



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:46 PM BST

PDB ID : 5K77  
Title : Dbr1 in complex with 7-mer branched RNA  
Authors : Clark, N.E.; Taylor, A.B.; Hart, P.J.  
Deposited on : 2016-05-25  
Resolution : 2.17 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 : 2.13.1  
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) : 2.13.1

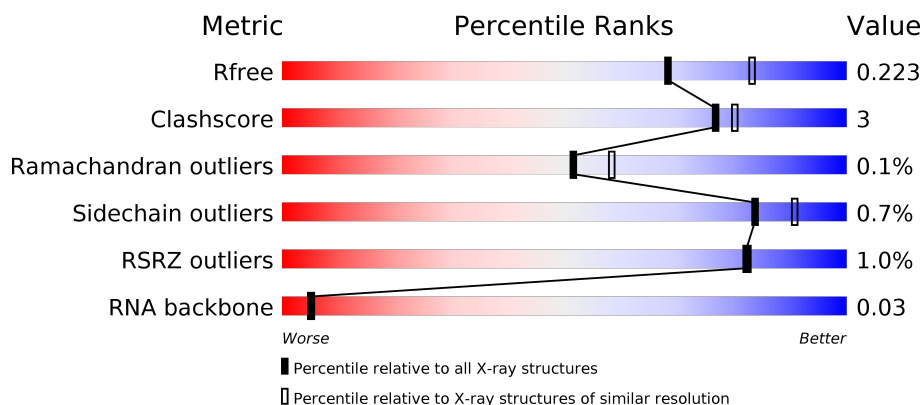
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)
RNA backbone	3102	1052 (2.60-1.76)

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	360	<div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	360	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	C	360	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	D	360	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	360	<div> <div></div> <div>%</div> <div>88%</div> <div>9%</div> <div></div> </div>
2	V	5	<div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
2	W	5	<div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
2	X	5	<div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
2	Y	5	<div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
2	Z	5	<div> <div></div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
3	v	2	<div> <div></div> <div>100%</div> </div>
3	w	2	<div> <div></div> <div>100%</div> </div>
3	x	2	<div> <div></div> <div>100%</div> </div>
3	y	2	<div> <div></div> <div>100%</div> </div>
3	z	2	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15513 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 RNA lariat debranching enzyme, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	5	0
			2882	1873	467	526	16			
1	B	349	Total	C	N	O	S	0	5	0
			2881	1872	467	526	16			
1	C	349	Total	C	N	O	S	0	5	0
			2887	1876	468	527	16			
1	D	349	Total	C	N	O	S	0	1	0
			2856	1858	463	520	15			
1	E	349	Total	C	N	O	S	0	5	0
			2889	1877	469	528	15			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ALA	HIS	conflict	UNP C4M1P9
A	355	HIS	-	expression tag	UNP C4M1P9
A	356	HIS	-	expression tag	UNP C4M1P9
A	357	HIS	-	expression tag	UNP C4M1P9
A	358	HIS	-	expression tag	UNP C4M1P9
A	359	HIS	-	expression tag	UNP C4M1P9
A	360	HIS	-	expression tag	UNP C4M1P9
B	91	ALA	HIS	engineered mutation	UNP C4M1P9
B	355	HIS	-	expression tag	UNP C4M1P9
B	356	HIS	-	expression tag	UNP C4M1P9
B	357	HIS	-	expression tag	UNP C4M1P9
B	358	HIS	-	expression tag	UNP C4M1P9
B	359	HIS	-	expression tag	UNP C4M1P9
B	360	HIS	-	expression tag	UNP C4M1P9
C	91	ALA	HIS	engineered mutation	UNP C4M1P9
C	355	HIS	-	expression tag	UNP C4M1P9
C	356	HIS	-	expression tag	UNP C4M1P9
C	357	HIS	-	expression tag	UNP C4M1P9
C	358	HIS	-	expression tag	UNP C4M1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	359	HIS	-	expression tag	UNP C4M1P9
C	360	HIS	-	expression tag	UNP C4M1P9
D	91	ALA	HIS	engineered mutation	UNP C4M1P9
D	355	HIS	-	expression tag	UNP C4M1P9
D	356	HIS	-	expression tag	UNP C4M1P9
D	357	HIS	-	expression tag	UNP C4M1P9
D	358	HIS	-	expression tag	UNP C4M1P9
D	359	HIS	-	expression tag	UNP C4M1P9
D	360	HIS	-	expression tag	UNP C4M1P9
E	91	ALA	HIS	engineered mutation	UNP C4M1P9
E	355	HIS	-	expression tag	UNP C4M1P9
E	356	HIS	-	expression tag	UNP C4M1P9
E	357	HIS	-	expression tag	UNP C4M1P9
E	358	HIS	-	expression tag	UNP C4M1P9
E	359	HIS	-	expression tag	UNP C4M1P9
E	360	HIS	-	expression tag	UNP C4M1P9

