WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 08:36 AM EDT

PDB ID	:	1XL9
Title	:	Crystal Structure of Dihydrodipicolinate Synthase DapA-2 (BA3935) from Bacillus Anthracis.
Authors	:	Blagova, E.; Levdikov, V.; Milioti, N.; Fogg, M.J.; Kalliomaa, A.K.; Brannigan, J.A.; Wilson, K.S.; Wilkinson, A.J.
Deposited on	:	2004-09-30
Resolution	:	2.23 Å(reported)

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

|		
MolProbity	:	4.02b-467
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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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.
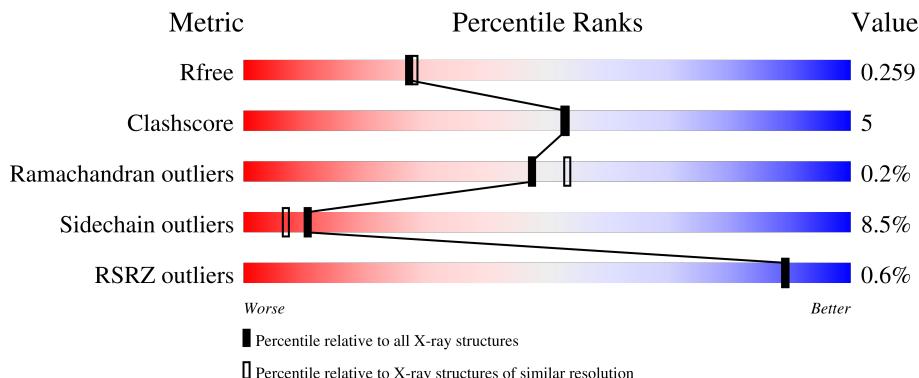
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	301	82% ... 12% ..
1	B	301	79% ... 15% ..
1	C	301	84% ... 12% ..
1	D	301	80% ... 14% ..
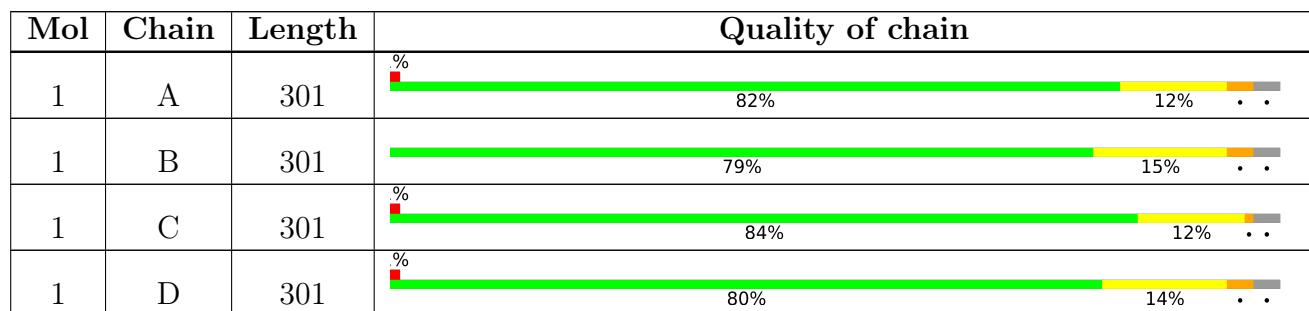
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9535 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 dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	1	0
			2195	1393	363	427	12			
1	B	292	Total	C	N	O	S	0	0	0
			2188	1388	361	427	12			
1	C	292	Total	C	N	O	S	0	1	0
			2194	1392	362	428	12			
1	D	292	Total	C	N	O	S	0	2	0
			2199	1395	362	430	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	cloning artifact	UNP Q81WN7
A	-7	SER	-	cloning artifact	UNP Q81WN7
A	-6	SER	-	cloning artifact	UNP Q81WN7
A	-5	HIS	-	expression tag	UNP Q81WN7
A	-4	HIS	-	expression tag	UNP Q81WN7
A	-3	HIS	-	expression tag	UNP Q81WN7
A	-2	HIS	-	expression tag	UNP Q81WN7
A	-1	HIS	-	expression tag	UNP Q81WN7
A	0	HIS	-	expression tag	UNP Q81WN7
B	-8	GLY	-	cloning artifact	UNP Q81WN7
B	-7	SER	-	cloning artifact	UNP Q81WN7
B	-6	SER	-	cloning artifact	UNP Q81WN7
B	-5	HIS	-	expression tag	UNP Q81WN7
B	-4	HIS	-	expression tag	UNP Q81WN7
B	-3	HIS	-	expression tag	UNP Q81WN7
B	-2	HIS	-	expression tag	UNP Q81WN7
B	-1	HIS	-	expression tag	UNP Q81WN7
B	0	HIS	-	expression tag	UNP Q81WN7
C	-8	GLY	-	cloning artifact	UNP Q81WN7
C	-7	SER	-	cloning artifact	UNP Q81WN7
C	-6	SER	-	cloning artifact	UNP Q81WN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP Q81WN7
C	-4	HIS	-	expression tag	UNP Q81WN7
C	-3	HIS	-	expression tag	UNP Q81WN7
C	-2	HIS	-	expression tag	UNP Q81WN7
C	-1	HIS	-	expression tag	UNP Q81WN7
C	0	HIS	-	expression tag	UNP Q81WN7
D	-8	GLY	-	cloning artifact	UNP Q81WN7
D	-7	SER	-	cloning artifact	UNP Q81WN7
D	-6	SER	-	cloning artifact	UNP Q81WN7
D	-5	HIS	-	expression tag	UNP Q81WN7
D	-4	HIS	-	expression tag	UNP Q81WN7
D	-3	HIS	-	expression tag	UNP Q81WN7
D	-2	HIS	-	expression tag	UNP Q81WN7
D	-1	HIS	-	expression tag	UNP Q81WN7
D	0	HIS	-	expression tag	UNP Q81WN7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	214	Total 214	O 214	0	0
2	B	221	Total 221	O 221	0	0
2	C	148	Total 148	O 148	0	0
2	D	176	Total 176	O 176	0	0

