



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:24 PM GMT

PDB ID : 4RIQ  
Title : Crystal structure of DPY-30 dimerization/docking domain in complex with Ash2L Sdc1-DPY-30 Interacting region (SDI)  
Authors : Tremblay, V.; Couture, J.-F.  
Deposited on : 2014-10-07  
Resolution : 2.23 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

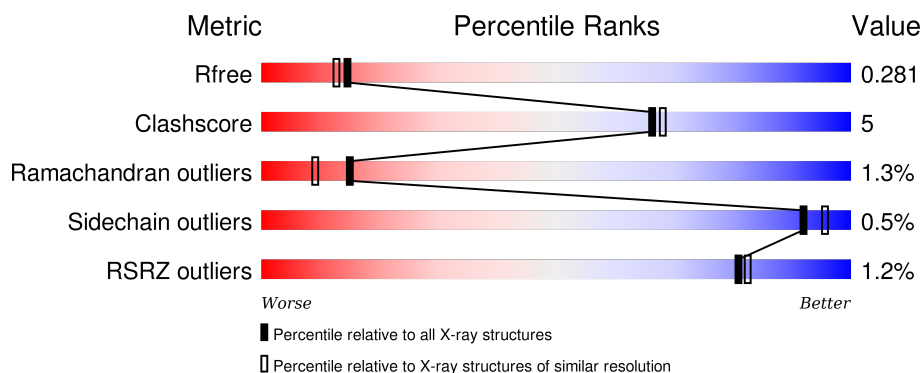
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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))
$R_{free}$	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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. 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	56	<div> <div></div> <div>75% 11% • 13%</div> </div>
1	B	56	<div> <div></div> <div>70% 13% • 16%</div> </div>
1	D	56	<div> <div>5%</div> <div>80% 11% 9%</div> </div>
1	E	56	<div> <div>4%</div> <div>71% 18% 11%</div> </div>
1	G	56	<div> <div></div> <div>77% 13% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	56	
1	J	56	
1	K	56	
1	M	56	
1	N	56	
1	P	56	
1	Q	56	
1	S	56	
1	T	56	
1	V	56	
1	Z	56	
2	C	27	
2	F	27	
2	I	27	
2	L	27	
2	O	27	
2	R	27	
2	U	27	
2	X	27	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7461 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 Protein dpy-30 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	49	Total	C	N	O	0	0	0
			361	240	59	62			
1	B	47	Total	C	N	O	0	0	0
			357	236	60	61			
1	D	51	Total	C	N	O	0	0	0
			387	255	64	68			
1	E	50	Total	C	N	O	0	0	0
			376	247	63	66			
1	G	50	Total	C	N	O	0	1	0
			390	258	64	68			
1	H	51	Total	C	N	O	0	0	0
			379	251	64	64			
1	J	49	Total	C	N	O	0	0	0
			368	243	60	65			
1	K	50	Total	C	N	O	0	0	0
			375	248	61	66			
1	M	50	Total	C	N	O	0	0	0
			366	243	60	63			
1	N	48	Total	C	N	O	0	0	0
			364	242	61	61			
1	P	45	Total	C	N	O	0	0	0
			341	227	56	58			
1	Q	49	Total	C	N	O	0	0	0
			368	242	61	65			
1	S	48	Total	C	N	O	0	0	0
			364	241	60	63			
1	T	49	Total	C	N	O	0	0	0
			370	246	61	63			
1	V	49	Total	C	N	O	0	0	0
			372	244	61	67			
1	Z	48	Total	C	N	O	0	0	0
			365	239	60	66			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	EXPRESSION TAG	UNP Q9C005
B	44	GLY	-	EXPRESSION TAG	UNP Q9C005
D	44	GLY	-	EXPRESSION TAG	UNP Q9C005
E	44	GLY	-	EXPRESSION TAG	UNP Q9C005
G	44	GLY	-	EXPRESSION TAG	UNP Q9C005
H	44	GLY	-	EXPRESSION TAG	UNP Q9C005
J	44	GLY	-	EXPRESSION TAG	UNP Q9C005
K	44	GLY	-	EXPRESSION TAG	UNP Q9C005
M	44	GLY	-	EXPRESSION TAG	UNP Q9C005
N	44	GLY	-	EXPRESSION TAG	UNP Q9C005
P	44	GLY	-	EXPRESSION TAG	UNP Q9C005
Q	44	GLY	-	EXPRESSION TAG	UNP Q9C005
S	44	GLY	-	EXPRESSION TAG	UNP Q9C005
T	44	GLY	-	EXPRESSION TAG	UNP Q9C005
V	44	GLY	-	EXPRESSION TAG	UNP Q9C005
Z	44	GLY	-	EXPRESSION TAG	UNP Q9C005

