



# wwPDB X-ray Structure Validation Summary Report

Feb 14, 2024 – 09:17 AM EST

PDB ID : 3KXY  
Title : Crystal Structure of the ExsC-ExsE Complex  
Authors : Vogelaar, N.J.; Robinson, H.H.; Schubot, F.D.  
Deposited on : 2009-12-04  
Resolution : 2.80 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

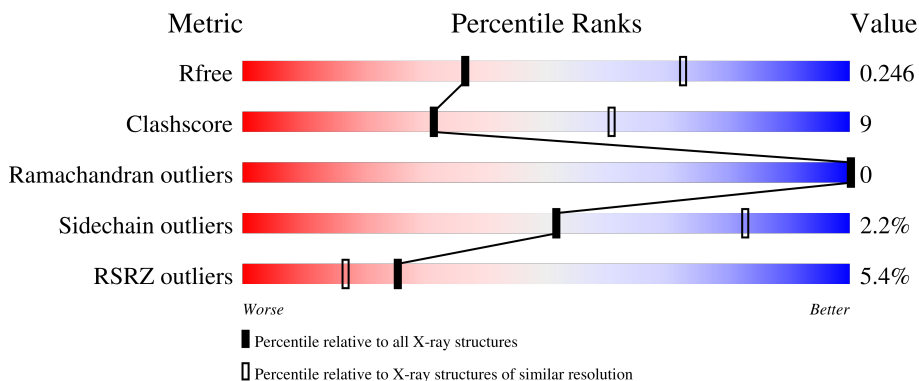
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	133	 83% 17%
1	B	133	 80% 19%
1	C	133	 83% 17%
1	D	133	 90% 7%
1	E	133	 77% 22%

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Mol	Chain	Length	Quality of chain
1	F	133	 5% 71% 27% ..
1	G	133	 2% 81% 19%
1	H	133	 12% 77% 20% ..
1	I	133	 2% 80% 20%
1	J	133	 9% 67% 29% ..
1	K	133	 % 80% 18% .
1	L	133	 8% 72% 26% .
2	T	66	 83% 15% .
2	U	66	 12% 80% 9% . 9%
2	V	66	 12% 83% 14% ..
2	W	66	 9% 45% 8% . 44%
2	X	66	 8% 44% 15% 41%
2	Y	66	 15% 48% 15% . 35%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15017 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 Exoenzyme S synthesis protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1055	678	178	195	4	0	0	0
1	B	132	1048	675	177	192	4	0	0	0
1	C	133	1055	678	178	195	4	0	0	0
1	D	130	1037	669	175	190	3	0	0	0
1	E	133	1055	678	178	195	4	0	0	0
1	F	132	1047	673	177	194	3	0	0	0
1	G	133	1055	678	178	195	4	0	0	0
1	H	130	1035	667	175	190	3	0	0	0
1	I	133	1055	678	178	195	4	0	0	0
1	J	129	1029	664	174	189	2	0	0	0
1	K	133	1055	678	178	195	4	0	0	0
1	L	130	1035	667	175	190	3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	VAL	ALA	engineered mutation	UNP P26995
A	132	ALA	ASP	engineered mutation	UNP P26995
B	59	VAL	ALA	engineered mutation	UNP P26995
B	132	ALA	ASP	engineered mutation	UNP P26995
C	59	VAL	ALA	engineered mutation	UNP P26995

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Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	ASP	engineered mutation	UNP P26995
D	59	VAL	ALA	engineered mutation	UNP P26995
D	132	ALA	ASP	engineered mutation	UNP P26995
E	59	VAL	ALA	engineered mutation	UNP P26995
E	132	ALA	ASP	engineered mutation	UNP P26995
F	59	VAL	ALA	engineered mutation	UNP P26995
F	132	ALA	ASP	engineered mutation	UNP P26995
G	59	VAL	ALA	engineered mutation	UNP P26995
G	132	ALA	ASP	engineered mutation	UNP P26995
H	59	VAL	ALA	engineered mutation	UNP P26995
H	132	ALA	ASP	engineered mutation	UNP P26995
I	59	VAL	ALA	engineered mutation	UNP P26995
I	132	ALA	ASP	engineered mutation	UNP P26995
J	59	VAL	ALA	engineered mutation	UNP P26995
J	132	ALA	ASP	engineered mutation	UNP P26995
K	59	VAL	ALA	engineered mutation	UNP P26995
K	132	ALA	ASP	engineered mutation	UNP P26995
L	59	VAL	ALA	engineered mutation	UNP P26995
L	132	ALA	ASP	engineered mutation	UNP P26995

