



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:06 pm BST

PDB ID : 2PZB
Title : NAD⁺ Synthetase from *Bacillus anthracis*
Authors : McDonald, H.M.; Pruetz, P.S.; Deivanayagam, C.; Protasevich, I.I.; Carson, W.M.; DeLucas, L.J.; Brouillette, W.J.; Brouillette, C.G.
Deposited on : 2007-05-17
Resolution : 1.90 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 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 : 2.11
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) : 2.11

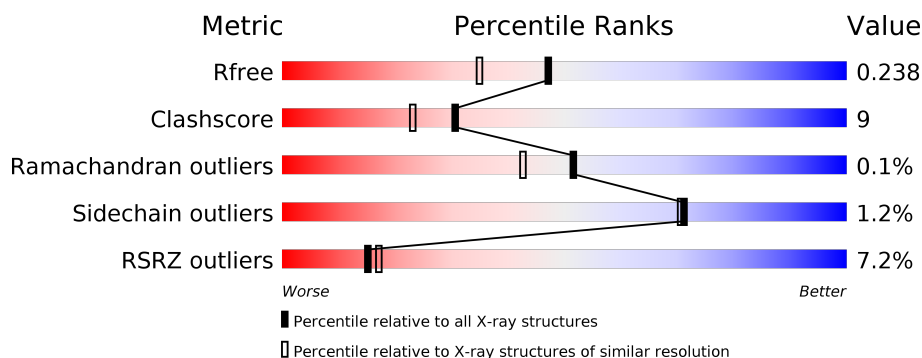
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 ≥ 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	284	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>12%</div> </div> </div>
1	B	284	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>12%</div> </div> </div>
1	C	284	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>13%</div> </div> </div>
1	D	284	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8319 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 NH(3)-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1955	1241	337	373	4			
1	B	249	Total	C	N	O	S	0	0	0
			1948	1236	336	372	4			
1	C	247	Total	C	N	O	S	0	0	0
			1931	1226	334	368	3			
1	D	250	Total	C	N	O	S	0	0	0
			1947	1236	335	372	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	LEU	-	CLONING ARTIFACT	UNP Q81RP3
A	274	ALA	-	CLONING ARTIFACT	UNP Q81RP3
A	275	ALA	-	CLONING ARTIFACT	UNP Q81RP3
A	276	ALA	-	CLONING ARTIFACT	UNP Q81RP3
A	277	LEU	-	CLONING ARTIFACT	UNP Q81RP3
A	278	GLU	-	CLONING ARTIFACT	UNP Q81RP3
A	279	HIS	-	CLONING ARTIFACT	UNP Q81RP3
A	280	HIS	-	CLONING ARTIFACT	UNP Q81RP3
A	281	HIS	-	CLONING ARTIFACT	UNP Q81RP3
A	282	HIS	-	CLONING ARTIFACT	UNP Q81RP3
A	283	HIS	-	CLONING ARTIFACT	UNP Q81RP3
A	284	HIS	-	CLONING ARTIFACT	UNP Q81RP3
B	273	LEU	-	CLONING ARTIFACT	UNP Q81RP3
B	274	ALA	-	CLONING ARTIFACT	UNP Q81RP3
B	275	ALA	-	CLONING ARTIFACT	UNP Q81RP3
B	276	ALA	-	CLONING ARTIFACT	UNP Q81RP3
B	277	LEU	-	CLONING ARTIFACT	UNP Q81RP3
B	278	GLU	-	CLONING ARTIFACT	UNP Q81RP3
B	279	HIS	-	CLONING ARTIFACT	UNP Q81RP3
B	280	HIS	-	CLONING ARTIFACT	UNP Q81RP3
B	281	HIS	-	CLONING ARTIFACT	UNP Q81RP3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	CLONING ARTIFACT	UNP Q81RP3
B	283	HIS	-	CLONING ARTIFACT	UNP Q81RP3
B	284	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	273	LEU	-	CLONING ARTIFACT	UNP Q81RP3
C	274	ALA	-	CLONING ARTIFACT	UNP Q81RP3
C	275	ALA	-	CLONING ARTIFACT	UNP Q81RP3
C	276	ALA	-	CLONING ARTIFACT	UNP Q81RP3
C	277	LEU	-	CLONING ARTIFACT	UNP Q81RP3
C	278	GLU	-	CLONING ARTIFACT	UNP Q81RP3
C	279	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	280	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	281	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	282	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	283	HIS	-	CLONING ARTIFACT	UNP Q81RP3
C	284	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	273	LEU	-	CLONING ARTIFACT	UNP Q81RP3
D	274	ALA	-	CLONING ARTIFACT	UNP Q81RP3
D	275	ALA	-	CLONING ARTIFACT	UNP Q81RP3
D	276	ALA	-	CLONING ARTIFACT	UNP Q81RP3
D	277	LEU	-	CLONING ARTIFACT	UNP Q81RP3
D	278	GLU	-	CLONING ARTIFACT	UNP Q81RP3
D	279	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	280	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	281	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	282	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	283	HIS	-	CLONING ARTIFACT	UNP Q81RP3
D	284	HIS	-	CLONING ARTIFACT	UNP Q81RP3

