



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 07:40 AM EDT

PDB ID : 3ETB
Title : Crystal structure of the engineered neutralizing antibody M18 complexed with anthrax protective antigen domain 4
Authors : Monzingo, A.F.; Leysath, C.E.; Barnett, J.; Iverson, B.L.; Georgiou, G.; Robertus, J.D.
Deposited on : unknown
Resolution : 3.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

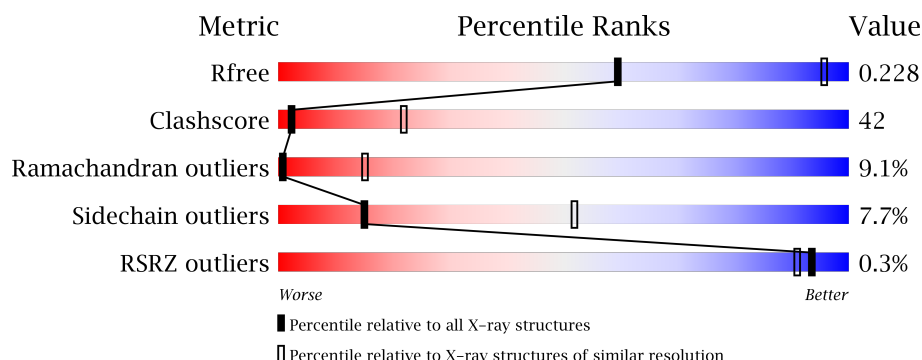
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	F	252	
1	G	252	
1	H	252	
1	I	252	
2	J	144	

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Mol	Chain	Length	Quality of chain
2	K	144	<div><div><div></div><div></div><div></div></div><div>2%42%47%10%•</div></div>
2	L	144	<div><div><div></div><div></div><div></div></div><div>%41%50%8%••</div></div>
2	M	144	<div><div><div></div><div></div><div></div></div><div>44%48%7%•</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11546 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 Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGS)₄ linker.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	228	Total	C	N	O	S	0	0	1
			1742	1091	296	347	8			
1	G	229	Total	C	N	O	S	0	0	1
			1743	1091	296	348	8			
1	H	229	Total	C	N	O	S	0	0	1
			1743	1091	296	348	8			
1	I	228	Total	C	N	O	S	0	0	1
			1742	1091	296	347	8			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	MET	-	EXPRESSION TAG	PDB 3ETB
F	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
F	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
F	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
F	0	LYS	-	EXPRESSION TAG	PDB 3ETB
F	21	VAL	ILE	ENGINEERED	PDB 3ETB
F	46	PHE	LEU	ENGINEERED	PDB 3ETB
F	56	PRO	SER	ENGINEERED	PDB 3ETB
F	76	ASN	SER	ENGINEERED	PDB 3ETB
F	78	LEU	GLN	ENGINEERED	PDB 3ETB
F	94	PRO	LEU	ENGINEERED	PDB 3ETB
F	109	GLY	-	LINKER	PDB 3ETB
F	110	GLY	-	LINKER	PDB 3ETB
F	111	GLY	-	LINKER	PDB 3ETB
F	112	GLY	-	LINKER	PDB 3ETB
F	113	SER	-	LINKER	PDB 3ETB
F	114	GLY	-	LINKER	PDB 3ETB
F	115	GLY	-	LINKER	PDB 3ETB
F	116	GLY	-	LINKER	PDB 3ETB
F	117	GLY	-	LINKER	PDB 3ETB