- Molecule 2 is a RNA chain called branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	4	Total 64	C 29	N 13	O 19	P 3	0	0	1
2	W	4	Total 64	C 29	N 13	O 19	P 3	0	0	1
2	X	4	Total 64	C 29	N 13	O 19	P 3	0	0	1
2	Y	4	Total 64	C 29	N 13	O 19	P 3	0	0	1
2	Z	4	Total 64	C 29	N 13	O 19	P 3	0	0	1

- Molecule 3 is a RNA chain called brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	v	2	Total 28	C 10	N 5	O 11	P 2	0	0	0
3	w	2	Total 28	C 10	N 5	O 11	P 2	0	0	0
3	x	2	Total 28	C 10	N 5	O 11	P 2	0	0	0
3	y	2	Total 28	C 10	N 5	O 11	P 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	z	2	Total	C	N	O	P	0	0	0
			28	10	5	11	2			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Fe	0	0
			1	1		
5	A	1	Total	Fe	0	0
			1	1		
5	D	1	Total	Fe	0	0
			1	1		
5	C	1	Total	Fe	0	0
			1	1		
5	E	1	Total	Fe	0	0
			1	1		

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



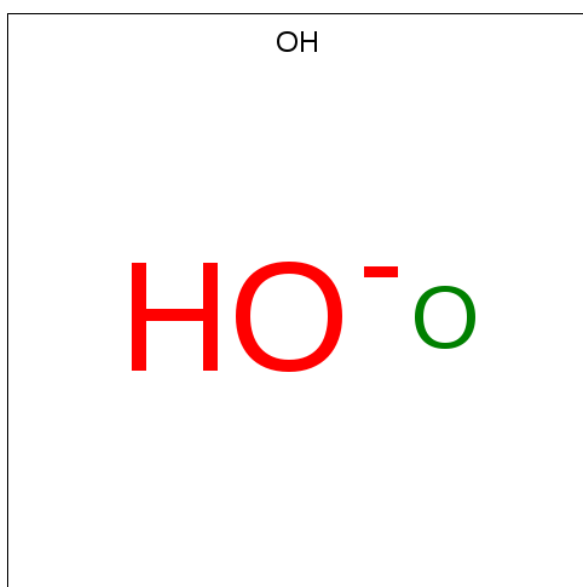
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	B	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0
7	D	1	Total O 1 1	0	0
7	E	1	Total O 1 1	0	0

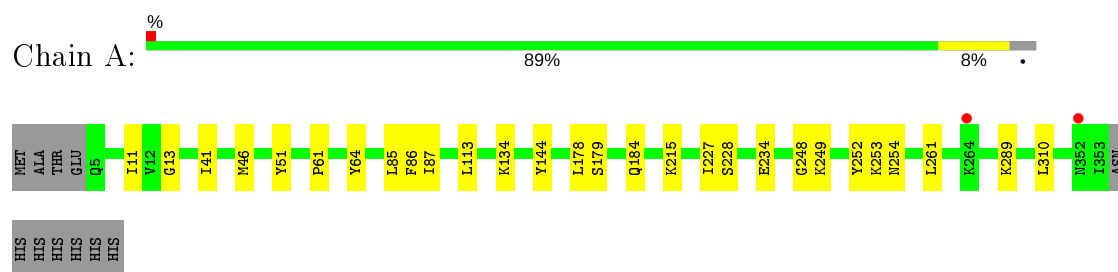
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	88	Total O 88 88	0	0
8	B	101	Total O 101 101	0	0
8	C	122	Total O 122 122	0	0
8	D	110	Total O 110 110	0	0
8	E	89	Total O 89 89	0	0
8	v	1	Total O 1 1	0	0
8	w	1	Total O 1 1	0	0
8	X	3	Total O 3 3	0	0
8	x	1	Total O 1 1	0	0
8	Z	2	Total O 2 2	0	0