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

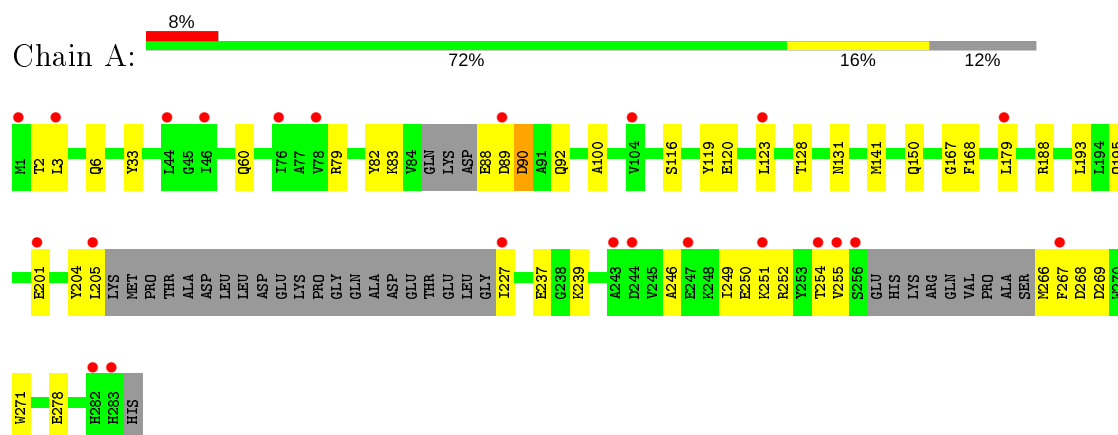
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	124	Total 124	O 124	0	0
3	C	104	Total 104	O 104	0	0
3	D	127	Total 127	O 127	0	0

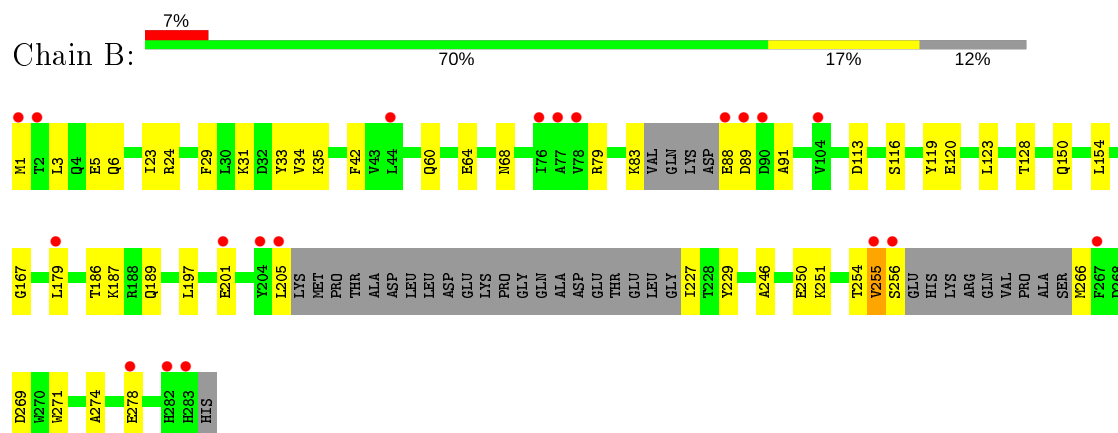
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