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Chain	Residue	Modelled	Actual	Comment	Reference
F	118	SER	-	LINKER	PDB 3ETB
F	119	GLY	-	LINKER	PDB 3ETB
F	120	GLY	-	LINKER	PDB 3ETB
F	121	GLY	-	LINKER	PDB 3ETB
F	122	GLY	-	LINKER	PDB 3ETB
F	123	SER	-	LINKER	PDB 3ETB
F	124	GLY	-	LINKER	PDB 3ETB
F	125	GLY	-	LINKER	PDB 3ETB
F	126	GLY	-	LINKER	PDB 3ETB
F	127	GLY	-	LINKER	PDB 3ETB
F	128	SER	-	LINKER	PDB 3ETB
F	1030	ASN	SER	ENGINEERED	PDB 3ETB
F	1057	SER	THR	ENGINEERED	PDB 3ETB
F	1064	GLU	LYS	ENGINEERED	PDB 3ETB
F	1068	ILE	THR	ENGINEERED	PDB 3ETB
G	-4	MET	-	EXPRESSION TAG	PDB 3ETB
G	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
G	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
G	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
G	0	LYS	-	EXPRESSION TAG	PDB 3ETB
G	21	VAL	ILE	ENGINEERED	PDB 3ETB
G	46	PHE	LEU	ENGINEERED	PDB 3ETB
G	56	PRO	SER	ENGINEERED	PDB 3ETB
G	76	ASN	SER	ENGINEERED	PDB 3ETB
G	78	LEU	GLN	ENGINEERED	PDB 3ETB
G	94	PRO	LEU	ENGINEERED	PDB 3ETB
G	109	GLY	-	LINKER	PDB 3ETB
G	110	GLY	-	LINKER	PDB 3ETB
G	111	GLY	-	LINKER	PDB 3ETB
G	112	GLY	-	LINKER	PDB 3ETB
G	113	SER	-	LINKER	PDB 3ETB
G	114	GLY	-	LINKER	PDB 3ETB
G	115	GLY	-	LINKER	PDB 3ETB
G	116	GLY	-	LINKER	PDB 3ETB
G	117	GLY	-	LINKER	PDB 3ETB
G	118	SER	-	LINKER	PDB 3ETB
G	119	GLY	-	LINKER	PDB 3ETB
G	120	GLY	-	LINKER	PDB 3ETB
G	121	GLY	-	LINKER	PDB 3ETB
G	122	GLY	-	LINKER	PDB 3ETB
G	123	SER	-	LINKER	PDB 3ETB
G	124	GLY	-	LINKER	PDB 3ETB

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Chain	Residue	Modelled	Actual	Comment	Reference
G	125	GLY	-	LINKER	PDB 3ETB
G	126	GLY	-	LINKER	PDB 3ETB
G	127	GLY	-	LINKER	PDB 3ETB
G	128	SER	-	LINKER	PDB 3ETB
G	1030	ASN	SER	ENGINEERED	PDB 3ETB
G	1057	SER	THR	ENGINEERED	PDB 3ETB
G	1064	GLU	LYS	ENGINEERED	PDB 3ETB
G	1068	ILE	THR	ENGINEERED	PDB 3ETB
H	-4	MET	-	EXPRESSION TAG	PDB 3ETB
H	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
H	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
H	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
H	0	LYS	-	EXPRESSION TAG	PDB 3ETB
H	21	VAL	ILE	ENGINEERED	PDB 3ETB
H	46	PHE	LEU	ENGINEERED	PDB 3ETB
H	56	PRO	SER	ENGINEERED	PDB 3ETB
H	76	ASN	SER	ENGINEERED	PDB 3ETB
H	78	LEU	GLN	ENGINEERED	PDB 3ETB
H	94	PRO	LEU	ENGINEERED	PDB 3ETB
H	109	GLY	-	LINKER	PDB 3ETB
H	110	GLY	-	LINKER	PDB 3ETB
H	111	GLY	-	LINKER	PDB 3ETB
H	112	GLY	-	LINKER	PDB 3ETB
H	113	SER	-	LINKER	PDB 3ETB
H	114	GLY	-	LINKER	PDB 3ETB
H	115	GLY	-	LINKER	PDB 3ETB
H	116	GLY	-	LINKER	PDB 3ETB
H	117	GLY	-	LINKER	PDB 3ETB
H	118	SER	-	LINKER	PDB 3ETB
H	119	GLY	-	LINKER	PDB 3ETB
H	120	GLY	-	LINKER	PDB 3ETB
H	121	GLY	-	LINKER	PDB 3ETB
H	122	GLY	-	LINKER	PDB 3ETB
H	123	SER	-	LINKER	PDB 3ETB
H	124	GLY	-	LINKER	PDB 3ETB
H	125	GLY	-	LINKER	PDB 3ETB
H	126	GLY	-	LINKER	PDB 3ETB
H	127	GLY	-	LINKER	PDB 3ETB
H	128	SER	-	LINKER	PDB 3ETB
H	1030	ASN	SER	ENGINEERED	PDB 3ETB
H	1057	SER	THR	ENGINEERED	PDB 3ETB
H	1064	GLU	LYS	ENGINEERED	PDB 3ETB

