



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 5HUO / pdb_00005huo
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

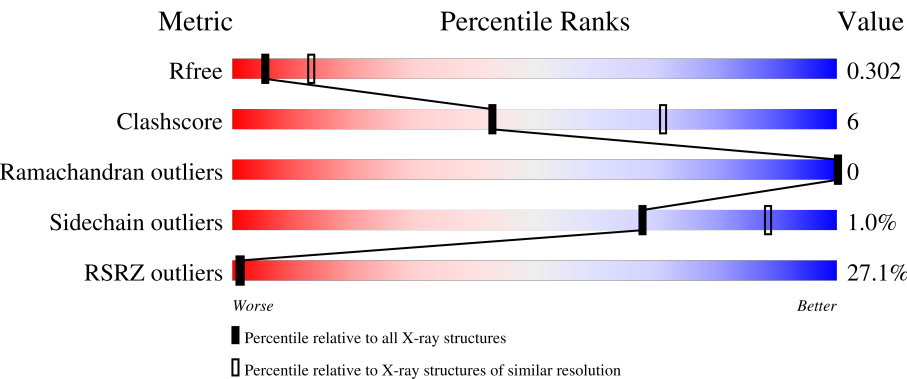
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	314	19% 80%10%10%
1	B	314	19% 77%13%10%
1	C	314	46% 73%15%•11%
1	E	314	36% 77%12%•10%
1	F	314	8% 79%11%•10%

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Mol	Chain	Length	Quality of chain
1	H	314	18% 77% 12% • 10%

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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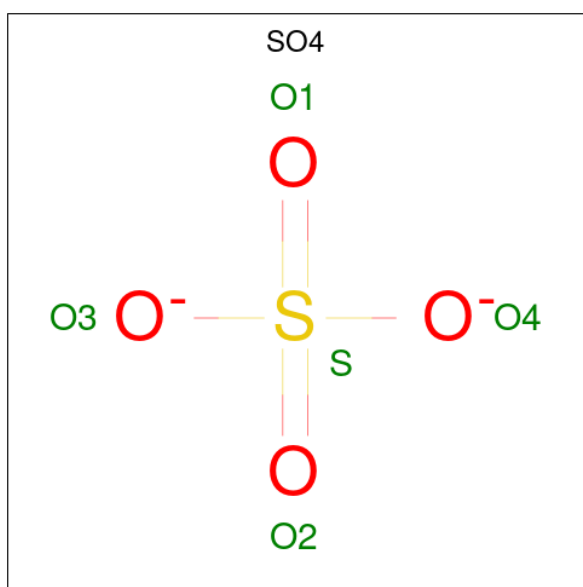
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A0A0H3BVM1
E	0	GLY	-	expression tag	UNP A0A0H3BVM1
E	?	-	UNK	deletion	UNP A0A0H3BVM1
F	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
F	-23	HIS	-	expression tag	UNP A0A0H3BVM1
F	-22	HIS	-	expression tag	UNP A0A0H3BVM1
F	-21	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 (CCD ID: SO4) (formula: O₄S).



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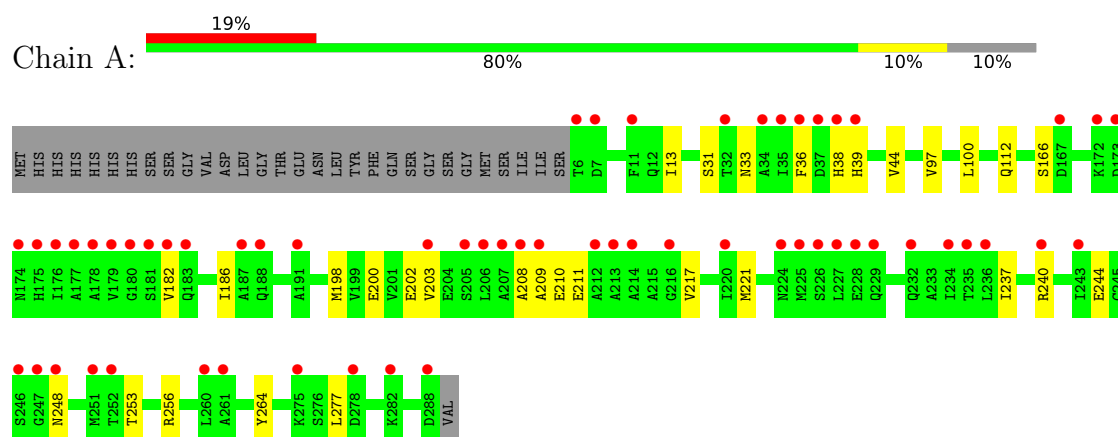
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	31	Total	O	0	0
			31	31		
3	H	29	Total	O	0	0
			29	29		

