



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2022 – 03:34 PM EDT

PDB ID : 8H4Z
Title : Crystal structure of carboxyspermidine dehydrogenase from *Helicobacter pylori* in space group P21212
Authors : Ko, K.Y.; Park, S.C.; Cho, S.Y.; Yoon, S.I.
Deposited on : 2022-10-11
Resolution : 2.20 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

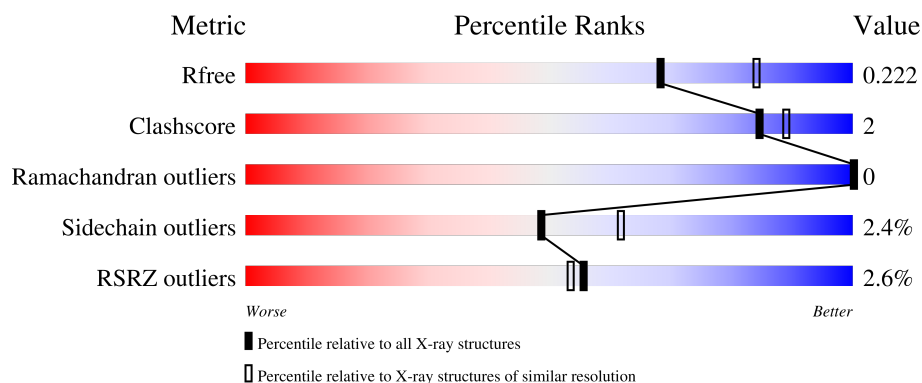
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	405	<div> <div>0%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	405	<div> <div>2%</div> <div>89%</div> <div>6%</div> <div>.</div> </div>
1	C	405	<div> <div>3%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
1	D	405	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12567 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 Carboxyspermidine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3070	1961	513	575	21			
1	B	388	Total	C	N	O	S	0	0	0
			3029	1935	506	567	21			
1	C	383	Total	C	N	O	S	0	0	0
			2974	1895	501	557	21			
1	D	393	Total	C	N	O	S	0	0	0
			3069	1961	509	578	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP E8QMS0
A	-4	SER	-	expression tag	UNP E8QMS0
A	-3	HIS	-	expression tag	UNP E8QMS0
A	-2	MET	-	expression tag	UNP E8QMS0
A	-1	ALA	-	expression tag	UNP E8QMS0
A	0	SER	-	expression tag	UNP E8QMS0
A	156	ARG	LYS	conflict	UNP E8QMS0
B	-5	GLY	-	expression tag	UNP E8QMS0
B	-4	SER	-	expression tag	UNP E8QMS0
B	-3	HIS	-	expression tag	UNP E8QMS0
B	-2	MET	-	expression tag	UNP E8QMS0
B	-1	ALA	-	expression tag	UNP E8QMS0
B	0	SER	-	expression tag	UNP E8QMS0
B	156	ARG	LYS	conflict	UNP E8QMS0
C	-5	GLY	-	expression tag	UNP E8QMS0
C	-4	SER	-	expression tag	UNP E8QMS0
C	-3	HIS	-	expression tag	UNP E8QMS0
C	-2	MET	-	expression tag	UNP E8QMS0
C	-1	ALA	-	expression tag	UNP E8QMS0
C	0	SER	-	expression tag	UNP E8QMS0
C	156	ARG	LYS	conflict	UNP E8QMS0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP E8QMS0
D	-4	SER	-	expression tag	UNP E8QMS0
D	-3	HIS	-	expression tag	UNP E8QMS0
D	-2	MET	-	expression tag	UNP E8QMS0
D	-1	ALA	-	expression tag	UNP E8QMS0
D	0	SER	-	expression tag	UNP E8QMS0
D	156	ARG	LYS	conflict	UNP E8QMS0

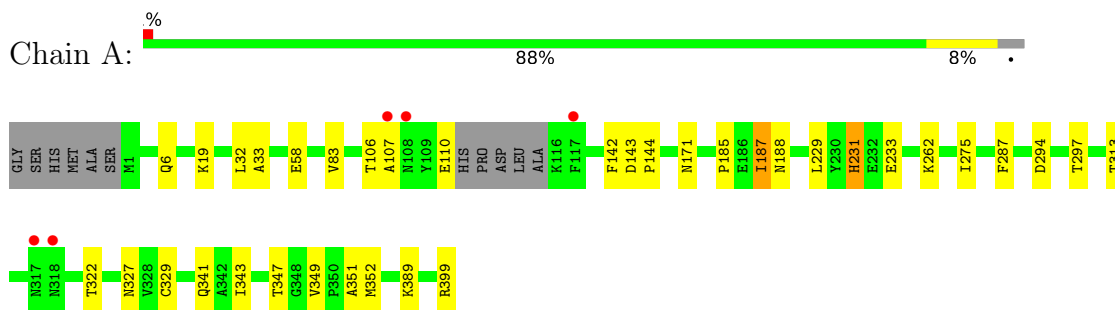
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total 111	O 111	0	0
2	B	122	Total 122	O 122	0	0
2	C	81	Total 81	O 81	0	0
2	D	111	Total 111	O 111	0	0