- Molecule 2 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	24	Total	C	N	O	S	0	1	0
			193	123	31	38	1			
2	F	24	Total	C	N	O	S	0	1	0
			193	123	31	38	1			
2	I	24	Total	C	N	O	S	0	1	0
			193	123	31	38	1			
2	L	24	Total	C	N	O		0	1	0
			182	117	31	34				
2	O	24	Total	C	N	O	S	0	1	0
			193	123	31	38	1			
2	R	24	Total	C	N	O		0	0	0
			175	112	29	34				
2	U	23	Total	C	N	O		0	1	0
			177	114	30	33				
2	X	24	Total	C	N	O	S	0	1	0
			189	121	31	36	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
C	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
C	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
C	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
C	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
C	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
C	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
C	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
C	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
C	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
F	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
F	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
F	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
F	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
F	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
F	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
F	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
F	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
F	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
F	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
F	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
I	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
I	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
I	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
I	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
I	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
I	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
I	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
I	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
I	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
I	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
I	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
L	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
L	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
L	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
L	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
L	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
L	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
L	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
L	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
L	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
L	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3

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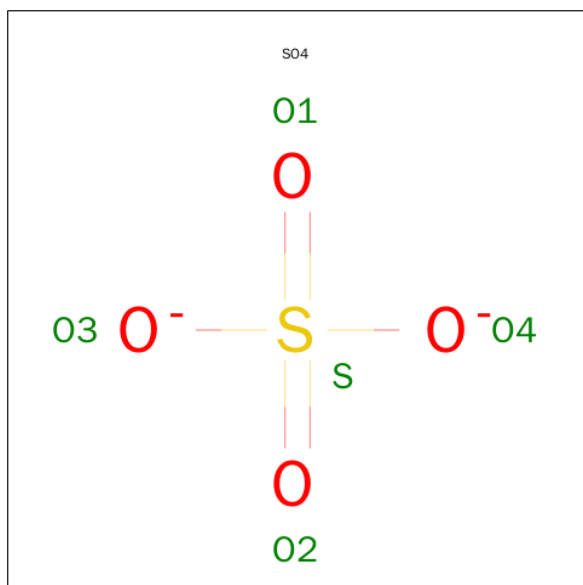
Chain	Residue	Modelled	Actual	Comment	Reference
L	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
O	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
O	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
O	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
O	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
O	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
O	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
O	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
O	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
O	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
O	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
O	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
R	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
R	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
R	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
R	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
R	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
R	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
R	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
R	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
R	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
R	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
R	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
U	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
U	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
U	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
U	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
U	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
U	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
U	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
U	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3
U	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
U	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
U	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3
X	504	GLY	-	EXPRESSION TAG	UNP Q9UBL3
X	505	ALA	-	EXPRESSION TAG	UNP Q9UBL3
X	506	MET	-	EXPRESSION TAG	UNP Q9UBL3
X	507	GLY	-	EXPRESSION TAG	UNP Q9UBL3
X	508	SER	-	EXPRESSION TAG	UNP Q9UBL3
X	525	GLU	-	EXPRESSION TAG	UNP Q9UBL3
X	526	ASN	-	EXPRESSION TAG	UNP Q9UBL3
X	527	LEU	-	EXPRESSION TAG	UNP Q9UBL3

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Chain	Residue	Modelled	Actual	Comment	Reference
X	528	TYR	-	EXPRESSION TAG	UNP Q9UBL3
X	529	PHE	-	EXPRESSION TAG	UNP Q9UBL3
X	530	GLN	-	EXPRESSION TAG	UNP Q9UBL3

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	U	1	Total O S 5 4 1	0	0

- Molecule 4 is water.