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: dihydrodipicolinate synthase
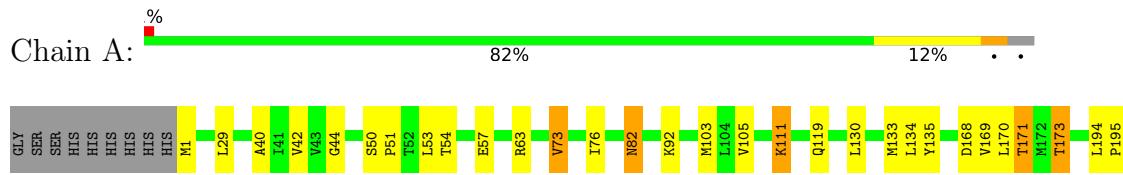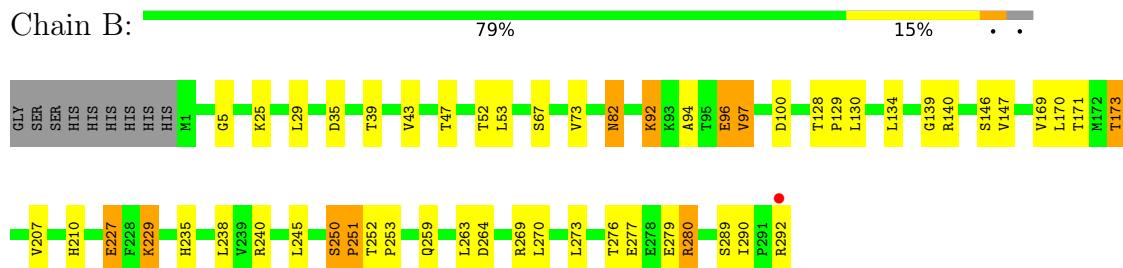