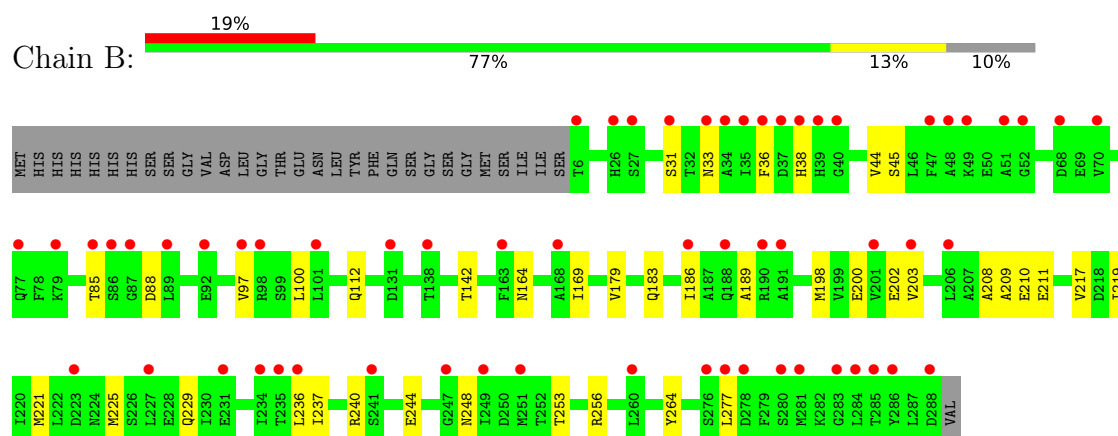
3 Residue-property plots

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.

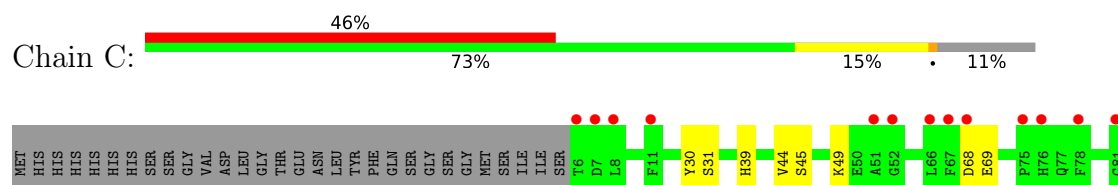
- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)



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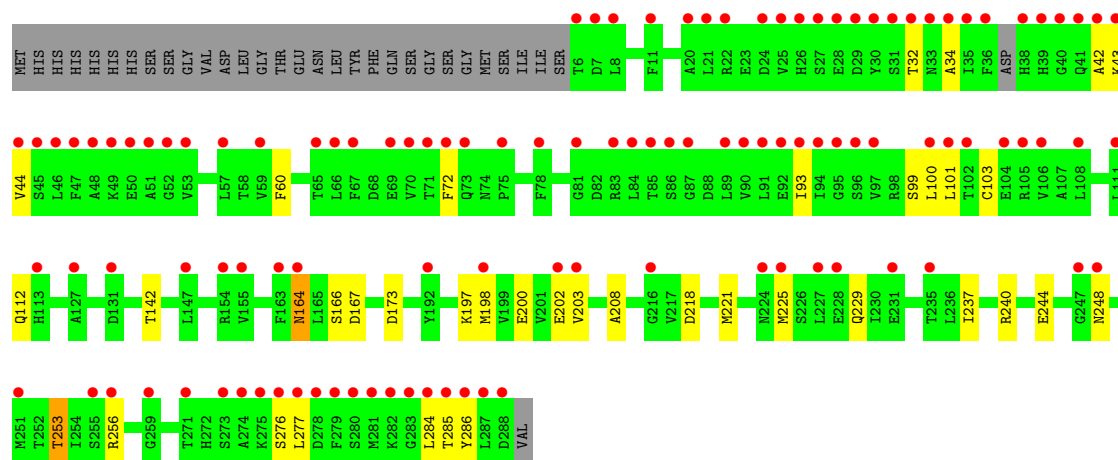
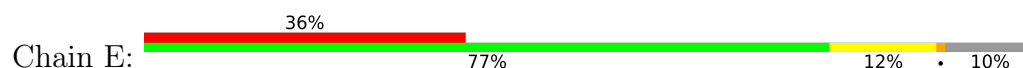


- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)

