



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2017 – 01:55 PM EST

PDB ID : 5HUO  
Title : Crystal Structure of NadC Deletion Mutant in C2221 Space Group  
Authors : Booth, W.T.; Chruszcz, M.  
Deposited on : 2016-01-27  
Resolution : 2.80 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

<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

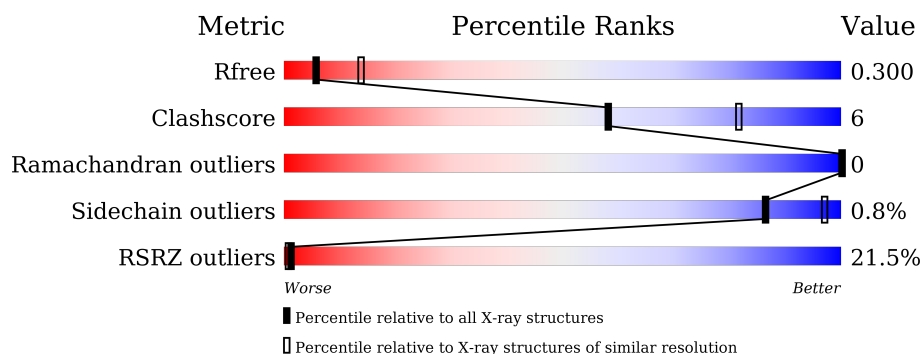
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	314	<div> <div>16%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	B	314	<div> <div>17%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
1	C	314	<div> <div>36%</div> <div>74%</div> <div>15%</div> <div>11%</div> </div>
1	E	314	<div> <div>23%</div> <div>78%</div> <div>11%</div> <div>10%</div> </div>
1	F	314	<div> <div>12%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
1	H	314	<div> <div>12%</div> <div>79%</div> <div>10%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	302	-	-	-	X
2	SO4	B	303	-	-	-	X
2	SO4	C	302	-	-	-	X
2	SO4	E	302	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13069 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 Nicotinate-nucleotide diphosphorylase (Carboxylating).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2152	1360	370	413	9			
1	B	283	Total	C	N	O	S	0	1	0
			2171	1370	373	418	10			
1	C	280	Total	C	N	O	S	0	0	0
			2072	1304	353	408	7			
1	E	282	Total	C	N	O	S	0	0	0
			2108	1328	360	411	9			
1	F	284	Total	C	N	O	S	0	0	0
			2161	1363	369	420	9			
1	H	282	Total	C	N	O	S	0	1	0
			2156	1361	371	415	9			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
A	-23	HIS	-	expression tag	UNP A0A0H3BVM1
A	-22	HIS	-	expression tag	UNP A0A0H3BVM1
A	-21	HIS	-	expression tag	UNP A0A0H3BVM1
A	-20	HIS	-	expression tag	UNP A0A0H3BVM1
A	-19	HIS	-	expression tag	UNP A0A0H3BVM1
A	-18	HIS	-	expression tag	UNP A0A0H3BVM1
A	-17	SER	-	expression tag	UNP A0A0H3BVM1
A	-16	SER	-	expression tag	UNP A0A0H3BVM1
A	-15	GLY	-	expression tag	UNP A0A0H3BVM1
A	-14	VAL	-	expression tag	UNP A0A0H3BVM1
A	-13	ASP	-	expression tag	UNP A0A0H3BVM1
A	-12	LEU	-	expression tag	UNP A0A0H3BVM1
A	-11	GLY	-	expression tag	UNP A0A0H3BVM1
A	-10	THR	-	expression tag	UNP A0A0H3BVM1
A	-9	GLU	-	expression tag	UNP A0A0H3BVM1
A	-8	ASN	-	expression tag	UNP A0A0H3BVM1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP A0A0H3BVM1
A	-6	TYR	-	expression tag	UNP A0A0H3BVM1
A	-5	PHE	-	expression tag	UNP A0A0H3BVM1
A	-4	GLN	-	expression tag	UNP A0A0H3BVM1
A	-3	SER	-	expression tag	UNP A0A0H3BVM1
A	-2	GLY	-	expression tag	UNP A0A0H3BVM1
A	-1	SER	-	expression tag	UNP A0A0H3BVM1
A	0	GLY	-	expression tag	UNP A0A0H3BVM1
A	?	-	UNK	deletion	UNP A0A0H3BVM1
B	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
B	-23	HIS	-	expression tag	UNP A0A0H3BVM1
B	-22	HIS	-	expression tag	UNP A0A0H3BVM1
B	-21	HIS	-	expression tag	UNP A0A0H3BVM1
B	-20	HIS	-	expression tag	UNP A0A0H3BVM1
B	-19	HIS	-	expression tag	UNP A0A0H3BVM1
B	-18	HIS	-	expression tag	UNP A0A0H3BVM1
B	-17	SER	-	expression tag	UNP A0A0H3BVM1
B	-16	SER	-	expression tag	UNP A0A0H3BVM1
B	-15	GLY	-	expression tag	UNP A0A0H3BVM1
B	-14	VAL	-	expression tag	UNP A0A0H3BVM1
B	-13	ASP	-	expression tag	UNP A0A0H3BVM1
B	-12	LEU	-	expression tag	UNP A0A0H3BVM1
B	-11	GLY	-	expression tag	UNP A0A0H3BVM1
B	-10	THR	-	expression tag	UNP A0A0H3BVM1
B	-9	GLU	-	expression tag	UNP A0A0H3BVM1
B	-8	ASN	-	expression tag	UNP A0A0H3BVM1
B	-7	LEU	-	expression tag	UNP A0A0H3BVM1
B	-6	TYR	-	expression tag	UNP A0A0H3BVM1
B	-5	PHE	-	expression tag	UNP A0A0H3BVM1
B	-4	GLN	-	expression tag	UNP A0A0H3BVM1
B	-3	SER	-	expression tag	UNP A0A0H3BVM1
B	-2	GLY	-	expression tag	UNP A0A0H3BVM1
B	-1	SER	-	expression tag	UNP A0A0H3BVM1
B	0	GLY	-	expression tag	UNP A0A0H3BVM1
B	?	-	UNK	deletion	UNP A0A0H3BVM1
C	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
C	-23	HIS	-	expression tag	UNP A0A0H3BVM1
C	-22	HIS	-	expression tag	UNP A0A0H3BVM1
C	-21	HIS	-	expression tag	UNP A0A0H3BVM1
C	-20	HIS	-	expression tag	UNP A0A0H3BVM1
C	-19	HIS	-	expression tag	UNP A0A0H3BVM1
C	-18	HIS	-	expression tag	UNP A0A0H3BVM1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A0H3BVM1
C	-16	SER	-	expression tag	UNP A0A0H3BVM1
C	-15	GLY	-	expression tag	UNP A0A0H3BVM1
C	-14	VAL	-	expression tag	UNP A0A0H3BVM1
C	-13	ASP	-	expression tag	UNP A0A0H3BVM1
C	-12	LEU	-	expression tag	UNP A0A0H3BVM1
C	-11	GLY	-	expression tag	UNP A0A0H3BVM1
C	-10	THR	-	expression tag	UNP A0A0H3BVM1
C	-9	GLU	-	expression tag	UNP A0A0H3BVM1
C	-8	ASN	-	expression tag	UNP A0A0H3BVM1
C	-7	LEU	-	expression tag	UNP A0A0H3BVM1
C	-6	TYR	-	expression tag	UNP A0A0H3BVM1
C	-5	PHE	-	expression tag	UNP A0A0H3BVM1
C	-4	GLN	-	expression tag	UNP A0A0H3BVM1
C	-3	SER	-	expression tag	UNP A0A0H3BVM1
C	-2	GLY	-	expression tag	UNP A0A0H3BVM1
C	-1	SER	-	expression tag	UNP A0A0H3BVM1
C	0	GLY	-	expression tag	UNP A0A0H3BVM1
C	?	-	UNK	deletion	UNP A0A0H3BVM1
E	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
E	-23	HIS	-	expression tag	UNP A0A0H3BVM1
E	-22	HIS	-	expression tag	UNP A0A0H3BVM1
E	-21	HIS	-	expression tag	UNP A0A0H3BVM1
E	-20	HIS	-	expression tag	UNP A0A0H3BVM1
E	-19	HIS	-	expression tag	UNP A0A0H3BVM1
E	-18	HIS	-	expression tag	UNP A0A0H3BVM1
E	-17	SER	-	expression tag	UNP A0A0H3BVM1
E	-16	SER	-	expression tag	UNP A0A0H3BVM1
E	-15	GLY	-	expression tag	UNP A0A0H3BVM1
E	-14	VAL	-	expression tag	UNP A0A0H3BVM1
E	-13	ASP	-	expression tag	UNP A0A0H3BVM1
E	-12	LEU	-	expression tag	UNP A0A0H3BVM1
E	-11	GLY	-	expression tag	UNP A0A0H3BVM1
E	-10	THR	-	expression tag	UNP A0A0H3BVM1
E	-9	GLU	-	expression tag	UNP A0A0H3BVM1
E	-8	ASN	-	expression tag	UNP A0A0H3BVM1
E	-7	LEU	-	expression tag	UNP A0A0H3BVM1
E	-6	TYR	-	expression tag	UNP A0A0H3BVM1
E	-5	PHE	-	expression tag	UNP A0A0H3BVM1
E	-4	GLN	-	expression tag	UNP A0A0H3BVM1
E	-3	SER	-	expression tag	UNP A0A0H3BVM1
E	-2	GLY	-	expression tag	UNP A0A0H3BVM1