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1068	ILE	THR	ENGINEERED	PDB 3ETB
I	-4	MET	-	EXPRESSION TAG	PDB 3ETB
I	-3	ALA	-	EXPRESSION TAG	PDB 3ETB
I	-2	ASP	-	EXPRESSION TAG	PDB 3ETB
I	-1	TYR	-	EXPRESSION TAG	PDB 3ETB
I	0	LYS	-	EXPRESSION TAG	PDB 3ETB
I	21	VAL	ILE	ENGINEERED	PDB 3ETB
I	46	PHE	LEU	ENGINEERED	PDB 3ETB
I	56	PRO	SER	ENGINEERED	PDB 3ETB
I	76	ASN	SER	ENGINEERED	PDB 3ETB
I	78	LEU	GLN	ENGINEERED	PDB 3ETB
I	94	PRO	LEU	ENGINEERED	PDB 3ETB
I	109	GLY	-	LINKER	PDB 3ETB
I	110	GLY	-	LINKER	PDB 3ETB
I	111	GLY	-	LINKER	PDB 3ETB
I	112	GLY	-	LINKER	PDB 3ETB
I	113	SER	-	LINKER	PDB 3ETB
I	114	GLY	-	LINKER	PDB 3ETB
I	115	GLY	-	LINKER	PDB 3ETB
I	116	GLY	-	LINKER	PDB 3ETB
I	117	GLY	-	LINKER	PDB 3ETB
I	118	SER	-	LINKER	PDB 3ETB
I	119	GLY	-	LINKER	PDB 3ETB
I	120	GLY	-	LINKER	PDB 3ETB
I	121	GLY	-	LINKER	PDB 3ETB
I	122	GLY	-	LINKER	PDB 3ETB
I	123	SER	-	LINKER	PDB 3ETB
I	124	GLY	-	LINKER	PDB 3ETB
I	125	GLY	-	LINKER	PDB 3ETB
I	126	GLY	-	LINKER	PDB 3ETB
I	127	GLY	-	LINKER	PDB 3ETB
I	128	SER	-	LINKER	PDB 3ETB
I	1030	ASN	SER	ENGINEERED	PDB 3ETB
I	1057	SER	THR	ENGINEERED	PDB 3ETB
I	1064	GLU	LYS	ENGINEERED	PDB 3ETB
I	1068	ILE	THR	ENGINEERED	PDB 3ETB

