



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:03 am BST

PDB ID : 5Y3A  
Title : Crystal structure of Ragulator complex (p18 49-161)  
Authors : Zhang, T.; Ding, J.  
Deposited on : 2017-07-28  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (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

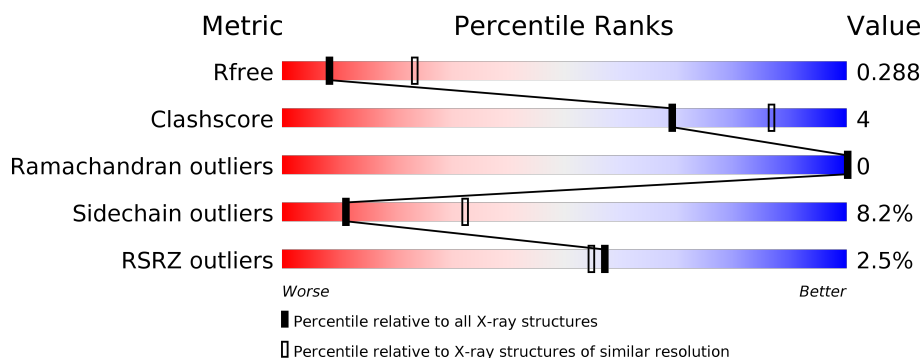
# 1 Overall quality at a glance

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	112	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>8%</div> <div>•</div> <div>34%</div> </div> </div>
1	F	112	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>6%</div> <div>•</div> <div>38%</div> </div> </div>
2	B	127	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
2	G	127	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div> </div>
3	C	124	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
3	H	124	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	101	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>78%</div><div>13%</div><div>• 7%</div></div></div>
4	I	101	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>77%</div><div>15%</div><div>8%</div></div></div>
5	E	93	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>86%</div><div>11%</div><div>•</div></div></div>
5	J	93	<div><div><div>3%</div><div><div></div><div></div><div></div></div><div>83%</div><div>13%</div><div>• •</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7463 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 Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			591	374	105	111	1			
1	F	70	Total	C	N	O	S	0	0	0
			558	355	98	104	1			

- Molecule 2 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			852	537	144	165	6			
2	G	110	Total	C	N	O	S	0	0	0
			828	521	141	160	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP Q9Y2Q5
B	0	ALA	-	expression tag	UNP Q9Y2Q5
G	-1	MET	-	expression tag	UNP Q9Y2Q5
G	0	ALA	-	expression tag	UNP Q9Y2Q5

- Molecule 3 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			934	601	157	175	1			
3	H	120	Total	C	N	O	S	0	0	0
			930	598	156	175	1			

- Molecule 4 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	94	Total	C	N	O	S	0	0	0
			701	437	126	135	3			
4	I	93	Total	C	N	O	S	0	0	0
			703	438	128	134	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	expression tag	UNP Q0VGL1
D	0	GLY	-	expression tag	UNP Q0VGL1
I	-1	MET	-	expression tag	UNP Q0VGL1
I	0	GLY	-	expression tag	UNP Q0VGL1

- Molecule 5 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	90	Total	C	N	O	S	0	0	0
			657	402	114	134	7			
5	J	90	Total	C	N	O	S	0	0	0
			657	402	114	134	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	81	MET	-	expression tag	UNP O43504
E	82	ALA	-	expression tag	UNP O43504
J	81	MET	-	expression tag	UNP O43504
J	82	ALA	-	expression tag	UNP O43504

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		
7	E	2	Total	O	0	0
			2	2		
7	G	1	Total	O	0	0
			1	1		

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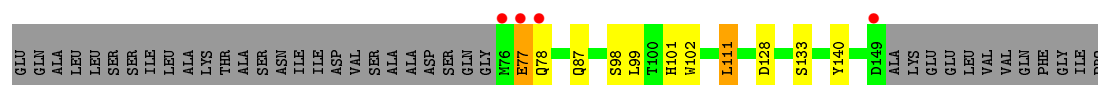
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	2	Total 2	O 2	0	0
7	I	1	Total 1	O 1	0	0
7	J	4	Total 4	O 4	0	0

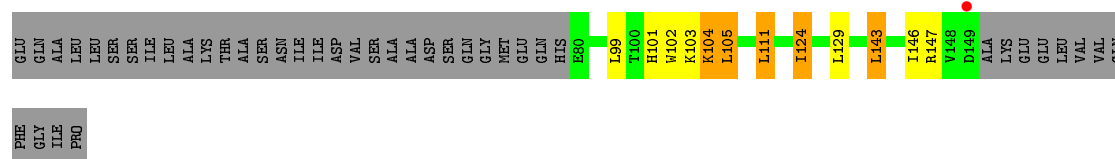
### 3 Residue-property plots [i](#)

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.