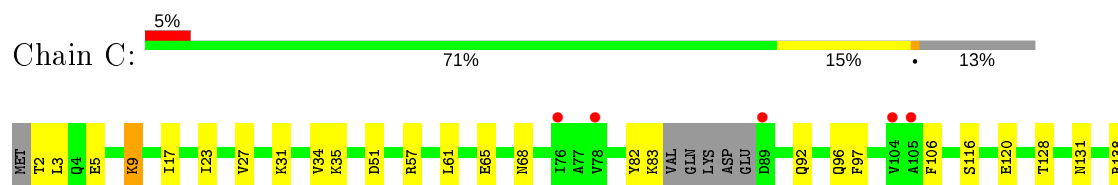
- Molecule 1: NH(3)-dependent NAD(+) synthetase

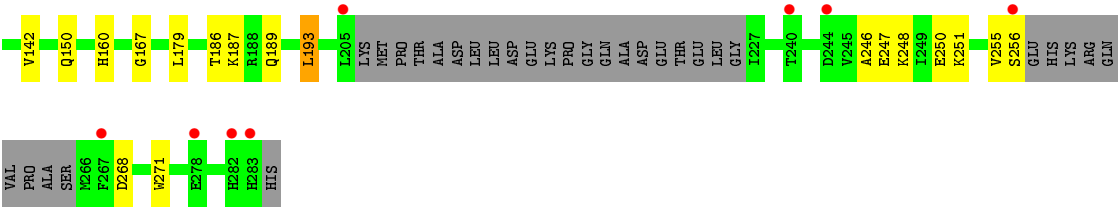


- Molecule 1: NH(3)-dependent NAD(+) synthetase

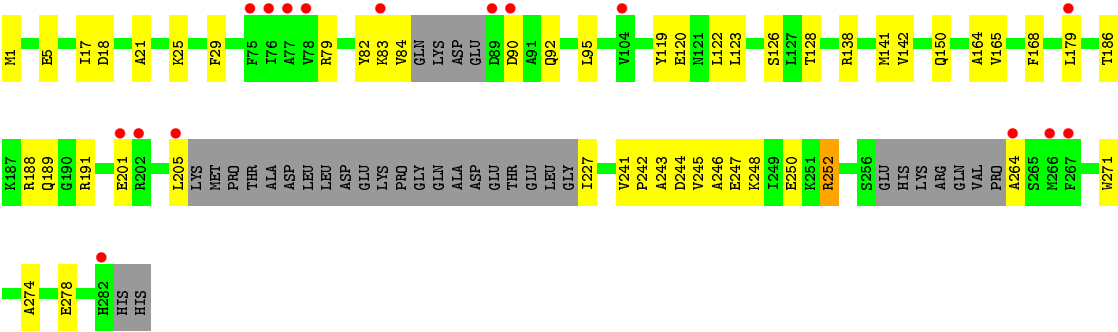


- Molecule 1: NH(3)-dependent NAD(+) synthetase





● Molecule 1: NH(3)-dependent NAD(+) synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.42Å 84.55Å 245.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.10 – 1.90 36.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (36.10-1.90) 94.6 (36.09-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.63	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.237 0.219 , 0.238	Depositor DCC
R_{free} test set	12582 reflections (9.54%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8319	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	0.32	0/1986	0.54	0/2678
1	B	0.32	0/1979	0.53	0/2668
1	C	0.32	0/1962	0.52	0/2646
1	D	0.32	0/1977	0.53	0/2666
All	All	0.32	0/7904	0.53	0/10658

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	1955	0	1946	43	0
1	B	1948	0	1937	40	0
1	C	1931	0	1919	35	0
1	D	1947	0	1943	40	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	123	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	124	0	0	1	0
3	C	104	0	0	3	0
3	D	127	0	0	4	0
All	All	8319	0	7745	143	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 9.

