



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:36 am BST

PDB ID : 6I8S  
Title : Discovery and characterisation of an antibody that selectively modulates the inhibitory activity of plasminogen activator inhibitor-1  
Authors : Vousden, K.A.; Lundqvist, T.; Popovic, B.  
Deposited on : 2018-11-21  
Resolution : 2.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

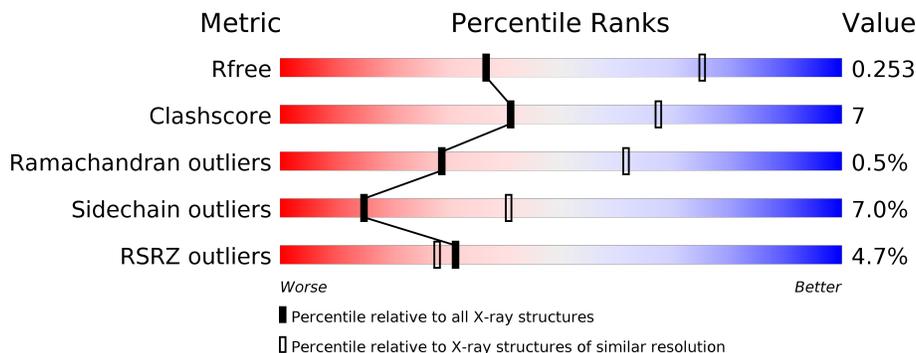
# 1 Overall quality at a glance

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.



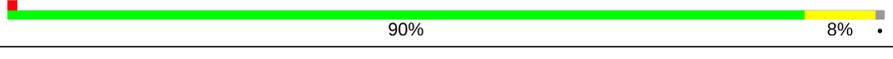
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	379	 3% 82% 13% . .
1	B	379	 5% 81% 14% . .
1	C	379	 4% 80% 15% . .
1	D	379	 10% 77% 15% . .
2	E	223	 6% 76% 17% . .
2	F	223	 6% 65% 28% . .

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Mol	Chain	Length	Quality of chain
2	G	223	 3% 84% 11% ..
2	H	223	 5% 83% 12% ..
3	I	214	 2% 86% 10% ..
3	J	214	 6% 75% 22% ..
3	K	214	 % 85% 13% ..
3	L	214	 % 90% 8% .

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 24618 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 Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2901	1862	495	529	15	0	0	0
1	B	363	2901	1862	495	529	15	0	0	0
1	C	363	2901	1862	495	529	15	0	0	0
1	D	363	2901	1862	495	529	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	engineered mutation	UNP P05121
A	154	THR	LYS	engineered mutation	UNP P05121
A	319	LEU	GLN	engineered mutation	UNP P05121
A	354	ILE	MET	engineered mutation	UNP P05121
B	150	HIS	ASN	engineered mutation	UNP P05121
B	154	THR	LYS	engineered mutation	UNP P05121
B	319	LEU	GLN	engineered mutation	UNP P05121
B	354	ILE	MET	engineered mutation	UNP P05121
C	150	HIS	ASN	engineered mutation	UNP P05121
C	154	THR	LYS	engineered mutation	UNP P05121
C	319	LEU	GLN	engineered mutation	UNP P05121
C	354	ILE	MET	engineered mutation	UNP P05121
D	150	HIS	ASN	engineered mutation	UNP P05121
D	154	THR	LYS	engineered mutation	UNP P05121
D	319	LEU	GLN	engineered mutation	UNP P05121
D	354	ILE	MET	engineered mutation	UNP P05121

- Molecule 2 is a protein called HEAVY CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	214	Total	C	N	O	S	0	0	0
			1614	1021	274	313	6			
2	F	214	Total	C	N	O	S	0	0	0
			1614	1021	274	313	6			
2	G	214	Total	C	N	O	S	0	0	0
			1614	1021	274	313	6			
2	H	214	Total	C	N	O	S	0	0	0
			1614	1021	274	313	6			

