain X:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.35Å 83.52Å 145.79Å 107.24° 106.53° 89.98°	Depositor
Resolution (Å)	23.97 – 3.00 24.59 – 1.68	Depositor EDS
% Data completeness (in resolution range)	86.4 (23.97-3.00) 62.9 (24.59-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.68Å)	Xtriage
Refinement program	PHENIX dev_2747	Depositor
R, R_{free}	0.235 , 0.260 0.238 , 0.263	Depositor DCC
R_{free} test set	12545 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 1.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,-h,h+l 0.000 for -k,h,k+l 0.054 for h,-k,-h-l 0.000 for -h,k,-k-l 0.014 for k,h,-h-k-l 0.000 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
Reported twinning fraction	0.120 for h,-k,-h-l	Depositor
Outliers	0 of 252856 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	50918	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 83.02 % 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 2.4133e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.31	0/1584	0.61	0/2168
1	C	0.33	0/1584	0.64	2/2168 (0.1%)
1	E	0.32	0/1588	0.63	0/2173
1	G	0.33	0/1588	0.63	0/2173
1	I	0.34	0/1584	0.66	0/2168
1	K	0.34	0/1588	0.66	0/2173
1	M	0.34	0/1584	0.66	0/2168
1	O	0.34	0/1588	0.65	0/2173
2	B	0.30	0/1669	0.60	0/2266
2	D	0.30	0/1669	0.57	0/2266
2	F	0.31	0/1669	0.58	0/2266
2	H	0.29	0/1669	0.57	0/2266
2	J	0.31	0/1661	0.60	0/2255
2	L	0.31	0/1652	0.58	0/2243
2	N	0.31	0/1652	0.59	0/2243
2	P	0.31	0/1660	0.60	0/2254
3	Q	0.26	0/43	0.43	0/55
3	R	0.30	0/43	0.61	0/55
3	S	0.25	0/43	0.41	0/55
3	T	0.27	0/43	0.41	0/55
3	U	0.26	0/43	0.40	0/55
3	V	0.30	0/43	0.62	0/55
3	W	0.24	0/39	0.53	0/50
3	X	0.26	0/43	0.42	0/55
All	All	0.32	0/26329	0.61	2/35858 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	50	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	C	50	PHE	CB-CG-CD2	5.62	124.73	120.80

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	1543	1528	1527	14	0
1	C	1543	1528	1527	13	0
1	E	1547	1531	1530	11	0
1	G	1547	1531	1530	5	0
1	I	1543	1528	1527	10	0
1	K	1547	1531	1530	8	0
1	M	1543	1528	1527	7	0
1	O	1547	1531	1530	5	0
2	B	1637	1589	1589	9	0
2	D	1637	1588	1589	9	0
2	F	1637	1589	1589	7	0
2	H	1637	1589	1589	7	0
2	J	1629	1583	1582	12	0
2	L	1620	1577	1576	10	0
2	N	1620	1577	1576	11	0
2	P	1628	1583	1583	7	0
3	Q	44	32	32	2	0
3	R	44	32	32	1	0
3	S	44	32	32	0	0
3	T	44	32	32	0	0
3	U	44	32	32	0	0
3	V	44	32	32	0	0
3	W	40	30	29	1	0
3	X	44	32	32	0	0
All	All	25753	25165	25154	135	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 3.