All (143) 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:79:ARG:HH11	1:B:88:GLU:HG3	1.40	0.85
1:A:131:ASN:HD22	1:B:150:GLN:HE21	1.25	0.84
1:C:131:ASN:HD22	1:D:150:GLN:HE21	1.25	0.83
1:C:248:LYS:HA	1:C:251:LYS:HE2	1.63	0.80
1:A:88:GLU:HG2	1:A:90:ASP:H	1.44	0.80
1:B:79:ARG:NH1	1:B:88:GLU:HG3	1.99	0.78
1:D:188:ARG:HA	1:D:191:ARG:NH1	1.99	0.78
1:A:141:MET:HE3	3:A:4816:HOH:O	1.86	0.76
1:A:246:ALA:O	1:A:250:GLU:HG3	1.86	0.76
1:B:274:ALA:O	1:B:278:GLU:HG2	1.86	0.76
1:D:243:ALA:O	1:D:247:GLU:HG3	1.86	0.75
1:C:2:THR:HG23	1:C:5:GLU:H	1.54	0.72
1:A:131:ASN:HD22	1:B:150:GLN:NE2	1.85	0.72
1:C:131:ASN:HD22	1:D:150:GLN:NE2	1.87	0.72
1:C:150:GLN:HE22	1:D:128:THR:H	1.36	0.72
1:A:128:THR:H	1:B:150:GLN:HE22	1.37	0.71
1:C:128:THR:H	1:D:150:GLN:HE22	1.39	0.70
1:D:252:ARG:HD2	1:D:271:TRP:CH2	2.26	0.70
1:A:150:GLN:HE22	1:B:128:THR:H	1.39	0.70
1:D:246:ALA:O	1:D:250:GLU:HG3	1.92	0.68
1:B:255:VAL:O	1:B:255:VAL:HG12	1.95	0.67
1:A:119:TYR:CZ	1:A:123:LEU:HD22	2.30	0.67
1:B:88:GLU:HB3	1:B:91:ALA:HB3	1.76	0.66
1:D:21:ALA:O	1:D:25:LYS:HG2	1.95	0.66
1:A:239:LYS:HE3	3:D:4875:HOH:O	1.95	0.65
1:B:119:TYR:CE2	1:B:123:LEU:HD13	2.31	0.65
1:A:3:LEU:HD23	1:A:250:GLU:HB3	1.78	0.64
1:C:189:GLN:O	1:C:193:LEU:HD23	1.98	0.64
1:B:116:SER:O	1:B:120:GLU:HG3	1.99	0.62
1:A:33:TYR:CG	1:A:179:LEU:HD21	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:THR:OG1	1:D:189:GLN:HG3	1.99	0.62
1:B:251:LYS:O	1:B:255:VAL:HG23	2.00	0.61
1:D:119:TYR:CE2	1:D:123:LEU:HD13	2.35	0.61
1:B:187:LYS:HG3	1:B:229:TYR:CE2	2.36	0.60
1:C:247:GLU:O	1:C:251:LYS:HG2	2.02	0.59
1:C:160:HIS:HD2	1:C:268:ASP:OD2	1.86	0.59
1:A:141:MET:CE	3:A:4783:HOH:O	2.50	0.58
1:A:119:TYR:OH	1:A:123:LEU:HD22	2.04	0.58
1:B:246:ALA:O	1:B:250:GLU:HG3	2.04	0.58
1:C:17:ILE:HD13	1:C:189:GLN:HB3	1.85	0.58
1:C:23:ILE:O	1:C:27:VAL:HG23	2.04	0.57
1:D:241:VAL:HB	1:D:242:PRO:HD2	1.85	0.57
1:D:274:ALA:O	1:D:278:GLU:HG3	2.05	0.56
1:B:31:LYS:O	1:B:35:LYS:HG2	2.04	0.56
1:B:1:MET:CE	1:B:6:GLN:HG2	2.35	0.56
1:A:150:GLN:NE2	1:B:128:THR:H	2.04	0.55
1:C:23:ILE:HG13	1:C:193:LEU:HD13	1.89	0.55
1:B:254:THR:C	1:B:256:SER:H	2.10	0.55
1:A:251:LYS:O	1:A:255:VAL:HG23	2.07	0.55
