W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 04:45 am GMT

PDB ID	:	5F1I
Title	:	MHC with 9-mer peptide
Authors	:	Liu, J.; Chai, Y.; QI, J.; Gao, G.F.
Deposited on	:	2015-11-30
Resolution	:	2.90 Å(reported)

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

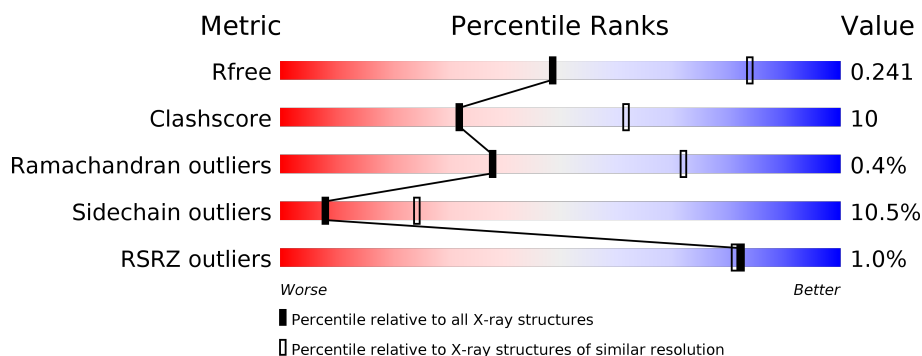|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.90 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		10.5%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 <=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	275	69% 25% • •
1	D	275	69% 28% • •
1	G	275	67% 28% • •
1	J	275	% 67% 26% 6% •
1	M	275	% 75% 21% • •
1	P	275	% 67% 28% • •

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Mol	Chain	Length	Quality of chain
1	S	275	69% 24% 6%
1	V	275	64% 32%
2	B	99	71% 23% 6%
2	E	99	76% 20%
2	H	99	69% 26% 5%
2	K	99	74% 21% 5%
2	N	99	69% 29%
2	Q	99	68% 31%
2	T	99	68% 27% 5%
2	W	99	76% 21%
3	C	9	100%
3	F	9	56% 22% 22%
3	I	9	67% 33%
3	L	9	78% 22%
3	O	9	78% 11% 11%
3	R	9	56% 33% 11%
3	U	9	33% 56% 11%
3	X	9	44% 44% 11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 24668 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 MHC class I DLA-88.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2177	1357	390	424	6			
1	D	271	Total	C	N	O	S	0	1	0
			2194	1368	394	426	6			
1	G	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	J	270	Total	C	N	O	S	0	0	0
			2177	1357	390	424	6			
1	M	271	Total	C	N	O	S	0	1	0
			2192	1366	393	427	6			
1	P	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	S	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			
1	V	271	Total	C	N	O	S	0	0	0
			2184	1362	391	425	6			

- Molecule 2 is a protein called Beta2M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	E	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	H	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	K	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	N	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	Q	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	W	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

- Molecule 3 is a protein called 9-mer peptide.

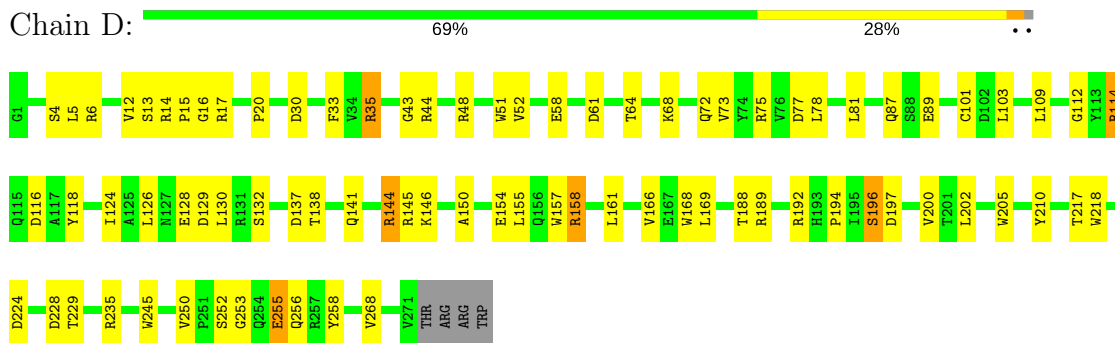| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	F	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	I	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	L	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	O	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	R	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	U	9	Total	C	N	O	0	0	0
			71	47	11	13			
3	X	9	Total	C	N	O	0	0	0
			71	47	11	13			