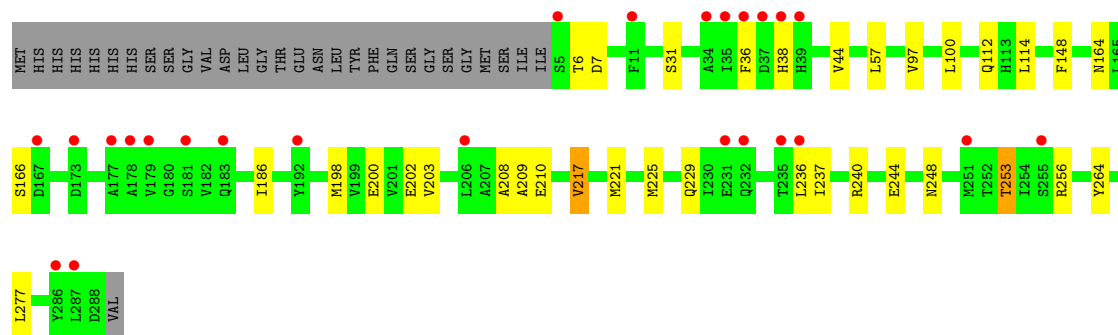
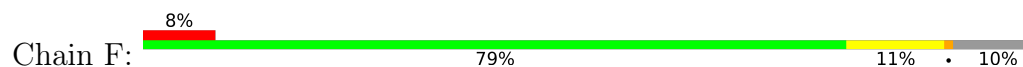




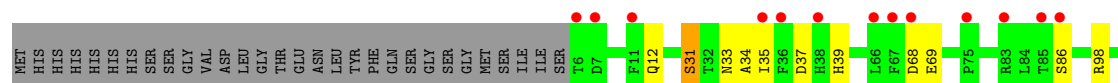
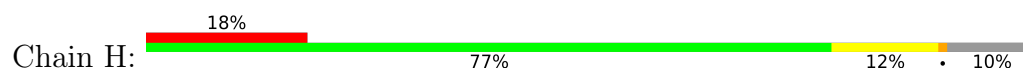
- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)

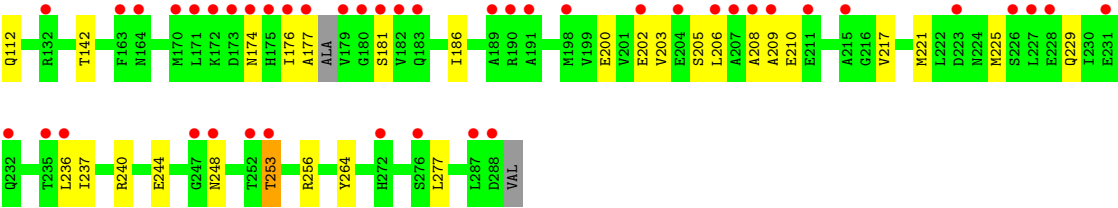


- Molecule 1: Nicotinate-nucleotide diphosphorylase (Carboxylating)



- 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, α , β , γ	106.20Å 186.26Å 221.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.80) 99.9 (40.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.216 , 0.255 0.263 , 0.302	Depositor DCC
R_{free} test set	2766 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.19	2/2185 (0.1%)	1.07	2/2957 (0.1%)
1	B	1.08	0/2207	1.04	3/2984 (0.1%)
1	C	1.08	1/2102 (0.0%)	1.09	6/2851 (0.2%)
1	E	1.08	1/2138 (0.0%)	1.06	5/2898 (0.2%)
1	F	1.19	1/2194 (0.0%)	1.08	3/2971 (0.1%)
1	H	1.17	1/2192 (0.0%)	1.07	3/2963 (0.1%)
All	All	1.13	6/13018 (0.0%)	1.07	22/17624 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	181	SER	CA-C	6.81	1.61	1.52
1	A	13	ILE	N-CA	6.32	1.52	1.46
1	C	281	MET	CA-C	-5.78	1.45	1.52
1	F	57	LEU	N-CA	5.57	1.53	1.46
1	E	173	ASP	CB-CG	5.36	1.65	1.52
1	A	166	SER	C-O	-5.09	1.17	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	12	GLN	N-CA-C	6.51	118.45	111.36
1	E	167	ASP	N-CA-C	6.44	118.38	111.36
1	H	176	ILE	N-CA-C	-6.26	103.22	111.05
1	C	211	GLU	N-CA-CB	6.23	119.22	109.94
1	H	253	THR	N-CA-C	6.01	117.91	111.36
1	A	39	HIS	N-CA-C	6.00	119.70	111.54
1	F	217	VAL	CB-CA-C	-5.94	104.80	111.45
1	E	285	THR	N-CA-C	-5.92	101.25	110.42
1	E	253	THR	N-CA-C	5.88	117.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	253	THR	N-CA-C	5.58	117.44	111.36
1	B	164	ASN	CB-CA-C	-5.57	100.25	110.62
1	A	33	ASN	N-CA-C	5.53	118.06	111.71
1	F	264	TYR	N-CA-C	5.44	116.55	108.60
1	C	167	ASP	N-CA-C	5.43	117.28	111.36
1	C	103	CYS	N-CA-C	5.42	119.73	113.18
1	C	171	LEU	N-CA-C	5.32	116.97	108.41
1	C	264	TYR	N-CA-C	5.31	116.35	108.60
1	C	172	LYS	N-CA-C	5.23	117.97	109.86
1	E	164	ASN	N-CA-C	5.15	116.67	108.79
1	B	33	ASN	N-CA-C	5.05	116.79	111.28
1	B	264	TYR	N-CA-C	5.04	115.96	108.60
1	E	164	ASN	CB-CA-C	-5.03	101.26	110.62

