



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 12:13 PM EDT

PDB ID : 3DV2  
Title : Crystal Structure of nicotinic acid mononucleotide adenylyltransferase from Bacillus anthracis  
Authors : Lu, S.; Smith, C.D.; Yang, Z.; Pruett, P.S.; Nagy, L.; McCombs, D.P.; DeLucas, L.J.; Brouillette, W.J.; Brouillette, C.G.  
Deposited on : 2008-07-18  
Resolution : 2.30 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.

The types of validation reports are described at

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

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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 : 2.35  
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) : 2.35

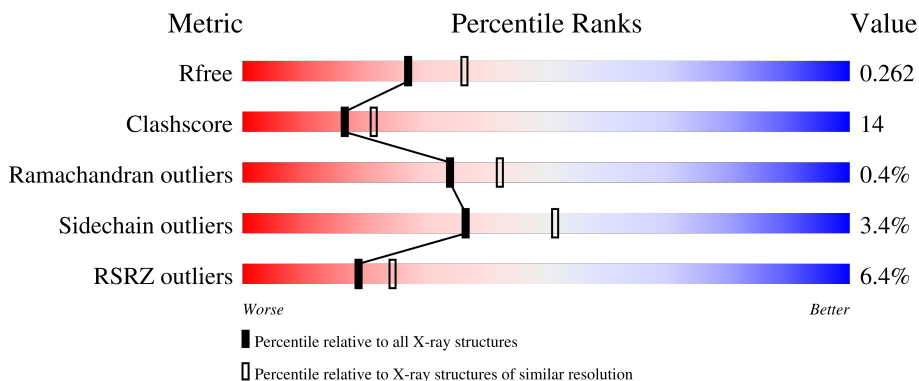
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	201	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      65%      27%      • 7%</p>
1	B	201	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">12%      64%      28%      • 6%</p>
1	C	201	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      69%      23%      • 7%</p>
1	D	201	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">7%      72%      21%      • 6%</p>

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6333 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 (Nicotinamide) nucleotide adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	187	Total 1536	C 1000	N 252	O 279	S 5	0	0	0
1	B	188	Total 1542	C 1003	N 253	O 281	S 5	0	0	0
1	C	187	Total 1536	C 1000	N 252	O 279	S 5	0	0	0
1	D	189	Total 1550	C 1008	N 254	O 282	S 6	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	LEU	-	expression tag	UNP Q6HT60
A	191	ALA	-	expression tag	UNP Q6HT60
A	192	ALA	-	expression tag	UNP Q6HT60
A	193	ALA	-	expression tag	UNP Q6HT60
A	194	LEU	-	expression tag	UNP Q6HT60
A	195	GLU	-	expression tag	UNP Q6HT60
A	196	HIS	-	expression tag	UNP Q6HT60
A	197	HIS	-	expression tag	UNP Q6HT60
A	198	HIS	-	expression tag	UNP Q6HT60
A	199	HIS	-	expression tag	UNP Q6HT60
A	200	HIS	-	expression tag	UNP Q6HT60
A	201	HIS	-	expression tag	UNP Q6HT60
B	190	LEU	-	expression tag	UNP Q6HT60
B	191	ALA	-	expression tag	UNP Q6HT60
B	192	ALA	-	expression tag	UNP Q6HT60
B	193	ALA	-	expression tag	UNP Q6HT60
B	194	LEU	-	expression tag	UNP Q6HT60
B	195	GLU	-	expression tag	UNP Q6HT60
B	196	HIS	-	expression tag	UNP Q6HT60
B	197	HIS	-	expression tag	UNP Q6HT60
B	198	HIS	-	expression tag	UNP Q6HT60