1:A:167:GLY:HA2	1:A:271:TRP:CD1	2.42	0.55
1:C:186:THR:OG1	1:C:189:GLN:HG3	2.07	0.55
1:D:242:PRO:HG2	1:D:245:VAL:CG2	2.37	0.55
1:D:1:MET:HG3	1:D:5:GLU:HB2	1.88	0.54
1:B:24:ARG:HD3	1:B:24:ARG:O	2.07	0.54
1:C:92:GLN:O	1:C:96:GLN:HG3	2.07	0.54
1:D:92:GLN:HG2	3:D:4894:HOH:O	2.07	0.54
1:A:141:MET:HE1	3:A:4783:HOH:O	2.07	0.54
1:D:18:ASP:HB3	1:D:21:ALA:HB3	1.90	0.54
1:A:33:TYR:HB3	1:A:179:LEU:HD11	1.89	0.54
1:A:128:THR:H	1:B:150:GLN:NE2	2.05	0.53
1:D:17:ILE:HD13	1:D:189:GLN:HB3	1.91	0.53
1:B:201:GLU:HB3	1:B:205:LEU:HD12	1.92	0.52
1:D:141:MET:CE	3:D:4809:HOH:O	2.57	0.52
1:C:246:ALA:O	1:C:250:GLU:HG3	2.09	0.51
1:C:116:SER:O	1:C:120:GLU:HG3	2.10	0.51
1:C:128:THR:H	1:D:150:GLN:NE2	2.08	0.51
1:C:82:TYR:O	1:C:83:LYS:HB2	2.10	0.51
1:C:3:LEU:HD23	1:C:250:GLU:HB3	1.93	0.51
1:B:1:MET:HG3	1:B:5:GLU:HB2	1.92	0.50
1:D:120:GLU:HG2	1:D:126:SER:HA	1.93	0.49
1:A:251:LYS:O	1:A:254:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ALA:O	1:D:25:LYS:HE2	2.12	0.49
1:D:82:TYR:O	1:D:83:LYS:HB2	2.13	0.49
1:A:168:PHE:CZ	1:A:252:ARG:HD3	2.47	0.49
1:D:201:GLU:CG	1:D:205:LEU:HD12	2.43	0.49
1:A:195:GLN:HG2	1:A:204:TYR:OH	2.14	0.48
1:A:3:LEU:HB3	1:A:250:GLU:OE1	2.14	0.48
1:A:266:MET:HB3	1:A:269:ASP:OD2	2.13	0.48
1:D:138:ARG:O	1:D:142:VAL:HG23	2.12	0.48
1:C:150:GLN:NE2	1:D:128:THR:H	2.07	0.47
1:B:60:GLN:O	1:B:64:GLU:HG3	2.13	0.47
1:D:201:GLU:HG2	1:D:205:LEU:HD12	1.96	0.47
1:C:256:SER:HB2	3:C:4884:HOH:O	2.14	0.47
1:A:2:THR:O	1:A:6:GLN:HG3	2.14	0.47
1:C:57:ARG:HG2	1:C:97:PHE:CZ	2.49	0.47
1:C:9:LYS:NZ	1:C:9:LYS:HB3	2.29	0.47
1:A:88:GLU:OE1	1:A:90:ASP:HB2	2.15	0.47
1:B:266:MET:HB3	1:B:269:ASP:OD2	2.15	0.47
1:B:3:LEU:HD23	1:B:250:GLU:HB3	1.97	0.47
1:D:25:LYS:HD3	1:D:25:LYS:N	2.30	0.46
1:C:61:LEU:O	1:C:65:GLU:HG3	2.16	0.46
1:A:131:ASN:ND2	1:B:150:GLN:HE21	2.03	0.46
1:C:179:LEU:HD23	1:C:179:LEU:N	2.31	0.46
1:C:138:ARG:O	1:C:142:VAL:HG23	2.16	0.46
1:B:186:THR:OG1	1:B:189:GLN:HG3	2.15	0.46
1:B:34:VAL:HG23	1:B:42:PHE:CZ	2.50	0.46
1:A:33:TYR:CB	1:A:179:LEU:HD11	2.46	0.45
1:B:167:GLY:HA2	1:B:271:TRP:CD1	2.51	0.45
1:B:23:ILE:HD13	1:B:197:LEU:HD21	1.98	0.45
1:C:248:LYS:HB2	1:C:248:LYS:HE3	1.81	0.45