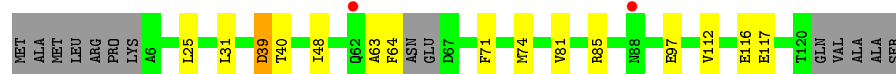
- Molecule 1: Regulator complex protein LAMTOR1



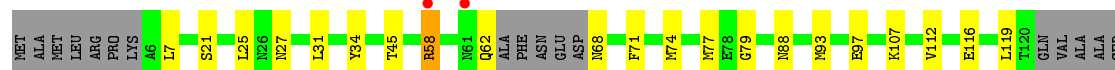
- Molecule 1: Regulator complex protein LAMTOR1



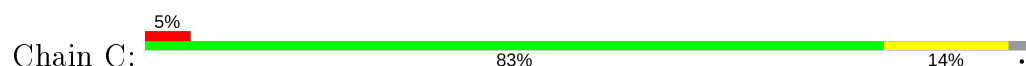
- Molecule 2: Regulator complex protein LAMTOR2



- Molecule 2: Regulator complex protein LAMTOR2

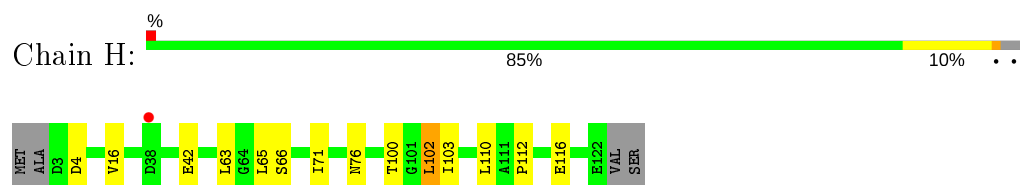


- Molecule 3: Regulator complex protein LAMTOR3

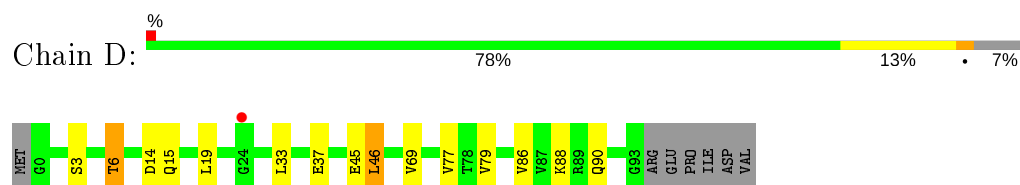




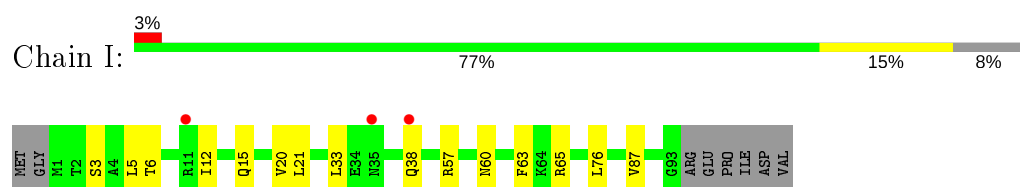
- Molecule 3: Regulator complex protein LAMTOR3



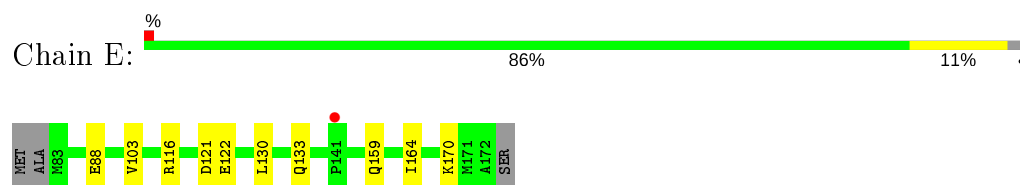
- Molecule 4: Regulator complex protein LAMTOR4



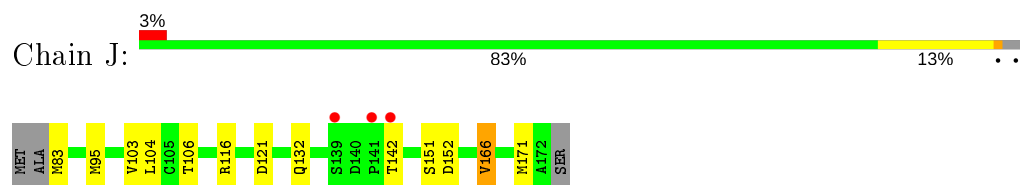
- Molecule 4: Regulator complex protein LAMTOR4