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HIS	-	expression tag	UNP Q6HT60
B	200	HIS	-	expression tag	UNP Q6HT60
B	201	HIS	-	expression tag	UNP Q6HT60
C	190	LEU	-	expression tag	UNP Q6HT60
C	191	ALA	-	expression tag	UNP Q6HT60
C	192	ALA	-	expression tag	UNP Q6HT60
C	193	ALA	-	expression tag	UNP Q6HT60
C	194	LEU	-	expression tag	UNP Q6HT60
C	195	GLU	-	expression tag	UNP Q6HT60
C	196	HIS	-	expression tag	UNP Q6HT60
C	197	HIS	-	expression tag	UNP Q6HT60
C	198	HIS	-	expression tag	UNP Q6HT60
C	199	HIS	-	expression tag	UNP Q6HT60
C	200	HIS	-	expression tag	UNP Q6HT60
C	201	HIS	-	expression tag	UNP Q6HT60
D	190	LEU	-	expression tag	UNP Q6HT60
D	191	ALA	-	expression tag	UNP Q6HT60
D	192	ALA	-	expression tag	UNP Q6HT60
D	193	ALA	-	expression tag	UNP Q6HT60
D	194	LEU	-	expression tag	UNP Q6HT60
D	195	GLU	-	expression tag	UNP Q6HT60
D	196	HIS	-	expression tag	UNP Q6HT60
D	197	HIS	-	expression tag	UNP Q6HT60
D	198	HIS	-	expression tag	UNP Q6HT60
D	199	HIS	-	expression tag	UNP Q6HT60
D	200	HIS	-	expression tag	UNP Q6HT60
D	201	HIS	-	expression tag	UNP Q6HT60

- Molecule 2 is SULFATE ION (three-letter code: SO4) (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	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	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

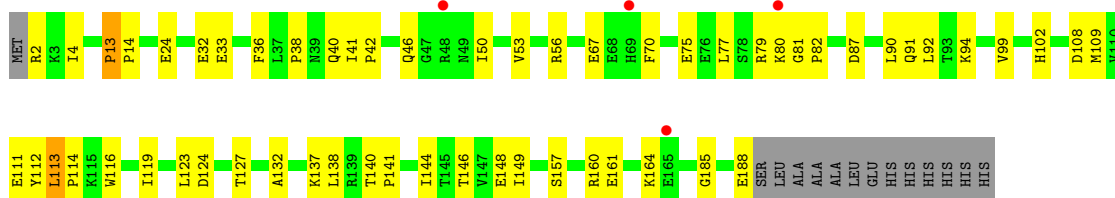
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	38	Total	O	0	0
			38	38		
3	C	27	Total	O	0	0
			27	27		
3	D	37	Total	O	0	0
			37	37		

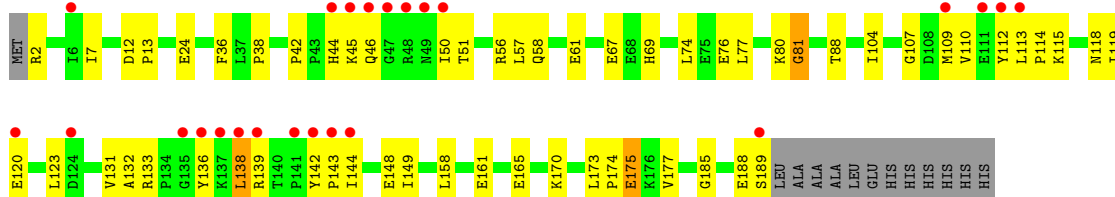
### 3 Residue-property plots [i](#)

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.

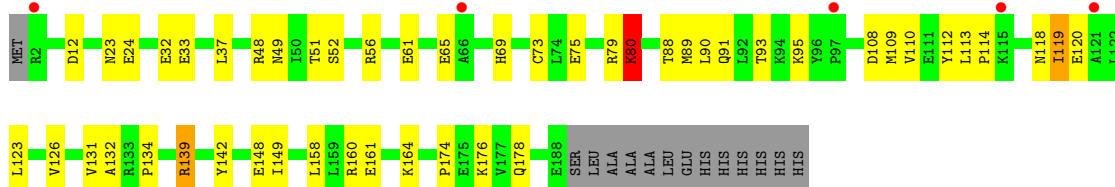
- Molecule 1: Nicotinate (Nicotinamide) nucleotide adenylyltransferase



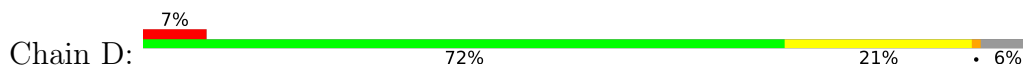
- Molecule 1: Nicotinate (Nicotinamide) nucleotide adenylyltransferase



