



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 11:59 PM EDT

PDB ID : 5XNB  
Title : Crystal structure of the IcmS-IcmW-DotL complex of the Legionella type IVb secretion system  
Authors : Xu, J.; Xu, D.; Zhu, Y.  
Deposited on : 2017-05-19  
Resolution : 2.59 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)

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<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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

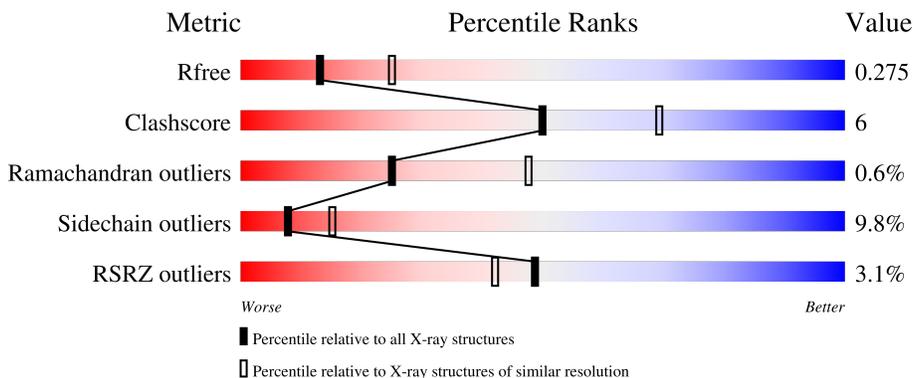
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	113	 4% 72% 17% 8%
1	D	113	 4% 71% 19% 5%
1	G	113	 3% 70% 16% 10%
1	J	113	 % 73% 13% 11%
1	M	113	 4% 65% 20% 9%

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Mol	Chain	Length	Quality of chain
1	P	113	 21% 62% 26% 12%
2	B	115	 83% 13% ..
2	E	115	 81% 16% ..
2	H	115	 87% 10% .
2	K	115	 86% 13% .
2	N	115	 81% 16% .
2	Q	115	 6% 83% 14% ..
3	C	151	 80% 17% ..
3	F	151	 79% 19% ..
3	I	151	 75% 21% ..
3	L	151	 77% 19% ..
3	O	151	 82% 13% ..
3	R	151	 7% 70% 24% 5% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17619 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 DotL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	104	798	506	133	158	1	0	0	0
1	D	107	815	518	135	161	1	0	0	0
1	G	102	788	500	131	156	1	0	0	0
1	J	101	783	497	130	155	1	0	0	0
1	M	103	799	507	132	159	1	0	0	0
1	P	100	779	495	129	154	1	0	0	0

- Molecule 2 is a protein called IcmS protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	114	882	557	142	173	10	0	0	0
2	E	114	882	557	142	173	10	0	0	0
2	H	115	887	560	143	174	10	0	0	0
2	K	115	887	560	143	174	10	0	0	0
2	N	115	887	560	143	174	10	0	0	0
2	Q	114	882	557	142	173	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP O54636

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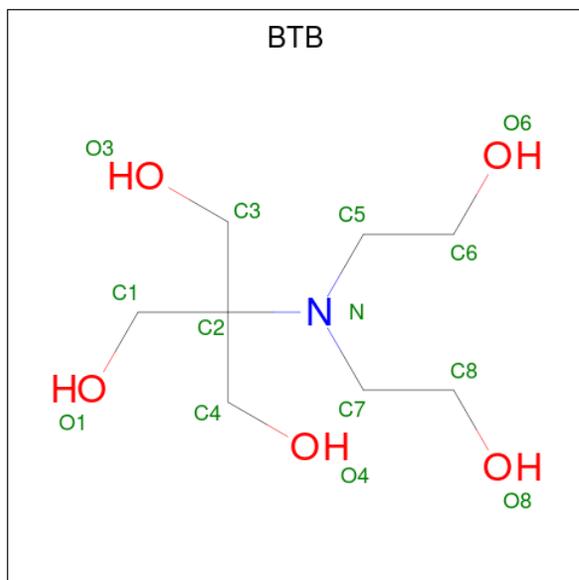
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ALA	-	expression tag	UNP O54636
H	0	ALA	-	expression tag	UNP O54636
K	0	ALA	-	expression tag	UNP O54636
N	0	ALA	-	expression tag	UNP O54636
Q	0	ALA	-	expression tag	UNP O54636