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.
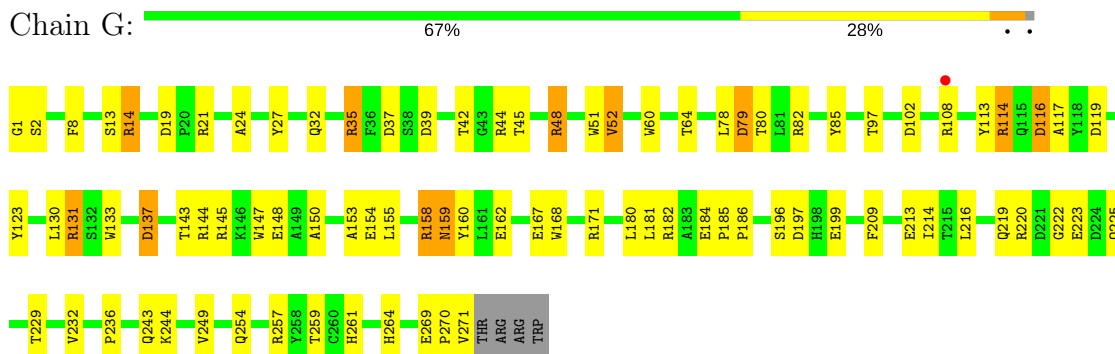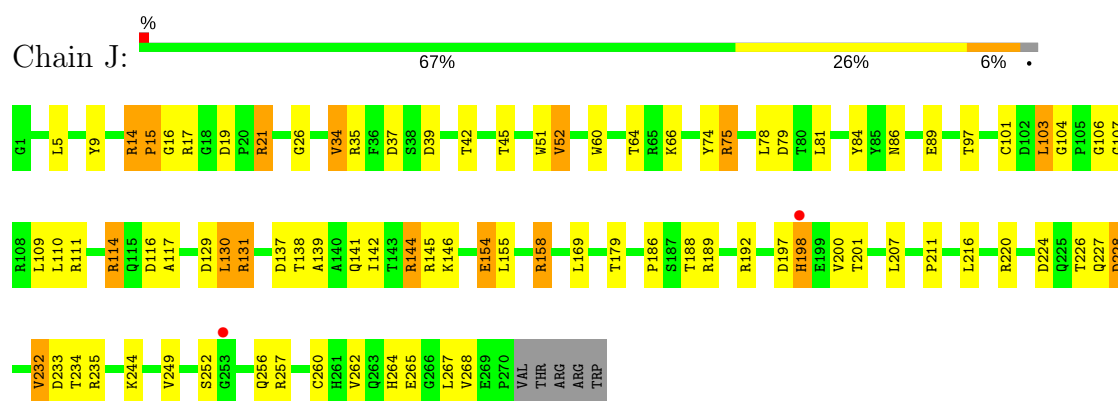
• Molecule 1: MHC class I DLA-88
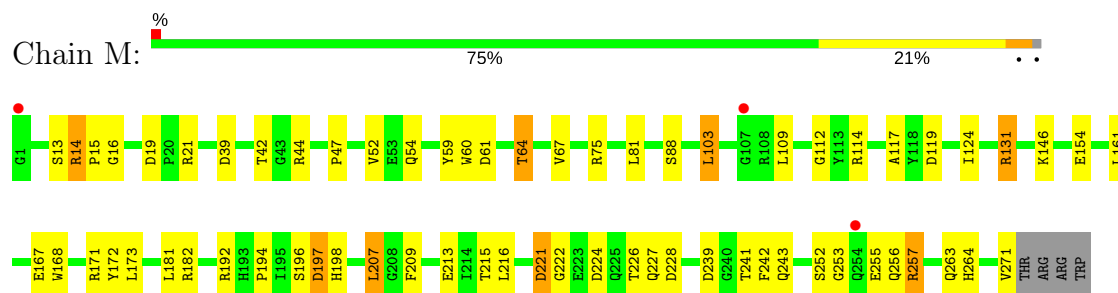
Chain A:

• Molecule 1: MHC class I DLA-88

Chain D:

• Molecule 1: MHC class I DLA-88

Chain G:

• Molecule 1: MHC class I DLA-88

Chain J:

67% 26% 6% ·

G1 L5 Y9 R14 P15 G16 R17 G18 D19 P20 R21 G26 V34 R35 F36 D37 S38 D39 T42 T45 W51 V52 W60 T64 R65 K66 Y74 R75 L78 D79 T80 L81 Y84 Y85 N86 E89 T97 C101 D102 L103 G104 P105 G106 G107

R108 L109 L110 R111 R114 Q115 D116 A117 D129 L130 R131 D137 T138 A139 A140 Q141 I142 T143 R144 R145 K146 E154 L155 R158 L169 L179 T179 P186 S187 T188 R189 R192 D197 H198 E199 V200 T201 L207 P211 L216 R220 D224 Q225 T226 Q227 D228

V232 D233 T234 R235 K244 V249 S252 G253 Q256 R257 C260 H261 V262 Q263 H264 E265 G266 L267 V268 E269 P270 VAL THR ARG ARG TRP

• Molecule 1: MHC class I DLA-88

Chain M:

75% 21% · ·

G1 S13 R14 P15 G16 D19 P20 R21 D39 T42 G43 R44 P47 V52 E53 Q54 Y59 W60 D61 T64 V67 R75 L81 S88 L103 G107 R108 L109 G112 Y113 R114 A117 Y118 D119 I124 R131 K146 E154 L161

E167 W168 R171 Y172 L173 L181 R182 R192 H193 P194 I195 S196 D197 H198 L207 G208 F209 E213 I214 T215 L216 D221 G222 E223 D224 Q225 T226 Q227 D228 D239 T241 F242 Q243 S252 G253 Q254 E255 Q256 R257 Q263 H264 V271 THR ARG ARG TRP

• Molecule 1: MHC class I DLA-88

Chain P:

67% 28% · ·

G1 L5 S11 V12 S13 R14 P15 G16 R17 G18 D19 P20 Q32 F33 V34 R35 D39 R44 T45 R48 W51 V52 G56 Y59 W60 D61 T64 K68 R75 L78 L81 R82 E89 T94 I95 P105 G106 G107 R108 L109 R114 Q115

D116 Y123 N127 R131 S132 W133 T134 T143 R144 E148 A149 A150 G151 V152 L155 Q156 W157 R158 L161 E162 T163 E167 W168 L169 Q170 L180 E184 P185 R189 P194 D197 V200 T201 L202 L207 T215 L216 L217 R220 Q225 T226 Q227

R235 P236 K244 V250 P251 S252 G253 Q254 E255 T259 C260 H261 V262 Q263 H264 E265 P270 V271 THR ARG ARG TRP

• Molecule 1: MHC class I DLA-88

Chain S:

69% 24% 6% ·

G1 S2 H3 S4 V12 S13 R14 P15 G16 D19 P20 R21 R35 D39 T42 G43 R44 T45 E46 P47 R48 V52 W60 D61 T64 R65 K66 Y74 L81 R82 Q87 T94 I95 Q96 T97 C101 D102 L103 G104 P105 G106 G107 R108 L109 L110 R111 G112

Y113 R114 Q115 D116 D122 Y123 I124 D129 L130 R131 S132 T138 R144 R145 K146 G151 V152 A153 E154 W157 R158 E162 W168 L169 Q170 R171 Y172 L173 L180 P186 S187 T188 R189 V190 T191 R192 H193 P194 H198 E199 V200 L207 G208 F209 Q219 R220

Q227 T234 R235 Q243 K244 S252 R257 Y258 T259 C260 H261 V262 V268 E269 P270 V271 THR ARG ARG TRP

• Molecule 1: MHC class I DLA-88

Chain V:

64% 32%

G1 S2 H3 S4 L5 S11 R14 P15 G16 D19 P20 R21 F22 I23 A24 V25 D29 D30 T31 R35 F36 D37 A40 A41 T42 G43 R44 R48 V52 W60 D61 T64 R65 K66 V67 K68 E69 R75 L78 D79 T97 C101 D102 L103 L109

R114 Q115 D116 A117 Y118 D119 Y123 I124 N127 E128 D129 L130 R131 S132 W133 T143 R144 R145 K146 W147 A150 G151 V152 A153 Q156 W157 R158 E162 T163 T164 E167 W168 L169 Q170 R171 Y172 M175 R182 P185 P186 P194 V200 W205 A206 L207 G208

F209 Y210 E213 I214 T215 L216 T217 R220 T226 Q227 T241 S252 G253 Q256 R257 Y258 T259 C260 H261 V262 Q263 H264 E265 G266 L267 V268 E269 P270 V271 THR ARG ARG TRP