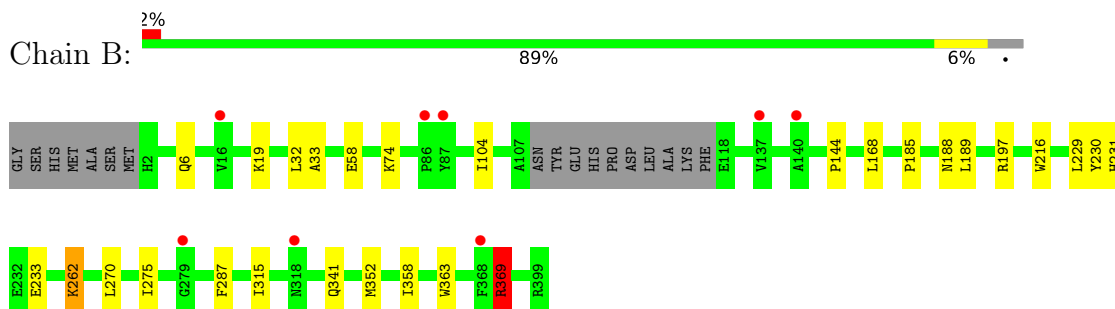
3 Residue-property plots

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.

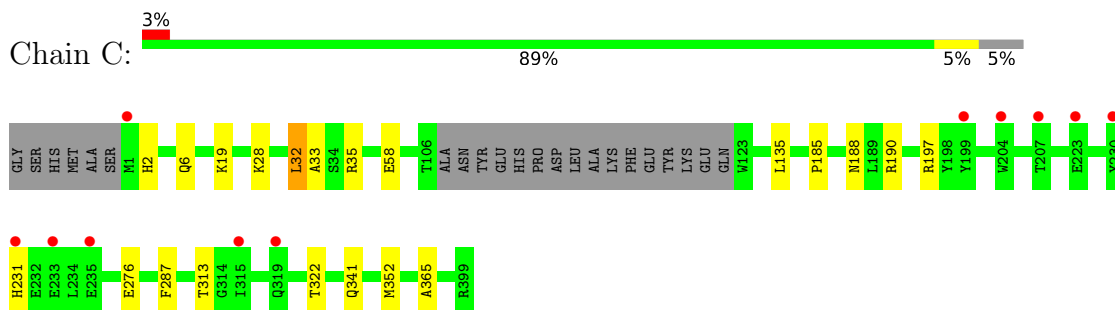
- Molecule 1: Carboxyspermidine dehydrogenase



- Molecule 1: Carboxyspermidine dehydrogenase

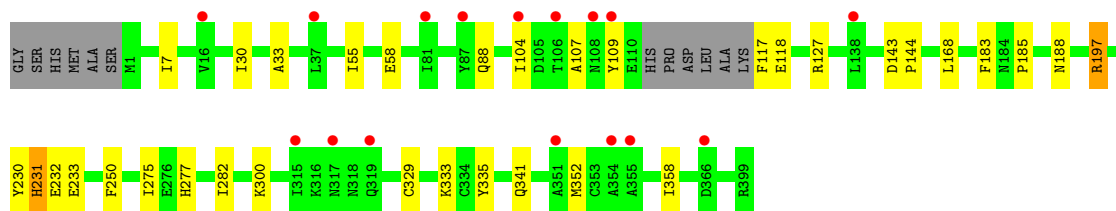


- Molecule 1: Carboxyspermidine dehydrogenase



- Molecule 1: Carboxyspermidine dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.88Å 153.15Å 97.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.20 30.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.98-2.20) 99.7 (30.01-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.185 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	4976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12567	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 3.14% 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](#)

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	0.42	0/3135	0.58	0/4248
1	B	0.42	0/3093	0.62	3/4192 (0.1%)
1	C	0.38	0/3035	0.56	0/4113
1	D	0.39	0/3135	0.57	0/4250
All	All	0.40	0/12398	0.58	3/16803 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ARG	CG-CD-NE	5.46	123.27	111.80
1	B	369	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	229	LEU	CA-CB-CG	5.32	127.54	115.30

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	3070	0	2977	17	0
1	B	3029	0	2959	17	0
1	C	2974	0	2904	8	0
1	D	3069	0	2978	16	0
2	A	111	0	0	1	0
2	B	122	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	81	0	0	1	0
2	D	111	0	0	2	0
All	All	12567	0	11818	54	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 2.