- Molecule 3 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			
3	F	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			
3	I	148	Total	C	N	O	S	0	0	0
			1194	763	204	223	4			
3	L	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			
3	O	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			
3	R	148	Total	C	N	O	S	0	0	0
			1194	763	204	223	4			

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	23	Total	O	0	0
			23	23		
5	C	34	Total	O	0	0
			34	34		
5	D	9	Total	O	0	0
			9	9		
5	E	28	Total	O	0	0
			28	28		
5	F	29	Total	O	0	0
			29	29		
5	G	11	Total	O	0	0
			11	11		
5	H	28	Total	O	0	0
			28	28		
5	I	20	Total	O	0	0
			20	20		
5	J	18	Total	O	0	0
			18	18		
5	K	26	Total	O	0	0
			26	26		
5	L	17	Total	O	0	0
			17	17		
5	M	6	Total	O	0	0
			6	6		
5	N	7	Total	O	0	0
			7	7		
5	O	6	Total	O	0	0
			6	6		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	P	1	Total O 1 1	0	0
5	Q	9	Total O 9 9	0	0
5	R	5	Total O 5 5	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.

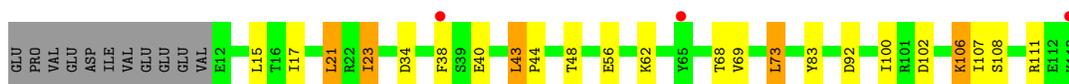
- Molecule 1: DotL



- Molecule 1: DotL



- Molecule 1: DotL



- Molecule 1: DotL

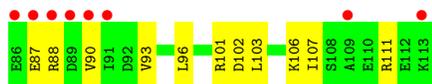
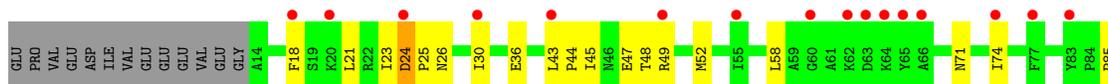


- Molecule 1: DotL

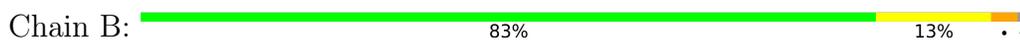




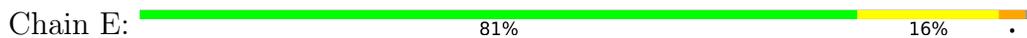
• Molecule 1: DotL



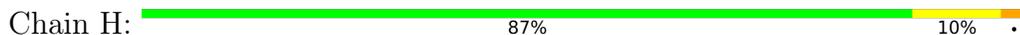
• Molecule 2: IcmS protein



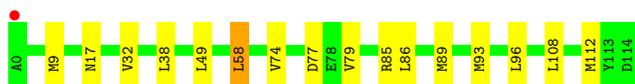
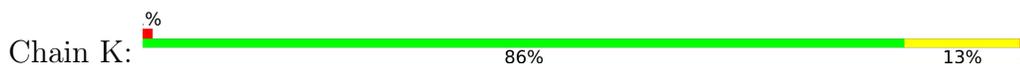
• Molecule 2: IcmS protein