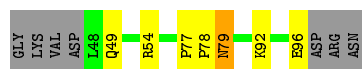
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0
4	K	1	Total O 1 1	0	0
4	L	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	3	Total O 3 3	0	0
4	P	1	Total O 1 1	0	0
4	R	2	Total O 2 2	0	0
4	S	1	Total O 1 1	0	0
4	T	3	Total O 3 3	0	0
4	U	3	Total O 3 3	0	0
4	V	1	Total O 1 1	0	0
4	X	1	Total O 1 1	0	0
4	Z	1	Total O 1 1	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 errors 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.

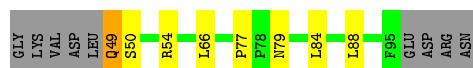
- Molecule 1: Protein dpy-30 homolog

Chain A: 




- Molecule 1: Protein dpy-30 homolog

Chain B: 



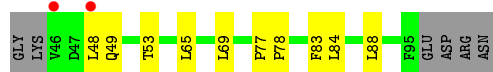
- Molecule 1: Protein dpy-30 homolog

Chain D: 




- Molecule 1: Protein dpy-30 homolog

Chain E: 



- Molecule 1: Protein dpy-30 homolog

Chain G: 



- Molecule 1: Protein dpy-30 homolog

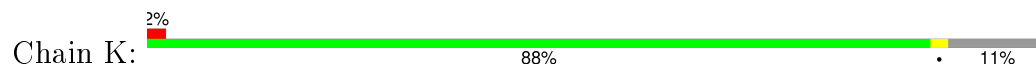
Chain H: 



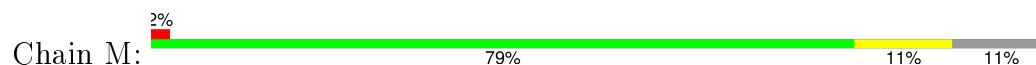
- Molecule 1: Protein dpy-30 homolog



- Molecule 1: Protein dpy-30 homolog



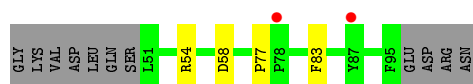
- Molecule 1: Protein dpy-30 homolog



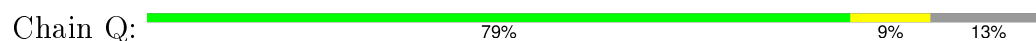
- Molecule 1: Protein dpy-30 homolog



- Molecule 1: Protein dpy-30 homolog



- Molecule 1: Protein dpy-30 homolog

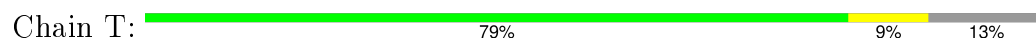


- Molecule 1: Protein dpy-30 homolog





- Molecule 1: Protein dpy-30 homolog



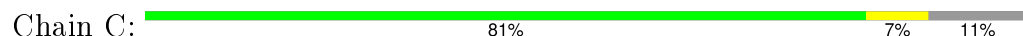
- Molecule 1: Protein dpy-30 homolog



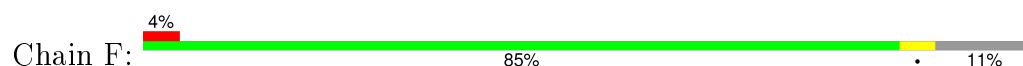
- Molecule 1: Protein dpy-30 homolog



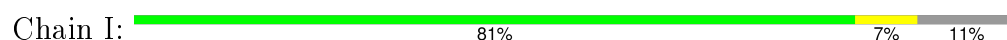
- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2