- Molecule 1: dihydrodipicolinate synthase


- Molecule 1: dihydrodipicolinate synthase

- Molecule 1: dihydrodipicolinate synthase

I145 S146 V147 V150 V151 V169 L170 T173 E174 E177 K178 V205 Q217 E218 E227 F228 K229 K233 L234 H235 L238 L245 T252 L263 D264 L275 R280 R292
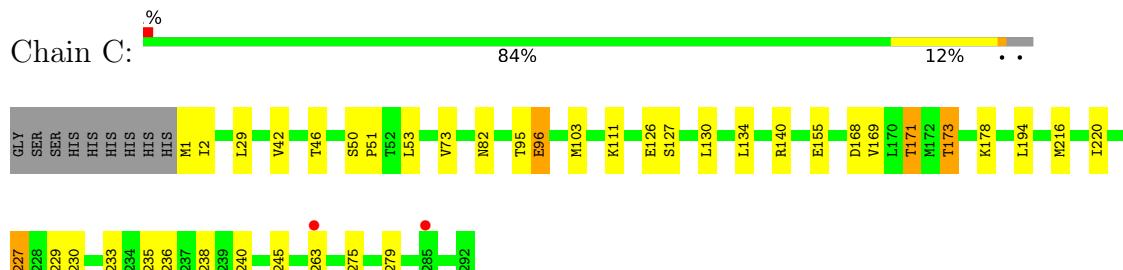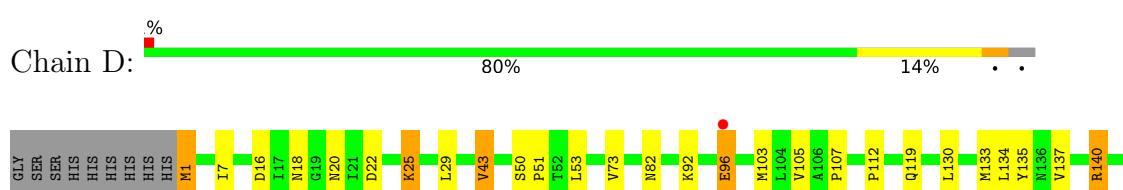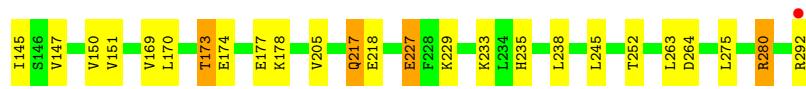
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.46Å 126.56Å 134.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 2.23 46.11 – 2.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.13-2.23) 99.3 (46.11-2.23)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.51 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.254 0.203 , 0.259	Depositor DCC
R_{free} test set	3609 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9535	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.88	1/2233 (0.0%)	0.87	2/3040 (0.1%)
1	B	0.91	2/2222 (0.1%)	0.91	3/3025 (0.1%)
1	C	0.81	3/2231 (0.1%)	0.78	2/3037 (0.1%)
1	D	0.83	1/2239 (0.0%)	0.79	3/3048 (0.1%)
All	All	0.86	7/8925 (0.1%)	0.84	10/12150 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	227	GLU	CD-OE2	9.57	1.36	1.25
1	B	227	GLU	CD-OE2	7.74	1.34	1.25
1	A	227	GLU	CD-OE2	7.11	1.33	1.25
1	C	227	GLU	CD-OE2	7.02	1.33	1.25
1	C	227	GLU	CG-CD	6.78	1.62	1.51
1	B	96	GLU	CG-CD	5.54	1.60	1.51
1	C	227	GLU	CB-CG	5.27	1.62	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	B	140	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	A	63	ARG	NE-CZ-NH2	-8.69	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	43	VAL	CB-CA-C	-6.21	99.60	111.40
1	C	140	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	D	140	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	140	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	100	ASP	CB-CG-OD2	5.56	123.31	118.30
1	C	140	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	269	ARG	NE-CZ-NH2	5.30	122.95	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	SER	Peptide
1	B	270	LEU	Peptide
1	B	97	VAL	Peptide
1	D	205	VAL	Peptide

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2253	24	0
1	B	2188	0	2246	29	0
1	C	2194	0	2254	15	0
1	D	2199	0	2258	32	0
2	A	214	0	0	3	0
2	B	221	0	0	4	0
2	C	148	0	0	1	0
2	D	176	0	0	7	0
All	All	9535	0	9011	96	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 5.