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	2152	0	2128	17	0
1	B	2171	0	2155	32	0
1	C	2072	0	1971	38	0
1	E	2108	0	2049	33	0
1	F	2161	0	2124	21	0
1	H	2156	0	2121	30	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	31	0	0	0	0
3	H	29	0	0	0	0
All	All	13069	0	12548	157	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 (157) 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:198:MET:HE3	1:E:218:ASP:HB3	1.65	0.78
1:H:225:MET:HE3	1:H:229:GLN:HB3	1.69	0.74
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:H:206:LEU:HD23	1:H:206:LEU:C	2.14	0.72
1:F:225:MET:HE3	1:F:229:GLN:HB3	1.71	0.72
1:A:203:VAL:HG13	1:A:208:ALA:HB3	1.72	0.71
1:E:225:MET:HE3	1:E:229:GLN:HB3	1.71	0.71
1:C:198:MET:HE3	1:C:218:ASP:HB3	1.73	0.71
1:B:225:MET:HE3	1:B:229:GLN:HB3	1.73	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: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:H:37:ASP:OD1	1:H:37:ASP:C	2.42	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:36:PHE:C	1:B:38:HIS:H	2.11	0.58
1:F:7:ASP:O	1:H:98:ARG:NH2	2.28	0.58
1:E:198:MET:HE3	1:E:218:ASP:CB	2.31	0.58
1:B:44:VAL:HG23	1:B:100:LEU:HD13	1.85	0.57
1:C:202:GLU:HB3	1:C:221:MET:HE3	1.87	0.57
1:A:44:VAL:HG23	1:A:100:LEU:HD13	1.86	0.56
1:A:237:ILE:O	1:A:240:ARG:HD3	2.03	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: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
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:F:6:THR:HG21	1:H:33:ASN:HB3	1.87	0.55
1:H:253:THR:O	1:H:256:ARG:HG2	2.06	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: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: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:C:198:MET:CE	1:C:218:ASP:HB3	2.37	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:PHE:HE2	1:E:93:ILE:HD11	1.76	0.49
1:E:112:GLN:HG2	1:E:277:LEU:O	2.13	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
1:E:42:ALA:HB1	1:E:284:LEU:HD11	1.94	0.48
1:E:93:ILE:HG22	1:E:100:LEU:CD2	2.44	0.48
1:E:203:VAL:HG13	1:E:208:ALA:CB	2.40	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:C:254:ILE:HD11	1:C:265:VAL:HG21	1.97	0.47
1:E:202:GLU:HG2	1:E:221:MET:SD	2.54	0.47
1:H:206:LEU:C	1:H:206:LEU:CD2	2.83	0.47
1:A:248:ASN:O	1:A:253:THR:HG21	2.15	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:C:133:ILE:CG2	1:C:134:LYS:N	2.78	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:142:THR:HG21	1:E:142:THR:HG21	1.97	0.45
1:C:202:GLU:HA	1:C:221:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:210:GLU:OE1	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
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:68:ASP:CG	1:H:69:GLU:H	2.28	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: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:36:PHE:C	1:B:38:HIS:N	2.75	0.41
1:B:203:VAL:HG11	1:B:209:ALA:N	2.36	0.41
1:C:68:ASP:CG	1:C:69:GLU:H	2.28	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:A:182:VAL:HB	1:A:211:GLU:CD	2.46	0.41
1:B:44:VAL:HG12	1:B: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:HD23	1:C:165:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	225/260 (86%)	223 (99%)	2 (1%)	70	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	230/260 (88%)	229 (100%)	1 (0%)	84	94
1	C	207/260 (80%)	204 (99%)	3 (1%)	59	85
1	E	217/260 (84%)	216 (100%)	1 (0%)	81	93
1	F	227/260 (87%)	225 (99%)	2 (1%)	70	89
1	H	226/260 (87%)	222 (98%)	4 (2%)	51	82
All	All	1332/1560 (85%)	1319 (99%)	13 (1%)	68	88