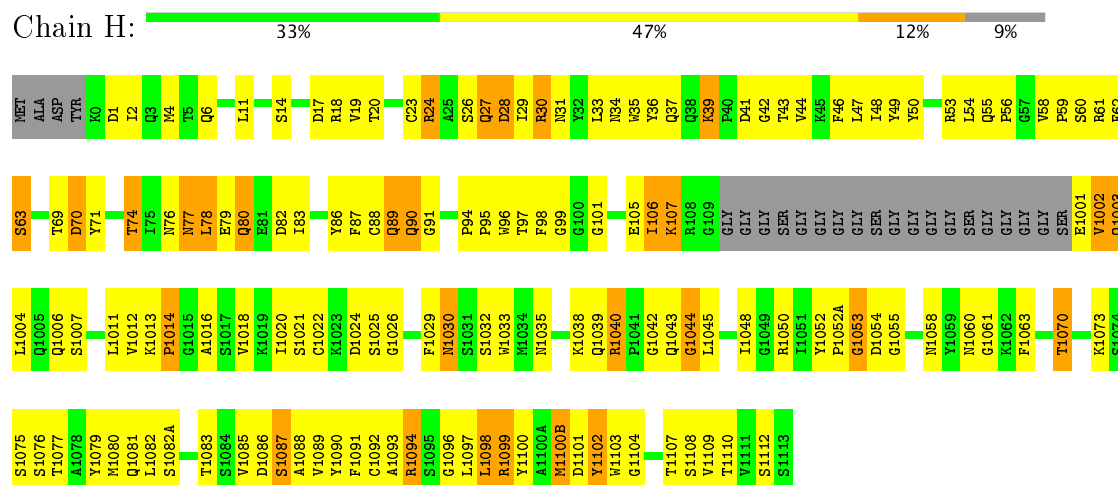
- Molecule 2 is a protein called Anthrax Protective Antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			

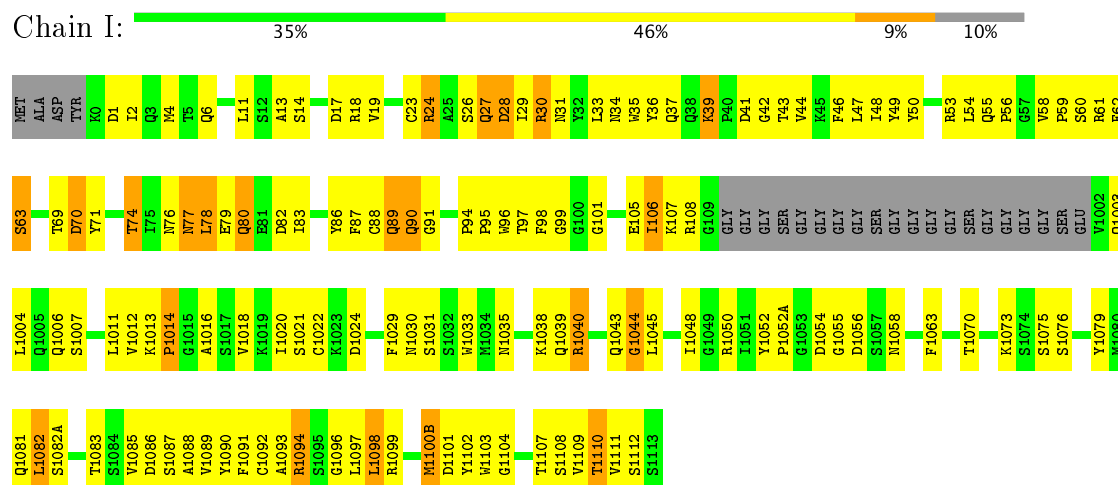
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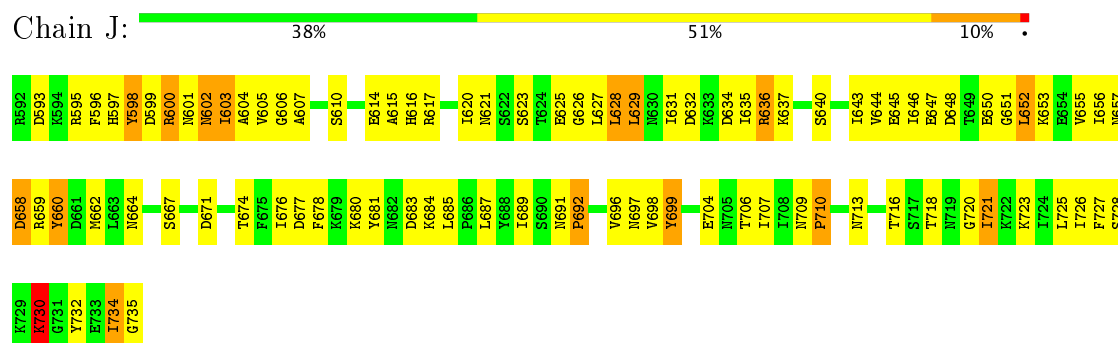
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			
2	L	143	Total	C	N	O	S	0	0	0
			1138	718	191	228	1			
2	M	144	Total	C	N	O	S	0	0	0
			1146	722	192	231	1			