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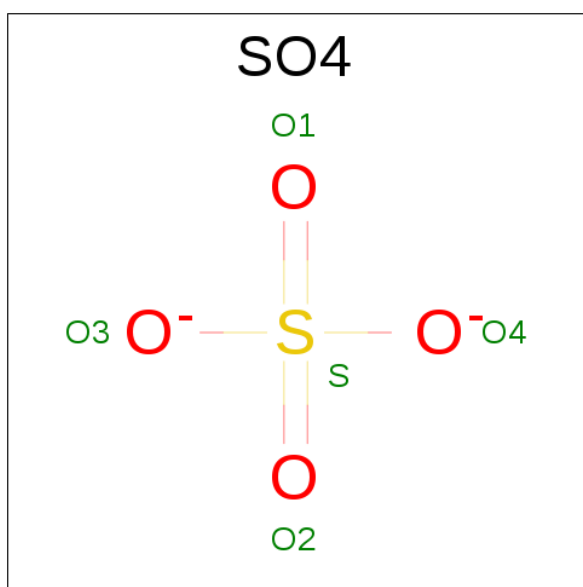
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A0A0H3BVM1
E	0	GLY	-	expression tag	UNP A0A0H3BVM1
E	?	-	UNK	deletion	UNP A0A0H3BVM1
F	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
F	-23	HIS	-	expression tag	UNP A0A0H3BVM1
F	-22	HIS	-	expression tag	UNP A0A0H3BVM1
F	-21	HIS	-	expression tag	UNP A0A0H3BVM1
F	-20	HIS	-	expression tag	UNP A0A0H3BVM1
F	-19	HIS	-	expression tag	UNP A0A0H3BVM1
F	-18	HIS	-	expression tag	UNP A0A0H3BVM1
F	-17	SER	-	expression tag	UNP A0A0H3BVM1
F	-16	SER	-	expression tag	UNP A0A0H3BVM1
F	-15	GLY	-	expression tag	UNP A0A0H3BVM1
F	-14	VAL	-	expression tag	UNP A0A0H3BVM1
F	-13	ASP	-	expression tag	UNP A0A0H3BVM1
F	-12	LEU	-	expression tag	UNP A0A0H3BVM1
F	-11	GLY	-	expression tag	UNP A0A0H3BVM1
F	-10	THR	-	expression tag	UNP A0A0H3BVM1
F	-9	GLU	-	expression tag	UNP A0A0H3BVM1
F	-8	ASN	-	expression tag	UNP A0A0H3BVM1
F	-7	LEU	-	expression tag	UNP A0A0H3BVM1
F	-6	TYR	-	expression tag	UNP A0A0H3BVM1
F	-5	PHE	-	expression tag	UNP A0A0H3BVM1
F	-4	GLN	-	expression tag	UNP A0A0H3BVM1
F	-3	SER	-	expression tag	UNP A0A0H3BVM1
F	-2	GLY	-	expression tag	UNP A0A0H3BVM1
F	-1	SER	-	expression tag	UNP A0A0H3BVM1
F	0	GLY	-	expression tag	UNP A0A0H3BVM1
F	?	-	UNK	deletion	UNP A0A0H3BVM1
H	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
H	-23	HIS	-	expression tag	UNP A0A0H3BVM1
H	-22	HIS	-	expression tag	UNP A0A0H3BVM1
H	-21	HIS	-	expression tag	UNP A0A0H3BVM1
H	-20	HIS	-	expression tag	UNP A0A0H3BVM1
H	-19	HIS	-	expression tag	UNP A0A0H3BVM1
H	-18	HIS	-	expression tag	UNP A0A0H3BVM1
H	-17	SER	-	expression tag	UNP A0A0H3BVM1
H	-16	SER	-	expression tag	UNP A0A0H3BVM1
H	-15	GLY	-	expression tag	UNP A0A0H3BVM1
H	-14	VAL	-	expression tag	UNP A0A0H3BVM1
H	-13	ASP	-	expression tag	UNP A0A0H3BVM1
H	-12	LEU	-	expression tag	UNP A0A0H3BVM1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	GLY	-	expression tag	UNP A0A0H3BVM1
H	-10	THR	-	expression tag	UNP A0A0H3BVM1
H	-9	GLU	-	expression tag	UNP A0A0H3BVM1
H	-8	ASN	-	expression tag	UNP A0A0H3BVM1
H	-7	LEU	-	expression tag	UNP A0A0H3BVM1
H	-6	TYR	-	expression tag	UNP A0A0H3BVM1
H	-5	PHE	-	expression tag	UNP A0A0H3BVM1
H	-4	GLN	-	expression tag	UNP A0A0H3BVM1
H	-3	SER	-	expression tag	UNP A0A0H3BVM1
H	-2	GLY	-	expression tag	UNP A0A0H3BVM1
H	-1	SER	-	expression tag	UNP A0A0H3BVM1
H	0	GLY	-	expression tag	UNP A0A0H3BVM1
H	?	-	UNK	deletion	UNP A0A0H3BVM1