- Molecule 1: Nicotinate (Nicotinamide) nucleotide adenylyltransferase



- Molecule 1: Nicotinate (Nicotinamide) nucleotide adenylyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.07Å 100.59Å 73.07Å 90.00° 110.42° 90.00°	Depositor
Resolution (Å)	25.15 – 2.30 25.15 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.4 (25.15-2.30) 92.9 (25.15-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.28Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.227 , 0.264 0.228 , 0.262	Depositor DCC
$R_{free}$ test set	1857 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtrriage
Anisotropy	0.630	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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	0.37	0/1578	0.59	0/2143
1	B	0.35	0/1584	0.59	0/2151
1	C	0.34	0/1578	0.58	0/2143
1	D	0.37	0/1592	0.59	0/2161
All	All	0.36	0/6332	0.59	0/8598

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	1536	0	1538	53	0
1	B	1542	0	1543	55	0
1	C	1536	0	1538	39	0
1	D	1550	0	1555	36	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	0	2	0
3	C	27	0	0	0	0
3	D	37	0	0	0	0
All	All	6333	0	6174	175	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 14.

All (175) 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:B:132:ALA:HB2	1:B:138:LEU:HD11	1.49	0.93
1:C:80:LYS:H	1:C:80:LYS:HE2	1.33	0.93
1:A:157:SER:OG	1:D:139:ARG:HD3	1.75	0.86
1:A:109:MET:CE	1:A:112:TYR:HB2	2.07	0.84
1:B:161:GLU:O	1:B:165:GLU:HG2	1.78	0.84
1:D:131:VAL:HG13	1:D:149:ILE:HD12	1.63	0.80
1:A:109:MET:HE3	1:A:112:TYR:HB2	1.65	0.79
1:D:138:LEU:HD22	1:D:138:LEU:H	1.48	0.78
1:D:2:ARG:HB3	1:D:2:ARG:NH2	1.98	0.78
1:B:131:VAL:HG13	1:B:149:ILE:HD12	1.66	0.78
1:D:113:LEU:O	1:D:119:ILE:HD12	1.84	0.77
1:C:134:PRO:HA	1:C:148:GLU:OE1	1.88	0.74
1:D:2:ARG:HB3	1:D:2:ARG:HH21	1.51	0.74
1:A:87:ASP:O	1:A:91:GLN:HG2	1.88	0.74
1:B:110:VAL:HG21	1:B:138:LEU:HD23	1.69	0.73
1:A:36:PHE:O	1:A:38:PRO:HD3	1.91	0.71
1:B:112:TYR:CE1	1:B:115:LYS:HD3	2.26	0.71
1:A:40:GLN:HE21	1:A:41:ILE:H	1.39	0.70
1:C:80:LYS:H	1:C:80:LYS:CE	2.02	0.70
1:D:43:PRO:HA	1:D:46:GLN:HG2	1.73	0.69
1:B:138:LEU:N	1:B:138:LEU:HD12	2.07	0.69
1:B:188:GLU:O	1:B:189:SER:HB2	1.92	0.69
1:B:132:ALA:O	1:B:148:GLU:HA	1.95	0.67
1:B:24:GLU:HG3	1:B:149:ILE:HG23	1.76	0.66
1:D:87:ASP:O	1:D:91:GLN:HG2	1.96	0.66
1:C:113:LEU:N	1:C:114:PRO:HD2	2.11	0.66
1:C:37:LEU:HD12	1:C:73:CYS:O	1.95	0.66
1:A:113:LEU:N	1:A:114:PRO:HD2	2.12	0.65
1:C:90:LEU:O	1:C:93:THR:HG22	1.96	0.65
1:D:132:ALA:HB2	1:D:138:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG21	1:B:138:LEU:CD2	2.26	0.65
1:A:40:GLN:NE2	1:A:56:ARG:HH22	1.94	0.65
1:C:32:GLU:HG3	1:C:33:GLU:HG2	1.79	0.65
1:B:80:LYS:HG2	1:B:81:GLY:N	2.13	0.63
1:C:23:ASN:ND2	1:D:170:LYS:HD3	2.14	0.63
1:A:109:MET:CE	1:A:116:TRP:HE1	2.10	0.62
1:C:80:LYS:HE2	1:C:80:LYS:N	2.11	0.62
1:D:131:VAL:CG1	1:D:149:ILE:HD12	2.30	0.62
1:D:24:GLU:HG3	1:D:149:ILE:HG23	1.81	0.61
1:A:157:SER:O	1:A:161:GLU:HG2	2.01	0.61
1:A:161:GLU:HG3	1:D:139:ARG:HH22	1.64	0.61
1:A:138:LEU:HD23	1:A:146:THR:OG1	2.00	0.61