All (96) 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:D:218:GLU:HG2	2:D:407:HOH:O	1.72	0.87
1:D:1:MET:HE1	2:D:442:HOH:O	1.81	0.81
1:D:103:MET:SD	1:D:133:MET:HE3	2.24	0.78
1:D:22:ASP:OD2	1:D:25:LYS:HE2	1.85	0.76
1:A:170:LEU:HA	1:A:173:THR:HG23	1.68	0.74
1:D:169:VAL:O	1:D:173:THR:HG22	1.88	0.73
1:D:25:LYS:HD2	1:D:264:ASP:O	1.94	0.68
1:B:250:SER:OG	1:B:251:PRO:HA	1.94	0.67
1:B:252:THR:HB	1:B:253:PRO:HD3	1.75	0.66
1:B:169:VAL:O	1:B:173:THR:HG22	1.95	0.66
1:C:169:VAL:O	1:C:173:THR:HG23	1.96	0.66
1:D:103:MET:SD	1:D:133:MET:CE	2.84	0.66
1:D:170:LEU:HA	1:D:173:THR:HG23	1.79	0.64
1:B:171:THR:HG21	2:B:298:HOH:O	1.98	0.64
1:B:96:GLU:HG3	2:B:378:HOH:O	1.97	0.63
1:D:96:GLU:HG3	2:D:426:HOH:O	1.99	0.62
1:D:169:VAL:O	1:D:173:THR:CG2	2.49	0.61
1:B:207:VAL:O	1:B:210:HIS:HD2	1.83	0.60
1:B:235:HIS:NE2	1:C:173:THR:HG21	2.16	0.60
1:A:103:MET:SD	1:A:133:MET:CE	2.92	0.58
1:A:169:VAL:O	1:A:173:THR:CG2	2.52	0.57
1:C:96:GLU:HG3	2:C:415:HOH:O	2.04	0.57
1:C:42:VAL:HG11	1:C:103:MET:HE1	1.87	0.55
1:B:252:THR:HG21	1:B:273:LEU:O	2.06	0.55
1:A:1:MET:HE1	2:A:477:HOH:O	2.07	0.55
1:B:170:LEU:HA	1:B:173:THR:HG23	1.88	0.54
1:A:119:GLN:NE2	2:A:300:HOH:O	2.35	0.54
1:C:169:VAL:O	1:C:173:THR:CG2	2.56	0.54
1:D:119:GLN:NE2	2:D:335:HOH:O	2.39	0.54
1:D:22:ASP:OD2	1:D:25:LYS:CE	2.55	0.53
1:D:7:ILE:HD12	1:D:217[A]:GLN:HG2	1.91	0.53
1:C:168:ASP:O	1:C:171:THR:HG22	2.09	0.52
1:C:42:VAL:HG11	1:C:103:MET:CE	2.39	0.52
1:A:173:THR:HG21	1:D:235:HIS:NE2	2.24	0.52
1:A:103:MET:SD	1:A:133:MET:HE3	2.50	0.51
1:B:240:ARG:NH1	1:B:289:SER:OG	2.43	0.51
1:B:94:ALA:O	1:B:97:VAL:HG22	2.11	0.51
1:D:217[A]:GLN:HE21	1:D:217[A]:GLN:HA	1.74	0.51
1:A:217:GLN:HA	1:A:217:GLN:NE2	2.26	0.51
1:A:169:VAL:O	1:A:173:THR:HG22	2.11	0.51
1:B:207:VAL:O	1:B:210:HIS:CD2	2.62	0.51
1:D:252:THR:HG22	1:D:275:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LYS:HG2	2:D:298:HOH:O	2.10	0.51
1:A:40:ALA:HA	1:A:73:VAL:HG13	1.93	0.51
1:B:290:ILE:O	1:B:292:ARG:HD3	2.11	0.50
1:A:169:VAL:O	1:A:173:THR:HG23	2.12	0.50
1:A:54:THR:OG1	1:A:57:GLU:HG3	2.12	0.49
1:B:128:THR:OG1	1:B:129:PRO:HD2	2.12	0.49
1:A:42:VAL:HA	1:A:76:ILE:O	2.12	0.49
1:A:103:MET:SD	1:A:133:MET:HE2	2.53	0.49
1:A:82:ASN:HD22	1:A:82:ASN:N	2.11	0.48