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	20	Total	O	0	0
			20	20		
3	C	20	Total	O	0	0
			20	20		
3	E	18	Total	O	0	0
			18	18		

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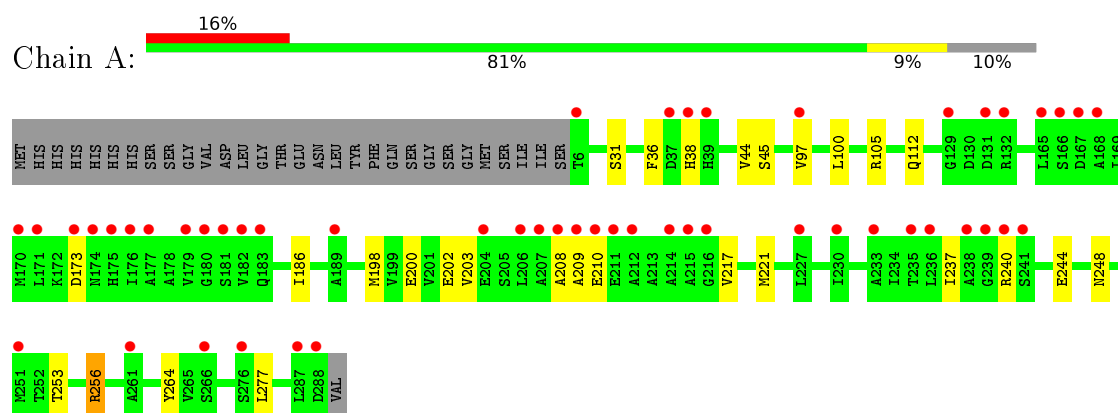
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	31	Total	O	0	0
			31	31		
3	H	29	Total	O	0	0
			29	29		

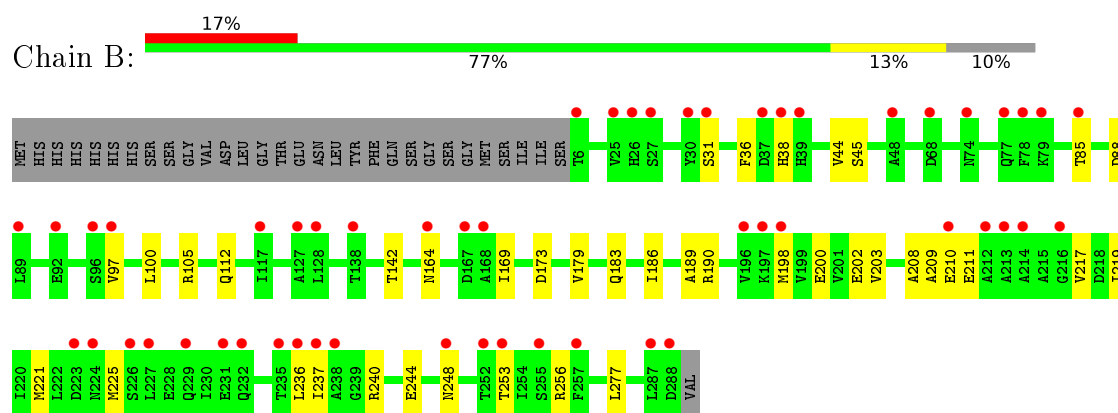
### 3 Residue-property plots [i](#)

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.

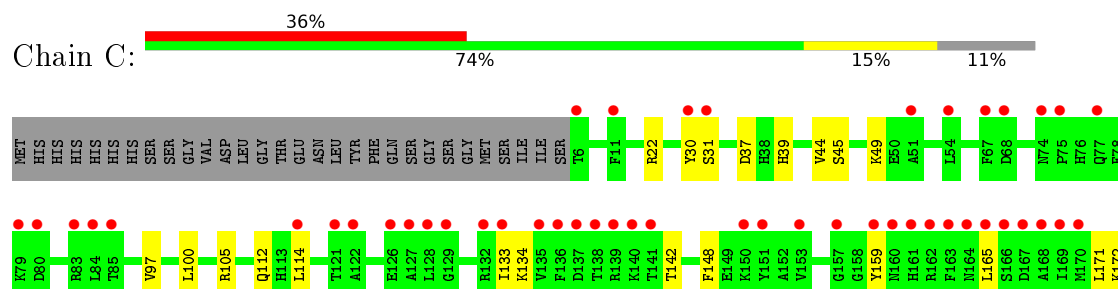
- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)

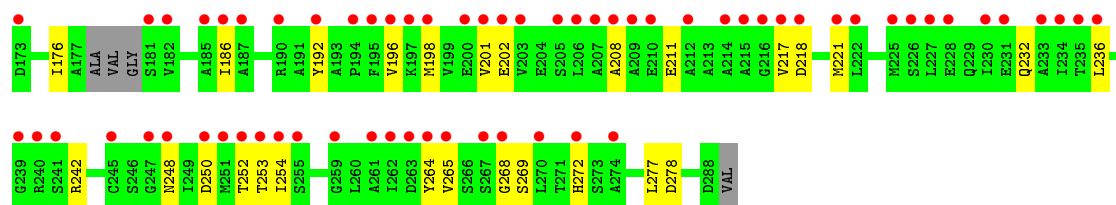


- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)

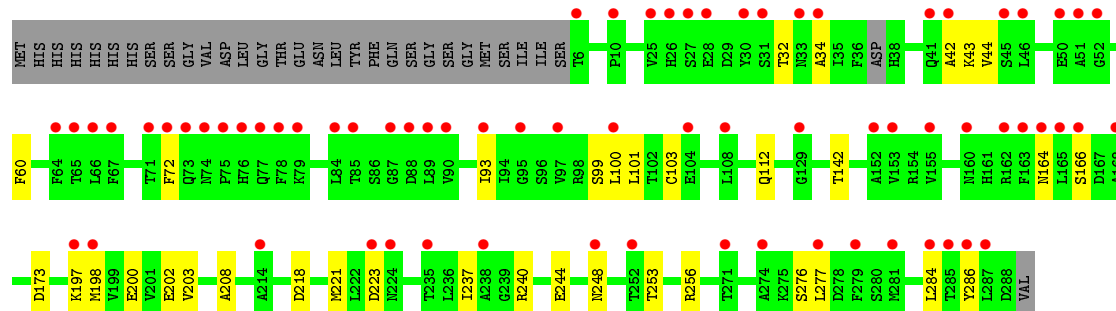
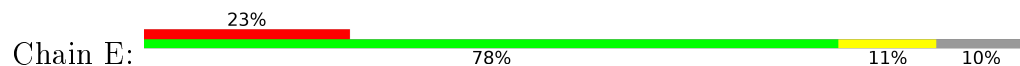


- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)