1:A:2:ARG:HB3	1:A:2:ARG:NH2	2.16	0.60
1:D:4:ILE:HD12	1:D:33:GLU:HG3	1.82	0.60
1:A:109:MET:HE1	1:A:112:TYR:HB2	1.83	0.59
1:D:2:ARG:HH22	1:D:100:GLN:HB2	1.66	0.59
1:D:43:PRO:HA	1:D:46:GLN:CG	2.32	0.59
1:A:137:LYS:HE2	1:C:139:ARG:HG3	1.84	0.59
1:B:123:LEU:HD23	1:B:123:LEU:O	2.03	0.59
1:C:48:ARG:HG3	1:C:49:ASN:OD1	2.02	0.58
1:B:46:GLN:O	1:B:46:GLN:HG3	2.04	0.58
1:B:12:ASP:HB2	1:B:56:ARG:HD3	1.85	0.57
1:A:185:GLY:HA2	1:A:188:GLU:OE2	2.05	0.57
1:D:100:GLN:HE21	1:D:102:HIS:CE1	2.23	0.57
1:D:132:ALA:HB2	1:D:138:LEU:CD2	2.36	0.56
1:B:133:ARG:HG2	1:B:136:TYR:HB3	1.88	0.55
1:A:160:ARG:O	1:A:164:LYS:HG3	2.07	0.54
1:C:79:ARG:NE	1:C:91:GLN:HG2	2.22	0.54
1:C:174:PRO:O	1:C:178:GLN:HG3	2.09	0.53
1:D:133:ARG:HH11	1:D:133:ARG:HB2	1.74	0.53
1:B:42:PRO:HB2	1:B:44:HIS:CE1	2.43	0.53
1:A:32:GLU:O	1:A:33:GLU:HG3	2.09	0.53
1:B:175:GLU:HA	1:B:175:GLU:OE1	2.09	0.53
1:B:50:ILE:HG13	3:B:212:HOH:O	2.08	0.52
1:A:46:GLN:HA	1:A:50:ILE:HD13	1.90	0.52
1:B:50:ILE:HG12	1:B:51:THR:N	2.25	0.52
1:C:123:LEU:HD11	1:C:142:TYR:HD2	1.74	0.52
1:B:109:MET:O	1:B:109:MET:HG2	2.09	0.51
1:B:158:LEU:C	1:B:158:LEU:HD23	2.30	0.51
1:D:26:TYR:HA	1:D:31:LEU:HD12	1.91	0.51
1:B:7:ILE:CG1	1:B:104:ILE:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:O	1:B:123:LEU:HB2	2.10	0.51
1:D:113:LEU:N	1:D:114:PRO:HD2	2.26	0.51
1:A:109:MET:HE2	1:A:116:TRP:NE1	2.25	0.51
1:B:114:PRO:HG3	1:B:142:TYR:CE2	2.46	0.51
1:A:2:ARG:O	1:A:99:VAL:HG13	2.12	0.50
1:D:41:ILE:HG21	1:D:50:ILE:HD11	1.94	0.50
1:C:37:LEU:HD21	1:C:88:THR:HG21	1.93	0.50
1:C:123:LEU:HD11	1:C:142:TYR:CD2	2.46	0.50
1:D:159:LEU:HD13	1:D:173:LEU:HD13	1.92	0.50
1:A:42:PRO:O	1:A:46:GLN:HG3	2.12	0.50
1:B:12:ASP:HB2	1:B:56:ARG:CD	2.42	0.50
1:B:57:LEU:O	1:B:61:GLU:HG3	2.11	0.49
1:A:140:THR:HG21	1:A:144:ILE:HG22	1.93	0.49
1:B:113:LEU:C	1:B:115:LYS:H	2.14	0.49
1:C:131:VAL:HG13	1:C:149:ILE:HD12	1.94	0.49
1:B:144:ILE:O	1:B:144:ILE:HG23	2.12	0.49
1:A:138:LEU:HD22	1:A:138:LEU:N	2.28	0.49
1:A:40:GLN:HE21	1:A:56:ARG:HH22	1.59	0.49
1:B:57:LEU:HD22	1:B:74:LEU:HD21	1.95	0.49
1:C:89:MET:CE	1:C:126:VAL:HG11	2.43	0.49
1:C:132:ALA:O	1:C:148:GLU:HA	2.12	0.48
1:A:140:THR:CG2	1:A:144:ILE:HG22	2.43	0.48
1:C:65:GLU:OE2	1:C:176:LYS:HE2	2.14	0.48
1:C:79:ARG:CZ	1:C:91:GLN:HG2	2.44	0.48
1:C:112:TYR:C	1:C:114:PRO:HD2	2.34	0.48
1:D:3:LYS:O	1:D:4:ILE:HD13	2.14	0.48
1:A:109:MET:HE1	1:A:116:TRP:HE1	1.77	0.47
1:A:140:THR:HG21	1:A:144:ILE:CG2	2.45	0.47
1:A:79:ARG:C	1:A:81:GLY:H	2.18	0.47
1:A:132:ALA:O	1:A:148:GLU:HA	2.15	0.47
1:B:138:LEU:HD12	1:B:138:LEU:H	1.77	0.47
1:A:2:ARG:HB3	1:A:2:ARG:CZ	2.45	0.47
1:A:113:LEU:N	1:A:114:PRO:CD	2.78	0.47
1:B:110:VAL:CG2	1:B:138:LEU:HD23	2.41	0.46
1:B:113:LEU:C	1:B:115:LYS:N	2.68	0.46
1:A:140:THR:OG1	1:A:141:PRO:HD2	2.15	0.46
1:B:74:LEU:HD22	1:B:77:LEU:HD22	1.97	0.46
1:B:69:HIS:HE1	3:B:231:HOH:O	1.97	0.46
1:B:173:LEU:HD23	1:B:173:LEU:N	2.31	0.46
1:A:102:HIS:HA	1:A:127:THR:O	2.15	0.46
1:A:119:ILE:O	1:A:123:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLU:O	1:D:114:PRO:HD2	2.16	0.45
