



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:41 am BST

PDB ID : 5DFR
Title : CRYSTAL STRUCTURE OF UNLIGANDED ESCHERICHIA COLI DIHYDROFOLATE REDUCTASE. LIGAND-INDUCED CONFORMATIONAL CHANGES AND COOPERATIVITY IN BINDING
Authors : Bystroff, C.; Kraut, J.
Deposited on : 1988-10-21
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

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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

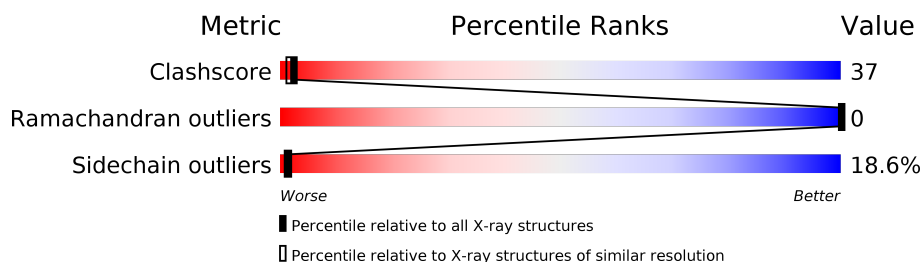
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1343 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 DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1220	779	210	226	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	CONFLICT	UNP P0ABQ4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		

- Molecule 3 is water.

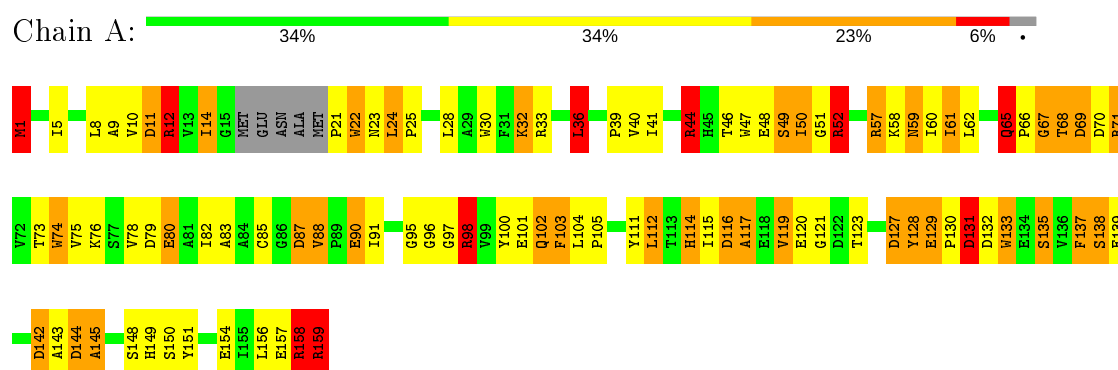
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.73Å 68.73Å 83.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1343	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.43	5/1253 (0.4%)	2.55	81/1702 (4.8%)