1:B:29:PHE:CZ	1:B:179:LEU:HD11	2.51	0.45
1:D:164:ALA:HA	1:D:168:PHE:O	2.16	0.45
1:A:82:TYR:O	1:A:83:LYS:HB2	2.17	0.45
1:B:3:LEU:CD2	1:B:250:GLU:HB3	2.47	0.45
1:B:227:ILE:N	3:B:4842:HOH:O	2.50	0.45
1:D:227:ILE:N	3:D:4859:HOH:O	2.50	0.44
1:D:244:ASP:O	1:D:248:LYS:HG3	2.18	0.44
1:A:188:ARG:HG2	1:A:237:GLU:OE1	2.17	0.44
1:A:201:GLU:HB2	1:A:205:LEU:HD12	2.00	0.44
1:A:88:GLU:HG2	1:A:89:ASP:N	2.32	0.44
1:A:128:THR:HG23	1:B:150:GLN:HE22	1.83	0.44
1:D:17:ILE:CD1	1:D:189:GLN:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CG	1:B:179:LEU:HD13	2.53	0.44
1:C:167:GLY:HA2	1:C:271:TRP:CD1	2.53	0.43
1:C:51:ASP:OD1	1:C:187:LYS:HE2	2.18	0.43
1:A:266:MET:HG3	1:A:268:ASP:H	1.83	0.43
1:D:29:PHE:CE2	1:D:179:LEU:HG	2.53	0.43
1:D:79:ARG:HG3	1:D:95:LEU:HD11	2.00	0.43
1:A:267:PHE:HD1	1:A:267:PHE:H	1.66	0.43
1:C:255:VAL:O	1:C:256:SER:HB3	2.18	0.43
1:C:106:PHE:HA	1:D:122:LEU:CD1	2.49	0.43
1:B:83:LYS:NZ	1:B:113:ASP:OD2	2.52	0.42
1:A:79:ARG:NH1	1:A:92:GLN:HE22	2.17	0.42
1:B:1:MET:HE2	1:B:6:GLN:HG2	1.99	0.42
1:C:68:ASN:ND2	3:C:4861:HOH:O	2.53	0.42
1:D:165:VAL:HG13	1:D:264:ALA:O	2.19	0.42
1:D:252:ARG:HD2	1:D:271:TRP:CZ2	2.55	0.42
1:A:116:SER:O	1:A:120:GLU:HG3	2.19	0.42
1:D:227:ILE:HD11	1:D:248:LYS:HD2	2.02	0.42
1:A:79:ARG:HH11	1:A:92:GLN:HE22	1.66	0.42
1:B:1:MET:HG2	1:B:6:GLN:HG3	2.01	0.42
1:C:17:ILE:CD1	1:C:189:GLN:HB3	2.49	0.42
1:A:60:GLN:OE1	1:A:100:ALA:HA	2.20	0.41
1:A:33:TYR:CD2	1:A:179:LEU:HD21	2.55	0.41
1:B:33:TYR:HD2	1:B:154:LEU:HD13	1.84	0.41
1:A:168:PHE:CE2	1:A:252:ARG:HD3	2.56	0.41
1:A:227:ILE:HD13	1:A:249:ILE:HG12	2.01	0.41
1:C:2:THR:N	3:C:4873:HOH:O	2.54	0.41
1:C:31:LYS:O	1:C:35:LYS:HG3	2.20	0.41
1:A:204:TYR:CD1	1:A:205:LEU:HG	2.55	0.41
1:D:227:ILE:HD12	1:D:245:VAL:HG13	2.03	0.41
1:D:83:LYS:O	1:D:84:VAL:HG23	2.21	0.41
1:B:23:ILE:HD13	1:B:197:LEU:CD2	2.51	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	242/284 (85%)	240 (99%)	2 (1%)	0	100	100
1	B	241/284 (85%)	238 (99%)	2 (1%)	1 (0%)	34	24
1	C	239/284 (84%)	234 (98%)	5 (2%)	0	100	100
1	D	242/284 (85%)	238 (98%)	4 (2%)	0	100	100
All	All	964/1136 (85%)	950 (98%)	13 (1%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	VAL