1:B:80:LYS:CG	1:B:81:GLY:N	2.79	0.45
1:B:114:PRO:HG3	1:B:142:TYR:OH	2.16	0.45
1:B:115:LYS:HG2	1:B:115:LYS:O	2.17	0.45
1:C:80:LYS:H	1:C:80:LYS:CD	2.28	0.45
1:B:113:LEU:O	1:B:115:LYS:N	2.50	0.45
1:B:131:VAL:CG1	1:B:149:ILE:HD12	2.42	0.45
1:C:24:GLU:HG3	1:C:149:ILE:HG23	1.98	0.45
1:A:40:GLN:HE22	1:A:56:ARG:HH12	1.64	0.44
1:A:67:GLU:OE1	1:B:170:LYS:NZ	2.51	0.44
1:A:24:GLU:HG3	1:A:149:ILE:HG23	1.99	0.44
1:B:138:LEU:N	1:B:138:LEU:CD1	2.78	0.44
1:B:174:PRO:HB2	1:B:177:VAL:HG23	1.98	0.44
1:C:75:GLU:OE2	1:C:95:LYS:NZ	2.46	0.44
1:A:109:MET:HE2	1:A:116:TRP:HE1	1.75	0.44
1:A:157:SER:CB	1:D:139:ARG:HD3	2.47	0.44
1:B:118:ASN:HD22	1:B:118:ASN:HA	1.61	0.44
1:D:140:THR:OG1	1:D:141:PRO:HD2	2.18	0.44
1:A:112:TYR:C	1:A:114:PRO:HD2	2.37	0.44
1:B:185:GLY:HA2	1:B:188:GLU:OE2	2.17	0.44
1:D:133:ARG:HB2	1:D:133:ARG:NH1	2.33	0.44
1:D:38:PRO:HG3	1:D:60:LEU:CD2	2.47	0.44
1:B:139:ARG:NH1	1:C:160:ARG:HH11	2.15	0.43
1:D:2:ARG:NH2	1:D:100:GLN:HB2	2.33	0.43
1:D:186:LEU:HD23	1:D:186:LEU:N	2.33	0.43
1:B:46:GLN:O	1:B:46:GLN:CG	2.65	0.43
1:A:111:GLU:HA	1:A:111:GLU:OE1	2.19	0.43
1:D:132:ALA:O	1:D:148:GLU:HA	2.18	0.43
1:B:119:ILE:HG23	1:B:120:GLU:N	2.34	0.42
1:C:119:ILE:CG2	1:C:120:GLU:N	2.82	0.42
1:C:160:ARG:O	1:C:164:LYS:HG3	2.18	0.42
1:A:148:GLU:OE2	1:C:139:ARG:HD3	2.19	0.42
1:C:113:LEU:N	1:C:114:PRO:CD	2.81	0.42
1:A:75:GLU:HG3	1:A:92:LEU:CD2	2.49	0.42
1:C:113:LEU:O	1:C:119:ILE:HG13	2.20	0.42
1:A:53:VAL:HG13	1:A:77:LEU:HD21	2.01	0.42
1:A:108:ASP:HB2	3:A:220:HOH:O	2.19	0.42
1:C:12:ASP:HB2	1:C:56:ARG:HD3	2.02	0.42
1:D:109:MET:SD	1:D:112:TYR:HB2	2.60	0.42
1:D:4:ILE:HG12	1:D:99:VAL:HG13	2.01	0.42
1:B:114:PRO:HG3	1:B:142:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:O	1:A:81:GLY:N	2.53	0.41
1:B:158:LEU:HD23	1:B:158:LEU:O	2.20	0.41
1:C:108:ASP:OD1	1:C:109:MET:N	2.52	0.41
1:A:90:LEU:HG	1:A:94:LYS:HE2	2.02	0.41
1:C:79:ARG:HG2	1:C:79:ARG:NH2	2.35	0.41
1:A:4:ILE:CD1	1:A:33:GLU:HB2	2.50	0.41
1:C:158:LEU:C	1:C:158:LEU:HD23	2.41	0.41
1:A:4:ILE:HD12	1:A:33:GLU:HB2	2.01	0.41
1:A:13:PRO:HB2	1:A:14:PRO:HD2	2.02	0.41
1:A:67:GLU:HG3	1:A:70:PHE:CE2	2.56	0.41
1:D:79:ARG:HH21	1:D:79:ARG:HG3	1.85	0.41
1:B:76:GLU:HG3	1:B:88:THR:OG1	2.21	0.40
1:B:36:PHE:O	1:B:38:PRO:HD3	2.21	0.40
1:B:142:TYR:HA	1:B:143:PRO:HD3	1.93	0.40
1:C:119:ILE:O	1:C:119:ILE:HD13	2.22	0.40
1:A:81:GLY:HA2	1:A:82:PRO:HD3	1.94	0.40
1:C:51:THR:HG22	1:C:52:SER:O	2.22	0.40
1:B:42:PRO:HG2	1:B:45:LYS:HB3	2.03	0.40
1:B:107:GLY:HA3	1:B:131:VAL:O	2.21	0.40
1:C:89:MET:HE2	1:C:126:VAL:HG11	2.02	0.40
1:C:110:VAL:O	1:C:110:VAL:HG12	2.21	0.40
1:D:188:GLU:O	1:D:189:SER:HB2	2.22	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	185/201 (92%)	179 (97%)	5 (3%)	1 (0%)	29	35
1	B	186/201 (92%)	170 (91%)	15 (8%)	1 (0%)	29	35
1	C	185/201 (92%)	176 (95%)	8 (4%)	1 (0%)	29	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	187/201 (93%)	176 (94%)	11 (6%)	0	100	100
All	All	743/804 (92%)	701 (94%)	39 (5%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	80	LYS
1	A	80	LYS
1	B	81	GLY