- Molecule 2: Beta2M

Chain B:

%

71% 23% 6%

I1 T4 A15 E16 G29 S33 D34 L39 I46 V49 E50 H51 S52 D53 L54 S55 K58 D59 W60 S61 F62 L65 T68 E69 F70 T73 E74 K75 D76 E77 Y78 N83 L87 M99

- Molecule 2: Beta2M

Chain E:

2%

76% 20%

I1 P5 K6 Y10 S11 N24 V27 F30 S33 V37 R45 E50 K58 L65 Y66 Y67 T68 E69 F70 T73 E74 K75 R81 V82 I92 V93 K94 R97 D98 M99

- Molecule 2: Beta2M

Chain H:

4%

69% 26% 5%

I1 Q2 R3 Q8 S11 A15 S20 L23 G29 D34 I35 E36 L39 I46 E47 K48 V49 S55 F56 S57 K58 D59 W60 S61 L65 Y66 Y67 T68 E69 F70 T71 P72 T73 D76 E77 Y78 R81 Q89 P90 R97 D98 M99

- Molecule 2: Beta2M

Chain K:

%

74% 21% 5%

I1 T4 P5 K6 I7 Q8 V9 Y10 E16 N21 F22 L23 G29 F30 H31 L39 E44 E47 K48 S57 K58 D59 W60 S61 Y67 F70 Y78 V82 N83 H84 V85 T86 L87 M99

- Molecule 2: Beta2M

Chain N:

2%

69% 29%

I1 P5 K6 I7 A15 E16 N17 N21 F22 L23 N24 G29 F30 L39 I46 E47 K48 V49 E50 K58 D59 W60 S61 L65 T68 E69 F70 T71 P72 T73 E74 K75 D76 E77 R81 V82 N83 H84 L87 S88 Q89 I92 M99

- Molecule 2: Beta2M

Chain Q:

3%

68% 31%

I1 Q2 R3 K6 I7 Y10 A15 E16 N17 N21 F22 C25 G29 S33 D34 I35 E36 V37 D38 L39 L40 K41 E44 R45 I46 E47 K48 S52 D53 L54 F62 L65 Y66 F70 A79 C80 R81 V82 L87 S88 Q89 R97 D98 M99

• Molecule 2: Beta2M

Chain T:

2%
68%　　　　27%　　　5%

I1 Q2 R3 T4 P5 R12 K19 S20 N21 F22 L23 N24 C25 Y26 V27 H31 D34 V37 D38 L39 L40 K41 E44 H51 S52 F56 S57 K58 F62 Y63 L64 L65 Y66 F70 T73 D76 E77 Y78 V85 I92 M99

• Molecule 2: Beta2M

Chain W:

%
76%　　　　21%　・

I1 Q2 R3 T4 P5 E16 N17 N24 P32 V37 E50 H51 K58 D59 W60 L65 F70 Y78 A79 V82 N83 H84 V85 T86 K91 K94 M99

• Molecule 3: 9-mer peptide

Chain C:

100%

There are no outlier residues recorded for this chain.

• Molecule 3: 9-mer peptide

Chain F:

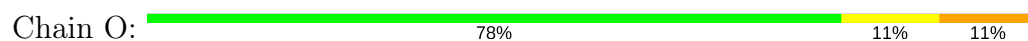56%　　　　22%　　　22%

K1 E6 L7 T8 K9

• Molecule 3: 9-mer peptide

Chain I:

67%　　　　33%

K1 L2 F3 L7 T8 K9

• Molecule 3: 9-mer peptide

Chain L:

78%　　　　22%

K1 L2 T8 K9

• Molecule 3: 9-mer peptide

Chain O:

78%　　　11%　　11%

K1 E6 L7 T8 K9
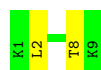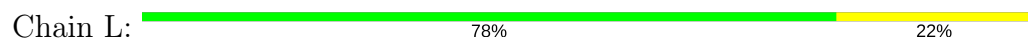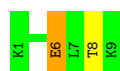
• Molecule 3: 9-mer peptide
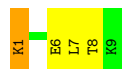
Chain R:

• Molecule 3: 9-mer peptide
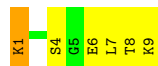
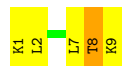Chain U:

• Molecule 3: 9-mer peptide

Chain X:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.10Å 94.63Å 124.36Å 84.60° 72.79° 81.61°	Depositor
Resolution (Å)	41.55 – 2.90 48.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.55-2.90) 95.0 (48.90-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.208 , 0.240 0.209 , 0.241	Depositor DCC
R_{free} test set	3817 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 28.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24668	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.46	0/2234	0.65	0/3043
1	D	0.48	0/2252	0.65	0/3068
1	G	0.45	0/2241	0.64	0/3053
1	J	0.44	0/2234	0.65	0/3043
1	M	0.47	0/2249	0.65	0/3064
1	P	0.41	0/2241	0.60	0/3053
1	S	0.43	0/2241	0.63	0/3053
1	V	0.42	0/2241	0.61	0/3053
2	B	0.53	0/851	0.66	0/1152
2	E	0.51	0/851	0.59	0/1152
2	H	0.53	0/851	0.64	0/1152
2	K	0.45	0/851	0.60	0/1152
2	N	0.48	0/851	0.62	0/1152
2	Q	0.44	0/851	0.58	0/1152
2	T	0.46	0/851	0.62	0/1152
2	W	0.45	0/851	0.61	0/1152
3	C	0.42	0/71	0.57	0/92
3	F	0.47	0/71	0.62	0/92
3	I	0.48	0/71	0.53	0/92
3	L	0.48	0/71	0.64	0/92
3	O	0.58	0/71	0.73	0/92
3	R	0.51	0/71	0.65	0/92
3	U	0.56	0/71	0.67	0/92
3	X	0.46	0/71	0.83	0/92
All	All	0.46	0/25309	0.63	0/34382

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	2177	0	2040	46	0
1	D	2194	0	2055	48	0
1	G	2184	0	2049	62	0
1	J	2177	0	2040	47	0
1	M	2192	0	2054	37	0
1	P	2184	0	2049	57	0
1	S	2184	0	2049	49	0
1	V	2184	0	2049	60	0
2	B	828	0	794	15	0
2	E	828	0	794	13	0
2	H	828	0	794	18	1
2	K	828	0	794	11	1
2	N	828	0	794	14	0
2	Q	828	0	794	20	0
2	T	828	0	794	18	0
2	W	828	0	794	13	0
3	C	71	0	80	0	0
3	F	71	0	80	6	0
3	I	71	0	80	4	0
3	L	71	0	80	2	0
3	O	71	0	80	3	0
3	R	71	0	80	1	0
3	U	71	0	80	5	0
3	X	71	0	80	6	0
All	All	24668	0	23377	484	1

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 10.

The worst 5 of 484 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:S:227:GLN:HB3	1:V:144:ARG:HH22	1.35	0.91
1:P:45:THR:H	1:P:64:THR:HG22	1.37	0.90
1:S:35:ARG:HD2	1:S:48:ARG:HD2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:24:ASN:HB3	2:N:65:LEU:HD11	1.62	0.82
2:B:4:THR:H	2:E:1:ILE:HD12	1.44	0.82

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:ARG:NH2	2:K:44:GLU:OE1[1_545]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	268/275 (98%)	245 (91%)	21 (8%)	2 (1%)	25	60
1	D	270/275 (98%)	245 (91%)	24 (9%)	1 (0%)	38	72
1	G	269/275 (98%)	246 (91%)	21 (8%)	2 (1%)	25	60
1	J	268/275 (98%)	245 (91%)	22 (8%)	1 (0%)	38	72
1	M	270/275 (98%)	241 (89%)	28 (10%)	1 (0%)	38	72
1	P	269/275 (98%)	250 (93%)	17 (6%)	2 (1%)	25	60
1	S	269/275 (98%)	246 (91%)	22 (8%)	1 (0%)	38	72
1	V	269/275 (98%)	246 (91%)	22 (8%)	1 (0%)	38	72
2	B	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	H	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	K	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	N	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
2	Q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
2	W	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
3	L	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	U	7/9 (78%)	7 (100%)	0	0	100	100
3	X	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	2984/3064 (97%)	2751 (92%)	222 (7%)	11 (0%)	38	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	196	SER
1	D	196	SER
1	S	270	PRO
1	G	254	GLN
1	A	266	GLY