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	202/231 (87%)	199 (98%)	3 (2%)	65	62
1	B	201/231 (87%)	199 (99%)	2 (1%)	76	76
1	C	199/231 (86%)	196 (98%)	3 (2%)	65	62
1	D	201/231 (87%)	199 (99%)	2 (1%)	76	76
All	All	803/924 (87%)	793 (99%)	10 (1%)	71	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	193	LEU
1	A	278	GLU
1	B	68	ASN
1	B	89	ASP
1	C	9	LYS
1	C	34	VAL

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Mol	Chain	Res	Type
1	C	193	LEU
1	D	90	ASP
1	D	252	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	117	ASN
1	A	144	GLN
1	A	150	GLN
1	A	280	HIS
1	A	281	HIS
1	A	282	HIS
1	B	68	ASN
1	B	131	ASN
1	B	150	GLN
1	B	281	HIS
1	B	282	HIS
1	C	68	ASN
1	C	92	GLN
1	C	117	ASN
1	C	150	GLN
1	C	160	HIS
1	D	131	ASN
1	D	144	GLN
1	D	150	GLN
1	D	281	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	C	4776	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	B	4775	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	4780	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	C	4772	-	4,4,4	0.29	0	6,6,6	0.04	0
2	SO4	D	4777	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	A	4778	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	A	4774	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	D	4773	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	A	4770	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	D	4781	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	B	4771	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	B	4779	-	4,4,4	0.28	0	6,6,6	0.15	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, 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	250/284 (88%)	0.50	23 (9%) 9 10	19, 31, 57, 72	0
1	B	249/284 (87%)	0.46	20 (8%) 12 13	19, 33, 58, 71	0
1	C	247/284 (86%)	0.43	13 (5%) 26 29	19, 34, 58, 65	0
1	D	250/284 (88%)	0.40	16 (6%) 19 22	20, 33, 56, 67	0
All	All	996/1136 (87%)	0.45	72 (7%) 15 17	19, 33, 58, 72	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	7.9
1	B	205	LEU	7.2
1	D	205	LEU	6.7
1	C	205	LEU	6.4
1	B	1	MET	5.1
1	A	267	PHE	5.1
1	B	267	PHE	5.1
1	A	255	VAL	4.8
1	C	282	HIS	4.8
1	B	282	HIS	4.6
1	D	89	ASP	4.4
1	D	266	MET	4.4
1	B	88	GLU	4.4
1	B	255	VAL	4.3
1	C	267	PHE	4.0
1	A	254	THR	3.8
1	A	1	MET	3.7
1	B	89	ASP	3.5
1	D	282	HIS	3.4
1	A	256	SER	3.3
1	A	76	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	104	VAL	3.2
1	C	256	SER	3.1
1	D	76	ILE	3.1
1	A	244	ASP	3.0
1	A	104	VAL	3.0
1	B	201	GLU	3.0
1	A	247	GLU	3.0
1	D	264	ALA	3.0
1	A	89	ASP	3.0
1	C	76	ILE	2.9
1	C	89	ASP	2.9
1	A	282	HIS	2.9
1	C	244	ASP	2.9
1	B	104	VAL	2.8
1	C	104	VAL	2.8
1	B	44	LEU	2.8
1	B	77	ALA	2.8
1	B	283	HIS	2.8
1	D	201	GLU	2.8
1	A	78	VAL	2.6
1	B	256	SER	2.6
1	B	179	LEU	2.6
1	D	78	VAL	2.6
1	D	267	PHE	2.6
1	A	179	LEU	2.6
1	A	201	GLU	2.5
1	A	243	ALA	2.5
1	A	283	HIS	2.5
1	C	283	HIS	2.4
1	B	78	VAL	2.4
1	D	90	ASP	2.3
1	D	202	ARG	2.3
1	A	44	LEU	2.3
1	B	204	TYR	2.2
1	A	3	LEU	2.2
1	A	123	LEU	2.2
1	B	76	ILE	2.1
1	B	278	GLU	2.1
1	A	46	ILE	2.1
1	A	227	ILE	2.1
1	D	75	PHE	2.1
1	B	2	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	278	GLU	2.1
1	C	240	THR	2.0
1	C	78	VAL	2.0
1	D	83	LYS	2.0
1	D	179	LEU	2.0
1	C	105	ALA	2.0
1	D	77	ALA	2.0
1	B	90	ASP	2.0
1	A	251	LYS	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. 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(\AA^2)	Q<0.9
2	SO4	C	4772	5/5	0.97	0.10	48,48,50,50	0
2	SO4	A	4778	5/5	0.97	0.12	37,39,42,42	0
2	SO4	C	4780	5/5	0.98	0.12	40,40,42,44	0
2	SO4	D	4773	5/5	0.98	0.11	41,43,45,45	0
2	SO4	D	4781	5/5	0.98	0.09	41,42,44,44	0
2	SO4	B	4771	5/5	0.98	0.07	43,44,46,46	0
2	SO4	A	4774	5/5	0.99	0.09	35,35,37,37	0
2	SO4	B	4775	5/5	0.99	0.10	30,32,34,34	0
2	SO4	A	4770	5/5	0.99	0.08	42,43,46,46	0
2	SO4	D	4777	5/5	0.99	0.09	34,35,39,39	0
2	SO4	C	4776	5/5	0.99	0.07	35,36,39,40	0
2	SO4	B	4779	5/5	0.99	0.09	38,42,44,45	0

6.5 Other polymers

There are no such residues in this entry.