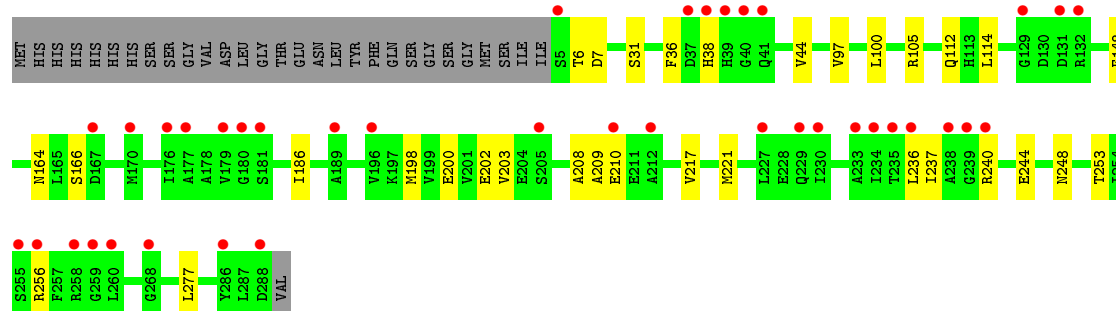
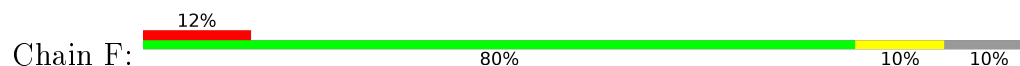




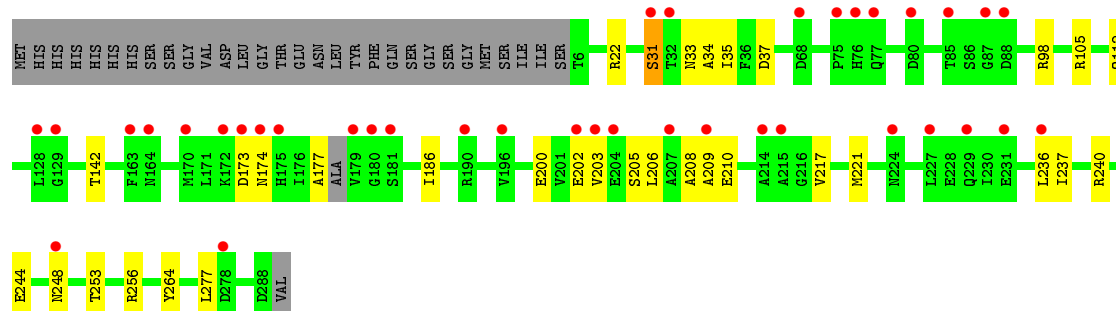
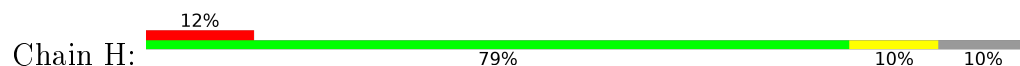
• Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)



• Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)



• Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.20Å 186.26Å 221.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 36.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.80) 100.0 (36.98-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.216 , 0.255 0.261 , 0.300	Depositor DCC
$R_{free}$ test set	2766 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.012 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	0.86	0/2185	0.87	3/2957 (0.1%)
1	B	0.79	0/2207	0.85	5/2984 (0.2%)
1	C	0.76	0/2102	0.87	3/2851 (0.1%)
1	E	0.78	1/2138 (0.0%)	0.83	2/2898 (0.1%)
1	F	0.85	0/2194	0.85	2/2971 (0.1%)
1	H	0.85	0/2192	0.91	5/2963 (0.2%)
All	All	0.82	1/13018 (0.0%)	0.86	20/17624 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	ASP	CB-CG	6.52	1.65	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	H	22	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	H	105	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	22	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	H	22	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	190	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	F	105	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	H	105	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	173	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	105	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	F	105	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	37	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	256	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	173	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	223	ASP	CB-CG-OD1	-5.35	113.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	105	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	190	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	164	ASN	CB-CA-C	-5.07	100.25	110.40
1	B	105	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	H	173	ASP	CB-CG-OD1	5.06	122.85	118.30

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	2152	0	2128	17	0
1	B	2171	0	2155	31	0
1	C	2072	0	1971	36	0
1	E	2108	0	2049	32	0
1	F	2161	0	2124	20	0
1	H	2156	0	2121	28	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	10	0	0	0	0
2	E	20	0	0	0	0
2	F	15	0	0	0	0
2	H	15	0	0	0	0
3	A	31	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	1	0
3	E	18	0	0	0	0
3	F	31	0	0	0	0
3	H	29	0	0	0	0
All	All	13069	0	12548	150	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.