1:A:111:LYS:HE3	1:B:139:GLY:O	2.12	0.48
1:D:147:VAL:O	1:D:151:VAL:HG23	2.12	0.48
1:B:229:LYS:HZ3	1:B:229:LYS:N	2.10	0.48
1:D:16:ASP:OD2	1:D:20:ASN:HB2	2.13	0.48
1:A:82:ASN:HD22	1:A:82:ASN:H	1.61	0.48
1:A:105:VAL:HA	1:A:135:TYR:HB3	1.95	0.48
1:D:280:ARG:NH1	1:D:280:ARG:HB3	2.29	0.47
1:D:25:LYS:HG3	2:D:401:HOH:O	2.14	0.47
1:C:1:MET:HG3	1:C:2:ILE:H	1.79	0.47
1:C:194:LEU:HD22	1:C:235:HIS:HB2	1.95	0.47
1:B:171:THR:CG2	2:B:298:HOH:O	2.59	0.47
1:A:50:SER:N	1:A:51:PRO:CD	2.79	0.46
1:D:105:VAL:HA	1:D:135:TYR:HB3	1.99	0.45
1:C:50:SER:OG	1:C:51:PRO:HD3	2.16	0.45
1:B:92:LYS:CD	2:B:455:HOH:O	2.65	0.45
1:C:111:LYS:HE2	1:D:140:ARG:HG2	1.99	0.45
1:B:169:VAL:O	1:B:173:THR:CG2	2.64	0.44
1:D:177:GLU:OE2	2:D:362:HOH:O	2.21	0.44
1:B:82:ASN:C	1:B:82:ASN:HD22	2.21	0.44
1:B:280:ARG:HB3	1:B:280:ARG:NH1	2.32	0.44
1:B:146:SER:O	1:B:147:VAL:C	2.56	0.44
1:D:16:ASP:OD1	1:D:18:ASN:N	2.52	0.43
1:C:216:MET:O	1:C:220:ILE:HG13	2.18	0.43
1:D:145:ILE:HG22	1:D:150:VAL:HG23	1.99	0.43
1:C:275:LEU:HG	1:C:279:GLU:HB3	2.00	0.43
1:B:47:THR:O	1:B:251:PRO:HG3	2.18	0.43
1:D:50:SER:N	1:D:51:PRO:CD	2.82	0.43
1:A:194:LEU:HB3	1:A:195:PRO:HD3	2.00	0.43
1:C:95:THR:HG23	1:C:130:LEU:HD13	2.01	0.42
1:D:174:GLU:OE2	1:D:178:LYS:NZ	2.42	0.42
1:B:252:THR:N	1:B:253:PRO:CD	2.81	0.42
1:D:107:PRO:HB2	1:D:112:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ASP:OD1	1:D:22:ASP:C	2.57	0.42
1:A:168:ASP:O	1:A:171:THR:HG22	2.20	0.42
1:A:44:GLY:O	1:A:50:SER:HB3	2.20	0.41
1:B:290:ILE:O	1:B:292:ARG:CD	2.67	0.41
1:B:52:THR:O	1:B:269:ARG:NH1	2.53	0.41
1:B:276:THR:O	1:B:279:GLU:N	2.53	0.41
1:D:137:VAL:O	1:D:137:VAL:HG13	2.21	0.41
1:C:50:SER:N	1:C:51:PRO:HD2	2.36	0.41
1:D:263:LEU:HD23	1:D:263:LEU:HA	1.88	0.41
1:A:42:VAL:HG11	1:A:103:MET:HE1	2.03	0.41
1:B:259:GLN:HG3	1:B:264:ASP:OD2	2.21	0.41
1:A:233:LYS:HG2	2:A:490:HOH:O	2.21	0.40
1:B:5:GLY:HA3	1:B:39:THR:OG1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	291/301 (97%)	282 (97%)	9 (3%)	0	100	100
1	B	290/301 (96%)	275 (95%)	13 (4%)	2 (1%)	22	20
1	C	291/301 (97%)	277 (95%)	14 (5%)	0	100	100
1	D	292/301 (97%)	281 (96%)	11 (4%)	0	100	100
All	All	1164/1204 (97%)	1115 (96%)	47 (4%)	2 (0%)	47	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	277	GLU
1	B	251	PRO