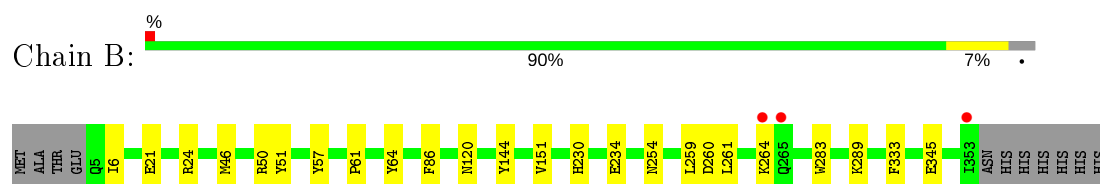
### 3 Residue-property plots

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.

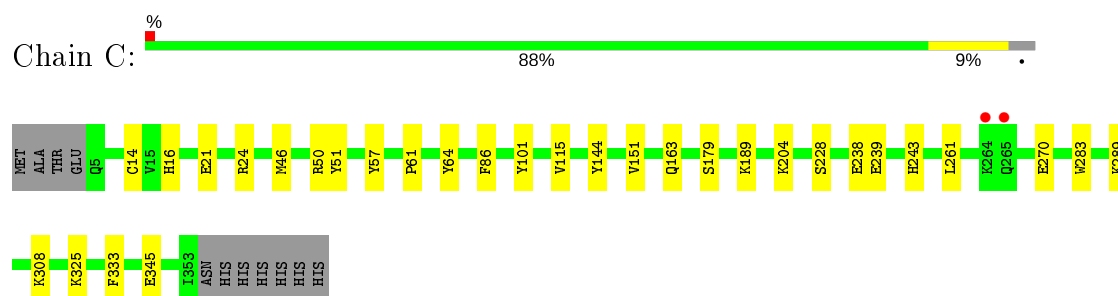
- Molecule 1: RNA lariat debranching enzyme, putative



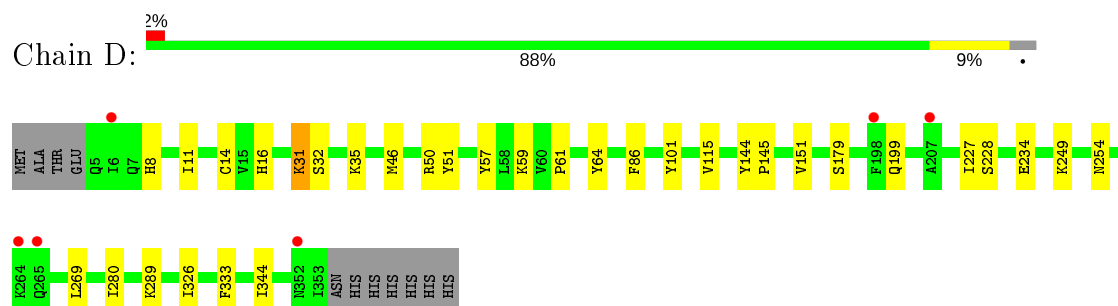
- Molecule 1: RNA lariat debranching enzyme, putative



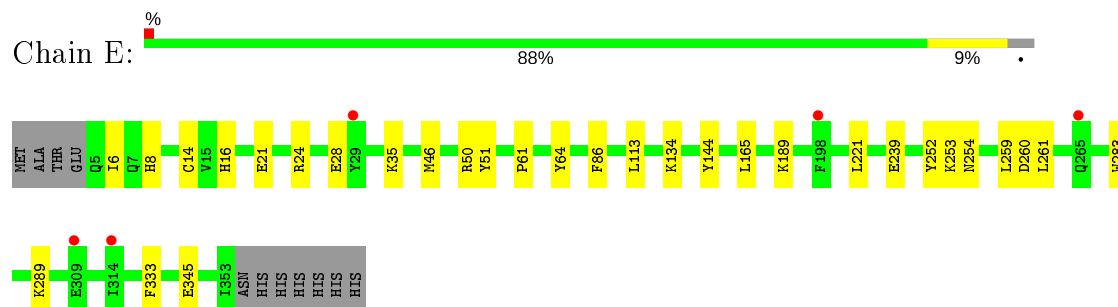
- Molecule 1: RNA lariat debranching enzyme, putative



- Molecule 1: RNA lariat debranching enzyme, putative



- Molecule 1: RNA lariat debranching enzyme, putative



- Molecule 2: branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'



- Molecule 2: branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'



- Molecule 2: branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'



- Molecule 2: branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'



- Molecule 2: branch 1 of branched RNA 5'-UAA(-2'GU)CA-3'



- Molecule 3: brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'



There are no outlier residues recorded for this chain.