All (13) 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
1	F	31	SER
1	F	38	HIS
1	H	31	SER
1	H	39	HIS
1	H	86	SER
1	H	205	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	GLN
1	C	77	GLN
1	F	61	GLN
1	H	160	ASN
1	H	188	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	H	302	-	4,4,4	0.56	0	6,6,6	0.51	0
2	SO4	A	301	-	4,4,4	0.45	0	6,6,6	0.26	0
2	SO4	F	302	-	4,4,4	0.51	0	6,6,6	0.59	0
2	SO4	H	303	-	4,4,4	0.45	0	6,6,6	0.29	0
2	SO4	E	301	-	4,4,4	0.46	0	6,6,6	0.23	0
2	SO4	B	302	-	4,4,4	0.40	0	6,6,6	0.27	0
2	SO4	A	304	-	4,4,4	0.49	0	6,6,6	0.65	0
2	SO4	H	301	-	4,4,4	0.48	0	6,6,6	0.72	0
2	SO4	C	302	-	4,4,4	0.46	0	6,6,6	0.18	0
2	SO4	B	303	-	4,4,4	0.54	0	6,6,6	0.46	0
2	SO4	C	301	-	4,4,4	0.42	0	6,6,6	0.35	0
2	SO4	A	303	-	4,4,4	0.30	0	6,6,6	0.59	0
2	SO4	F	303	-	4,4,4	0.50	0	6,6,6	0.31	0
2	SO4	A	302	-	4,4,4	0.61	0	6,6,6	0.50	0
2	SO4	B	301	-	4,4,4	0.37	0	6,6,6	0.62	0
2	SO4	F	301	-	4,4,4	0.46	0	6,6,6	0.53	0
2	SO4	E	303	-	4,4,4	0.38	0	6,6,6	0.89	0
2	SO4	E	302	-	4,4,4	0.53	0	6,6,6	0.46	0
2	SO4	E	304	-	4,4,4	0.37	0	6,6,6	0.26	0
2	SO4	B	304	-	4,4,4	0.49	0	6,6,6	0.20	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, 95th 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 ²)	Q<0.9
1	A	283/314 (90%)	1.30	60 (21%) 2 2	87, 105, 179, 236	0
1	B	283/314 (90%)	1.33	61 (21%) 2 2	60, 117, 159, 194	1 (0%)
1	C	280/314 (89%)	2.18	143 (51%) 0 0	91, 154, 268, 297	0
1	E	282/314 (89%)	1.86	113 (40%) 0 0	92, 131, 219, 316	0
1	F	284/314 (90%)	0.99	25 (8%) 15 11	89, 101, 141, 201	0
1	H	282/314 (89%)	1.32	57 (20%) 3 2	56, 105, 152, 175	1 (0%)
All	All	1694/1884 (89%)	1.49	459 (27%) 1 1	56, 115, 211, 316	2 (0%)