- Molecule 2 is a protein called ExsE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	65	Total	C	N	O	0	0	0
			497	295	107	95			
2	U	60	Total	C	N	O	0	0	0
			460	274	99	87			
2	V	65	Total	C	N	O	0	0	0
			497	295	107	95			
2	W	37	Total	C	N	O	0	0	0
			285	166	63	56			
2	X	39	Total	C	N	O	0	0	0
			298	173	65	60			
2	Y	43	Total	C	N	O	0	0	0
			329	194	71	64			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	17	THR	ALA	engineered mutation	UNP Q9I322
U	17	THR	ALA	engineered mutation	UNP Q9I322
V	17	THR	ALA	engineered mutation	UNP Q9I322

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Chain	Residue	Modelled	Actual	Comment	Reference
W	17	THR	ALA	engineered mutation	UNP Q9I322
X	17	THR	ALA	engineered mutation	UNP Q9I322
Y	17	THR	ALA	engineered mutation	UNP Q9I322

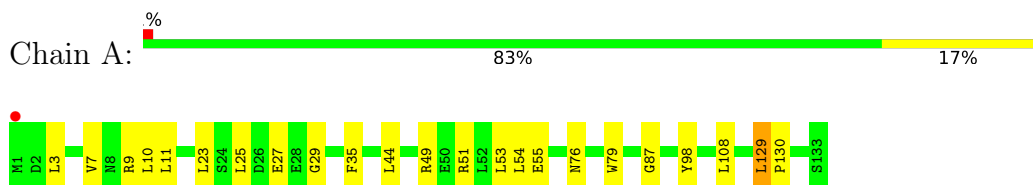
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	7	Total O 7 7	0	0
3	T	9	Total O 9 9	0	0
3	C	15	Total O 15 15	0	0
3	D	4	Total O 4 4	0	0
3	U	7	Total O 7 7	0	0
3	E	7	Total O 7 7	0	0
3	F	1	Total O 1 1	0	0
3	V	4	Total O 4 4	0	0
3	W	3	Total O 3 3	0	0
3	I	4	Total O 4 4	0	0
3	J	1	Total O 1 1	0	0
3	X	1	Total O 1 1	0	0
3	K	6	Total O 6 6	0	0
3	L	3	Total O 3 3	0	0
3	Y	1	Total O 1 1	0	0

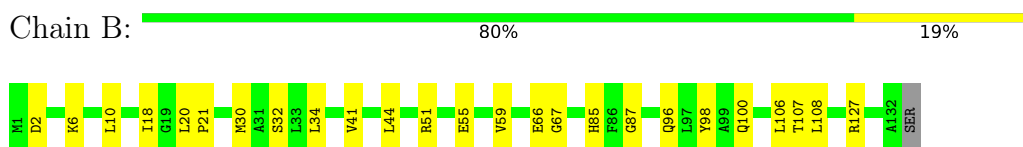
### 3 Residue-property plots [i](#)

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 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.

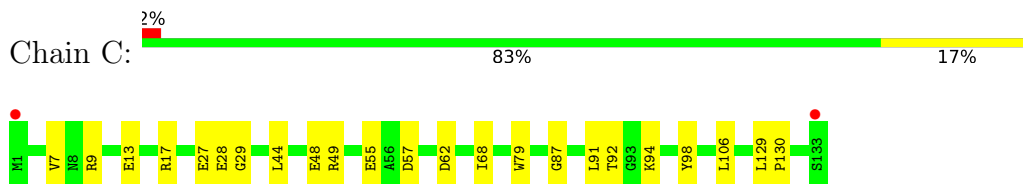
- Molecule 1: Exoenzyme S synthesis protein C