- Molecule 3: brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: brnch 2 of branched RNA 5'-UAA(-2'GU)CA-3'

Chain z:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.15Å 141.89Å 212.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.00 – 2.17 118.01 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.7 (118.00-2.17) 98.3 (118.01-2.17)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, $R_{free}$	0.182 , 0.223 0.182 , 0.223	Depositor DCC
$R_{free}$ test set	5763 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FE2, SO4, OH

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	0/2968	0.42	0/4012
1	B	0.24	0/2967	0.41	0/4011
1	C	0.24	0/2971	0.42	0/4016
1	D	0.24	0/2936	0.42	0/3969
1	E	0.24	0/2973	0.42	0/4019
2	V	0.27	0/71	0.64	0/109
2	W	0.24	0/71	0.65	0/109
2	X	0.22	0/71	0.65	0/109
2	Y	0.20	0/71	0.65	0/109
2	Z	0.23	0/71	0.64	0/109
3	v	0.16	0/30	0.56	0/44
3	w	0.15	0/30	0.57	0/44
3	x	0.16	0/30	0.55	0/44
3	y	0.18	0/30	0.56	0/44
3	z	0.17	0/30	0.57	0/44
All	All	0.24	0/15320	0.43	0/20792

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	2882	0	2861	15	0
1	B	2881	0	2859	14	0
1	C	2887	0	2859	16	0
1	D	2856	0	2838	17	0
1	E	2889	0	2860	17	0
2	V	64	0	34	1	0
2	W	64	0	34	0	0
2	X	64	0	34	0	0
2	Y	64	0	34	0	0
2	Z	64	0	34	1	0
3	v	28	0	11	0	0
3	w	28	0	11	0	0
3	x	28	0	11	0	0
3	y	28	0	11	0	0
3	z	28	0	11	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	25	0	0	0	0
6	B	20	0	0	0	0
6	C	35	0	0	1	0
6	D	25	0	0	1	0
6	E	20	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	88	0	0	0	0
8	B	101	0	0	1	0
8	C	122	0	0	0	0
8	D	110	0	0	0	0
8	E	89	0	0	0	0
8	X	3	0	0	0	0
8	Z	2	0	0	0	0
8	v	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	w	1	0	0	0	0
8	x	1	0	0	0	0
All	All	15513	0	14502	79	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 3.