All (135) 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)
2:J:67:SER:OG	2:J:74:THR:OG1	2.06	0.73
1:C:30:ARG:NH1	1:C:31:TYR:OH	2.25	0.70
2:D:69:SER:O	2:D:71:THR:N	2.25	0.69
2:D:154:ASP:OD1	2:D:192:HIS:ND1	2.24	0.69
1:C:146:ASP:OD2	1:C:173:GLN:NE2	2.27	0.67
1:G:146:ASP:OD1	1:G:173:GLN:NE2	2.27	0.67
2:L:154:ASP:OD2	2:L:192:HIS:ND1	2.26	0.67
2:B:154:ASP:OD1	2:B:192:HIS:ND1	2.30	0.65
2:J:154:ASP:OD2	2:J:192:HIS:ND1	2.27	0.64
1:C:200:VAL:HB	1:C:209:VAL:HG23	1.86	0.58
2:F:154:ASP:OD1	2:F:192:HIS:ND1	2.34	0.57
1:A:146:ASP:OD1	1:A:173:GLN:NE2	2.37	0.56
2:L:42:ARG:HB2	2:L:168:GLU:HG3	1.88	0.55
2:J:69:SER:O	2:J:71:THR:N	2.37	0.55
1:I:81:THR:O	1:I:82:SER:C	2.45	0.55
2:P:154:ASP:OD1	2:P:192:HIS:ND1	2.40	0.54
2:L:69:SER:O	2:L:71:THR:N	2.36	0.54
1:A:65:ARG:NH2	1:A:87:ASP:OD1	2.41	0.54
1:I:50:PHE:CE2	1:I:70:LYS:HE3	2.43	0.53
2:N:69:SER:O	2:N:71:THR:N	2.35	0.53
2:F:69:SER:O	2:F:71:THR:N	2.35	0.53
2:D:42:ARG:HB2	2:D:168:GLU:HG3	1.91	0.53
2:P:69:SER:O	2:P:71:THR:N	2.39	0.52
2:J:67:SER:HB3	3:R:30:GLY:N	2.24	0.51
2:J:190:GLU:O	2:J:214:ARG:NH2	2.44	0.51
1:I:32:ALA:O	1:I:95:ARG:NE	2.44	0.50
2:B:190:GLU:O	2:B:214:ARG:NH2	2.45	0.49
2:N:123:PRO:HD3	2:N:135:VAL:HG22	1.95	0.49
1:G:32:ALA:O	1:G:95:ARG:NE	2.45	0.49
1:I:146:ASP:OD1	1:I:173:GLN:NE2	2.43	0.49
2:J:139:LEU:HD21	2:J:199:VAL:HG13	1.95	0.49
1:C:96:MET:HG3	2:D:38:TYR:OH	2.13	0.48
1:I:21:CYS:HB2	1:I:35:TRP:CZ2	2.48	0.48
2:L:123:PRO:HD3	2:L:135:VAL:HG22	1.95	0.48
2:L:148:LYS:CE	2:L:150:GLN:OE1	2.61	0.48
2:N:15:VAL:HG12	1:O:117:SER:OG	2.12	0.48
2:J:36:LYS:HD3	2:J:38:TYR:CZ	2.49	0.47
2:B:36:LYS:HD3	2:B:38:TYR:CZ	2.49	0.47
1:C:96:MET:O	1:C:96:MET:HG2	2.14	0.47
2:L:189:TYR:HA	2:L:195:TYR:OH	2.14	0.47
1:E:97:PRO:O	2:F:36:LYS:NZ	2.39	0.47
2:D:2:ILE:HG21	2:D:94:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:NE2	2:D:88:TYR:O	2.41	0.47
1:K:81:THR:O	1:K:82:SER:HB3	2.16	0.46
2:J:123:PRO:HD3	2:J:135:VAL:HG22	1.96	0.46
1:M:146:ASP:OD1	1:M:173:GLN:NE2	2.47	0.46
2:N:154:ASP:OD1	2:N:192:HIS:ND1	2.43	0.46
2:B:69:SER:O	2:B:71:THR:N	2.44	0.46
1:G:186:VAL:HG11	1:G:196:TYR:CE2	2.51	0.46
1:C:1:GLN:OE1	1:C:104:PHE:CZ	2.67	0.46
1:A:186:VAL:HG11	1:A:196:TYR:CE2	2.51	0.46
2:B:123:PRO:HD3	2:B:135:VAL:HG22	1.97	0.46
1:C:30:ARG:O	1:C:30:ARG:HG2	2.15	0.46
2:H:123:PRO:HD3	2:H:135:VAL:HG22	1.97	0.46
1:K:21:CYS:HB2	1:K:35:TRP:CZ2	2.50	0.46
2:L:63:ARG:NH1	2:L:84:ASP:OD2	2.48	0.45
1:E:146:ASP:OD1	1:E:173:GLN:NE2	2.47	0.45
2:B:139:LEU:HD21	2:B:199:VAL:HG13	1.97	0.45
1:K:32:ALA:O	1:K:95:ARG:NE	2.48	0.45
2:P:36:LYS:HD3	2:P:38:TYR:CZ	2.51	0.45
1:M:123:VAL:O	1:M:211:LYS:HE3	2.17	0.45
2:F:17:GLY:O	2:F:80:LEU:HD23	2.17	0.45
1:A:32:ALA:O	1:A:95:ARG:NE	2.47	0.45
1:E:203:LYS:N	1:E:204:PRO:CD	2.80	0.45
2:J:63:ARG:NH1	2:J:84:ASP:OD2	2.48	0.45
1:O:96:MET:O	1:O:96:MET:HG2	2.17	0.45