All (150) 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:C:186:ILE:HD11	1:C:201:VAL:HG21	1.53	0.90
1:B:85:THR:O	1:B:88:ASP:OD2	1.90	0.89
1:A:198:MET:SD	1:E:198:MET:SD	2.72	0.88
1:C:186:ILE:HD11	1:C:201:VAL:CG2	2.04	0.86
1:H:206:LEU:HD23	1:H:206:LEU:O	1.80	0.81
1:E:60:PHE:CE2	1:E:93:ILE:HD11	2.23	0.74
1:E:203:VAL:HG13	1:E:208:ALA:HB3	1.71	0.72
1:F:203:VAL:HG13	1:F:208:ALA:HB3	1.70	0.72
1:B:203:VAL:HG13	1:B:208:ALA:HB3	1.72	0.72
1:A:203:VAL:HG13	1:A:208:ALA:HB3	1.72	0.71
1:H:203:VAL:HG13	1:H:208:ALA:HB3	1.74	0.69
1:B:179:VAL:CG2	1:H:35:ILE:HG23	2.22	0.69
1:H:206:LEU:HD23	1:H:206:LEU:C	2.14	0.67
1:E:60:PHE:CZ	1:E:93:ILE:HD11	2.30	0.66
1:H:174:ASN:O	1:H:177:ALA:HB3	1.96	0.65
1:C:269:SER:HA	1:C:272:HIS:HB3	1.77	0.65
1:E:44:VAL:HG23	1:E:100:LEU:HD13	1.79	0.63
1:B:142:THR:HG21	1:H:142:THR:HG21	1.80	0.63
1:C:272:HIS:CE1	1:E:276:SER:HB2	2.34	0.63
1:E:198:MET:CE	1:E:218:ASP:HB3	2.28	0.62
1:C:208:ALA:HA	1:C:211:GLU:HG2	1.80	0.62
1:F:253:THR:O	1:F:256:ARG:HG2	1.98	0.62
1:E:253:THR:O	1:E:256:ARG:HG2	2.00	0.62
1:C:172:LYS:O	1:C:176:ILE:N	2.32	0.61
1:C:134:LYS:HE2	1:C:159:TYR:CE2	2.36	0.61
1:B:183:GLN:CG	1:B:211:GLU:HG2	2.32	0.60
1:F:237:ILE:O	1:F:240:ARG:HD3	2.02	0.59
1:C:196:VAL:HG12	1:C:196:VAL:O	2.01	0.59
1:B:198[A]:MET:SD	1:F:198:MET:SD	3.01	0.59
1:F:7:ASP:O	1:H:98:ARG:NH2	2.28	0.58
1:B:44:VAL:HG23	1:B:100:LEU:HD13	1.85	0.57
1:A:237:ILE:O	1:A:240:ARG:HD3	2.03	0.56
1:A:44:VAL:HG23	1:A:100:LEU:HD13	1.86	0.56
1:C:250:ASP:OD1	1:C:252:THR:N	2.38	0.56
1:C:44:VAL:HG23	1:C:100:LEU:HD13	1.87	0.56
1:H:37:ASP:C	1:H:37:ASP:OD1	2.42	0.56
1:C:248:ASN:O	1:C:253:THR:HG21	2.05	0.56
1:B:36:PHE:CD2	1:B:97:VAL:HG11	2.41	0.56
1:H:237:ILE:O	1:H:240:ARG:HD3	2.06	0.56
1:E:237:ILE:O	1:E:240:ARG:HD3	2.05	0.56
1:H:206:LEU:HD21	1:H:236:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG23	1:H:35:ILE:HG23	1.86	0.56
1:B:237:ILE:O	1:B:240:ARG:HD3	2.05	0.55
1:H:253:THR:O	1:H:256:ARG:HG2	2.06	0.55
1:F:6:THR:HG21	1:H:33:ASN:HB3	1.87	0.55
1:E:198:MET:HE1	1:E:218:ASP:HB3	1.88	0.55
1:F:44:VAL:HG23	1:F:100:LEU:HD13	1.88	0.55
1:B:179:VAL:HG21	1:H:35:ILE:HD12	1.88	0.54
1:C:134:LYS:HE2	1:C:159:TYR:CZ	2.43	0.54
1:C:192:TYR:CD2	1:E:34:ALA:HB2	2.43	0.54
1:B:183:GLN:HG2	1:B:211:GLU:HG2	1.89	0.54
1:B:36:PHE:C	1:B:38:HIS:H	2.11	0.54
1:C:133:ILE:HG22	1:C:134:LYS:N	2.22	0.53
1:C:186:ILE:HD12	1:C:217:VAL:CG1	2.39	0.53
1:E:44:VAL:HG22	1:E:284:LEU:HD13	1.90	0.53
1:C:198:MET:CE	1:C:218:ASP:HB3	2.37	0.53
1:F:203:VAL:HG13	1:F:208:ALA:CB	2.38	0.53
1:B:210:GLU:HB2	1:B:236:LEU:HD21	1.90	0.53
1:E:72:PHE:CE1	1:E:93:ILE:HG12	2.45	0.52
1:H:206:LEU:CD2	1:H:236:LEU:HD22	2.40	0.52
1:C:30:TYR:CE2	1:E:197:LYS:HE3	2.44	0.52
1:F:36:PHE:CD1	1:F:97:VAL:HG11	2.44	0.52
1:B:198[B]:MET:SD	1:B:219:ILE:HD12	2.49	0.52
1:E:198:MET:HE3	1:E:218:ASP:HB3	1.92	0.51
1:A:112:GLN:HG2	1:A:277:LEU:O	2.09	0.51
1:A:203:VAL:HG13	1:A:208:ALA:CB	2.40	0.51
1:B:203:VAL:HG13	1:B:208:ALA:CB	2.39	0.51
1:H:203:VAL:HG13	1:H:208:ALA:CB	2.41	0.50
1:B:253:THR:HG22	1:B:256:ARG:HE	1.77	0.50
1:B:85:THR:N	1:B:88:ASP:OD2	2.39	0.50
1:C:133:ILE:HG23	1:C:264:TYR:HA	1.93	0.50
1:H:112:GLN:HG2	1:H:277:LEU:O	2.12	0.50
1:E:43:LYS:O	1:E:284:LEU:HD12	2.11	0.50
1:C:268:GLY:O	1:C:272:HIS:HB2	2.12	0.49
1:B:169:ILE:HG23	1:H:31:SER:HB3	1.94	0.49
1:E:112:GLN:HG2	1:E:277:LEU:O	2.13	0.49
1:E:60:PHE:HE2	1:E:93:ILE:HD11	1.76	0.49
1:F:112:GLN:HG2	1:F:277:LEU:O	2.12	0.49
1:F:210:GLU:OE1	1:F:236:LEU:HD11	2.13	0.49
1:H:210:GLU:HB2	1:H:236:LEU:HD21	1.94	0.49
1:C:112:GLN:HG2	1:C:277:LEU:O	2.12	0.49
1:F:253:THR:HG22	1:F:256:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ALA:HB1	1:E:284:LEU:HD11	1.94	0.48
1:E:203:VAL:HG13	1:E:208:ALA:CB	2.40	0.48
1:E:93:ILE:HG22	1:E:100:LEU:CD2	2.44	0.48
1:E:43:LYS:O	1:E:284:LEU:HA	2.13	0.48
1:F:186:ILE:HD13	1:F:217:VAL:HG13	1.95	0.48
1:A:186:ILE:HD13	1:A:217:VAL:HG13	1.95	0.48
1:B:112:GLN:HG2	1:B:277:LEU:O	2.14	0.47
1:C:202:GLU:O	1:C:202:GLU:HG3	2.15	0.47
1:E:202:GLU:HG2	1:E:221:MET:SD	2.54	0.47
1:C:254:ILE:HD11	1:C:265:VAL:HG21	1.97	0.47
1:C:198:MET:HE1	1:C:218:ASP:HB3	1.96	0.47
1:A:248:ASN:O	1:A:253:THR:HG21	2.15	0.46
1:C:133:ILE:CG2	1:C:134:LYS:N	2.78	0.46
1:E:93:ILE:HG22	1:E:100:LEU:HD21	1.97	0.46
1:E:200:GLU:OE2	1:E:244:GLU:OE2	2.33	0.46
1:F:248:ASN:O	1:F:253:THR:HG21	2.15	0.46
1:A:200:GLU:OE2	1:A:244:GLU:OE2	2.34	0.46
1:E:248:ASN:O	1:E:253:THR:HG21	2.15	0.46
1:E:202:GLU:HA	1:E:221:MET:HB3	1.98	0.46
1:E:32:THR:HG23	1:E:101:LEU:HD22	1.98	0.45
1:H:200:GLU:OE2	1:H:244:GLU:OE2	2.34	0.45
1:B:200:GLU:OE2	1:B:244:GLU:OE2	2.34	0.45
1:F:200:GLU:OE2	1:F:244:GLU:OE2	2.34	0.45
1:C:202:GLU:HA	1:C:221:MET:HB3	1.98	0.45
1:C:142:THR:HG21	1:E:142:THR:HG21	1.97	0.45
1:F:203:VAL:HG11	1:F:209:ALA:N	2.32	0.45
1:B:202:GLU:HA	1:B:221:MET:HB3	1.98	0.45
1:H:202:GLU:HG2	1:H:221:MET:SD	2.57	0.45
1:E:99:SER:O	1:E:103:CYS:HB2	2.16	0.44
1:H:186:ILE:HD13	1:H:217:VAL:HG13	1.99	0.44
1:A:210:GLU:OE1	1:A:210:GLU:HA	2.18	0.44
1:F:202:GLU:HA	1:F:221:MET:HB3	1.99	0.44
1:B:248:ASN:O	1:B:253:THR:HG21	2.17	0.44
1:H:248:ASN:O	1:H:253:THR:HG21	2.18	0.44
1:B:202:GLU:HG2	1:B:221:MET:SD	2.57	0.43
1:H:202:GLU:HA	1:H:221:MET:HB3	1.98	0.43
1:A:202:GLU:HA	1:A:221:MET:HB3	2.00	0.43
1:B:189:ALA:HA	1:H:34:ALA:HB1	2.00	0.43
1:C:171:LEU:O	1:C:202:GLU:HG2	2.17	0.43
1:C:232:GLN:O	1:C:236:LEU:HD13	2.17	0.43
1:H:244:GLU:HB2	1:H:264:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:VAL:HG11	1:H:209:ALA:N	2.34	0.43
1:A:36:PHE:CD2	1:A:97:VAL:HG11	2.54	0.43
1:C:196:VAL:O	1:C:196:VAL:CG1	2.64	0.42
1:H:206:LEU:C	1:H:206:LEU:CD2	2.83	0.42
1:A:244:GLU:HB2	1:A:264:TYR:CZ	2.55	0.42
1:C:97:VAL:HG23	3:C:407:HOH:O	2.19	0.42
1:C:44:VAL:HG12	1:C:45:SER:N	2.35	0.42
1:B:225:MET:HE2	1:B:225:MET:HB3	1.81	0.42
1:F:164:ASN:HB3	1:F:166:SER:H	1.85	0.42
1:F:114:LEU:HD21	1:F:148:PHE:HB3	2.01	0.42
1:A:253:THR:HG22	1:A:256:ARG:HE	1.85	0.41
1:C:49:LYS:HE3	1:C:278:ASP:OD2	2.20	0.41
1:E:164:ASN:HB3	1:E:166:SER:H	1.85	0.41
1:F:202:GLU:HG2	1:F:221:MET:SD	2.60	0.41
1:B:203:VAL:HG11	1:B:209:ALA:N	2.36	0.41
1:A:202:GLU:HG2	1:A:221:MET:SD	2.60	0.41
1:B:186:ILE:HD13	1:B:217:VAL:HG13	2.03	0.41
1:C:186:ILE:HD12	1:C:217:VAL:HG11	2.03	0.41
1:B:44:VAL:HG12	1:B:45:SER:N	2.36	0.41
1:A:44:VAL:HG12	1:A:45:SER:N	2.36	0.41
1:B:183:GLN:HG3	1:B:211:GLU:HG2	2.01	0.41
1:E:112:GLN:HB3	1:E:276:SER:HB3	2.02	0.41
1:A:203:VAL:HG11	1:A:209:ALA:N	2.36	0.41
1:C:165:LEU:HA	1:C:165:LEU:HD23	1.88	0.41
1:C:208:ALA:HA	1:C:211:GLU:CG	2.50	0.40
1:C:114:LEU:HD21	1:C:148:PHE:HB3	2.03	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	281/314 (90%)	274 (98%)	7 (2%)	0	100	100
1	B	282/314 (90%)	274 (97%)	8 (3%)	0	100	100
1	C	276/314 (88%)	268 (97%)	8 (3%)	0	100	100
1	E	278/314 (88%)	270 (97%)	8 (3%)	0	100	100
1	F	282/314 (90%)	275 (98%)	7 (2%)	0	100	100
1	H	279/314 (89%)	271 (97%)	8 (3%)	0	100	100
All	All	1678/1884 (89%)	1632 (97%)	46 (3%)	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	225/260 (86%)	223 (99%)	2 (1%)	84	96
1	B	230/260 (88%)	229 (100%)	1 (0%)	93	98
1	C	207/260 (80%)	204 (99%)	3 (1%)	74	94
1	E	217/260 (84%)	216 (100%)	1 (0%)	92	98
1	F	227/260 (87%)	225 (99%)	2 (1%)	84	96
1	H	226/260 (87%)	224 (99%)	2 (1%)	84	96
All	All	1332/1560 (85%)	1321 (99%)	11 (1%)	86	97