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	246/253 (97%)	222 (90%)	24 (10%)	8	4
1	B	245/253 (97%)	227 (93%)	18 (7%)	14	10
1	C	246/253 (97%)	224 (91%)	22 (9%)	9	6
1	D	247/253 (98%)	227 (92%)	20 (8%)	11	8
All	All	984/1012 (97%)	900 (92%)	84 (8%)	10	7

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	53	LEU
1	A	73	VAL
1	A	82	ASN
1	A	92	LYS
1	A	111	LYS
1	A	130	LEU
1	A	134	LEU
1	A	171	THR
1	A	173	THR
1	A	202	LYS
1	A	217	GLN
1	A	218	GLU
1	A	227	GLU
1	A	229	LYS
1	A	233	LYS
1	A	238	LEU
1	A	245	LEU
1	A	263	LEU
1	A	278	GLU
1	A	282	THR
1	A	284	GLN
1	A	288	GLN
1	A	292	ARG

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Mol	Chain	Res	Type
1	B	25	LYS
1	B	29	LEU
1	B	35	ASP
1	B	43	VAL
1	B	53	LEU
1	B	67	SER
1	B	73	VAL
1	B	82	ASN
1	B	92	LYS
1	B	130	LEU
1	B	134	LEU
1	B	173	THR
1	B	227	GLU
1	B	229	LYS
1	B	238	LEU
1	B	245	LEU
1	B	263	LEU
1	B	280	ARG
1	C	29	LEU
1	C	46	THR
1	C	53	LEU
1	C	73	VAL
1	C	82	ASN
1	C	96	GLU
1	C	126	GLU
1	C	127	SER
1	C	134	LEU
1	C	155	GLU
1	C	171	THR
1	C	173	THR
1	C	178	LYS
1	C	227	GLU
1	C	229	LYS
1	C	230	LYS
1	C	233	LYS
1	C	236	GLN
1	C	238	LEU
1	C	240	ARG
1	C	245	LEU
1	C	263	LEU
1	D	1	MET
1	D	25	LYS

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Mol	Chain	Res	Type
1	D	29	LEU
1	D	43	VAL
1	D	53	LEU
1	D	73	VAL
1	D	82	ASN
1	D	96	GLU
1	D	130	LEU
1	D	134	LEU
1	D	173	THR
1	D	217[A]	GLN
1	D	217[B]	GLN
1	D	227	GLU
1	D	229	LYS
1	D	233	LYS
1	D	238	LEU
1	D	245	LEU
1	D	280	ARG
1	D	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	ASN
1	A	119	GLN
1	A	217	GLN
1	A	236	GLN
1	B	64	HIS
1	B	82	ASN
1	B	119	GLN
1	B	210	HIS
1	C	64	HIS
1	C	82	ASN
1	C	85	HIS
1	C	119	GLN
1	D	64	HIS
1	D	82	ASN
1	D	119	GLN
1	D	210	HIS
1	D	236	GLN
1	D	288	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	292/301 (97%)	-0.27	2 (0%)	87	87	32, 41, 60, 78	2 (0%)
1	B	292/301 (97%)	-0.45	1 (0%)	94	94	32, 39, 54, 72	2 (0%)
1	C	292/301 (97%)	-0.27	2 (0%)	87	87	38, 48, 62, 74	2 (0%)
1	D	292/301 (97%)	-0.27	2 (0%)	87	87	37, 45, 61, 81	2 (0%)
All	All	1168/1204 (97%)	-0.32	7 (0%)	89	89	32, 44, 60, 81	8 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	292	ARG	3.5
1	C	263	LEU	2.8
1	C	285	SER	2.6
1	A	292	ARG	2.4
1	A	280	ARG	2.3
1	B	292	ARG	2.2
1	D	96	GLU	2.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.