- Molecule 3 is a protein called LIGHT CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	211	Total	C	N	O	S	0	0	0
			1628	1022	274	327	5			
3	J	211	Total	C	N	O	S	0	0	0
			1628	1022	274	327	5			
3	K	211	Total	C	N	O	S	0	0	0
			1628	1022	274	327	5			
3	L	211	Total	C	N	O	S	0	0	0
			1628	1022	274	327	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total 6 6	0	0
4	B	5	Total 5 5	0	0
4	C	7	Total 7 7	0	0
4	D	5	Total 5 5	0	0
4	F	2	Total 2 2	0	0
4	H	3	Total 3 3	0	0
4	I	4	Total 4 4	0	0
4	J	3	Total 3 3	0	0
4	K	7	Total 7 7	0	0

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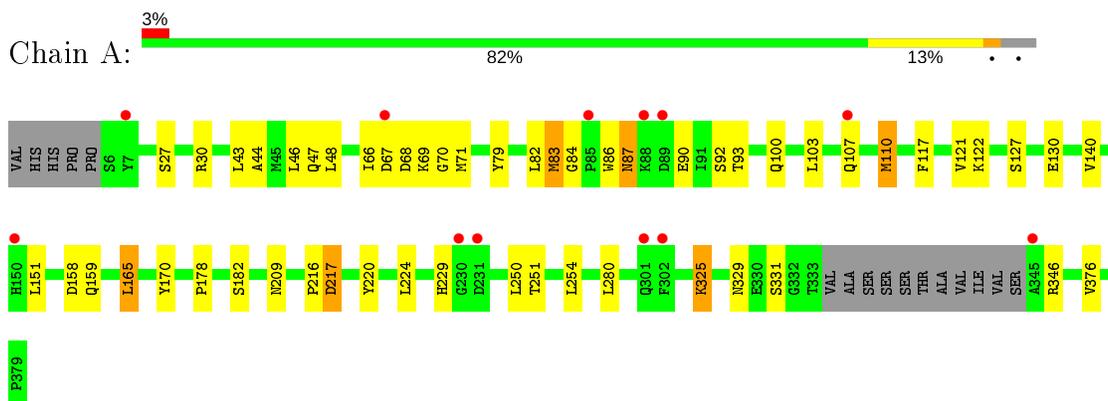
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	L	4	Total	O	0	0
			4	4		

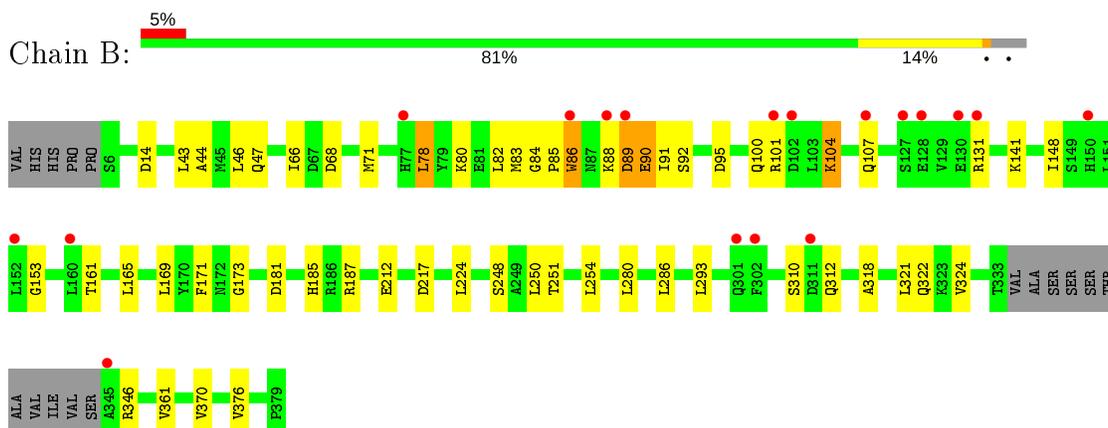
### 3 Residue-property plots [i](#)

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.