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

Mol	Chain	Res	Type
1	A	31	SER
1	A	38	HIS
1	B	31	SER
1	C	31	SER
1	C	39	HIS
1	C	242	ARG
1	E	286	TYR

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Mol	Chain	Res	Type
1	F	31	SER
1	F	38	HIS
1	H	31	SER
1	H	205	SER

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	160	ASN
1	F	160	ASN
1	H	188	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](#)

20 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	$\# Z  > 2$
2	SO4	A	301	-	4,4,4	0.39	0	6,6,6	0.23	0
2	SO4	A	302	-	4,4,4	0.62	0	6,6,6	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	303	-	4,4,4	0.31	0	6,6,6	0.42	0
2	SO4	A	304	-	4,4,4	0.38	0	6,6,6	0.43	0
2	SO4	B	301	-	4,4,4	0.34	0	6,6,6	0.69	0
2	SO4	B	302	-	4,4,4	0.38	0	6,6,6	0.37	0
2	SO4	B	303	-	4,4,4	0.68	0	6,6,6	0.53	0
2	SO4	B	304	-	4,4,4	0.45	0	6,6,6	0.14	0
2	SO4	C	301	-	4,4,4	0.32	0	6,6,6	0.42	0
2	SO4	C	302	-	4,4,4	0.38	0	6,6,6	0.18	0
2	SO4	E	301	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	E	302	-	4,4,4	0.54	0	6,6,6	0.36	0
2	SO4	E	303	-	4,4,4	0.34	0	6,6,6	1.12	0
2	SO4	E	304	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	F	301	-	4,4,4	0.39	0	6,6,6	0.39	0
2	SO4	F	302	-	4,4,4	0.52	0	6,6,6	0.70	0
2	SO4	F	303	-	4,4,4	0.47	0	6,6,6	0.36	0
2	SO4	H	301	-	4,4,4	0.37	0	6,6,6	0.53	0
2	SO4	H	302	-	4,4,4	0.52	0	6,6,6	0.65	0
2	SO4	H	303	-	4,4,4	0.37	0	6,6,6	0.27	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
2	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	303	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	SO4	E	301	-	-	0/0/0/0	0/0/0/0
2	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	SO4	E	303	-	-	0/0/0/0	0/0/0/0
2	SO4	E	304	-	-	0/0/0/0	0/0/0/0
2	SO4	F	301	-	-	0/0/0/0	0/0/0/0
2	SO4	F	302	-	-	0/0/0/0	0/0/0/0
2	SO4	F	303	-	-	0/0/0/0	0/0/0/0
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	H	302	-	-	0/0/0/0	0/0/0/0
2	SO4	H	303	-	-	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