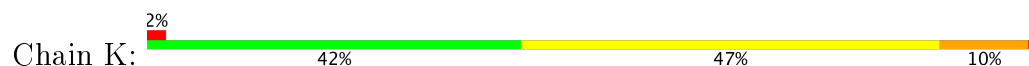
- Molecule 1: Antibody M18 light chain and antibody M18 heavy chain linked with a synthetic (GGGS)₄ linker

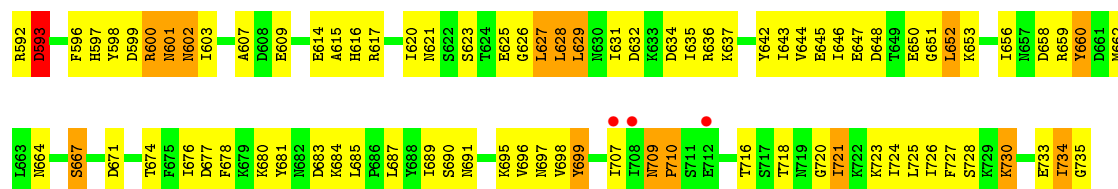


- Molecule 2: Anthrax Protective Antigen

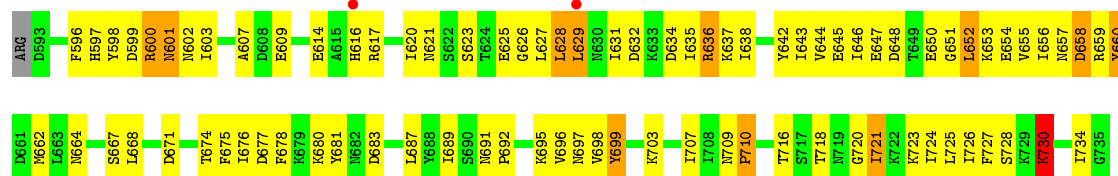


- Molecule 2: Anthrax Protective Antigen

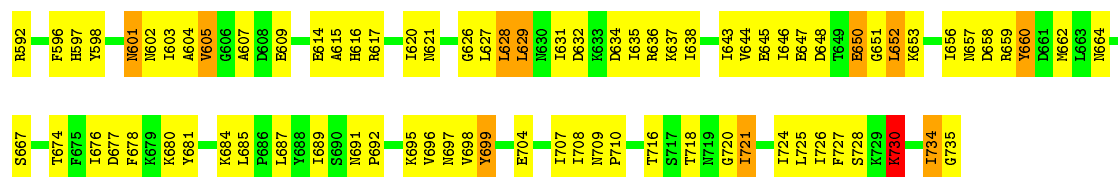




• Molecule 2: Anthrax Protective Antigen



• Molecule 2: Anthrax Protective Antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.94Å 299.72Å 68.95Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	20.00 – 3.80 43.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	83.8 (20.00-3.80) 89.8 (43.84-3.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.276 0.222 , 0.228	Depositor DCC
R_{free} test set	884 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 1.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	F	0.48	0/1781	0.70	0/2413
1	G	0.49	0/1782	0.71	0/2416
1	H	0.49	0/1782	0.70	0/2416
1	I	0.49	0/1781	0.70	0/2413
2	J	0.44	0/1162	0.66	0/1566
2	K	0.47	0/1162	0.69	0/1566
2	L	0.47	0/1154	0.70	0/1555
2	M	0.47	0/1162	0.68	0/1566
All	All	0.48	0/11766	0.69	0/15911

There are no bond length outliers.