1:E:123:VAL:O	1:E:211:LYS:HE3	2.16	0.45
2:F:123:PRO:HD3	2:F:135:VAL:HG22	2.00	0.45
1:A:96:MET:HG2	1:A:96:MET:O	2.18	0.44
1:E:212:LYS:HE2	1:E:214:GLU:OE2	2.16	0.44
1:C:201:ASN:OD1	1:C:203:LYS:HG2	2.16	0.44
2:J:15:VAL:HG12	1:K:117:SER:OG	2.17	0.44
1:M:30:ARG:O	1:M:30:ARG:HG2	2.17	0.44
2:J:42:ARG:HG3	2:J:168:GLU:HB3	1.99	0.44
2:P:123:PRO:HD3	2:P:135:VAL:HG22	1.99	0.44
1:I:186:VAL:HG11	1:I:196:TYR:CE2	2.53	0.44
2:L:145:ARG:NH2	2:L:166:VAL:HG21	2.33	0.43
1:O:88:THR:HG23	1:O:112:THR:HA	2.00	0.43
1:A:123:VAL:O	1:A:211:LYS:HE3	2.18	0.43
2:F:154:ASP:HA	2:F:194:VAL:HG22	2.00	0.43
1:I:209:VAL:CG2	2:P:8:PRO:HB3	2.47	0.43
1:E:88:THR:HG23	1:E:112:THR:HA	2.01	0.43
2:N:189:TYR:HA	2:N:195:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:VAL:HG23	2:H:80:LEU:HD11	1.99	0.43
1:C:61:TRP:O	1:C:65:ARG:HD3	2.19	0.43
1:C:186:VAL:HG11	1:C:196:TYR:CE2	2.54	0.43
2:L:186:LYS:HE3	2:L:190:GLU:OE1	2.18	0.43
1:E:1:GLN:HA	1:E:24:SER:O	2.19	0.43
2:H:36:LYS:HD3	2:H:38:TYR:CZ	2.54	0.43
1:A:203:LYS:N	1:A:204:PRO:CD	2.82	0.42
2:D:123:PRO:HD3	2:D:135:VAL:HG22	2.00	0.42
1:E:118:THR:HA	1:E:148:PHE:O	2.19	0.42
2:H:188:ASP:HA	2:H:191:LYS:HD3	2.00	0.42
2:F:189:TYR:HA	2:F:195:TYR:OH	2.19	0.42
1:O:186:VAL:HG11	1:O:196:TYR:CE2	2.54	0.42
1:A:32:ALA:HB2	3:Q:33:GLU:O	2.19	0.42
1:K:186:VAL:HG11	1:K:196:TYR:CE2	2.54	0.42
1:M:21:CYS:HB2	1:M:35:TRP:CZ2	2.53	0.42
2:D:56:LEU:HD21	2:D:60:VAL:O	2.20	0.42
1:E:30:ARG:O	1:E:30:ARG:HG2	2.19	0.42
1:G:123:VAL:O	1:G:211:LYS:HE3	2.19	0.42
2:H:192:HIS:O	2:H:214:ARG:NE	2.40	0.42
1:I:203:LYS:N	1:I:204:PRO:CD	2.83	0.42
2:P:85:ALA:HB2	2:P:109:ILE:HG12	2.01	0.42
1:E:66:PHE:HB3	1:E:78:LEU:HD11	2.02	0.42
1:G:88:THR:HG23	1:G:112:THR:HA	2.02	0.42
1:K:203:LYS:N	1:K:204:PRO:CD	2.82	0.42
1:A:71:THR:HB	2:H:206:SER:HB3	2.02	0.41
1:I:123:VAL:O	1:I:211:LYS:HE3	2.20	0.41
2:L:148:LYS:HE2	2:L:150:GLN:OE1	2.20	0.41
1:O:123:VAL:O	1:O:211:LYS:HE3	2.19	0.41
2:D:189:TYR:HA	2:D:195:TYR:OH	2.20	0.41
2:N:110:LYS:HA	2:N:143:TYR:OH	2.20	0.41
1:A:51:GLY:HA3	3:Q:33:GLU:HB3	2.02	0.41
2:B:63:ARG:NH1	2:B:84:ASP:OD2	2.53	0.41
2:J:126:GLU:HG3	2:P:72:GLN:OE1	2.20	0.41
1:M:97:PRO:O	2:N:36:LYS:NZ	2.44	0.41
2:N:30:ALA:HB1	3:W:32:LEU:HD11	2.02	0.41
1:A:81:THR:O	1:A:82:SER:C	2.58	0.41
1:M:203:LYS:N	1:M:204:PRO:CD	2.84	0.41
1:A:1:GLN:OE1	1:A:104:PHE:CZ	2.74	0.41
1:M:185:THR:HG21	2:N:140:ASN:ND2	2.36	0.41
2:N:170:ASP:HB3	2:N:173:ASP:OD1	2.21	0.41
2:B:193:LYS:HE3	2:B:213:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PHE:CE2	1:C:70:LYS:HB2	2.56	0.41
1:C:128:PRO:HG3	1:C:140:LEU:HB3	2.02	0.41
1:A:21:CYS:O	1:A:75:THR:HA	2.21	0.40
2:H:195:TYR:O	2:H:211:SER:HA	2.21	0.40
1:E:1:GLN:HG2	1:E:25:GLY:O	2.21	0.40
1:K:146:ASP:OD1	1:K:173:GLN:NE2	2.49	0.40
1:A:96:MET:HG3	2:B:38:TYR:OH	2.22	0.40
1:I:19:LEU:HD12	1:I:78:LEU:HD23	2.03	0.40
1:K:61:TRP:O	1:K:65:ARG:HD3	2.21	0.40