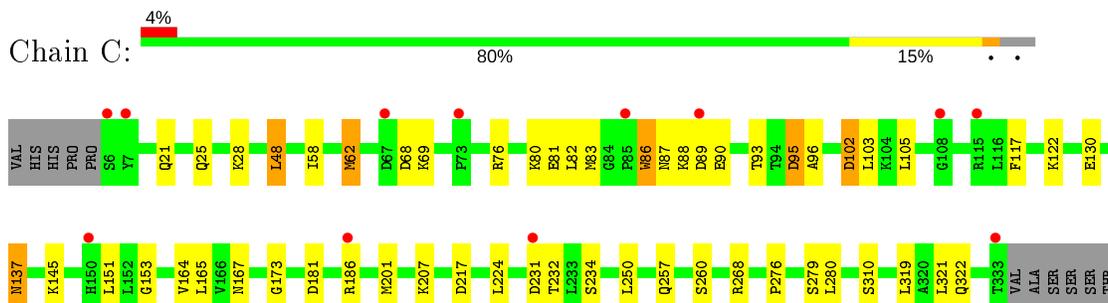
- Molecule 1: Plasminogen activator inhibitor 1

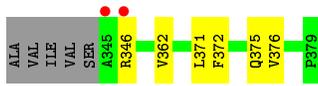


- Molecule 1: Plasminogen activator inhibitor 1

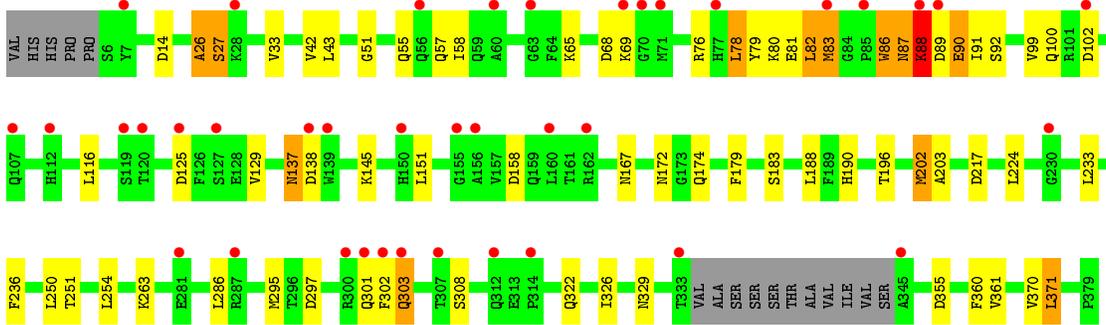


- Molecule 1: Plasminogen activator inhibitor 1

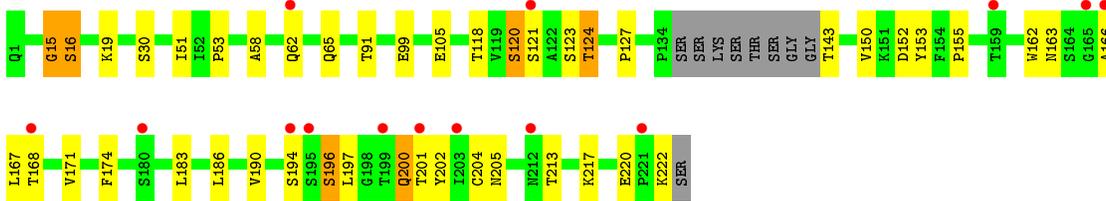
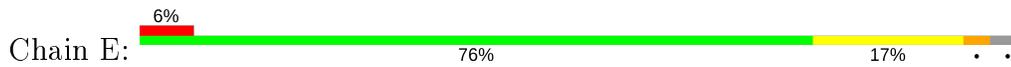




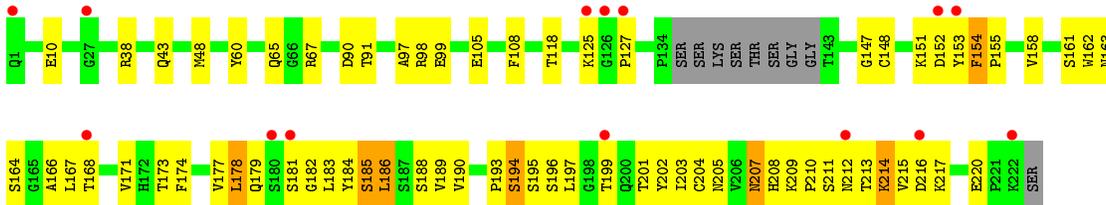
- Molecule 1: Plasminogen activator inhibitor 1