- Molecule 5: Regulator complex protein LAMTOR5



- Molecule 5: Regulator complex protein LAMTOR5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 89.63Å 232.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90 30.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.01-2.90) 84.5 (30.39-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.72 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.246 , 0.288 0.246 , 0.288	Depositor DCC
$R_{free}$ test set	1457 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 10.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.83% 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: SO4

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	0.40	0/606	0.63	0/826
1	F	0.48	0/572	0.70	0/780
2	B	0.41	0/861	0.70	0/1165
2	G	0.40	0/836	0.69	0/1131
3	C	0.40	0/951	0.65	0/1290
3	H	0.39	0/947	0.64	0/1286
4	D	0.38	0/709	0.67	0/957
4	I	0.39	0/711	0.70	0/959
5	E	0.35	0/663	0.62	0/899
5	J	0.34	0/663	0.62	0/899
All	All	0.39	0/7519	0.66	0/10192

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

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	591	0	584	8	0
1	F	558	0	561	10	0
2	B	852	0	854	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	828	0	836	9	0
3	C	934	0	958	7	0
3	H	930	0	947	10	0
4	D	701	0	708	9	0
4	I	703	0	716	5	0
5	E	657	0	656	8	0
5	J	657	0	656	5	0
6	A	20	0	0	0	0
6	E	5	0	0	0	0
6	F	5	0	0	0	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	2	0	0	0	0
7	G	1	0	0	0	0
7	H	2	0	0	0	0
7	I	1	0	0	0	0
7	J	4	0	0	0	0
All	All	7463	0	7476	55	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 4.

All (55) 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)
4:D:46:LEU:HD22	5:E:130:LEU:HD23	1.71	0.73
4:D:46:LEU:HD23	5:E:133:GLN:OE1	1.89	0.71
2:G:74:MET:HG2	3:H:71:ILE:HG12	1.75	0.69
1:F:104:LYS:HZ2	1:F:105:LEU:H	1.42	0.67
4:D:46:LEU:CD2	5:E:130:LEU:HD23	2.26	0.65
5:J:95:MET:HG3	5:J:116:ARG:HG2	1.84	0.60
1:F:146:ILE:O	1:F:146:ILE:HG22	2.02	0.60
2:B:63:ALA:HA	3:C:43:HIS:HB3	1.85	0.57
4:D:14:ASP:HB3	4:D:90:GLN:HB3	1.88	0.56
1:A:99:LEU:HD22	3:C:116:GLU:HG2	1.89	0.54
4:I:3:SER:HA	4:I:6:THR:HG22	1.90	0.54
2:G:77:MET:HB2	3:H:66:SER:HB2	1.91	0.53
2:G:93:MET:HE1	2:G:107:LYS:HB3	1.91	0.52
1:F:111:LEU:HG	4:I:63:PHE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:65:ARG:HD3	4:I:76:LEU:HD23	1.93	0.51
2:G:79:GLY:HA3	3:H:65:LEU:HD22	1.92	0.51
2:G:58:ARG:O	2:G:62:GLN:HB3	2.11	0.50
1:F:103:LYS:HD2	3:H:4:ASP:HB3	1.94	0.49
1:A:101:HIS:HB3	1:A:102:TRP:CE3	2.48	0.49
2:B:112:VAL:O	2:B:116:GLU:HG2	2.12	0.49
4:I:63:PHE:HA	5:J:151:SER:HB3	1.95	0.48
1:F:124:ILE:H	1:F:124:ILE:HD13	1.79	0.48
1:A:133:SER:HA	5:E:159:GLN:NE2	2.28	0.48
2:G:31:LEU:HD11	2:G:34:TYR:HB3	1.96	0.47
1:F:99:LEU:HD11	3:H:116:GLU:HG2	1.96	0.47
1:F:124:ILE:HG13	1:F:129:LEU:HD21	1.97	0.47
1:F:146:ILE:HA	5:J:83:MET:HG3	1.98	0.45
5:J:104:LEU:HD21	5:J:106:THR:HG23	1.99	0.45
3:C:83:PHE:HB2	3:C:90:VAL:HB	1.99	0.44
1:A:133:SER:HA	5:E:159:GLN:HE22	1.83	0.44
5:E:88:GLU:HG3	5:E:116:ARG:NH1	2.33	0.44
5:E:88:GLU:HG3	5:E:116:ARG:HH12	1.83	0.43
1:F:143:LEU:HA	1:F:146:ILE:HD12	2.01	0.42
2:B:48:ILE:HG23	3:C:59:GLN:HB3	2.00	0.42
1:A:77:GLU:OE1	1:A:78:GLN:N	2.51	0.42
1:F:102:TRP:HZ2	3:H:112:PRO:HB2	1.84	0.42
2:B:74:MET:HB2	2:B:81:VAL:HB	2.01	0.42
4:D:19:LEU:HB3	4:D:86:VAL:HB	2.01	0.42
1:A:140:TYR:HB2	5:E:164:ILE:HG21	2.01	0.42
3:H:16:VAL:HG22	3:H:102:LEU:HD13	2.01	0.42
2:B:39:ASP:OD1	2:B:39:ASP:N	2.52	0.42
3:C:16:VAL:HG22	3:C:102:LEU:HD13	2.02	0.42
2:B:74:MET:HG2	3:C:71:ILE:HG12	2.01	0.42
4:D:3:SER:HA	4:D:6:THR:HG22	2.01	0.42
2:G:112:VAL:O	2:G:116:GLU:HB2	2.19	0.42
4:I:12:ILE:HG21	4:I:87:VAL:HG11	2.01	0.41
1:A:101:HIS:HB3	1:A:102:TRP:CD2	2.56	0.41
1:A:111:LEU:HD22	4:D:79:VAL:H	1.85	0.41
2:B:64:PHE:HE1	3:C:41:PRO:HG2	1.86	0.41
4:D:33:LEU:HD21	4:D:88:LYS:HB2	2.03	0.40
4:D:77:VAL:HG13	4:D:86:VAL:HG22	2.03	0.40
3:H:100:THR:HA	3:H:103:ILE:HD12	2.03	0.40
5:J:104:LEU:O	5:J:166:VAL:HA	2.21	0.40
2:G:45:THR:HA	3:H:63:LEU:CD2	2.51	0.40
2:G:45:THR:HA	3:H:63:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