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	283/314 (90%)	1.26	51 (18%) 2 1	87, 105, 179, 236	0
1	B	283/314 (90%)	1.23	53 (18%) 2 1	90, 117, 159, 194	0
1	C	280/314 (89%)	1.95	112 (40%) 0 0	91, 154, 268, 297	0
1	E	282/314 (89%)	1.50	71 (25%) 1 0	92, 131, 219, 316	0
1	F	284/314 (90%)	1.05	39 (13%) 4 2	89, 101, 141, 201	0
1	H	282/314 (89%)	1.05	38 (13%) 4 2	91, 105, 152, 175	0
All	All	1694/1884 (89%)	1.34	364 (21%) 1 1	87, 115, 211, 316	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	VAL	10.2
1	C	239	GLY	9.3
1	C	215	ALA	9.0
1	C	206	LEU	8.2
1	A	38	HIS	8.1
1	C	241	SER	7.9
1	A	288	ASP	7.4
1	C	214	ALA	7.2
1	E	89	LEU	6.9
1	C	85	THR	6.8
1	F	38	HIS	6.6
1	F	288	ASP	6.3
1	C	209	ALA	6.2
1	C	167	ASP	6.0
1	C	161	HIS	6.0
1	C	132	ARG	5.6
1	B	79	LYS	5.3
1	A	216	GLY	5.3
1	C	202	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	5.2
1	C	216	GLY	5.1
1	E	42	ALA	5.1
1	B	235	THR	5.0
1	C	261	ALA	5.0
1	C	240	ARG	4.9
1	C	259	GLY	4.9
1	E	78	PHE	4.8
1	A	39	HIS	4.8
1	E	79	LYS	4.7
1	A	210	GLU	4.7
1	A	236	LEU	4.7
1	E	64	PHE	4.7
1	C	252	THR	4.6
1	C	133	ILE	4.6
1	C	164	ASN	4.6
1	E	71	THR	4.6
1	E	285	THR	4.6
1	C	196	VAL	4.5
1	C	234	ILE	4.5
1	E	88	ASP	4.5
1	E	287	LEU	4.4
1	H	173	ASP	4.4
1	E	85	THR	4.4
1	H	214	ALA	4.4
1	E	30	TYR	4.3
1	C	227	LEU	4.3
1	A	214	ALA	4.3
1	B	288	ASP	4.3
1	A	235	THR	4.3
1	C	205	SER	4.3
1	H	174	ASN	4.3
1	A	181	SER	4.2
1	C	201	VAL	4.2
1	F	236	LEU	4.2
1	C	162	ARG	4.2
1	C	268	GLY	4.2
1	C	208	ALA	4.1
1	E	284	LEU	4.1
1	C	166	SER	4.1
1	E	27	SER	4.1
1	A	180	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	236	LEU	4.1
1	H	85	THR	4.0
1	B	128	LEU	4.0
1	B	38	HIS	4.0
1	C	187	ALA	4.0
1	B	212	ALA	4.0
1	E	248	ASN	4.0
1	A	261	ALA	4.0
1	C	235	THR	3.9
1	F	5	SER	3.9
1	B	37	ASP	3.9
1	C	226	SER	3.9
1	B	78	PHE	3.9
1	H	203	VAL	3.8
1	A	182	VAL	3.8
1	C	182	VAL	3.8
1	F	181	SER	3.8
1	B	224	ASN	3.8
1	H	215	ALA	3.8
1	B	257	PHE	3.8
1	E	33	ASN	3.8
1	H	227	LEU	3.7
1	A	239	GLY	3.7
1	A	179	VAL	3.7
1	F	131	ASP	3.7
1	C	263	ASP	3.7
1	H	202	GLU	3.7
1	C	173	ASP	3.7
1	C	197	LYS	3.7
1	C	198	MET	3.6
1	C	272	HIS	3.6
1	E	41	GLN	3.6
1	C	255	SER	3.6
1	F	176	ILE	3.6
1	H	129	GLY	3.6
1	B	237	ILE	3.6
1	C	141	THR	3.5
1	C	221	MET	3.5
1	C	218	ASP	3.5
1	E	87	GLY	3.5
1	B	223	ASP	3.5
1	A	132	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	3.4
1	B	89	LEU	3.4
1	E	90	VAL	3.4
1	C	267	SER	3.4
1	A	208	ALA	3.4
1	H	204	GLU	3.3
1	E	77	GLN	3.3
1	E	46	LEU	3.3
1	B	231	GLU	3.3
1	C	192	TYR	3.3
1	C	190	ARG	3.3
1	C	210	GLU	3.3
1	H	207	ALA	3.3
1	B	287	LEU	3.2
1	B	198[A]	MET	3.2
1	F	235	THR	3.2
1	C	11	PHE	3.2
1	E	45	SER	3.2
1	F	256	ARG	3.2
1	F	39	HIS	3.2
1	B	238	ALA	3.2
1	A	206	LEU	3.2
1	C	231	GLU	3.2
1	C	128	LEU	3.2
1	A	175	HIS	3.2
1	A	174	ASN	3.2
1	E	165	LEU	3.2
1	C	248	ASN	3.1
1	E	224	ASN	3.1
1	E	286	TYR	3.1
1	A	170	MET	3.1
1	C	253	THR	3.1
1	E	235	THR	3.1
1	C	264	TYR	3.1
1	C	230	ILE	3.1
1	C	122	ALA	3.1
1	C	222	LEU	3.1
1	F	210	GLU	3.1
1	A	215	ALA	3.1
1	C	168	ALA	3.1
1	B	77	GLN	3.0
1	C	262	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	27	SER	3.0
1	C	195	PHE	3.0
1	E	74	ASN	3.0
1	F	189	ALA	3.0
1	H	164	ASN	3.0
1	C	251	MET	3.0
1	E	84	LEU	3.0
1	F	40	GLY	3.0
1	E	223	ASP	3.0
1	E	214	ALA	3.0
1	A	167	ASP	3.0
1	C	186	ILE	3.0
1	C	121	THR	3.0
1	A	227	LEU	2.9
1	C	163	PHE	2.9
1	C	6	THR	2.9
1	E	31	SER	2.9
1	H	31	SER	2.9
1	C	170	MET	2.9
1	A	173	ASP	2.9
1	E	76	HIS	2.9
1	C	84	LEU	2.9
1	C	139	ARG	2.9
1	B	216	GLY	2.9
1	B	39	HIS	2.9
1	F	238	ALA	2.9
1	F	37	ASP	2.8
1	A	131	ASP	2.8
1	C	129	GLY	2.8
1	C	138	THR	2.8
1	B	213	ALA	2.8
1	C	126	GLU	2.8
1	B	31	SER	2.8
1	A	176	ILE	2.8
1	A	230	ILE	2.8
1	F	179	VAL	2.8
1	H	231	GLU	2.8
1	H	229	GLN	2.8
1	C	265	VAL	2.8
1	A	240	ARG	2.8
1	C	150	LYS	2.7
1	B	97	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	207	ALA	2.7
1	C	80	ASP	2.7
1	A	211	GLU	2.7
1	B	226	SER	2.7
1	E	104	GLU	2.7
1	E	25	VAL	2.7
1	C	245	CYS	2.7
1	C	159	TYR	2.7
1	A	207	ALA	2.7
1	E	162	ARG	2.7
1	C	77	GLN	2.7
1	E	163	PHE	2.6
1	C	225	MET	2.6
1	E	93	ILE	2.6