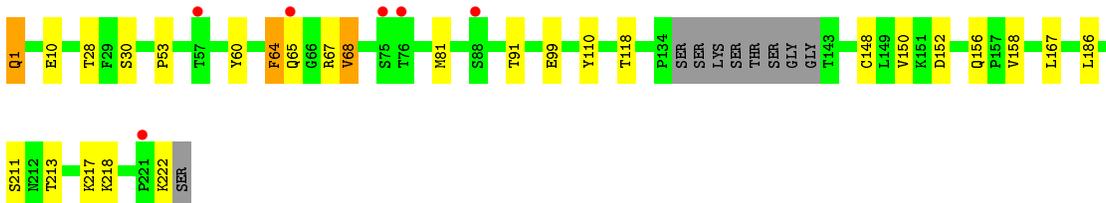
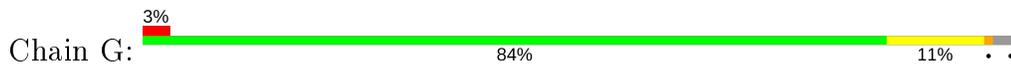
- Molecule 2: HEAVY CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



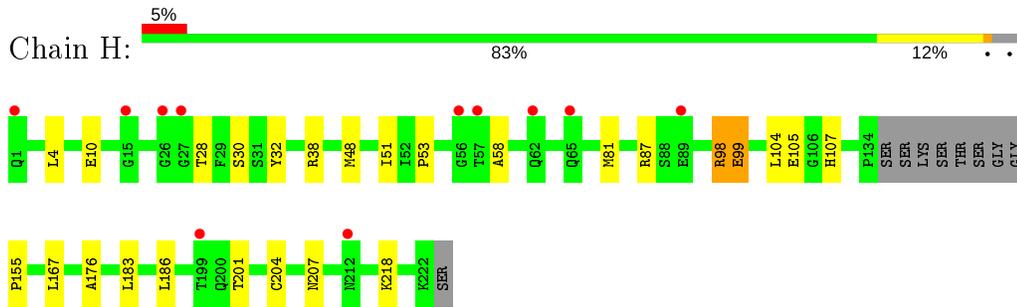
- Molecule 2: HEAVY CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



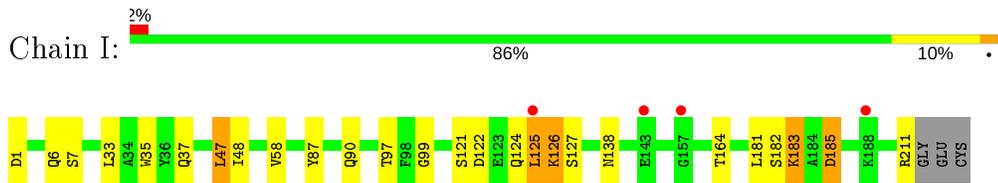
- Molecule 2: HEAVY CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



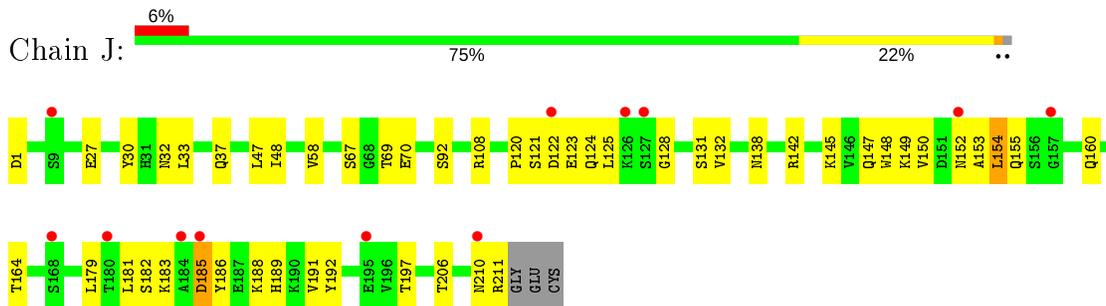
- Molecule 2: HEAVY CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