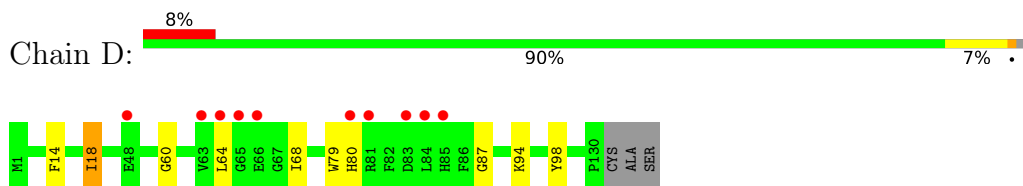
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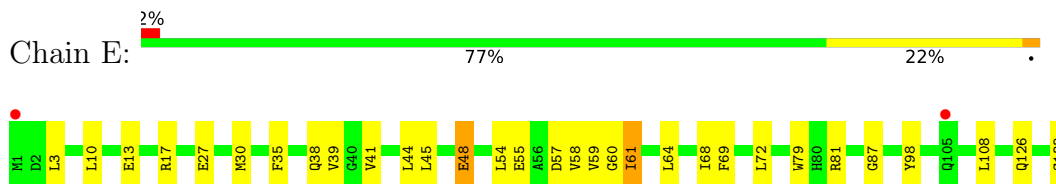
- Molecule 1: Exoenzyme S synthesis protein C



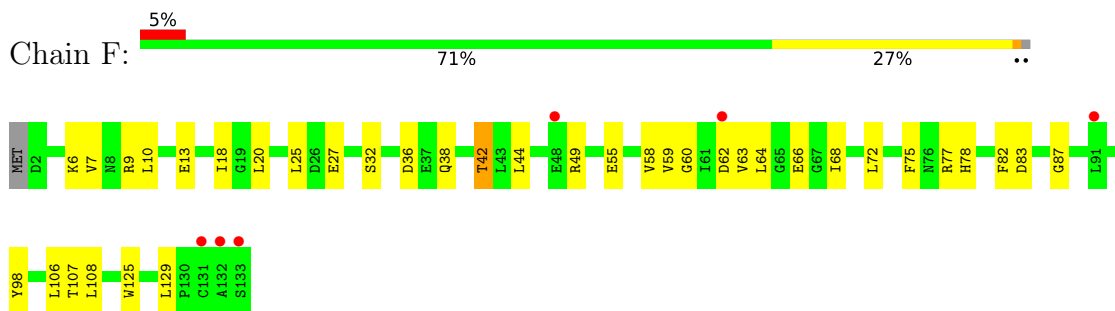
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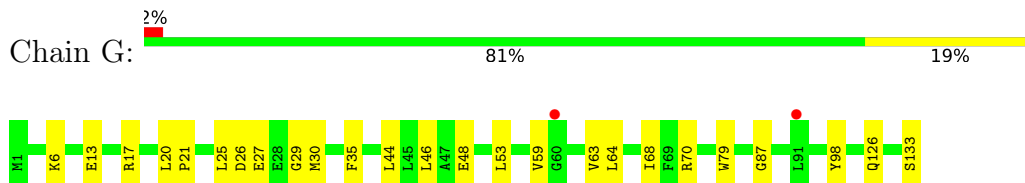
- Molecule 1: Exoenzyme S synthesis protein C



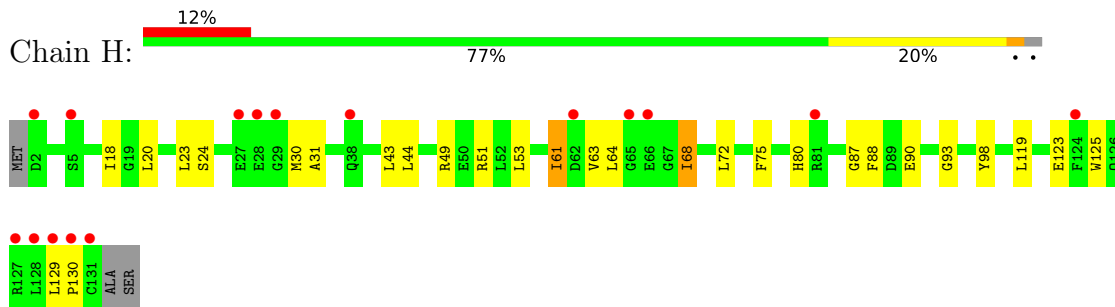
- Molecule 1: Exoenzyme S synthesis protein C