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	A	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLY	N-CA	12.68	1.65	1.46
1	A	90	GLU	CD-OE2	-8.06	1.16	1.25
1	A	111	TYR	CG-CD2	-6.59	1.30	1.39
1	A	100	TYR	CE1-CZ	-5.05	1.31	1.38
1	A	138	SER	CA-CB	5.02	1.60	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-25.95	107.33	120.30
1	A	70	ASP	CB-CG-OD1	13.23	130.21	118.30
1	A	159	ARG	NE-CZ-NH1	-12.81	113.89	120.30
1	A	71	ARG	CD-NE-CZ	9.61	137.05	123.60
1	A	80	GLU	CA-CB-CG	9.46	134.21	113.40
1	A	145	ALA	CB-CA-C	9.42	124.23	110.10
1	A	98	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	95	GLY	N-CA-C	8.61	134.63	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	THR	CA-CB-CG2	8.41	124.18	112.40
1	A	96	GLY	C-N-CA	-8.15	105.18	122.30
1	A	142	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	71	ARG	NH1-CZ-NH2	8.12	128.34	119.40
1	A	100	TYR	CB-CG-CD1	8.10	125.86	121.00
1	A	151	TYR	CB-CG-CD1	-7.99	116.20	121.00
1	A	69	ASP	CB-CG-OD1	7.82	125.33	118.30
1	A	71	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	80	GLU	OE1-CD-OE2	-7.73	114.03	123.30
1	A	22	TRP	N-CA-CB	-7.68	96.78	110.60
1	A	65	GLN	CB-CA-C	7.53	125.46	110.40
1	A	90	GLU	CG-CD-OE1	7.53	133.35	118.30
1	A	22	TRP	CB-CA-C	7.33	125.06	110.40
1	A	28	LEU	O-C-N	-7.32	110.98	122.70
1	A	90	GLU	OE1-CD-OE2	-7.21	114.64	123.30
1	A	131	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	150	SER	CA-CB-OG	-6.97	92.37	111.20
1	A	138	SER	N-CA-CB	-6.96	100.06	110.50
1	A	96	GLY	CA-C-O	-6.90	108.19	120.60
1	A	80	GLU	CG-CD-OE1	6.85	132.00	118.30
1	A	1	MET	CG-SD-CE	-6.85	89.24	100.20
1	A	24	LEU	CA-CB-CG	6.84	131.04	115.30
1	A	157	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	83	ALA	N-CA-CB	-6.81	100.56	110.10
1	A	112	LEU	O-C-N	6.70	133.42	122.70
1	A	97	GLY	N-CA-C	-6.60	96.61	113.10
1	A	158	ARG	CA-CB-CG	6.58	127.89	113.40
1	A	70	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	28	LEU	CA-C-N	6.49	131.47	117.20
1	A	44	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	137	PHE	CD1-CE1-CZ	-6.42	112.39	120.10
1	A	48	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	A	116	ASP	CB-CA-C	6.32	123.04	110.40
1	A	70	ASP	O-C-N	6.31	132.80	122.70
1	A	87	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	36	LEU	CB-CA-C	6.25	122.08	110.20
1	A	1	MET	N-CA-CB	-6.24	99.36	110.60
1	A	117	ALA	CB-CA-C	6.24	119.45	110.10
1	A	114	HIS	N-CA-CB	6.17	121.71	110.60
1	A	137	PHE	CG-CD1-CE1	6.12	127.53	120.80
1	A	47	TRP	O-C-N	-6.04	113.04	122.70
1	A	95	GLY	CA-C-N	-6.03	104.13	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	TRP	O-C-N	6.03	132.35	122.70
1	A	138	SER	CB-CA-C	-6.02	98.66	110.10
1	A	100	TYR	CG-CD2-CE2	5.90	126.02	121.30
1	A	133	TRP	CA-CB-CG	-5.90	102.49	113.70
1	A	142	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	135	SER	N-CA-CB	5.81	119.21	110.50
1	A	74	TRP	O-C-N	5.76	131.92	122.70
1	A	11	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	30	TRP	CA-CB-CG	5.65	124.44	113.70
1	A	79	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	103	PHE	CB-CG-CD2	5.52	124.66	120.80
1	A	49	SER	CA-C-O	-5.51	108.53	120.10
1	A	11	ASP	O-C-N	5.50	131.50	122.70
1	A	52	ARG	CD-NE-CZ	5.46	131.25	123.60
1	A	68	THR	N-CA-CB	-5.46	99.94	110.30
1	A	57	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	139	GLU	CG-CD-OE2	-5.43	107.43	118.30
1	A	144	ASP	CB-CA-C	5.33	121.06	110.40
1	A	51	GLY	CA-C-O	-5.32	111.02	120.60
1	A	101	GLU	CA-CB-CG	5.26	124.98	113.40
1	A	78	VAL	CA-CB-CG1	5.25	118.78	110.90
1	A	59	ASN	O-C-N	5.23	131.06	122.70
1	A	127	ASP	O-C-N	5.20	131.01	122.70
1	A	67	GLY	O-C-N	5.18	130.99	122.70
1	A	131	ASP	CB-CA-C	5.17	120.75	110.40
1	A	48	GLU	CG-CD-OE1	5.17	128.65	118.30
1	A	121	GLY	O-C-N	5.13	130.90	122.70
1	A	30	TRP	CH2-CZ2-CE2	-5.12	112.28	117.40
1	A	49	SER	N-CA-CB	5.03	118.05	110.50
1	A	91	ILE	CG1-CB-CG2	5.03	122.47	111.40
1	A	88	VAL	CA-CB-CG2	5.01	118.42	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	137	PHE	Mainchain
1	A	158	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	44	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	52	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	98	ARG	Sidechain

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	1220	0	1178	89	0
2	A	3	0	0	2	0
3	A	120	0	0	15	0
All	All	1343	0	1178	90	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 37.