2:N:145:ARG:NH2	2:N:166:VAL:HG11	2.37	0.40
1:C:32:ALA:O	1:C:95:ARG:NE	2.53	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	204/219 (93%)	198 (97%)	6 (3%)	0	100	100
1	C	204/219 (93%)	200 (98%)	4 (2%)	0	100	100
1	E	205/219 (94%)	201 (98%)	4 (2%)	0	100	100
1	G	205/219 (94%)	201 (98%)	4 (2%)	0	100	100
1	I	204/219 (93%)	200 (98%)	3 (2%)	1 (0%)	29	68
1	K	205/219 (94%)	201 (98%)	4 (2%)	0	100	100
1	M	204/219 (93%)	199 (98%)	5 (2%)	0	100	100
1	O	205/219 (94%)	201 (98%)	4 (2%)	0	100	100
2	B	214/217 (99%)	204 (95%)	8 (4%)	2 (1%)	17	55
2	D	214/217 (99%)	204 (95%)	9 (4%)	1 (0%)	29	68
2	F	214/217 (99%)	204 (95%)	9 (4%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	214/217 (99%)	206 (96%)	8 (4%)	0	100	100
2	J	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	29	68
2	L	212/217 (98%)	203 (96%)	8 (4%)	1 (0%)	29	68
2	N	212/217 (98%)	202 (95%)	9 (4%)	1 (0%)	29	68
2	P	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	29	68
3	Q	4/6 (67%)	4 (100%)	0	0	100	100
3	R	4/6 (67%)	4 (100%)	0	0	100	100
3	S	4/6 (67%)	4 (100%)	0	0	100	100
3	T	4/6 (67%)	4 (100%)	0	0	100	100
3	U	4/6 (67%)	4 (100%)	0	0	100	100
3	V	4/6 (67%)	4 (100%)	0	0	100	100
3	W	3/6 (50%)	3 (100%)	0	0	100	100
3	X	4/6 (67%)	4 (100%)	0	0	100	100
All	All	3373/3536 (95%)	3265 (97%)	99 (3%)	9 (0%)	41	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	70	GLY
2	B	70	GLY
2	F	70	GLY
2	J	70	GLY
2	N	70	GLY
2	P	70	GLY
2	B	42	ARG
2	L	70	GLY
1	I	82	SER

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	175/185 (95%)	175 (100%)	0	100 100
1	C	175/185 (95%)	175 (100%)	0	100 100
1	E	175/185 (95%)	175 (100%)	0	100 100
1	G	175/185 (95%)	174 (99%)	1 (1%)	86 95
1	I	175/185 (95%)	175 (100%)	0	100 100
1	K	175/185 (95%)	175 (100%)	0	100 100
1	M	175/185 (95%)	175 (100%)	0	100 100
1	O	175/185 (95%)	175 (100%)	0	100 100
2	B	184/185 (100%)	184 (100%)	0	100 100
2	D	184/185 (100%)	183 (100%)	1 (0%)	88 96
2	F	184/185 (100%)	184 (100%)	0	100 100
2	H	184/185 (100%)	184 (100%)	0	100 100
2	J	183/185 (99%)	182 (100%)	1 (0%)	88 96
2	L	182/185 (98%)	182 (100%)	0	100 100
2	N	182/185 (98%)	182 (100%)	0	100 100
2	P	183/185 (99%)	183 (100%)	0	100 100
3	Q	5/5 (100%)	5 (100%)	0	100 100
3	R	5/5 (100%)	5 (100%)	0	100 100
3	S	5/5 (100%)	5 (100%)	0	100 100
3	T	5/5 (100%)	4 (80%)	1 (20%)	1 7
3	U	5/5 (100%)	5 (100%)	0	100 100
3	V	5/5 (100%)	5 (100%)	0	100 100
3	W	5/5 (100%)	5 (100%)	0	100 100
3	X	5/5 (100%)	5 (100%)	0	100 100
All	All	2906/3000 (97%)	2902 (100%)	4 (0%)	93 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	183	THR
1	G	102	ARG
2	J	216	GLU
3	T	31	ASP

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

sidechains are listed below:

Mol	Chain	Res	Type
1	K	166	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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.