## 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	72/112 (64%)	70 (97%)	2 (3%)	0	100	100
1	F	68/112 (61%)	66 (97%)	2 (3%)	0	100	100
2	B	109/127 (86%)	105 (96%)	4 (4%)	0	100	100
2	G	106/127 (84%)	99 (93%)	7 (7%)	0	100	100
3	C	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
3	H	118/124 (95%)	115 (98%)	3 (2%)	0	100	100
4	D	92/101 (91%)	87 (95%)	5 (5%)	0	100	100
4	I	91/101 (90%)	88 (97%)	3 (3%)	0	100	100
5	E	88/93 (95%)	82 (93%)	6 (7%)	0	100	100
5	J	88/93 (95%)	83 (94%)	5 (6%)	0	100	100
All	All	950/1114 (85%)	906 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	66/97 (68%)	61 (92%)	5 (8%)	13	36
1	F	63/97 (65%)	56 (89%)	7 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/99 (89%)	80 (91%)	8 (9%)	9	28
2	G	86/99 (87%)	76 (88%)	10 (12%)	5	16
3	C	105/108 (97%)	97 (92%)	8 (8%)	13	36
3	H	104/108 (96%)	100 (96%)	4 (4%)	33	67
4	D	76/84 (90%)	70 (92%)	6 (8%)	12	34
4	I	77/84 (92%)	69 (90%)	8 (10%)	7	21
5	E	75/78 (96%)	71 (95%)	4 (5%)	22	54
5	J	75/78 (96%)	68 (91%)	7 (9%)	9	27
All	All	815/932 (87%)	748 (92%)	67 (8%)	11	32

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	87	GLN
1	A	98	SER
1	A	111	LEU
1	A	128	ASP
2	B	25	LEU
2	B	31	LEU
2	B	39	ASP
2	B	40	THR
2	B	71	PHE
2	B	85	ARG
2	B	97	GLU
2	B	117	GLU
3	C	28	ASP
3	C	39	ASN
3	C	42	GLU
3	C	77	THR
3	C	79	GLN
3	C	86	LEU
3	C	110	LEU
3	C	118	ARG
4	D	6	THR
4	D	15	GLN
4	D	37	GLU
4	D	45	GLU
4	D	46	LEU