All (79) 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:E:134:LYS:HE3	2:Z:503:A:H5'	1.77	0.65
1:C:189:LYS:NZ	6:C:407:SO4:O4	2.32	0.63
1:E:21[B]:GLU:OE1	1:E:24:ARG:NH1	2.31	0.62
1:E:189:LYS:HG3	1:E:239:GLU:HG2	1.85	0.59
1:C:21[B]:GLU:OE1	1:C:24:ARG:NH1	2.36	0.59
1:A:41:ILE:HG23	1:A:178:LEU:HD21	1.85	0.58
1:A:134:LYS:HE3	2:V:503:A:H5'	1.86	0.58
1:A:234:GLU:HB2	1:A:254:ASN:HB3	1.84	0.58
1:C:61:PRO:HG2	1:C:64:TYR:HD2	1.69	0.56
1:E:6:ILE:HD12	1:E:260:ASP:HB3	1.87	0.56
1:B:6:ILE:HD12	1:B:260:ASP:HB3	1.87	0.56
1:E:189:LYS:NZ	1:E:239:GLU:OE2	2.39	0.56
1:D:46:MET:HG3	1:D:86:PHE:CD2	2.42	0.55
1:E:259:LEU:HB3	1:E:261:LEU:HD13	1.90	0.54
1:C:46:MET:HG3	1:C:86:PHE:CD2	2.43	0.54
1:A:61:PRO:HG2	1:A:64:TYR:HD2	1.71	0.53
1:D:234:GLU:HB2	1:D:254:ASN:HB2	1.91	0.53
1:E:252:TYR:O	1:E:254[A]:ASN:N	2.42	0.53
1:B:46:MET:HG3	1:B:86:PHE:CD2	2.44	0.53
1:E:46:MET:HG3	1:E:86:PHE:CD1	2.43	0.53
1:D:61:PRO:HG2	1:D:64:TYR:HD2	1.73	0.53
1:B:259:LEU:HB3	1:B:261:LEU:HD13	1.91	0.52
1:C:238:GLU:OE1	1:C:243:HIS:ND1	2.42	0.52
1:E:61:PRO:HG2	1:E:64:TYR:HD2	1.75	0.52
1:A:46:MET:HG3	1:A:86:PHE:CD2	2.45	0.52
1:C:101:TYR:HB2	1:C:115:VAL:HG23	1.93	0.51
1:D:269:LEU:HG	1:D:326:ILE:HD12	1.93	0.49
1:C:189:LYS:NZ	1:C:239:GLU:OE1	2.46	0.49
1:C:270:GLU:HG2	1:C:325:LYS:HD3	1.93	0.48
1:A:87:ILE:HD13	1:A:178:LEU:HB3	1.95	0.48
1:B:61:PRO:HG2	1:B:64:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:TYR:HA	1:D:151[A]:VAL:HG12	1.95	0.47
1:D:31:LYS:HG3	1:D:32:SER:N	2.30	0.47
1:B:283:TRP:CZ2	1:B:345:GLU:HB2	2.51	0.46
1:D:144:TYR:HB3	1:D:289:LYS:O	2.15	0.46
1:E:144:TYR:HB3	1:E:289:LYS:O	2.16	0.46
1:D:8:HIS:CE1	1:D:35:LYS:HD2	2.51	0.46
1:E:252:TYR:O	1:E:254[B]:ASN:N	2.48	0.46
1:A:179:SER:O	1:A:228:SER:HA	2.15	0.46
1:E:8:HIS:CE1	1:E:35:LYS:HD3	2.50	0.45
1:B:234:GLU:HB2	1:B:254[B]:ASN:HB3	1.98	0.45
1:B:57:TYR:HA	1:B:151[A]:VAL:HG12	1.99	0.45
1:B:57:TYR:HA	1:B:151[B]:VAL:HG22	1.99	0.45
1:B:120:ASN:ND2	8:B:503:HOH:O	2.41	0.44
1:C:144:TYR:HB3	1:C:289:LYS:O	2.17	0.44
1:C:57:TYR:HA	1:C:151[A]:VAL:HG12	2.00	0.44
1:D:101:TYR:HB2	1:D:115:VAL:HG23	1.99	0.44
1:B:21[B]:GLU:OE1	1:B:24:ARG:NH1	2.46	0.43
1:D:14:CYS:HB3	1:D:16:HIS:CD2	2.53	0.43
1:A:253:LYS:HD3	1:A:254:ASN:H	1.82	0.43
1:D:50:ARG:HD3	1:D:333:PHE:CE2	2.53	0.43
1:D:249:LYS:NZ	6:D:407:SO4:O3	2.36	0.43
1:B:144:TYR:HB3	1:B:289:LYS:O	2.19	0.42
1:C:179:SER:O	1:C:228:SER:HA	2.18	0.42
1:E:50:ARG:HD3	1:E:333:PHE:CE2	2.55	0.42
1:E:14:CYS:HB3	1:E:16:HIS:CD2	2.54	0.42
1:C:14:CYS:HB3	1:C:16:HIS:CD2	2.55	0.42
1:A:13:GLY:HA3	1:A:248:GLY:O	2.20	0.42
1:C:204:LYS:HB3	1:C:204:LYS:HE3	1.81	0.42
1:C:283:TRP:CZ2	1:C:345:GLU:HB2	2.55	0.42
1:D:144:TYR:CG	1:D:145:PRO:HA	2.55	0.42
1:A:249:LYS:HE3	1:A:252:TYR:CE1	2.55	0.41
1:B:230:HIS:HA	7:B:407:OH:O	2.19	0.41
1:D:11:ILE:HG21	1:D:227:ILE:HD13	2.03	0.41
1:A:184:GLN:HB3	1:A:215:LYS:HE2	2.02	0.41
1:D:59:LYS:HB2	1:D:151[B]:VAL:HG12	2.03	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD23	1.94	0.41
1:A:85:LEU:HB3	1:A:113:LEU:HD11	2.03	0.41
1:C:50:ARG:HD3	1:C:333:PHE:CE2	2.55	0.41
1:B:264:LYS:H	1:B:264:LYS:HG2	1.50	0.41
1:E:24:ARG:O	1:E:28:GLU:HG2	2.20	0.41
1:E:283:TRP:CZ2	1:E:345:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG21	1:A:227:ILE:HD13	2.02	0.41
1:A:144:TYR:HB3	1:A:289:LYS:O	2.21	0.40
1:B:50:ARG:HD3	1:B:333:PHE:CE2	2.56	0.40
1:E:165:LEU:O	1:E:221:LEU:HD21	2.21	0.40
1:C:308:LYS:HB2	1:C:308:LYS:HE3	1.83	0.40
1:D:179:SER:O	1:D:228:SER:HA	2.21	0.40
1:D:280:ILE:HD13	1:D:344:ILE:HG23	2.04	0.40