All (54) 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:A:144:PRO:HB3	1:A:233:GLU:HB3	1.56	0.88
1:B:144:PRO:HB3	1:B:233:GLU:HB3	1.62	0.78
1:D:144:PRO:HB3	1:D:233:GLU:HB3	1.74	0.68
1:B:262:LYS:HE3	1:B:262:LYS:HA	1.76	0.66
1:D:117:PHE:CD1	1:D:232:GLU:HG2	2.31	0.64
1:B:185:PRO:HA	1:B:188:ASN:HD22	1.66	0.61
1:C:185:PRO:HA	1:C:188:ASN:HD22	1.68	0.58
1:A:294:ASP:HB3	1:A:297:THR:HG23	1.86	0.57
1:C:6:GLN:HB3	1:C:32:LEU:HD12	1.87	0.56
1:D:104:ILE:HD11	1:D:358:ILE:HD12	1.89	0.54
1:C:19:LYS:HB3	1:C:352:MET:HE2	1.91	0.53
1:C:313:THR:HG22	1:C:322:THR:HG22	1.91	0.52
1:D:277:HIS:HB3	1:D:282:ILE:HD12	1.91	0.51
1:A:185:PRO:HA	1:A:188:ASN:HD22	1.75	0.51
1:C:2:HIS:ND1	2:C:404:HOH:O	2.35	0.50
1:D:107:ALA:HA	1:D:109:TYR:CE2	2.47	0.50
1:B:363:TRP:O	1:B:369:ARG:NH1	2.46	0.49
1:D:30:ILE:HB	1:D:55:ILE:HG22	1.93	0.49
1:A:83:VAL:HG12	1:A:106:THR:HG23	1.94	0.49
1:D:185:PRO:HA	1:D:188:ASN:HD22	1.79	0.48
1:B:104:ILE:HD11	1:B:358:ILE:HD12	1.96	0.47
1:B:6:GLN:NE2	1:B:32:LEU:HD11	2.30	0.47
1:C:135:LEU:HG	1:C:365:ALA:HB2	1.96	0.47
1:A:19:LYS:HG3	1:A:349:VAL:HG22	1.96	0.47
1:D:33:ALA:HA	1:D:58:GLU:O	2.15	0.47
1:A:33:ALA:HA	1:A:58:GLU:O	2.16	0.46
1:A:275:ILE:HD11	1:B:287:PHE:CE2	2.51	0.45
1:C:33:ALA:HA	1:C:58:GLU:O	2.17	0.44
1:D:197:ARG:HB3	1:D:230:TYR:HB2	1.99	0.44
1:B:369:ARG:CG	1:B:369:ARG:HH11	2.30	0.44
1:D:127:ARG:NE	2:D:409:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HB3	1:B:352:MET:HE2	1.99	0.44
1:C:287:PHE:CE2	1:D:275:ILE:HD11	2.53	0.44
1:A:107:ALA:HB2	1:A:347:THR:HG21	2.00	0.43
1:A:229:LEU:HD22	2:A:431:HOH:O	2.18	0.43
1:B:32:LEU:HD12	1:B:32:LEU:HA	1.72	0.43
1:A:142:PHE:CZ	1:A:327:ASN:HB3	2.54	0.43
1:B:33:ALA:HA	1:B:58:GLU:O	2.19	0.43
1:A:106:THR:HG21	1:A:351:ALA:HB2	2.01	0.43
1:A:287:PHE:CE2	1:B:275:ILE:HD11	2.54	0.43
1:B:185:PRO:HA	1:B:188:ASN:ND2	2.32	0.42
1:B:74:LYS:O	1:D:127:ARG:NH2	2.52	0.42
1:D:168:LEU:HD23	1:D:250:PHE:HB2	2.01	0.42
1:B:168:LEU:HD13	1:B:216:TRP:CE2	2.55	0.42
1:A:110:GLU:HA	1:A:187:ILE:HD11	2.02	0.41
1:D:232:GLU:HG3	2:D:423:HOH:O	2.19	0.41
1:B:197:ARG:HB3	1:B:230:TYR:HB2	2.03	0.41
1:A:313:THR:HG22	1:A:322:THR:HG22	2.03	0.41
1:A:171:ASN:ND2	1:A:343:ILE:HD11	2.36	0.41
1:D:143:ASP:O	1:D:231:HIS:HE1	2.04	0.41
1:D:300:LYS:HB3	1:D:335:TYR:CZ	2.56	0.41
1:B:189:LEU:HD13	1:B:270:LEU:HB3	2.03	0.41
1:A:6:GLN:NE2	1:A:32:LEU:HD21	2.36	0.40
1:A:143:ASP:O	1:A:231:HIS:HE1	2.04	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	390/405 (96%)	384 (98%)	6 (2%)	0	100	100
1	B	384/405 (95%)	378 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	379/405 (94%)	374 (99%)	5 (1%)	0	100	100
1	D	389/405 (96%)	383 (98%)	6 (2%)	0	100	100
All	All	1542/1620 (95%)	1519 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/346 (92%)	309 (98%)	8 (2%)	47	60
1	B	318/346 (92%)	313 (98%)	5 (2%)	62	76
1	C	312/346 (90%)	304 (97%)	8 (3%)	46	58
1	D	321/346 (93%)	311 (97%)	10 (3%)	40	51
All	All	1268/1384 (92%)	1237 (98%)	31 (2%)	49	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ILE
1	A	231	HIS
1	A	262	LYS
1	A	329	CYS
1	A	341	GLN
1	A	352	MET
1	A	389	LYS
1	A	399	ARG
1	B	231	HIS
1	B	262	LYS
1	B	315	ILE
1	B	341	GLN
1	B	369	ARG
1	C	28	LYS