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Mol	Chain	Res	Type
4	D	69	VAL
5	E	103	VAL
5	E	121	ASP
5	E	122	GLU
5	E	170	LYS
1	F	101	HIS
1	F	104	LYS
1	F	105	LEU
1	F	111	LEU
1	F	124	ILE
1	F	143	LEU
1	F	147	ARG
2	G	7	LEU
2	G	21	SER
2	G	25	LEU
2	G	27	ASN
2	G	58	ARG
2	G	68	ASN
2	G	71	PHE
2	G	88	ASN
2	G	97	GLU
2	G	119	LEU
3	H	42	GLU
3	H	76	ASN
3	H	102	LEU
3	H	110	LEU
4	I	5	LEU
4	I	15	GLN
4	I	20	VAL
4	I	21	LEU
4	I	33	LEU
4	I	38	GLN
4	I	57	ARG
4	I	60	ASN
5	J	103	VAL
5	J	121	ASP
5	J	132	GLN
5	J	142	THR
5	J	152	ASP
5	J	166	VAL
5	J	171	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such



sidechains are listed below:

Mol	Chain	Res	Type
3	C	68	ASN
3	C	84	ASN
4	D	56	HIS
5	E	159	GLN
3	H	119	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](#)

8 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	$\# Z  > 2$
6	SO4	A	204	-	4,4,4	0.26	0	6,6,6	0.33	0
6	SO4	E	201	-	4,4,4	0.33	0	6,6,6	0.05	0
6	SO4	F	201	-	4,4,4	0.33	0	6,6,6	0.05	0
6	SO4	A	202	-	4,4,4	0.32	0	6,6,6	0.04	0
6	SO4	A	201	-	4,4,4	0.32	0	6,6,6	0.05	0
6	SO4	J	201	-	4,4,4	0.29	0	6,6,6	0.05	0
6	SO4	A	203	-	4,4,4	0.28	0	6,6,6	0.09	0
6	SO4	I	101	-	4,4,4	0.32	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 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, 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	74/112 (66%)	0.11	4 (5%)	25 22	27, 40, 79, 116	0
1	F	70/112 (62%)	-0.16	1 (1%)	75 75	26, 40, 61, 66	0
2	B	113/127 (88%)	-0.02	2 (1%)	68 67	29, 38, 81, 104	0
2	G	110/127 (86%)	-0.03	2 (1%)	68 67	28, 37, 75, 98	0
3	C	120/124 (96%)	0.06	6 (5%)	28 25	28, 39, 75, 116	0
3	H	120/124 (96%)	-0.22	1 (0%)	86 86	23, 33, 56, 85	0
4	D	94/101 (93%)	-0.08	1 (1%)	80 80	23, 34, 72, 83	0
4	I	93/101 (92%)	0.03	3 (3%)	47 43	25, 40, 91, 103	0
5	E	90/93 (96%)	-0.20	1 (1%)	80 80	24, 29, 50, 68	0
5	J	90/93 (96%)	-0.22	3 (3%)	46 41	24, 30, 72, 99	0
All	All	974/1114 (87%)	-0.07	24 (2%)	57 55	23, 37, 75, 116	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	43	HIS	4.5
1	A	76	MET	3.9
1	A	78	GLN	3.2
2	G	61	ASN	3.0
1	F	149	ASP	2.7
4	I	11	ARG	2.4
1	A	77	GLU	2.4
3	C	40	ALA	2.4
5	J	142	THR	2.4
4	I	38	GLN	2.3
4	I	35	ASN	2.3
1	A	149	ASP	2.3
2	G	58	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	38	ASP	2.3
3	C	66	SER	2.2
3	C	37	ASN	2.2
2	B	88	ASN	2.2
3	C	77	THR	2.2
3	H	38	ASP	2.2
5	J	141	PRO	2.2
5	J	139	SER	2.1
5	E	141	PRO	2.1
4	D	24	GLY	2.1
2	B	62	GLN	2.0

## 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](#)

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
6	SO4	A	202	5/5	0.81	0.27	66,67,68,77	1
6	SO4	I	101	5/5	0.84	0.29	63,63,63,64	2
6	SO4	E	201	5/5	0.85	0.22	64,65,65,75	1
6	SO4	A	204	5/5	0.86	0.33	66,67,67,67	2
6	SO4	F	201	5/5	0.88	0.21	74,74,76,80	1
6	SO4	A	203	5/5	0.91	0.24	83,83,84,85	3
6	SO4	A	201	5/5	0.91	0.18	55,55,55,55	1
6	SO4	J	201	5/5	0.93	0.16	52,52,52,52	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.