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	352/360 (98%)	344 (98%)	8 (2%)	0	100	100
1	B	352/360 (98%)	341 (97%)	11 (3%)	0	100	100
1	C	352/360 (98%)	342 (97%)	10 (3%)	0	100	100
1	D	348/360 (97%)	339 (97%)	9 (3%)	0	100	100
1	E	352/360 (98%)	343 (97%)	8 (2%)	1 (0%)	41	43
All	All	1756/1800 (98%)	1709 (97%)	46 (3%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	LYS

### 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	320/325 (98%)	318 (99%)	2 (1%)	86	92
1	B	320/325 (98%)	319 (100%)	1 (0%)	92	96
1	C	320/325 (98%)	317 (99%)	3 (1%)	78	87
1	D	316/325 (97%)	313 (99%)	3 (1%)	78	87
1	E	320/325 (98%)	318 (99%)	2 (1%)	86	92
All	All	1596/1625 (98%)	1585 (99%)	11 (1%)	84	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	261	LEU
1	B	51	TYR
1	C	51	TYR
1	C	163	GLN
1	C	261	LEU
1	D	31	LYS
1	D	51	TYR
1	D	199	GLN
1	E	51	TYR
1	E	113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	V	1/5 (20%)	0	0
2	W	2/5 (40%)	1 (50%)	0
2	X	2/5 (40%)	1 (50%)	0
2	Y	2/5 (40%)	1 (50%)	0
2	Z	2/5 (40%)	0	0
3	v	0/2	-	-
3	w	0/2	-	-
3	x	0/2	-	-
3	y	0/2	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	z	0/2	-	-
All	All	9/35 (25%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	W	502	C
2	X	502	C
2	Y	503	A

There are no RNA pucker outliers to report.

## 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](#)

Of 40 ligands modelled in this entry, 5 are modelled with single atom and 10 are monoatomic - leaving 25 for Mogul analysis.

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	D	405	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	A	406	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	D	407	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	C	409	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	B	406	-	4,4,4	0.13	0	6,6,6	0.05	0
6	SO4	C	405	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	C	408	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	D	406	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	B	405	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	E	403	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	C	407	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	E	404	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	E	405	-	4,4,4	0.13	0	6,6,6	0.06	0
6	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	E	406	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.04	0
6	SO4	A	407	-	4,4,4	0.14	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	407	SO4	1	0
6	C	407	SO4	1	0