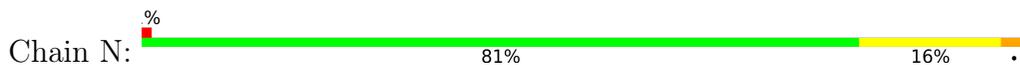
• Molecule 2: IcmS protein



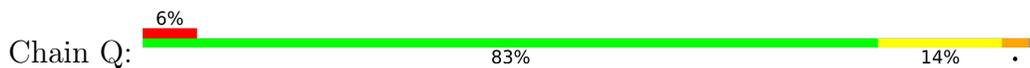
• Molecule 2: IcmS protein



• Molecule 2: IcmS protein



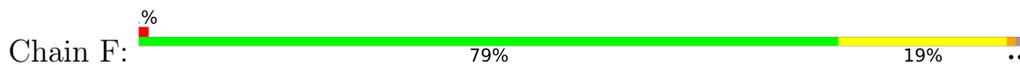
- Molecule 2: IcmS protein



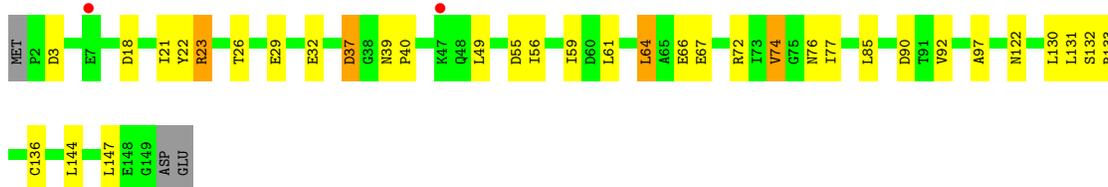
- Molecule 3: IcmW



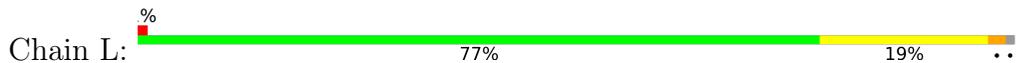
- Molecule 3: IcmW



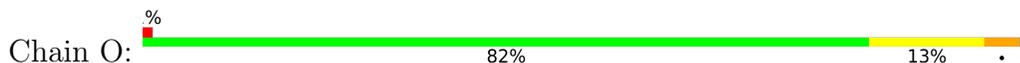
- Molecule 3: IcmW



- Molecule 3: IcmW

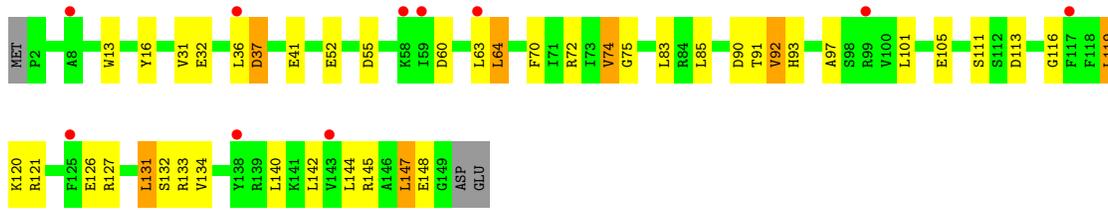


- Molecule 3: IcmW



- Molecule 3: IcmW





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.86Å 135.86Å 125.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.27 – 2.59 46.13 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.27-2.59) 99.5 (46.13-2.59)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.223 , 0.282 0.215 , 0.275	Depositor DCC
$R_{free}$ test set	4012 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 20.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l 0.258 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB

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	0.24	0/809	0.47	0/1098
1	D	0.23	0/826	0.43	0/1122
1	G	0.23	0/799	0.43	0/1084
1	J	0.24	0/794	0.44	0/1077
1	M	0.23	0/810	0.42	0/1099
1	P	0.22	0/790	0.41	0/1072
2	B	0.25	0/895	0.42	0/1208
2	E	0.25	0/895	0.42	0/1208
2	H	0.25	0/900	0.44	0/1215
2	K	0.26	0/900	0.44	0/1215
2	N	0.23	0/900	0.39	0/1215
2	Q	0.22	0/895	0.39	0/1208
3	C	0.23	0/1224	0.38	0/1650
3	F	0.24	0/1224	0.38	0/1650
3	I	0.23	0/1216	0.38	0/1639
3	L	0.23	0/1224	0.38	0/1650
3	O	0.22	0/1224	0.38	0/1650
3	R	0.21	0/1216	0.37	0/1639
All	All	0.23	0/17541	0.41	0/23699