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	VAL	6.1
1	F	5	SER	5.7
1	E	284	LEU	5.6
1	H	179	VAL	5.4
1	E	286	TYR	5.4
1	C	195	PHE	5.3
1	C	189	ALA	5.2
1	C	169	ILE	5.1
1	E	35	ILE	5.1
1	C	204	GLU	5.1
1	E	31	SER	5.1
1	C	245	CYS	5.0
1	C	6	THR	5.0
1	H	183	GLN	4.9
1	B	26	HIS	4.8
1	B	235	THR	4.8
1	A	34	ALA	4.8
1	E	30	TYR	4.8
1	B	6	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	248	ASN	4.6
1	B	36	PHE	4.6
1	C	161	HIS	4.6
1	C	194	PRO	4.5
1	C	168	ALA	4.4
1	E	25	VAL	4.4
1	A	37	ASP	4.4
1	C	67	PHE	4.4
1	E	36	PHE	4.3
1	C	7	ASP	4.3
1	A	224	ASN	4.3
1	E	198	MET	4.2
1	C	165	LEU	4.1
1	C	203	VAL	4.1
1	H	181	SER	4.1
1	H	180	GLY	4.1
1	A	173	ASP	4.1
1	C	257	PHE	4.1
1	C	247	GLY	4.1
1	C	288	ASP	4.1
1	E	288	ASP	4.1
1	A	6	THR	4.0
1	H	182	VAL	4.0
1	H	173	ASP	4.0
1	H	204	GLU	4.0
1	A	178	ALA	3.9
1	E	97	VAL	3.9
1	C	261	ALA	3.9
1	E	6	THR	3.9
1	C	135	VAL	3.8
1	A	174	ASN	3.8
1	C	256	ARG	3.8
1	A	227	LEU	3.8
1	E	101	LEU	3.8
1	C	262	ILE	3.8
1	C	185	ALA	3.8
1	C	236	LEU	3.8
1	C	182	VAL	3.7
1	C	159	TYR	3.7
1	C	220	ILE	3.7
1	E	75	PRO	3.7
1	H	207	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	281	MET	3.7
1	C	11	PHE	3.7
1	E	47	PHE	3.7
1	C	162	ARG	3.7
1	E	33	ASN	3.7
1	C	138	THR	3.7
1	C	175	HIS	3.7
1	C	157	GLY	3.7
1	F	37	ASP	3.6
1	E	285	THR	3.6
1	E	34	ALA	3.6
1	C	129	GLY	3.6
1	C	164	ASN	3.6
1	H	6	THR	3.6
1	H	202	GLU	3.6
1	C	198	MET	3.6
1	C	287	LEU	3.6
1	E	38	HIS	3.6
1	C	270	LEU	3.6
1	A	175	HIS	3.5
1	C	267	SER	3.5
1	E	280	SER	3.5
1	C	249	ILE	3.5
1	H	174	ASN	3.5
1	C	200	GLU	3.5
1	C	248	ASN	3.5
1	H	227	LEU	3.5
1	C	183	GLN	3.4
1	C	251	MET	3.4
1	E	92	GLU	3.4
1	C	209	ALA	3.4
1	C	136	PHE	3.4
1	C	197	LYS	3.4
1	C	201	VAL	3.4
1	C	191	ALA	3.4
1	C	241	SER	3.4
1	H	288	ASP	3.4
1	C	206	LEU	3.4
1	C	265	VAL	3.4
1	A	181	SER	3.4
1	C	205	SER	3.4
1	C	243	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	94	ILE	3.4
1	C	264	TYR	3.4
1	E	279	PHE	3.4
1	C	199	VAL	3.3
1	E	93	ILE	3.3
1	C	227	LEU	3.3
1	E	227	LEU	3.3
1	C	158	GLY	3.3
1	A	214	ALA	3.3
1	E	277	LEU	3.3
1	F	232	GLN	3.3
1	E	26	HIS	3.3
1	E	127	ALA	3.3
1	H	67	PHE	3.2
1	C	231	GLU	3.2
1	E	42	ALA	3.2
1	E	46	LEU	3.2
1	E	283	GLY	3.2
1	C	167	ASP	3.2
1	C	177	ALA	3.2
1	E	39	HIS	3.2
1	C	186	ILE	3.2
1	C	237	ILE	3.2
1	C	260	LEU	3.1
1	E	27	SER	3.1
1	F	38	HIS	3.1
1	H	85	THR	3.1
1	E	100	LEU	3.1
1	H	206	LEU	3.1
1	B	33	ASN	3.1
1	B	35	ILE	3.1
1	E	71	THR	3.1
1	C	222	LEU	3.1
1	F	178	ALA	3.1
1	H	177	ALA	3.1
1	C	125	VAL	3.1
1	A	179	VAL	3.1
1	E	28	GLU	3.1
1	C	163	PHE	3.0
1	H	198	MET	3.0
1	A	176	ILE	3.0
1	A	228	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	235	THR	3.0
1	H	253	THR	3.0
1	E	90	VAL	3.0
1	C	8	LEU	3.0
1	A	182	VAL	3.0
1	B	97	VAL	3.0
1	C	275	LYS	3.0
1	H	176	ILE	3.0
1	A	206	LEU	3.0
1	C	212	ALA	3.0
1	H	208	ALA	3.0
1	C	134	LYS	3.0
1	A	35	ILE	3.0
1	C	284	LEU	3.0
1	B	27	SER	3.0
1	C	160	ASN	3.0
1	B	191	ALA	3.0
1	H	36	PHE	3.0
1	H	287	LEU	2.9
1	C	263	ASP	2.9
1	E	248	ASN	2.9
1	C	266	SER	2.9
1	C	51	ALA	2.9
1	E	49	LYS	2.9
1	E	102	THR	2.9
1	C	259	GLY	2.9