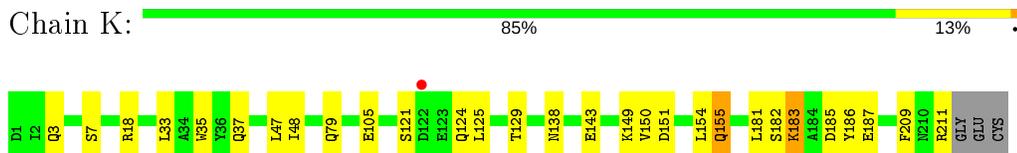
- Molecule 3: LIGHT CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



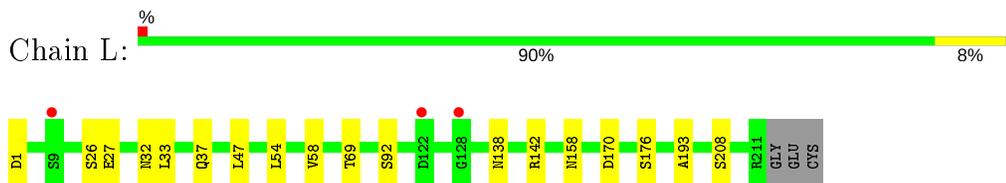
- Molecule 3: LIGHT CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



- Molecule 3: LIGHT CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



- Molecule 3: LIGHT CHAIN OF FAB FRAGMENT FROM AN PAI-1 ANTIBODY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.22Å 89.66Å 249.77Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	14.99 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (14.99-2.90) 99.2 (14.99-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.91Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.219 , 0.243 0.229 , 0.253	Depositor DCC
$R_{free}$ test set	4317 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.068	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.51	1/2971 (0.0%)	0.68	2/4025 (0.0%)
1	B	0.52	0/2971	0.65	0/4025
1	C	0.44	0/2971	0.64	0/4025
1	D	0.47	0/2971	0.68	2/4025 (0.0%)
2	E	0.55	0/1653	0.72	2/2250 (0.1%)
2	F	0.76	0/1653	0.81	0/2250
2	G	0.46	1/1653 (0.1%)	0.63	0/2250
2	H	0.35	0/1653	0.62	0/2250
3	I	0.46	0/1664	0.64	0/2259
3	J	0.47	0/1664	0.66	0/2259
3	K	0.54	0/1664	0.66	0/2259
3	L	0.40	0/1664	0.62	0/2259
All	All	0.50	2/25152 (0.0%)	0.67	6/34136 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	TYR	CE1-CZ	-5.13	1.31	1.38
2	G	60	TYR	CE1-CZ	-5.01	1.32	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASP	CB-CG-OD1	7.14	124.73	118.30
1	D	26	ALA	C-N-CA	6.19	137.17	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	120	SER	C-N-CA	5.49	135.42	121.70
1	D	90	GLU	N-CA-C	5.29	125.27	111.00
2	E	15	GLY	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	88	LYS	Peptide

## 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	2901	0	2891	26	0
1	B	2901	0	2891	39	0
1	C	2901	0	2891	29	0
1	D	2901	0	2891	58	0
2	E	1614	0	1589	23	0
2	F	1614	0	1589	77	0
2	G	1614	0	1589	10	0
2	H	1614	0	1589	9	0
3	I	1628	0	1591	14	0
3	J	1628	0	1591	43	0
3	K	1628	0	1591	21	0
3	L	1628	0	1591	4	0
4	A	6	0	0	0	0
4	B	5	0	0	0	0
4	C	7	0	0	0	0
4	D	5	0	0	0	0
4	F	2	0	0	0	0
4	H	3	0	0	0	0
4	I	4	0	0	0	0
4	J	3	0	0	0	0
4	K	7	0	0	0	0
4	L	4	0	0	0	0
All	All	24618	0	24284	345	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 7.