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	GLU	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	798	0	807	14	0
1	D	815	0	817	13	0
1	G	788	0	803	14	0
1	J	783	0	801	11	0
1	M	799	0	816	17	0
1	P	779	0	798	16	0
2	B	882	0	874	7	0
2	E	882	0	874	8	0
2	H	887	0	879	5	0
2	K	887	0	879	6	0
2	N	887	0	879	9	0
2	Q	882	0	874	12	0
3	C	1202	0	1206	15	0
3	F	1202	0	1206	14	0
3	I	1194	0	1202	19	0
3	L	1202	0	1206	17	0
3	O	1202	0	1206	18	0
3	R	1194	0	1202	24	0
4	C	14	0	19	2	0
4	F	14	0	19	0	0
4	I	14	0	19	2	0
4	L	14	0	19	2	0
4	R	14	0	19	3	0
5	A	7	0	0	0	0
5	B	23	0	0	0	0
5	C	34	0	0	0	0
5	D	9	0	0	1	0
5	E	28	0	0	0	0
5	F	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	11	0	0	0	0
5	H	28	0	0	0	0
5	I	20	0	0	0	0
5	J	18	0	0	1	0
5	K	26	0	0	0	0
5	L	17	0	0	0	0
5	M	6	0	0	0	0
5	N	7	0	0	0	0
5	O	6	0	0	0	0
5	P	1	0	0	0	0
5	Q	9	0	0	0	0
5	R	5	0	0	0	0
All	All	17619	0	17424	203	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 6.

The worst 5 of 203 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:J:107:ILE:HG22	3:L:64:LEU:HD11	1.71	0.71
2:H:58:LEU:O	2:H:85:ARG:NH1	2.25	0.69
1:G:111:ARG:HH21	3:I:55:ASP:HB3	1.56	0.68
1:M:93:VAL:HG12	3:O:36:LEU:HD22	1.74	0.68
1:P:107:ILE:HG22	3:R:64:LEU:HD11	1.76	0.68

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	102/113 (90%)	95 (93%)	6 (6%)	1 (1%)	15	32
1	D	105/113 (93%)	96 (91%)	5 (5%)	4 (4%)	3	4
1	G	100/113 (88%)	97 (97%)	3 (3%)	0	100	100
1	J	99/113 (88%)	94 (95%)	2 (2%)	3 (3%)	4	7
1	M	101/113 (89%)	92 (91%)	9 (9%)	0	100	100
1	P	98/113 (87%)	88 (90%)	7 (7%)	3 (3%)	4	6
2	B	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
2	E	112/115 (97%)	112 (100%)	0	0	100	100
2	H	113/115 (98%)	113 (100%)	0	0	100	100
2	K	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
2	N	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
2	Q	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
3	C	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
3	F	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
3	I	146/151 (97%)	142 (97%)	4 (3%)	0	100	100
3	L	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
3	O	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	22	43
3	R	146/151 (97%)	141 (97%)	5 (3%)	0	100	100
All	All	2160/2274 (95%)	2084 (96%)	64 (3%)	12 (1%)	25	47

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	33	ALA
1	P	25	PRO
1	D	11	VAL
1	D	12	GLU
1	D	33	ALA

### 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	86/99 (87%)	77 (90%)	9 (10%)	7	13
1	D	86/99 (87%)	76 (88%)	10 (12%)	5	10
1	G	86/99 (87%)	78 (91%)	8 (9%)	9	17
1	J	86/99 (87%)	78 (91%)	8 (9%)	9	17
1	M	88/99 (89%)	76 (86%)	12 (14%)	3	6
1	P	86/99 (87%)	80 (93%)	6 (7%)	15	30
2	B	97/97 (100%)	86 (89%)	11 (11%)	6	10
2	E	97/97 (100%)	83 (86%)	14 (14%)	3	5
2	H	97/97 (100%)	88 (91%)	9 (9%)	9	17
2	K	97/97 (100%)	88 (91%)	9 (9%)	9	17
2	N	97/97 (100%)	87 (90%)	10 (10%)	7	13
2	Q	97/97 (100%)	92 (95%)	5 (5%)	23	46
3	C	131/133 (98%)	117 (89%)	14 (11%)	6	12
3	F	131/133 (98%)	121 (92%)	10 (8%)	13	26
3	I	130/133 (98%)	118 (91%)	12 (9%)	9	17
3	L	131/133 (98%)	121 (92%)	10 (8%)	13	26
3	O	131/133 (98%)	121 (92%)	10 (8%)	13	26
3	R	130/133 (98%)	113 (87%)	17 (13%)	4	7
All	All	1884/1974 (95%)	1700 (90%)	184 (10%)	8	15