1	E	216	GLY	2.9
1	C	173	ASP	2.9
1	A	177	ALA	2.9
1	E	44	VAL	2.9
1	H	215	ALA	2.9
1	E	41	GLN	2.9
1	F	286	TYR	2.9
1	C	68	ASP	2.9
1	E	89	LEU	2.9
1	C	184	LYS	2.8
1	C	238	ALA	2.8
1	B	163	PHE	2.8
1	E	131	ASP	2.8
1	C	246	SER	2.8
1	E	287	LEU	2.8
1	C	192	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	236	LEU	2.8
1	C	166	SER	2.8
1	C	255	SER	2.8
1	C	139	ARG	2.8
1	E	70	VAL	2.8
1	B	39	HIS	2.8
1	E	224	ASN	2.8
1	C	181	SER	2.8
1	C	170	MET	2.8
1	H	35	ILE	2.8
1	A	216	GLY	2.8
1	C	75	PRO	2.8
1	E	69	GLU	2.7
1	E	163	PHE	2.7
1	A	225	MET	2.7
1	A	288	ASP	2.7
1	E	87	GLY	2.7
1	C	202	GLU	2.7
1	A	207	ALA	2.7
1	A	213	ALA	2.7
1	A	236	LEU	2.7
1	C	274	ALA	2.7
1	E	21	LEU	2.7
1	F	35	ILE	2.7
1	E	86	SER	2.7
1	E	273	SER	2.7
1	C	217	VAL	2.7
1	A	260	LEU	2.7
1	B	251	MET	2.7
1	B	286	TYR	2.7
1	C	272	HIS	2.7
1	E	7	ASP	2.7
1	A	36	PHE	2.7
1	C	225	MET	2.7
1	C	208	ALA	2.6
1	E	78	PHE	2.6
1	E	274	ALA	2.6
1	F	39	HIS	2.6
1	C	232	GLN	2.6
1	H	68	ASP	2.6
1	C	230	ILE	2.6
1	A	209	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	105	ARG	2.6
1	B	85	THR	2.6
1	F	236	LEU	2.6
1	H	231	GLU	2.6
1	C	187	ALA	2.6
1	E	20	ALA	2.6
1	C	151	TYR	2.6
1	E	106	VAL	2.6
1	H	235	THR	2.6
1	E	73	GLN	2.6
1	E	202	GLU	2.6
1	H	175	HIS	2.6
1	H	83	ARG	2.6
1	A	180	GLY	2.6
1	C	81	GLY	2.6
1	B	34	ALA	2.6
1	E	45	SER	2.5
1	C	128	LEU	2.5
1	C	240	ARG	2.5
1	F	167	ASP	2.5
1	A	205	SER	2.5
1	B	283	GLY	2.5
1	A	229	GLN	2.5
1	F	11	PHE	2.5
1	E	48	ALA	2.5
1	C	174	ASN	2.5
1	A	261	ALA	2.5
1	B	188	GLN	2.5
1	A	38	HIS	2.5
1	A	278	ASP	2.5
1	C	278	ASP	2.5
1	B	227	LEU	2.5
1	A	226	SER	2.5
1	E	255	SER	2.5
1	H	75	PRO	2.5
1	H	228	GLU	2.5
1	A	183	GLN	2.5
1	C	215	ALA	2.5
1	E	32	THR	2.5
1	B	79	LYS	2.5
1	E	164	ASN	2.5
1	C	137	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	8	LEU	2.4
1	B	52	GLY	2.4
1	B	247	GLY	2.4
1	E	276	SER	2.4
1	F	179	VAL	2.4
1	B	98	ARG	2.4
1	C	83	ARG	2.4
1	E	22	ARG	2.4
1	B	101	LEU	2.4
1	E	57	LEU	2.4
1	E	66	LEU	2.4
1	E	91	LEU	2.4
1	H	7	ASP	2.4
1	C	153	VAL	2.4
1	E	40	GLY	2.4
1	E	155	VAL	2.4
1	A	240	ARG	2.4
1	C	154	ARG	2.4
1	C	190	ARG	2.4
1	C	258	ARG	2.4
1	C	269	SER	2.4
1	E	231	GLU	2.4
1	C	233	ALA	2.4
1	H	191	ALA	2.4
1	C	252	THR	2.4
1	H	66	LEU	2.4
1	B	37	ASP	2.4
1	A	11	PHE	2.4
1	H	232	GLN	2.4
1	C	253	THR	2.4
1	E	271	THR	2.4
1	E	282	LYS	2.4
1	B	47	PHE	2.4
1	B	276	SER	2.4
1	B	260	LEU	2.4
1	H	38	HIS	2.4
1	A	220	ILE	2.4
1	C	223	ASP	2.3
1	E	11	PHE	2.3
1	H	86	SER	2.3
1	A	235	THR	2.3
1	B	89	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	286	TYR	2.3
1	E	84	LEU	2.3
1	H	236	LEU	2.3
1	E	43	LYS	2.3
1	H	172	LYS	2.3
1	E	53	VAL	2.3
1	F	173	ASP	2.3
1	A	208	ALA	2.3
1	A	212	ALA	2.3
1	B	241	SER	2.3
1	F	287	LEU	2.3
1	C	254	ILE	2.3
1	E	275	LYS	2.3
1	E	154	ARG	2.3
1	E	256	ARG	2.3
1	C	52	GLY	2.3
1	C	144	ASN	2.3
1	E	51	ALA	2.3
1	C	131	ASP	2.3
1	A	188	GLN	2.3
1	A	234	ILE	2.3
1	B	234	ILE	2.3
1	F	181	SER	2.3
1	E	67	PHE	2.3
1	B	51	ALA	2.3
1	E	228	GLU	2.3
1	A	167	ASP	2.3
1	B	68	ASP	2.3
1	B	223	ASP	2.3
1	F	183	GLN	2.3
1	H	226	SER	2.3
1	B	203	VAL	2.3