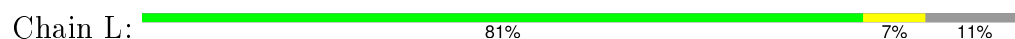
- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2



- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2



- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2





- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain O: 85% 11%



- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain R: 85% 11%



- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain U: 74% 11% 15%



- Molecule 2: Set1/Ash2 histone methyltransferase complex subunit ASH2

Chain X: 81% 7% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.27Å 56.27Å 95.09Å 90.08° 89.90° 115.39°	Depositor
Resolution (Å)	28.68 – 2.23 28.68 – 2.23	Depositor EDS
% Data completeness (in resolution range)	92.8 (28.68-2.23) 88.1 (28.68-2.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.236 , 0.284 0.236 , 0.281	Depositor DCC
$R_{free}$ test set	2283 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.4	EDS
Estimated twinning fraction	0.458 for -h,-k,l 0.012 for -k,-h,-l 0.016 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 47679 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.32	0/369	0.73	1/508 (0.2%)
1	B	0.28	0/365	0.53	0/501
1	D	0.29	0/395	0.53	0/541
1	E	0.29	0/384	0.55	0/527
1	G	0.31	0/401	0.54	0/549
1	H	0.33	0/387	0.60	1/531 (0.2%)
1	J	0.29	0/376	0.55	0/517
1	K	0.26	0/383	0.50	0/526
1	M	0.30	0/374	0.56	0/515
1	N	0.31	0/372	0.58	0/510
1	P	0.31	0/349	0.51	0/480
1	Q	0.40	0/376	0.56	0/518
1	S	0.28	0/372	0.51	0/511
1	T	0.31	0/378	0.51	0/518
1	V	0.30	0/380	0.51	0/523
1	Z	0.29	0/372	0.60	0/510
2	C	0.30	0/200	0.42	0/273
2	F	0.31	0/200	0.45	0/273
2	I	0.30	0/200	0.48	0/273
2	L	0.33	0/189	0.49	0/260
2	O	0.30	0/200	0.43	0/273
2	R	0.24	0/178	0.40	0/245
2	U	0.30	0/184	0.45	0/253
2	X	0.28	0/196	0.45	0/268
All	All	0.30	0/7580	0.54	2/10403 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PRO	C-N-CA	5.16	134.61	121.70
1	H	90	LYS	CB-CG-CD	5.05	124.74	111.60

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	361	0	364	5	0
1	B	357	0	367	6	0
1	D	387	0	395	3	0
1	E	376	0	377	7	0
1	G	390	0	408	4	0
1	H	379	0	387	5	0
1	J	368	0	372	8	0
1	K	375	0	378	1	0
1	M	366	0	366	3	0
1	N	364	0	381	10	0
1	P	341	0	350	4	0
1	Q	368	0	369	3	0
1	S	364	0	374	7	0
1	T	370	0	383	4	0
1	V	372	0	373	2	0
1	Z	365	0	378	5	0
2	C	193	0	178	2	0
2	F	193	0	178	1	0
2	I	193	0	178	2	0
2	L	182	0	163	2	0
2	O	193	0	178	1	0
2	R	175	0	156	1	0
2	U	177	0	158	3	0
2	X	189	0	174	2	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
3	I	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	O	5	0	0	0	0
3	R	5	0	0	0	0
3	U	5	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	3	0	0	0	0
4	P	1	0	0	0	0
4	R	2	0	0	0	0
4	S	1	0	0	0	0
4	T	3	0	0	0	0
4	U	3	0	0	0	0
4	V	1	0	0	0	0
4	X	1	0	0	0	0
4	Z	1	0	0	0	0
All	All	7461	0	7385	72	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 5.