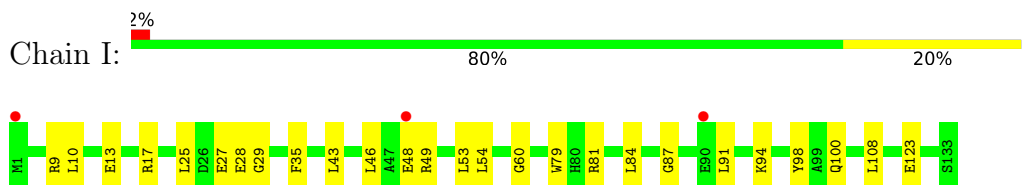
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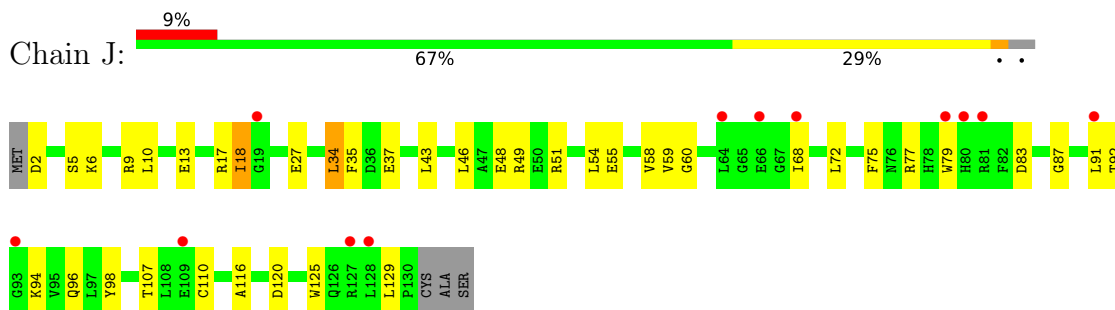
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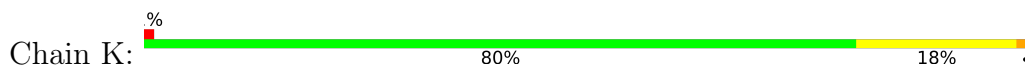
- Molecule 1: Exoenzyme S synthesis protein C



- Molecule 1: Exoenzyme S synthesis protein C



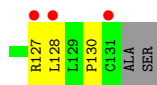
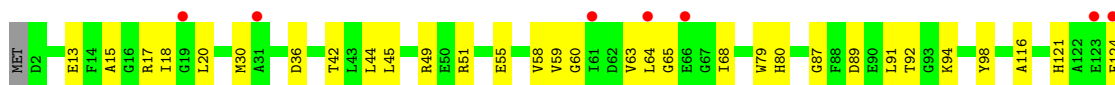
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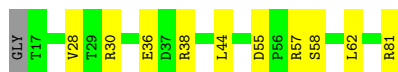
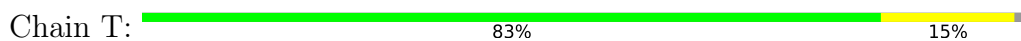




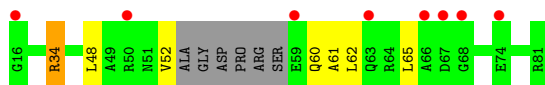
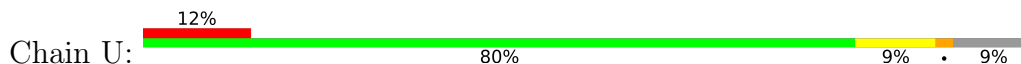
- Molecule 1: Exoenzyme S synthesis protein C



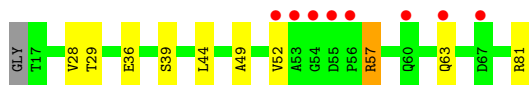
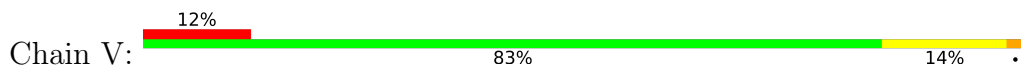
- Molecule 2: ExsE



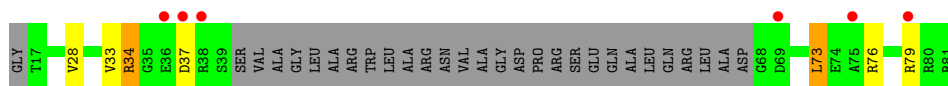
- Molecule 2: ExsE



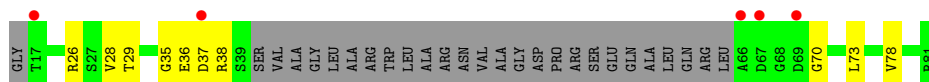
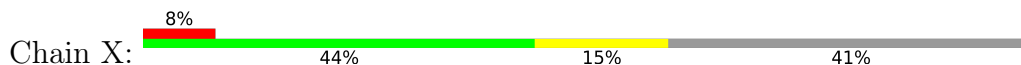
- Molecule 2: ExsE