1	B	40	GLY	2.3
1	H	189	ALA	2.2
1	C	84	LEU	2.2
1	C	218	ASP	2.2
1	E	29	ASP	2.2
1	B	190	ARG	2.2
1	F	255	SER	2.2
1	C	268	GLY	2.2
1	E	104	GLU	2.2
1	F	177	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	209	ALA	2.2
1	E	147	LEU	2.2
1	H	211	GLU	2.2
1	C	140	LYS	2.2
1	A	39	HIS	2.2
1	C	76	HIS	2.2
1	C	130	ASP	2.2
1	E	113	HIS	2.2
1	E	85	THR	2.2
1	E	96	SER	2.2
1	E	192	TYR	2.2
1	F	251	MET	2.2
1	H	11	PHE	2.2
1	C	171	LEU	2.2
1	H	164	ASN	2.2
1	B	131	ASP	2.2
1	E	203	VAL	2.2
1	A	32	THR	2.2
1	E	235	THR	2.2
1	A	172	LYS	2.2
1	E	72	PHE	2.2
1	B	284	LEU	2.2
1	E	108	LEU	2.2
1	C	214	ALA	2.2
1	E	83	ARG	2.2
1	A	232	GLN	2.2
1	B	38	HIS	2.2
1	A	203	VAL	2.2
1	B	288	ASP	2.2
1	E	24	ASP	2.2
1	E	251	MET	2.2
1	B	87	GLY	2.2
1	A	246	SER	2.2
1	C	78	PHE	2.2
1	B	206	LEU	2.2
1	B	280	SER	2.2
1	H	276	SER	2.2
1	B	168	ALA	2.2
1	C	224	ASN	2.1
1	B	70	VAL	2.1
1	C	155	VAL	2.1
1	A	7	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	251	MET	2.1
1	H	170	MET	2.1
1	A	247	GLY	2.1
1	B	285	THR	2.1
1	E	259	GLY	2.1
1	F	235	THR	2.1
1	H	247	GLY	2.1
1	H	163[A]	PHE	2.1
1	C	124	TYR	2.1
1	B	48	ALA	2.1
1	B	231	GLU	2.1
1	C	133	ILE	2.1
1	H	272	HIS	2.1
1	B	278	ASP	2.1
1	E	278	ASP	2.1
1	H	223	ASP	2.1
1	E	65	THR	2.1
1	C	66	LEU	2.1
1	C	148	PHE	2.1
1	E	111	LEU	2.1
1	F	36	PHE	2.1
1	F	34	ALA	2.1
1	B	31	SER	2.1
1	C	219	ILE	2.1
1	F	231	GLU	2.1
1	A	248	ASN	2.1
1	E	81	GLY	2.1
1	A	252	THR	2.1
1	A	191	ALA	2.1
1	B	249	ILE	2.1
1	C	244	GLU	2.1
1	F	206	LEU	2.1
1	E	52	GLY	2.1
1	E	95	GLY	2.1
1	C	242	ARG	2.1
1	H	190	ARG	2.1
1	H	252	THR	2.1
1	A	187	ALA	2.1
1	B	186	ILE	2.1
1	C	234	ILE	2.1
1	A	282	LYS	2.0
1	B	86	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	276	SER	2.0
1	H	171	LEU	2.0
1	C	87	GLY	2.0
1	E	247	GLY	2.0
1	H	132	ARG	2.0
1	A	243	ILE	2.0
1	C	211	GLU	2.0
1	E	50	GLU	2.0
1	B	49	LYS	2.0
1	F	192	TYR	2.0
1	B	77	GLN	2.0
1	B	201	VAL	2.0
1	E	59	VAL	2.0
1	B	277	LEU	2.0
1	B	138	THR	2.0
1	A	275	LYS	2.0
1	B	92	GLU	2.0
1	B	281	MET	2.0
1	C	281	MET	2.0
1	E	225	MET	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	SO4	B	304	5/5	0.25	0.17	122,124,132,135	0
2	SO4	H	303	5/5	0.48	0.20	113,117,132,134	0
2	SO4	B	303	5/5	0.58	0.29	99,105,130,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	302	5/5	0.65	0.25	117,121,123,127	0
2	SO4	A	301	5/5	0.67	0.26	113,113,124,127	0
2	SO4	F	303	5/5	0.69	0.27	100,105,113,119	0
2	SO4	A	302	5/5	0.77	0.30	90,92,97,119	0
2	SO4	E	301	5/5	0.82	0.26	100,104,113,121	0
2	SO4	C	301	5/5	0.83	0.32	88,88,97,98	0
2	SO4	H	301	5/5	0.84	0.30	73,81,84,87	0
2	SO4	A	304	5/5	0.84	0.28	90,95,104,111	0
2	SO4	E	302	5/5	0.86	0.31	77,80,92,95	0
2	SO4	H	302	5/5	0.90	0.26	63,65,71,80	0
2	SO4	F	301	5/5	0.90	0.27	76,77,85,91	0
2	SO4	F	302	5/5	0.92	0.25	67,70,78,82	0
2	SO4	A	303	5/5	0.93	0.26	62,71,77,79	0
2	SO4	E	303	5/5	0.93	0.28	59,63,66,70	0
2	SO4	B	301	5/5	0.94	0.27	63,63,70,72	0
2	SO4	E	304	5/5	0.94	0.21	75,76,83,84	0
2	SO4	B	302	5/5	0.95	0.21	60,70,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.