The worst 5 of 72 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:A:54:ARG:NH2	2:L:521:GLU:OE2	2.23	0.71
1:P:54:ARG:NH1	1:P:58:ASP:OD2	2.23	0.71
1:D:47:ASP:OD1	1:D:48:LEU:N	2.25	0.69
1:A:77:PRO:HB2	1:A:79:ASN:HB2	1.74	0.69
1:J:49:GLN:OE1	1:J:49:GLN:N	2.30	0.65

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	47/56 (84%)	44 (94%)	1 (2%)	2 (4%)	3	1
1	B	45/56 (80%)	44 (98%)	1 (2%)	0	100	100
1	D	49/56 (88%)	46 (94%)	2 (4%)	1 (2%)	9	4
1	E	48/56 (86%)	44 (92%)	2 (4%)	2 (4%)	3	1
1	G	49/56 (88%)	46 (94%)	2 (4%)	1 (2%)	9	4
1	H	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
1	J	47/56 (84%)	45 (96%)	1 (2%)	1 (2%)	9	3
1	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
1	M	48/56 (86%)	45 (94%)	2 (4%)	1 (2%)	9	3
1	N	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
1	P	43/56 (77%)	42 (98%)	1 (2%)	0	100	100
1	Q	47/56 (84%)	44 (94%)	2 (4%)	1 (2%)	9	3
1	S	46/56 (82%)	44 (96%)	2 (4%)	0	100	100
1	T	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
1	V	47/56 (84%)	44 (94%)	2 (4%)	1 (2%)	9	3
1	Z	46/56 (82%)	43 (94%)	1 (2%)	2 (4%)	3	1
2	C	23/27 (85%)	23 (100%)	0	0	100	100
2	F	23/27 (85%)	23 (100%)	0	0	100	100
2	I	23/27 (85%)	23 (100%)	0	0	100	100
2	L	23/27 (85%)	23 (100%)	0	0	100	100
2	O	23/27 (85%)	23 (100%)	0	0	100	100
2	R	22/27 (82%)	22 (100%)	0	0	100	100
2	U	22/27 (82%)	22 (100%)	0	0	100	100
2	X	23/27 (85%)	23 (100%)	0	0	100	100
All	All	934/1112 (84%)	896 (96%)	26 (3%)	12 (1%)	15	9

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	49	GLN
1	Q	49	GLN
1	V	48	LEU
1	Z	48	LEU
1	A	79	ASN

### 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	36/49 (74%)	36 (100%)	0	100	100
1	B	37/49 (76%)	36 (97%)	1 (3%)	52	63
1	D	40/49 (82%)	40 (100%)	0	100	100
1	E	38/49 (78%)	38 (100%)	0	100	100
1	G	42/49 (86%)	42 (100%)	0	100	100
1	H	38/49 (78%)	38 (100%)	0	100	100
1	J	38/49 (78%)	38 (100%)	0	100	100
1	K	38/49 (78%)	38 (100%)	0	100	100
1	M	36/49 (74%)	35 (97%)	1 (3%)	51	61
1	N	38/49 (78%)	37 (97%)	1 (3%)	54	64
1	P	35/49 (71%)	35 (100%)	0	100	100
1	Q	38/49 (78%)	38 (100%)	0	100	100
1	S	38/49 (78%)	38 (100%)	0	100	100
1	T	38/49 (78%)	38 (100%)	0	100	100
1	V	39/49 (80%)	38 (97%)	1 (3%)	54	64
1	Z	39/49 (80%)	39 (100%)	0	100	100
2	C	21/23 (91%)	21 (100%)	0	100	100
2	F	21/23 (91%)	21 (100%)	0	100	100
2	I	21/23 (91%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	18/23 (78%)	18 (100%)	0	100	100
2	O	21/23 (91%)	21 (100%)	0	100	100
2	R	17/23 (74%)	17 (100%)	0	100	100
2	U	18/23 (78%)	18 (100%)	0	100	100
2	X	20/23 (87%)	20 (100%)	0	100	100
All	All	765/968 (79%)	761 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	M	78	PRO
1	N	91	ASN
1	V	49	GLN