## 5.7 Other polymers ⓘ

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 ⓘ

### 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	349/360 (96%)	0.03	2 (0%) 89 89	31, 44, 70, 105	0
1	B	349/360 (96%)	0.09	3 (0%) 84 84	29, 45, 72, 101	0
1	C	349/360 (96%)	0.03	2 (0%) 89 89	28, 41, 62, 101	0
1	D	349/360 (96%)	0.07	6 (1%) 70 70	29, 44, 78, 104	0
1	E	349/360 (96%)	0.17	5 (1%) 75 75	29, 48, 80, 109	0
2	V	4/5 (80%)	-0.27	0 100 100	61, 62, 84, 91	1 (25%)
2	W	4/5 (80%)	-0.05	0 100 100	64, 67, 85, 98	0
2	X	4/5 (80%)	-0.57	0 100 100	53, 64, 90, 91	0
2	Y	4/5 (80%)	-0.06	0 100 100	69, 70, 89, 106	0
2	Z	4/5 (80%)	0.23	0 100 100	60, 63, 90, 104	0
3	v	2/2 (100%)	-0.44	0 100 100	56, 56, 56, 78	0
3	w	2/2 (100%)	-0.15	0 100 100	67, 67, 67, 94	0
3	x	2/2 (100%)	-0.64	0 100 100	58, 58, 58, 96	0
3	y	2/2 (100%)	-0.56	0 100 100	68, 68, 68, 109	0
3	z	2/2 (100%)	-0.72	0 100 100	57, 57, 57, 88	0
All	All	1775/1835 (96%)	0.07	18 (1%) 82 82	28, 45, 76, 109	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	GLN	5.0
1	E	265	GLN	4.7
1	E	198	PHE	4.5
1	D	265	GLN	3.5
1	D	207	ALA	3.0
1	B	264	LYS	2.8
1	E	29	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	264	LYS	2.6
1	D	352	ASN	2.5
1	B	353	ILE	2.4
1	D	6	ILE	2.4
1	C	264	LYS	2.3
1	D	198	PHE	2.3
1	C	265	GLN	2.2
1	A	264	LYS	2.2
1	A	352	ASN	2.2
1	E	309	GLU	2.1
1	E	314	ILE	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 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
6	SO4	C	408	5/5	0.51	0.37	122,122,124,125	5
6	SO4	C	405	5/5	0.69	0.28	136,137,138,141	0
6	SO4	D	406	5/5	0.80	0.22	95,97,101,102	5
6	SO4	C	409	5/5	0.82	0.16	117,119,120,121	0
6	SO4	A	407	5/5	0.83	0.28	72,74,75,76	5
6	SO4	C	407	5/5	0.85	0.20	83,83,85,87	5
6	SO4	B	405	5/5	0.86	0.18	96,99,101,106	0
6	SO4	C	406	5/5	0.88	0.20	108,111,113,116	0
6	SO4	D	407	5/5	0.89	0.14	115,115,117,122	0
6	SO4	E	405	5/5	0.89	0.12	85,94,97,99	0
6	SO4	A	405	5/5	0.90	0.19	102,103,105,106	0
6	SO4	E	406	5/5	0.90	0.17	89,93,95,97	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	404	5/5	0.92	0.10	115,115,118,119	0
6	SO4	D	404	5/5	0.92	0.22	101,102,103,105	0
6	SO4	A	406	5/5	0.92	0.20	65,71,75,82	5
6	SO4	A	404	5/5	0.92	0.10	97,100,101,103	0
6	SO4	E	404	5/5	0.93	0.16	100,101,102,107	0
6	SO4	B	406	5/5	0.93	0.11	87,92,94,97	0
6	SO4	D	405	5/5	0.94	0.10	72,85,86,86	0
7	OH	D	408	1/1	0.95	0.12	45,45,45,45	0
6	SO4	C	404	5/5	0.96	0.14	47,54,56,65	5
7	OH	B	407	1/1	0.98	0.10	31,31,31,31	0
5	FE2	B	401	1/1	0.98	0.10	37,37,37,37	0
7	OH	A	408	1/1	0.98	0.12	31,31,31,31	0
6	SO4	A	403	5/5	0.98	0.17	49,53,62,64	0
4	ZN	D	402	1/1	0.98	0.09	50,50,50,50	0
5	FE2	D	401	1/1	0.99	0.13	39,39,39,39	0
6	SO4	B	403	5/5	0.99	0.18	51,54,57,60	0
7	OH	E	407	1/1	0.99	0.13	32,32,32,32	0
7	OH	C	410	1/1	0.99	0.12	34,34,34,34	0
4	ZN	E	402	1/1	0.99	0.11	41,41,41,41	0
6	SO4	E	403	5/5	0.99	0.17	45,46,50,62	0
4	ZN	A	401	1/1	0.99	0.09	44,44,44,44	0
6	SO4	C	403	5/5	0.99	0.18	53,54,62,63	0
6	SO4	D	403	5/5	0.99	0.18	43,49,53,56	0
5	FE2	E	401	1/1	1.00	0.13	35,35,35,35	0
4	ZN	B	402	1/1	1.00	0.10	44,44,44,44	0
5	FE2	A	402	1/1	1.00	0.14	34,34,34,34	0
4	ZN	C	401	1/1	1.00	0.13	45,45,45,45	0
5	FE2	C	402	1/1	1.00	0.18	35,35,35,35	0

## 6.5 Other polymers

There are no such residues in this entry.