There are no bond angle outliers.

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	F	1742	0	1655	151	0
1	G	1743	0	1646	141	0
1	H	1743	0	1646	151	0
1	I	1742	0	1655	142	0
2	J	1146	0	1134	104	0
2	K	1146	0	1134	94	0
2	L	1138	0	1130	100	0
2	M	1146	0	1134	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11546	0	11134	953	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 42.

The worst 5 of 953 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:G:1006:GLN:HE22	1:G:1091:PHE:HA	1.29	0.96
1:F:1006:GLN:HE22	1:F:1091:PHE:HA	1.27	0.95
1:G:1011:LEU:HD13	1:G:1110:THR:HG23	1.47	0.95
2:M:629:LEU:HD23	2:M:629:LEU:H	1.32	0.93
1:H:1050:ARG:HE	1:H:1058:ASN:HD22	1.18	0.90

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	F	224/252 (89%)	168 (75%)	36 (16%)	20 (9%)	1	15
1	G	225/252 (89%)	165 (73%)	37 (16%)	23 (10%)	1	12
1	H	225/252 (89%)	164 (73%)	40 (18%)	21 (9%)	1	14
1	I	224/252 (89%)	165 (74%)	39 (17%)	20 (9%)	1	15
2	J	142/144 (99%)	100 (70%)	28 (20%)	14 (10%)	1	12
2	K	142/144 (99%)	100 (70%)	28 (20%)	14 (10%)	1	12
2	L	141/144 (98%)	105 (74%)	26 (18%)	10 (7%)	1	21
2	M	142/144 (99%)	100 (70%)	30 (21%)	12 (8%)	1	16
All	All	1465/1584 (92%)	1067 (73%)	264 (18%)	134 (9%)	1	15

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1033	TRP
1	F	1098	LEU
1	G	1002	VAL
1	G	1033	TRP
1	G	1098	LEU

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	F	188/201 (94%)	171 (91%)	17 (9%)	11	45
1	G	187/201 (93%)	171 (91%)	16 (9%)	12	47
1	H	187/201 (93%)	171 (91%)	16 (9%)	12	47
1	I	188/201 (94%)	170 (90%)	18 (10%)	10	41
2	J	128/131 (98%)	119 (93%)	9 (7%)	18	55
2	K	128/131 (98%)	120 (94%)	8 (6%)	21	58
2	L	127/131 (97%)	120 (94%)	7 (6%)	25	63
2	M	128/131 (98%)	122 (95%)	6 (5%)	30	66
All	All	1261/1328 (95%)	1164 (92%)	97 (8%)	15	52

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1070	THR
1	I	74	THR
2	L	699	TYR
1	H	1099	ARG
1	I	1	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	38	GLN
2	J	630	ASN
2	M	697	ASN
1	I	77	ASN
1	I	1035	ASN

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 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 [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	F	228/252 (90%)	-0.35	0	100	100	10, 10, 25, 100	0
1	G	229/252 (90%)	-0.29	0	100	100	10, 10, 28, 70	0
1	H	229/252 (90%)	-0.34	0	100	100	10, 10, 23, 75	0
1	I	228/252 (90%)	-0.34	0	100	100	10, 10, 21, 64	0
2	J	144/144 (100%)	0.15	0	100	100	10, 10, 38, 87	0
2	K	144/144 (100%)	-0.21	3 (2%)	64	54	10, 10, 42, 78	0
2	L	143/144 (99%)	0.30	2 (1%)	75	67	10, 10, 53, 80	0
2	M	144/144 (100%)	-0.27	0	100	100	10, 10, 30, 75	0
All	All	1489/1584 (94%)	-0.21	5 (0%)	93	91	10, 10, 33, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	707	ILE	3.0
2	L	629	LEU	2.9
2	L	616	HIS	2.5
2	K	708	ILE	2.3
2	K	712	GLU	2.1

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.