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

Mol	Chain	Res	Type
1	A	79	ASN
2	L	526	ASN
1	N	91	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	SO4	C	601	-	4,4,4	0.20	0	6,6,6	0.08	0
3	SO4	F	601	-	4,4,4	0.21	0	6,6,6	0.10	0
3	SO4	I	601	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	K	101	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	L	601	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	O	601	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	R	601	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	U	601	-	4,4,4	0.21	0	6,6,6	0.09	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
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	SO4	F	601	-	-	0/0/0/0	0/0/0/0
3	SO4	I	601	-	-	0/0/0/0	0/0/0/0
3	SO4	K	101	-	-	0/0/0/0	0/0/0/0
3	SO4	L	601	-	-	0/0/0/0	0/0/0/0
3	SO4	O	601	-	-	0/0/0/0	0/0/0/0
3	SO4	R	601	-	-	0/0/0/0	0/0/0/0
3	SO4	U	601	-	-	0/0/0/0	0/0/0/0

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	49/56 (87%)	0.20	0 100 100	63, 81, 108, 115	0
1	B	47/56 (83%)	-0.04	0 100 100	54, 80, 110, 117	0
1	D	51/56 (91%)	-0.02	3 (5%) 26 27	54, 73, 89, 112	0
1	E	50/56 (89%)	-0.07	2 (4%) 42 44	53, 68, 90, 99	0
1	G	50/56 (89%)	-0.21	0 100 100	57, 71, 97, 114	0
1	H	51/56 (91%)	-0.10	1 (1%) 68 70	55, 72, 97, 110	0
1	J	49/56 (87%)	-0.16	0 100 100	54, 66, 100, 116	0
1	K	50/56 (89%)	-0.09	1 (2%) 68 70	49, 68, 89, 106	0
1	M	50/56 (89%)	-0.00	1 (2%) 68 70	61, 83, 99, 107	0
1	N	48/56 (85%)	-0.07	0 100 100	58, 81, 105, 117	0
1	P	45/56 (80%)	-0.02	2 (4%) 38 40	58, 71, 100, 106	0
1	Q	49/56 (87%)	-0.08	0 100 100	58, 80, 98, 125	0
1	S	48/56 (85%)	-0.27	0 100 100	54, 66, 91, 104	0
1	T	49/56 (87%)	-0.21	0 100 100	53, 67, 90, 97	0
1	V	49/56 (87%)	-0.00	0 100 100	63, 77, 113, 126	0
1	Z	48/56 (85%)	-0.06	1 (2%) 67 69	56, 78, 106, 119	0
2	C	24/27 (88%)	-0.05	0 100 100	55, 64, 76, 86	0
2	F	24/27 (88%)	-0.06	1 (4%) 40 42	53, 65, 82, 101	0
2	I	24/27 (88%)	-0.29	0 100 100	55, 65, 84, 96	0
2	L	24/27 (88%)	-0.04	0 100 100	54, 65, 83, 96	0
2	O	24/27 (88%)	-0.28	0 100 100	56, 65, 78, 80	0
2	R	24/27 (88%)	-0.10	0 100 100	59, 75, 90, 96	0
2	U	23/27 (85%)	-0.23	0 100 100	54, 64, 79, 92	0
2	X	24/27 (88%)	0.06	0 100 100	59, 70, 93, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	974/1112 (87%)	-0.09	12 (1%) 81 82	49, 72, 102, 126	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	83	PHE	3.7
1	E	46	VAL	3.0
2	F	505	ALA	2.7
1	K	46	VAL	2.7
1	E	48	LEU	2.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	O	601	5/5	0.88	0.12	-0.34	101,109,116,120	0
3	SO4	I	601	5/5	0.87	0.11	-0.41	123,123,129,129	0
3	SO4	C	601	5/5	0.95	0.08	-1.70	93,95,107,109	0
3	SO4	L	601	5/5	0.96	0.08	-1.99	102,105,108,109	0
3	SO4	K	101	5/5	0.94	0.08	-2.39	114,115,122,124	0
3	SO4	R	601	5/5	0.95	0.07	-2.79	115,121,126,129	0
3	SO4	U	601	5/5	0.96	0.06	-2.81	96,98,108,116	0
3	SO4	F	601	5/5	0.86	0.10	-3.96	121,125,126,127	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.