All (90) 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:12:ARG:HH11	1:A:127:ASP:HA	1.09	1.14
1:A:131:ASP:HB2	3:A:347:HOH:O	1.58	1.01
1:A:12:ARG:HB2	1:A:12:ARG:HH21	1.25	0.98
1:A:114:HIS:HB2	2:A:502:CL:CL	2.00	0.96
1:A:12:ARG:HH11	1:A:127:ASP:CA	1.81	0.94
1:A:24:LEU:N	3:A:426:HOH:O	2.01	0.93
1:A:12:ARG:NH1	1:A:127:ASP:HA	1.91	0.85
1:A:65:GLN:CG	1:A:66:PRO:HD3	2.07	0.83
1:A:65:GLN:HG2	1:A:66:PRO:HD3	1.58	0.83
1:A:12:ARG:CB	1:A:12:ARG:HH21	1.93	0.82
1:A:10:VAL:O	1:A:11:ASP:HB2	1.80	0.80
1:A:12:ARG:NH1	1:A:127:ASP:CA	2.47	0.76
1:A:104:LEU:O	1:A:158:ARG:NH2	2.20	0.75
1:A:23:ASN:O	1:A:25:PRO:HD3	1.89	0.73
1:A:159:ARG:OXT	1:A:159:ARG:HG3	1.89	0.72
1:A:69:ASP:OD1	1:A:71:ARG:HB2	1.89	0.72
1:A:129:GLU:O	1:A:132:ASP:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:HB2	3:A:389:HOH:O	1.91	0.70
1:A:9:ALA:HB1	1:A:117:ALA:O	1.94	0.67
1:A:21:PRO:HD3	3:A:370:HOH:O	1.93	0.67
1:A:62:LEU:HD23	1:A:103:PHE:HE2	1.61	0.66
1:A:12:ARG:HB2	1:A:12:ARG:NH2	2.07	0.63
1:A:8:LEU:HD12	1:A:14:ILE:HG22	1.81	0.62
1:A:60:ILE:C	1:A:61:ILE:HD13	2.21	0.61
1:A:24:LEU:C	3:A:426:HOH:O	2.39	0.60
1:A:24:LEU:CD2	1:A:115:ILE:HG12	2.30	0.60
1:A:12:ARG:HH21	1:A:12:ARG:CG	2.14	0.60
1:A:46:THR:HG22	1:A:50:ILE:HD12	1.84	0.60
1:A:76:LYS:HE2	3:A:339:HOH:O	2.02	0.59
1:A:67:GLY:C	1:A:68:THR:HG23	2.22	0.59
1:A:98:ARG:O	1:A:102:GLN:HG2	2.02	0.59
1:A:59:ASN:HD22	1:A:59:ASN:N	2.01	0.59
1:A:76:LYS:HD2	3:A:356:HOH:O	2.02	0.58
1:A:98:ARG:O	1:A:102:GLN:CG	2.52	0.58
1:A:129:GLU:O	1:A:132:ASP:HB2	2.05	0.57
1:A:143:ALA:O	1:A:144:ASP:HB3	2.06	0.56
1:A:62:LEU:CD2	1:A:103:PHE:HE2	2.18	0.56
1:A:145:ALA:CB	3:A:316:HOH:O	2.54	0.55
1:A:75:VAL:HG12	1:A:80:GLU:HG2	1.88	0.55
2:A:501:CL:CL	3:A:338:HOH:O	2.55	0.55
1:A:61:ILE:HD13	1:A:61:ILE:N	2.21	0.55
1:A:135:SER:HB2	1:A:154:GLU:OE1	2.08	0.54
1:A:12:ARG:NH2	1:A:12:ARG:CG	2.70	0.54
1:A:65:GLN:CA	3:A:348:HOH:O	2.56	0.54
1:A:1:MET:HG2	1:A:90:GLU:HG3	1.89	0.54
1:A:148:SER:HG	1:A:149:HIS:CE1	2.25	0.53
1:A:145:ALA:HB2	3:A:316:HOH:O	2.08	0.53
1:A:82:ILE:O	1:A:85:CYS:HB2	2.09	0.52
1:A:117:ALA:HB2	1:A:149:HIS:CD2	2.44	0.52
1:A:67:GLY:HA3	1:A:74:TRP:CE2	2.45	0.51
1:A:52:ARG:O	1:A:52:ARG:NH2	2.40	0.51
1:A:133:TRP:CZ2	1:A:158:ARG:HD3	2.46	0.51