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	41	GLU
2	N	96	LEU
3	L	85	LEU
1	M	68	THR
3	O	67	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
2	E	23	ASN
1	M	71	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BTB	F	201	-	13,13,13	0.97	1 (7%)	7,16,16	0.38	0
4	BTB	L	201	-	13,13,13	1.02	1 (7%)	7,16,16	0.47	0
4	BTB	C	201	-	13,13,13	1.06	1 (7%)	7,16,16	0.55	0
4	BTB	I	201	-	13,13,13	1.01	1 (7%)	7,16,16	0.49	0
4	BTB	R	201	-	13,13,13	1.10	1 (7%)	7,16,16	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	F	201	-	-	11/21/21/21	-
4	BTB	L	201	-	-	6/21/21/21	-
4	BTB	C	201	-	-	7/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	I	201	-	-	9/21/21/21	-
4	BTB	R	201	-	-	6/21/21/21	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	201	BTB	C1-C2	-2.95	1.49	1.53
4	C	201	BTB	C1-C2	-2.72	1.49	1.53
4	L	201	BTB	C1-C2	-2.65	1.49	1.53
4	I	201	BTB	C1-C2	-2.57	1.50	1.53
4	F	201	BTB	C1-C2	-2.45	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	BTB	O1-C1-C2-C4
4	C	201	BTB	O1-C1-C2-N
4	C	201	BTB	C1-C2-C4-O4
4	C	201	BTB	C3-C2-C4-O4
4	C	201	BTB	N-C2-C4-O4

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	201	BTB	2	0
4	C	201	BTB	2	0
4	I	201	BTB	2	0
4	R	201	BTB	3	0

## 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	104/113 (92%)	0.38	4 (3%) 40 33	24, 45, 66, 85	0
1	D	107/113 (94%)	0.31	5 (4%) 31 25	24, 44, 69, 81	0
1	G	102/113 (90%)	0.32	3 (2%) 51 45	24, 48, 75, 83	0
1	J	101/113 (89%)	0.27	1 (0%) 82 80	23, 37, 62, 78	0
1	M	103/113 (91%)	0.49	4 (3%) 39 32	37, 56, 83, 92	0
1	P	100/113 (88%)	1.42	24 (24%) 0 0	66, 86, 105, 113	0
2	B	114/115 (99%)	0.10	0 100 100	19, 30, 45, 63	0
2	E	114/115 (99%)	0.10	0 100 100	19, 30, 50, 60	0
2	H	115/115 (100%)	0.06	0 100 100	20, 30, 46, 65	0
2	K	115/115 (100%)	0.15	1 (0%) 84 82	18, 29, 45, 63	0
2	N	115/115 (100%)	0.23	1 (0%) 84 82	36, 45, 62, 73	0
2	Q	114/115 (99%)	0.60	7 (6%) 21 16	41, 61, 79, 93	0
3	C	149/151 (98%)	0.12	0 100 100	23, 32, 49, 76	0
3	F	149/151 (98%)	0.12	1 (0%) 87 86	24, 33, 49, 73	0
3	I	148/151 (98%)	0.26	2 (1%) 75 71	23, 46, 70, 88	0
3	L	149/151 (98%)	0.16	2 (1%) 77 73	22, 37, 58, 87	0
3	O	149/151 (98%)	0.38	2 (1%) 77 73	35, 51, 70, 83	0
3	R	148/151 (98%)	0.64	10 (6%) 17 12	51, 69, 80, 88	0
All	All	2196/2274 (96%)	0.33	67 (3%) 49 42	18, 42, 79, 113	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	90	VAL	6.6
1	P	91	ILE	6.2
1	P	60	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	3.9
1	D	90	VAL	3.9

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BTB	I	201	14/14	0.70	0.20	40,56,63,64	0
4	BTB	C	201	14/14	0.76	0.20	31,44,59,62	0
4	BTB	L	201	14/14	0.77	0.18	38,55,61,62	0
4	BTB	F	201	14/14	0.78	0.18	33,41,49,54	0
4	BTB	R	201	14/14	0.80	0.17	61,68,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.