### 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	169/180 (94%)	166 (98%)	3 (2%)	59	75
1	B	170/180 (94%)	164 (96%)	6 (4%)	36	50
1	C	169/180 (94%)	162 (96%)	7 (4%)	30	43
1	D	171/180 (95%)	164 (96%)	7 (4%)	30	43
All	All	679/720 (94%)	656 (97%)	23 (3%)	37	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	113	LEU
1	A	124	ASP
1	B	2	ARG
1	B	13	PRO
1	B	58	GLN
1	B	67	GLU
1	B	138	LEU
1	B	175	GLU
1	C	61	GLU
1	C	69	HIS

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Mol	Chain	Res	Type
1	C	80	LYS
1	C	118	ASN
1	C	119	ILE
1	C	139	ARG
1	C	161	GLU
1	D	13	PRO
1	D	68	GLU
1	D	69	HIS
1	D	123	LEU
1	D	133	ARG
1	D	138	LEU
1	D	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	40	GLN
1	B	27	HIS
1	B	30	ASN
1	B	39	ASN
1	B	69	HIS
1	B	118	ASN
1	B	184	ASN
1	C	23	ASN
1	C	30	ASN
1	C	39	ASN
1	C	44	HIS
1	C	91	GLN
1	C	178	GLN
1	D	39	ASN
1	D	49	ASN
1	D	102	HIS
1	D	178	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	D	203	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	202	-	4,4,4	0.29	0	6,6,6	0.12	0
2	SO4	B	203	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	B	202	-	4,4,4	0.31	0	6,6,6	0.05	0
2	SO4	C	203	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	A	202	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	D	202	-	4,4,4	0.24	0	6,6,6	0.20	0
2	SO4	A	203	-	4,4,4	0.28	0	6,6,6	0.08	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