1:A:40:VAL:O	1:A:40:VAL:HG23	2.10	0.50
1:A:22:TRP:C	3:A:344:HOH:O	2.51	0.50
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.94	0.49
1:A:130:PRO:C	1:A:132:ASP:H	2.15	0.49
1:A:24:LEU:HD21	1:A:115:ILE:HG12	1.95	0.49
1:A:62:LEU:HD13	1:A:75:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:CB	1:A:66:PRO:CD	2.91	0.48
1:A:12:ARG:NH1	1:A:127:ASP:N	2.61	0.48
1:A:133:TRP:HB3	1:A:156:LEU:HB3	1.96	0.48
1:A:115:ILE:HG22	1:A:117:ALA:HB3	1.96	0.47
1:A:59:ASN:ND2	1:A:59:ASN:N	2.63	0.47
1:A:65:GLN:N	3:A:348:HOH:O	2.47	0.47
1:A:65:GLN:CG	1:A:66:PRO:CD	2.89	0.46
1:A:39:PRO:HG2	1:A:88:VAL:HG21	1.96	0.46
1:A:23:ASN:C	1:A:25:PRO:HD3	2.36	0.45
1:A:12:ARG:NH2	1:A:12:ARG:HG3	2.31	0.45
1:A:116:ASP:O	1:A:117:ALA:HB2	2.16	0.45
1:A:129:GLU:HA	1:A:130:PRO:HD2	1.44	0.45
1:A:128:TYR:N	1:A:128:TYR:CD1	2.79	0.44
1:A:10:VAL:O	1:A:11:ASP:CB	2.55	0.44
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.89	0.44
1:A:119:VAL:HG12	1:A:120:GLU:H	1.83	0.44
1:A:62:LEU:CD2	1:A:103:PHE:CE2	3.00	0.44
1:A:104:LEU:N	1:A:105:PRO:CD	2.81	0.43
1:A:21:PRO:N	3:A:366:HOH:O	2.52	0.43
1:A:130:PRO:C	1:A:132:ASP:N	2.72	0.42
1:A:159:ARG:OXT	1:A:159:ARG:CG	2.62	0.42
1:A:67:GLY:HA3	1:A:74:TRP:CD2	2.54	0.42
1:A:148:SER:OG	1:A:149:HIS:ND1	2.37	0.42
1:A:65:GLN:HG2	1:A:66:PRO:CD	2.38	0.42
1:A:12:ARG:HG3	1:A:12:ARG:HH21	1.85	0.42
1:A:65:GLN:CB	1:A:66:PRO:HD3	2.50	0.41
1:A:112:LEU:HD12	1:A:156:LEU:CD1	2.51	0.41
1:A:32:LYS:O	1:A:36:LEU:HB2	2.21	0.41
1:A:12:ARG:CB	1:A:12:ARG:NH2	2.73	0.41
1:A:41:ILE:HG21	1:A:41:ILE:HD13	1.88	0.40
1:A:10:VAL:HG23	1:A:117:ALA:O	2.21	0.40
1:A:65:GLN:CB	3:A:389:HOH:O	2.59	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	150/159 (94%)	137 (91%)	13 (9%)	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	129/136 (95%)	105 (81%)	24 (19%)	1	1

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ILE
1	A	12	ARG
1	A	14	ILE
1	A	32	LYS
1	A	36	LEU
1	A	44	ARG
1	A	49	SER
1	A	50	ILE
1	A	52	ARG
1	A	58	LYS
1	A	61	ILE
1	A	65	GLN
1	A	87	ASP
1	A	98	ARG
1	A	102	GLN
1	A	119	VAL
1	A	123	THR
1	A	128	TYR

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	131	ASP
1	A	138	SER
1	A	142	ASP
1	A	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.