1	E	155	VAL	2.6
1	H	75	PRO	2.6
1	E	26	HIS	2.6
1	E	66	LEU	2.6
1	E	153	VAL	2.6
1	A	177	ALA	2.6
1	E	72	PHE	2.6
1	E	166	SER	2.6
1	E	6	THR	2.6
1	F	239	GLY	2.6
1	F	259	GLY	2.6
1	E	75	PRO	2.6
1	E	152	ALA	2.6
1	E	73	GLN	2.6
1	A	287	LEU	2.6
1	A	204	GLU	2.6
1	B	96	SER	2.6
1	H	278	ASP	2.6
1	C	136	PHE	2.6
1	E	34	ALA	2.6
1	E	274	ALA	2.6
1	A	212	ALA	2.6
1	C	51	ALA	2.6
1	E	252	THR	2.5
1	A	209	ALA	2.5
1	A	97	VAL	2.5
1	B	248	ASN	2.5
1	C	228	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	248	ASN	2.5
1	E	168	ALA	2.5
1	B	236	LEU	2.5
1	F	230	ILE	2.5
1	C	194	PRO	2.4
1	H	163[A]	PHE	2.4
1	E	238	ALA	2.4
1	F	129	GLY	2.4
1	H	209	ALA	2.4
1	C	140	LYS	2.4
1	H	224	ASN	2.4
1	B	168	ALA	2.4
1	A	165	LEU	2.4
1	H	128	LEU	2.4
1	B	6	THR	2.4
1	C	135	VAL	2.4
1	C	68	ASP	2.4
1	C	137	ASP	2.4
1	E	50	GLU	2.4
1	B	30	TYR	2.4
1	F	286	TYR	2.4
1	E	97	VAL	2.4
1	B	74	ASN	2.4
1	C	127	ALA	2.4
1	C	270	LEU	2.4
1	C	31	SER	2.4
1	A	6	THR	2.4
1	E	52	GLY	2.4
1	F	268	GLY	2.4
1	A	166	SER	2.4
1	H	87	GLY	2.4
1	B	253	THR	2.4
1	C	160	ASN	2.4
1	B	227	LEU	2.3
1	C	254	ILE	2.3
1	A	189	ALA	2.3
1	B	92	GLU	2.3
1	F	180	GLY	2.3
1	H	77	GLN	2.3
1	E	164	ASN	2.3
1	H	172	LYS	2.3
1	B	25	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	153	VAL	2.3
1	A	168	ALA	2.3
1	B	26	HIS	2.3
1	H	88	ASP	2.3
1	A	171	LEU	2.3
1	A	238	ALA	2.3
1	C	233	ALA	2.3
1	E	198	MET	2.3
1	F	177	ALA	2.3
1	F	240	ARG	2.3
1	A	37	ASP	2.3
1	B	68	ASP	2.3
1	C	250	ASP	2.3
1	C	75	PRO	2.3
1	H	190	ARG	2.3
1	A	183	GLN	2.3
1	F	132	ARG	2.2
1	A	129	GLY	2.2
1	C	169	ILE	2.2
1	E	95	GLY	2.2
1	H	180	GLY	2.2
1	F	234	ILE	2.2
1	A	233	ALA	2.2
1	F	227	LEU	2.2
1	H	236	LEU	2.2
1	F	212	ALA	2.2
1	F	255	SER	2.2
1	H	175	HIS	2.2
1	E	129	GLY	2.2
1	E	279	PHE	2.2
1	F	229	GLN	2.2
1	E	28	GLU	2.2
1	E	197	LYS	2.2
1	C	212	ALA	2.2
1	B	255	SER	2.2
1	E	271	THR	2.2
1	F	41	GLN	2.2
1	C	151	TYR	2.2
1	C	83	ARG	2.2
1	F	170	MET	2.2
1	C	114	LEU	2.1
1	E	108	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.1
1	B	214	ALA	2.1
1	A	266	SER	2.1
1	C	200	GLU	2.1
1	H	32	THR	2.1
1	C	30	TYR	2.1
1	B	127	ALA	2.1
1	C	274	ALA	2.1
1	H	76	HIS	2.1
1	B	252	THR	2.1
1	C	157	GLY	2.1
1	H	179	VAL	2.1
1	B	197	LYS	2.1
1	F	167	ASP	2.1
1	C	185	ALA	2.1
1	C	74	ASN	2.1
1	A	276	SER	2.1
1	F	196	VAL	2.1
1	H	170	MET	2.1
1	A	241	SER	2.1
1	B	167	ASP	2.1
1	B	210	GLU	2.1
1	E	277	LEU	2.1
1	E	281	MET	2.1
1	H	181	SER	2.1
1	B	85	THR	2.1
1	B	117	ILE	2.1
1	C	79	LYS	2.1
1	B	138	THR	2.1
1	B	232	GLN	2.1
1	F	233	ALA	2.1
1	H	80	ASP	2.1
1	E	51	ALA	2.1
1	F	258	ARG	2.1
1	E	10	PRO	2.1
1	E	160	ASN	2.1
1	H	196	VAL	2.1
1	E	67	PHE	2.1
1	E	65	THR	2.0
1	B	164	ASN	2.0
1	B	229	GLN	2.0
1	F	260	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	205	SER	2.0
1	H	68	ASP	2.0
1	C	247	GLY	2.0
1	C	67	PHE	2.0
1	E	100	LEU	2.0
1	C	181	SER	2.0
1	A	251	MET	2.0
1	B	196	VAL	2.0
1	C	54	LEU	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. 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
2	SO4	A	302	5/5	0.79	0.48	5.07	90,92,97,119	0
2	SO4	B	303	5/5	0.42	0.56	4.66	99,105,130,135	0
2	SO4	E	302	5/5	0.89	0.41	1.52	77,80,92,95	0
2	SO4	C	302	5/5	0.77	0.45	0.72	117,121,123,127	0
2	SO4	H	302	5/5	0.90	0.31	0.64	63,65,71,80	0
2	SO4	A	303	5/5	0.94	0.29	0.62	62,71,77,79	0
2	SO4	F	302	5/5	0.93	0.29	0.33	67,70,78,82	0
2	SO4	F	301	5/5	0.90	0.32	0.17	76,77,85,91	0
2	SO4	A	304	5/5	0.84	0.32	-0.18	90,95,104,111	0
2	SO4	B	301	5/5	0.92	0.29	-0.49	63,63,70,72	0
2	SO4	H	301	5/5	0.88	0.28	-0.55	73,81,84,87	0
2	SO4	E	304	5/5	0.94	0.22	-1.07	75,76,83,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	302	5/5	0.97	0.18	-1.48	60,70,72,72	0
2	SO4	E	303	5/5	0.95	0.20	-1.91	59,63,66,70	0
2	SO4	H	303	5/5	0.78	0.40	-	113,117,132,134	0
2	SO4	A	301	5/5	0.86	0.47	-	113,113,124,127	0
2	SO4	B	304	5/5	0.78	0.50	-	122,124,132,135	0
2	SO4	F	303	5/5	0.74	0.69	-	100,105,113,119	0
2	SO4	C	301	5/5	0.86	0.57	-	88,88,97,98	0
2	SO4	E	301	5/5	0.78	0.52	-	100,104,113,121	0

## 6.5 Other polymers

There are no such residues in this entry.