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	187/201 (93%)	0.24	4 (2%) 63 70	22, 39, 65, 76	0
1	B	188/201 (93%)	0.71	24 (12%) 3 5	19, 42, 85, 111	0
1	C	187/201 (93%)	0.35	5 (2%) 54 62	25, 41, 65, 82	0
1	D	189/201 (94%)	0.44	15 (7%) 12 17	18, 38, 72, 92	0
All	All	751/804 (93%)	0.44	48 (6%) 19 25	18, 40, 75, 111	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	TYR	5.8
1	B	48	ARG	5.1
1	B	46	GLN	4.9
1	B	139	ARG	4.8
1	D	138	LEU	4.8
1	B	138	LEU	4.6
1	B	112	TYR	4.4
1	B	141	PRO	4.4
1	B	136	TYR	4.2
1	B	143	PRO	4.2
1	B	109	MET	3.9
1	B	49	ASN	3.7
1	B	111	GLU	3.6
1	D	112	TYR	3.6
1	B	44	HIS	3.6
1	B	47	GLY	3.5
1	A	80	LYS	3.4
1	D	139	ARG	3.3
1	D	49	ASN	3.0
1	B	142	TYR	3.0
1	D	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	189	SER	2.9
1	B	135	GLY	2.8
1	C	121	ALA	2.8
1	B	113	LEU	2.8
1	D	141	PRO	2.8
1	B	45	LYS	2.7
1	D	140	THR	2.7
1	B	144	ILE	2.6
1	D	79	ARG	2.6
1	D	137	LYS	2.6
1	C	2	ARG	2.5
1	D	165	GLU	2.5
1	D	109	MET	2.3
1	B	189	SER	2.3
1	B	50	ILE	2.3
1	C	97	PRO	2.3
1	D	80	LYS	2.3
1	B	120	GLU	2.2
1	B	6	ILE	2.2
1	C	115	LYS	2.2
1	B	124	ASP	2.2
1	A	48	ARG	2.1
1	A	69	HIS	2.1
1	B	137	LYS	2.1
1	C	66	ALA	2.1
1	A	165	GLU	2.0
1	D	188	GLU	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
2	SO4	A	202	5/5	0.98	0.12	36,46,48,50	0
2	SO4	A	203	5/5	0.98	0.10	57,57,59,59	0
2	SO4	B	202	5/5	0.98	0.11	33,37,37,41	0
2	SO4	B	203	5/5	0.98	0.13	41,47,49,51	0
2	SO4	C	202	5/5	0.98	0.12	46,46,54,54	0
2	SO4	C	203	5/5	0.98	0.08	48,49,50,51	0
2	SO4	D	202	5/5	0.98	0.13	30,30,32,44	0
2	SO4	D	203	5/5	0.98	0.09	51,53,57,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.