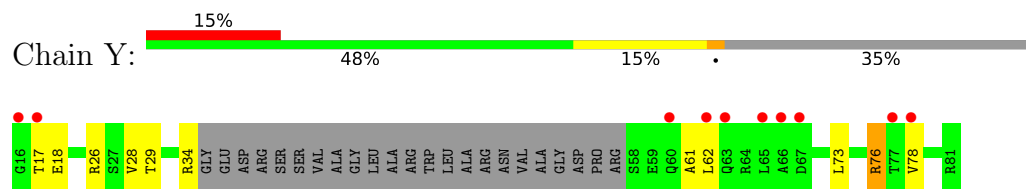
- Molecule 2: ExsE



- Molecule 2: ExsE



## ● Molecule 2: ExsE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.31Å 124.97Å 228.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (30.00-2.80) 89.3 (30.00-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, $R_{free}$	0.217 , 0.257 0.209 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.3	Xtrriage
Anisotropy	0.479	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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	0.22	0/1074	0.36	0/1452
1	B	0.22	0/1067	0.34	0/1444
1	C	0.22	0/1074	0.36	0/1452
1	D	0.21	0/1056	0.34	0/1429
1	E	0.21	0/1074	0.35	0/1452
1	F	0.21	0/1066	0.35	0/1442
1	G	0.21	0/1074	0.34	0/1452
1	H	0.21	0/1054	0.33	0/1427
1	I	0.21	0/1074	0.34	0/1452
1	J	0.21	0/1048	0.33	0/1419
1	K	0.21	0/1074	0.35	0/1452
1	L	0.21	0/1054	0.34	0/1427
2	T	0.20	0/502	0.38	0/674
2	U	0.20	0/463	0.38	0/619
2	V	0.19	0/502	0.38	0/674
2	W	0.19	0/286	0.38	0/379
2	X	0.19	0/299	0.37	0/397
2	Y	0.19	0/330	0.37	0/439
All	All	0.21	0/15171	0.35	0/20482

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	A	1055	0	1054	15	0
1	B	1048	0	1049	14	0
1	C	1055	0	1054	19	0
1	D	1037	0	1039	5	0
1	E	1055	0	1054	25	0
1	F	1047	0	1042	27	0
1	G	1055	0	1054	27	0
1	H	1035	0	1032	26	0
1	I	1055	0	1054	18	0
1	J	1029	0	1027	29	0
1	K	1055	0	1054	28	0
1	L	1035	0	1032	32	0
2	T	497	0	491	8	0
2	U	460	0	456	10	0
2	V	497	0	491	7	0
2	W	285	0	277	7	0
2	X	298	0	286	12	0
2	Y	329	0	325	14	0
3	A	17	0	0	0	0
3	B	7	0	0	0	0
3	C	15	0	0	0	0
3	D	4	0	0	0	0
3	E	7	0	0	0	0
3	F	1	0	0	0	0
3	I	4	0	0	0	0
3	J	1	0	0	0	0
3	K	6	0	0	0	0
3	L	3	0	0	0	0
3	T	9	0	0	0	0
3	U	7	0	0	0	0
3	V	4	0	0	0	0
3	W	3	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
All	All	15017	0	14871	268	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 9.

The worst 5 of 268 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:70:ARG:HH22	1:H:61:ILE:HG21	1.36	0.90
1:E:58:VAL:HG12	1:E:59:VAL:HG23	1.55	0.88
1:E:64:LEU:HD13	1:E:68:ILE:HD11	1.59	0.85
1:J:58:VAL:HG12	1:J:59:VAL:HG23	1.59	0.85
1:E:133:SER:HB2	1:K:81:ARG:HH21	1.42	0.84