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Mol	Chain	Res	Type
1	C	32	LEU
1	C	35	ARG
1	C	190	ARG
1	C	197	ARG
1	C	231	HIS
1	C	276	GLU
1	C	341	GLN
1	D	7	ILE
1	D	88	GLN
1	D	118	GLU
1	D	183	PHE
1	D	197	ARG
1	D	231	HIS
1	D	329	CYS
1	D	333	LYS
1	D	341	GLN
1	D	352	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	266	ASN
1	B	188	ASN
1	B	255	GLN
1	B	266	ASN
1	C	188	ASN
1	C	266	ASN
1	D	188	ASN
1	D	255	GLN
1	D	266	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	394/405 (97%)	-0.15	5 (1%) 77 75	18, 32, 52, 79	0
1	B	388/405 (95%)	-0.19	8 (2%) 63 61	17, 31, 53, 73	0
1	C	383/405 (94%)	-0.11	11 (2%) 51 49	22, 37, 62, 89	0
1	D	393/405 (97%)	-0.04	16 (4%) 37 35	21, 36, 56, 88	0
All	All	1558/1620 (96%)	-0.12	40 (2%) 56 53	17, 34, 58, 89	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLN	4.8
1	C	204	TRP	3.2
1	A	117	PHE	3.2
1	A	318	ASN	3.1
1	D	315	ILE	2.9
1	D	108	ASN	2.9
1	D	81	ILE	2.8
1	B	279	GLY	2.8
1	D	109	TYR	2.8
1	C	235	GLU	2.7
1	B	318	ASN	2.7
1	D	351	ALA	2.7
1	A	107	ALA	2.6
1	C	231	HIS	2.6
1	A	108	ASN	2.6
1	D	317	ASN	2.4
1	C	230	TYR	2.4
1	B	368	PHE	2.4
1	D	104	ILE	2.4
1	A	317	ASN	2.4
1	B	16	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.4
1	D	106	THR	2.3
1	B	140	ALA	2.3
1	D	366	ASP	2.3
1	B	87	TYR	2.3
1	C	315	ILE	2.3
1	D	354	ALA	2.2
1	B	137	VAL	2.2
1	C	223	GLU	2.2
1	D	138	LEU	2.2
1	C	207	THR	2.1
1	D	37	LEU	2.1
1	B	86	PRO	2.1
1	C	199	TYR	2.1
1	C	233	GLU	2.1
1	D	87	TYR	2.1
1	D	355	ALA	2.1
1	D	16	VAL	2.1
1	D	319	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.