The worst 5 of 345 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:F:203:ILE:HG23	2:F:217:LYS:O	1.44	1.18
2:E:200:GLN:NE2	2:E:201:THR:O	1.88	1.06
1:B:88:LYS:H	1:B:89:ASP:HA	1.28	0.98
3:J:125:LEU:HB3	3:J:183:LYS:HE2	1.46	0.96
1:A:84:GLY:H	1:A:87:ASN:HD21	1.08	0.96

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	359/379 (95%)	345 (96%)	14 (4%)	0	100	100
1	B	359/379 (95%)	345 (96%)	14 (4%)	0	100	100
1	C	359/379 (95%)	347 (97%)	11 (3%)	1 (0%)	41	71
1	D	359/379 (95%)	345 (96%)	10 (3%)	4 (1%)	14	42
2	E	210/223 (94%)	200 (95%)	8 (4%)	2 (1%)	15	45
2	F	210/223 (94%)	199 (95%)	11 (5%)	0	100	100
2	G	210/223 (94%)	197 (94%)	11 (5%)	2 (1%)	15	45
2	H	210/223 (94%)	200 (95%)	9 (4%)	1 (0%)	29	61
3	I	209/214 (98%)	198 (95%)	10 (5%)	1 (0%)	29	61
3	J	209/214 (98%)	193 (92%)	15 (7%)	1 (0%)	29	61
3	K	209/214 (98%)	193 (92%)	13 (6%)	3 (1%)	11	36
3	L	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	29	61
All	All	3112/3264 (95%)	2961 (95%)	135 (4%)	16 (0%)	29	61

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	124	THR
1	D	88	LYS
1	D	303	GLN
2	G	28	THR
3	J	138	ASN

### 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	319/333 (96%)	295 (92%)	24 (8%)	13	37
1	B	319/333 (96%)	298 (93%)	21 (7%)	16	44
1	C	319/333 (96%)	294 (92%)	25 (8%)	12	34
1	D	319/333 (96%)	294 (92%)	25 (8%)	12	34
2	E	179/186 (96%)	167 (93%)	12 (7%)	16	43
2	F	179/186 (96%)	164 (92%)	15 (8%)	11	31
2	G	179/186 (96%)	166 (93%)	13 (7%)	14	38
2	H	179/186 (96%)	168 (94%)	11 (6%)	18	48
3	I	185/187 (99%)	175 (95%)	10 (5%)	22	54
3	J	185/187 (99%)	172 (93%)	13 (7%)	15	41
3	K	185/187 (99%)	174 (94%)	11 (6%)	19	49
3	L	185/187 (99%)	175 (95%)	10 (5%)	22	54
All	All	2732/2824 (97%)	2542 (93%)	190 (7%)	15	41

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	138	ASP
2	E	222	LYS
3	K	155	GLN
1	D	202	MET

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Mol	Chain	Res	Type
2	E	99	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
2	E	179	GLN
3	J	147	GLN
1	D	172	ASN
2	E	156	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	363/379 (95%)	0.01	12 (3%) 46 41	34, 49, 73, 83	0
1	B	363/379 (95%)	0.17	18 (4%) 28 25	37, 53, 85, 99	0
1	C	363/379 (95%)	0.18	14 (3%) 39 35	44, 62, 88, 98	0
1	D	363/379 (95%)	0.46	39 (10%) 6 4	54, 72, 113, 127	0
2	E	214/223 (95%)	0.52	14 (6%) 18 14	52, 77, 109, 122	0
2	F	214/223 (95%)	0.45	14 (6%) 18 14	49, 75, 104, 121	0
2	G	214/223 (95%)	0.13	6 (2%) 53 49	44, 61, 83, 97	0
2	H	214/223 (95%)	0.25	11 (5%) 28 24	44, 63, 80, 90	0
3	I	211/214 (98%)	0.11	4 (1%) 66 65	37, 56, 82, 92	0
3	J	211/214 (98%)	0.30	12 (5%) 23 19	41, 57, 116, 130	0
3	K	211/214 (98%)	0.04	1 (0%) 91 91	32, 47, 97, 110	0
3	L	211/214 (98%)	-0.08	3 (1%) 75 75	35, 44, 74, 86	0
All	All	3152/3264 (96%)	0.21	148 (4%) 31 28	32, 61, 99, 130	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	212	ASN	5.5
1	D	70	GLY	5.0
1	D	150	HIS	4.9
3	J	157	GLY	4.9
1	C	67	ASP	4.5

### 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.