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	131/133 (98%)	130 (99%)	1 (1%)	0	100	100
1	B	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
1	C	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
1	D	128/133 (96%)	124 (97%)	4 (3%)	0	100	100
1	E	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
1	F	130/133 (98%)	125 (96%)	5 (4%)	0	100	100
1	G	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
1	H	128/133 (96%)	124 (97%)	4 (3%)	0	100	100
1	I	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
1	J	127/133 (96%)	124 (98%)	3 (2%)	0	100	100
1	K	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
1	L	128/133 (96%)	119 (93%)	9 (7%)	0	100	100
2	T	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
2	U	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
2	V	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
2	W	33/66 (50%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	35/66 (53%)	33 (94%)	2 (6%)	0	100	100
2	Y	39/66 (59%)	39 (100%)	0	0	100	100
All	All	1846/1992 (93%)	1785 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	111/111 (100%)	109 (98%)	2 (2%)	59	86
1	B	110/111 (99%)	107 (97%)	3 (3%)	44	78
1	C	111/111 (100%)	109 (98%)	2 (2%)	59	86
1	D	109/111 (98%)	107 (98%)	2 (2%)	59	86
1	E	111/111 (100%)	107 (96%)	4 (4%)	35	69
1	F	110/111 (99%)	107 (97%)	3 (3%)	44	78
1	G	111/111 (100%)	110 (99%)	1 (1%)	78	94
1	H	109/111 (98%)	107 (98%)	2 (2%)	59	86
1	I	111/111 (100%)	110 (99%)	1 (1%)	78	94
1	J	108/111 (97%)	103 (95%)	5 (5%)	27	60
1	K	111/111 (100%)	109 (98%)	2 (2%)	59	86
1	L	109/111 (98%)	109 (100%)	0	100	100
2	T	48/48 (100%)	48 (100%)	0	100	100
2	U	44/48 (92%)	43 (98%)	1 (2%)	50	82
2	V	48/48 (100%)	45 (94%)	3 (6%)	18	46
2	W	28/48 (58%)	26 (93%)	2 (7%)	14	39
2	X	29/48 (60%)	29 (100%)	0	100	100
2	Y	32/48 (67%)	31 (97%)	1 (3%)	40	74
All	All	1550/1620 (96%)	1516 (98%)	34 (2%)	52	83

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	34	LEU
1	J	48	GLU
1	K	68	ILE
1	E	61	ILE
1	E	57	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	85	HIS
1	L	80	HIS
1	L	121	HIS
1	C	126	GLN
1	F	78	HIS

### 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 monosaccharides 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

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	133/133 (100%)	-0.29	1 (0%) 86 81	38, 52, 87, 103	0
1	B	132/133 (99%)	-0.16	0 100 100	37, 65, 104, 118	0
1	C	133/133 (100%)	-0.19	2 (1%) 73 68	37, 52, 84, 149	0
1	D	130/133 (97%)	0.16	10 (7%) 13 7	42, 67, 111, 135	0
1	E	133/133 (100%)	-0.10	2 (1%) 73 68	46, 71, 105, 125	0
1	F	132/133 (99%)	0.18	6 (4%) 33 23	57, 84, 122, 161	0
1	G	133/133 (100%)	0.05	2 (1%) 73 68	47, 79, 122, 137	0
1	H	130/133 (97%)	0.65	16 (12%) 4 2	84, 119, 152, 183	0
1	I	133/133 (100%)	-0.10	3 (2%) 60 51	55, 81, 124, 143	0
1	J	129/133 (96%)	0.59	12 (9%) 8 4	81, 118, 151, 161	0
1	K	133/133 (100%)	-0.14	1 (0%) 86 81	51, 75, 117, 139	0
1	L	130/133 (97%)	0.52	10 (7%) 13 7	71, 105, 180, 220	0
2	T	65/66 (98%)	-0.43	0 100 100	39, 56, 85, 108	0
2	U	60/66 (90%)	0.55	8 (13%) 3 2	46, 92, 154, 177	0
2	V	65/66 (98%)	0.39	8 (12%) 4 2	52, 101, 147, 160	0
2	W	37/66 (56%)	0.78	6 (16%) 1 1	54, 126, 163, 169	0
2	X	39/66 (59%)	0.27	5 (12%) 3 2	61, 124, 173, 175	0
2	Y	43/66 (65%)	0.90	10 (23%) 0 0	51, 143, 189, 196	0
All	All	1890/1992 (94%)	0.14	102 (5%) 25 17	37, 81, 148, 220	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	38	ARG	8.5
2	U	67	ASP	7.6
2	U	68	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
2	Y	63	GLN	6.9
2	W	37	ASP	6.2

## 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 monosaccharides 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.