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	225/230 (98%)	202 (90%)	23 (10%)	8	26
1	D	227/230 (99%)	206 (91%)	21 (9%)	10	31
1	G	226/230 (98%)	207 (92%)	19 (8%)	13	36
1	J	225/230 (98%)	192 (85%)	33 (15%)	3	11
1	M	227/230 (99%)	203 (89%)	24 (11%)	8	24
1	P	226/230 (98%)	204 (90%)	22 (10%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	S	226/230 (98%)	202 (89%)	24 (11%)		8	24
1	V	226/230 (98%)	203 (90%)	23 (10%)		8	26
2	B	94/94 (100%)	83 (88%)	11 (12%)		6	18
2	E	94/94 (100%)	84 (89%)	10 (11%)		8	24
2	H	94/94 (100%)	84 (89%)	10 (11%)		8	24
2	K	94/94 (100%)	82 (87%)	12 (13%)		5	15
2	N	94/94 (100%)	85 (90%)	9 (10%)		10	29
2	Q	94/94 (100%)	87 (93%)	7 (7%)		16	42
2	T	94/94 (100%)	84 (89%)	10 (11%)		8	24
2	W	94/94 (100%)	87 (93%)	7 (7%)		16	42
3	C	8/8 (100%)	8 (100%)	0		100	100
3	F	8/8 (100%)	6 (75%)	2 (25%)		1	2
3	I	8/8 (100%)	8 (100%)	0		100	100
3	L	8/8 (100%)	8 (100%)	0		100	100
3	O	8/8 (100%)	7 (88%)	1 (12%)		5	16
3	R	8/8 (100%)	4 (50%)	4 (50%)		0	0
3	U	8/8 (100%)	6 (75%)	2 (25%)		1	2
3	X	8/8 (100%)	7 (88%)	1 (12%)		5	16
All	All	2624/2656 (99%)	2349 (90%)	275 (10%)		8	24

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	232	VAL
1	M	131	ARG
1	V	144	ARG
1	J	268	VAL
2	K	70	PHE

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

Mol	Chain	Res	Type
1	P	225	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 ⓘ

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, 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(Å²)	Q<0.9
1	A	270/275 (98%)	-0.19	0	100	100	34, 48, 78, 125	0
1	D	271/275 (98%)	-0.18	0	100	100	32, 47, 81, 130	0
1	G	271/275 (98%)	-0.16	1 (0%)	92	92	32, 49, 82, 111	0
1	J	270/275 (98%)	-0.11	2 (0%)	87	86	35, 50, 81, 104	0
1	M	271/275 (98%)	-0.14	3 (1%)	80	79	35, 48, 82, 107	0
1	P	271/275 (98%)	-0.12	3 (1%)	80	79	34, 54, 84, 110	0
1	S	271/275 (98%)	-0.01	3 (1%)	80	79	33, 50, 84, 106	0
1	V	271/275 (98%)	-0.12	1 (0%)	92	92	35, 55, 88, 118	0
2	B	99/99 (100%)	0.18	1 (1%)	82	81	34, 45, 68, 83	0
2	E	99/99 (100%)	-0.06	2 (2%)	65	62	34, 44, 73, 87	0
2	H	99/99 (100%)	0.18	4 (4%)	39	34	33, 45, 74, 90	0
2	K	99/99 (100%)	-0.13	1 (1%)	82	81	35, 47, 77, 97	0
2	N	99/99 (100%)	-0.12	2 (2%)	65	62	34, 46, 75, 98	0
2	Q	99/99 (100%)	0.13	3 (3%)	51	44	36, 51, 80, 105	0
2	T	99/99 (100%)	0.01	2 (2%)	65	62	34, 49, 73, 101	0
2	W	99/99 (100%)	0.08	1 (1%)	82	81	36, 50, 77, 101	0
3	C	9/9 (100%)	-0.10	0	100	100	40, 51, 60, 60	0
3	F	9/9 (100%)	-0.04	0	100	100	34, 45, 53, 77	0
3	I	9/9 (100%)	-0.19	0	100	100	37, 42, 55, 69	0
3	L	9/9 (100%)	0.02	0	100	100	42, 48, 56, 75	0
3	O	9/9 (100%)	-0.12	0	100	100	37, 44, 55, 70	0
3	R	9/9 (100%)	0.01	0	100	100	36, 48, 53, 74	0
3	U	9/9 (100%)	0.05	0	100	100	37, 48, 56, 65	0
3	X	9/9 (100%)	-0.18	0	100	100	42, 48, 61, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
All	All	3030/3064 (98%)	-0.09	29 (0%)	82	81	32, 49, 82, 130	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	79	ALA	4.9
2	N	68	THR	3.3
1	V	256	GLN	2.8
2	E	11	SER	2.8
2	H	23	LEU	2.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.