



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 5DFR / pdb_00005dfr
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

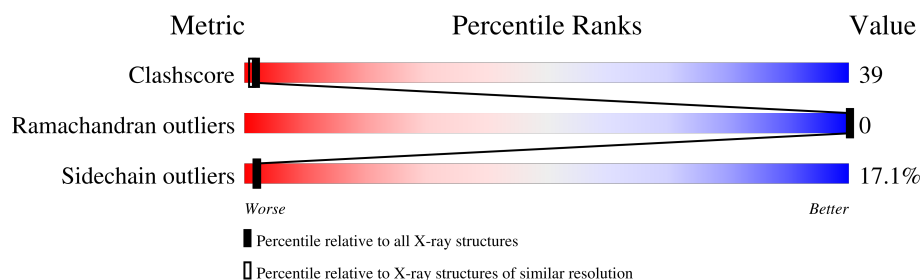
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

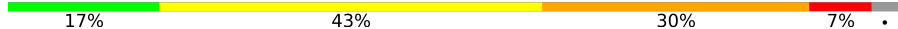
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 ≥ 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 (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is water.

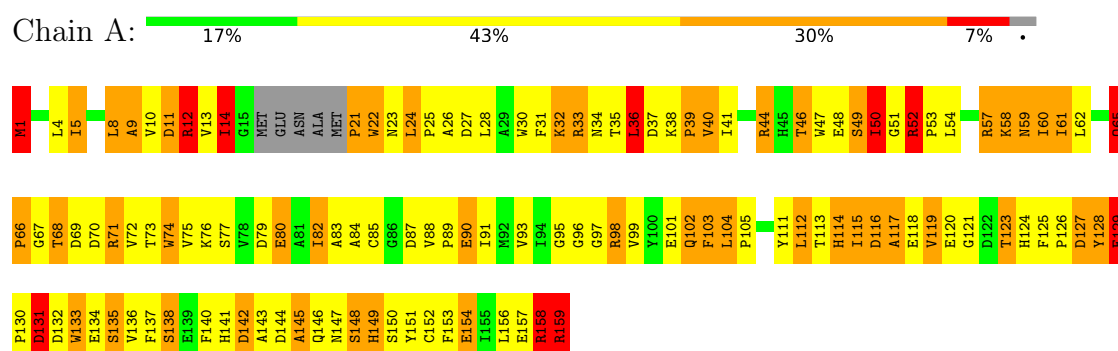
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		

3 Residue-property plots

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. 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

5.1 Standard geometry

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	1.80	15/1253 (1.2%)	3.06	183/1702 (10.8%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLY	N-CA	13.58	1.65	1.45
1	A	138	SER	C-N	-7.00	1.24	1.33
1	A	140	PHE	N-CA	-6.79	1.37	1.46
1	A	52	ARG	N-CA	6.68	1.52	1.45
1	A	22	TRP	N-CA	6.53	1.53	1.45
1	A	147	ASN	C-N	-6.25	1.25	1.33
1	A	114	HIS	CG-ND1	5.98	1.44	1.38
1	A	36	LEU	N-CA	5.68	1.53	1.46
1	A	57	ARG	C-O	5.38	1.30	1.23
1	A	123	THR	CA-CB	5.30	1.61	1.53
1	A	31	PHE	C-N	-5.27	1.27	1.33
1	A	35	THR	CA-CB	5.19	1.61	1.54
1	A	157	GLU	C-N	-5.19	1.26	1.33
1	A	103	PHE	N-CA	5.11	1.52	1.46
1	A	113	THR	CA-C	5.05	1.58	1.52

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	NE-CZ-NH2	-13.19	107.33	119.20
1	A	38	LYS	O-C-N	11.36	129.94	121.65
1	A	52	ARG	O-C-N	10.13	129.04	121.65
1	A	80	GLU	CA-CB-CG	10.05	134.21	114.10
1	A	28	LEU	O-C-N	-9.84	110.98	122.20
1	A	26	ALA	N-CA-C	-9.75	100.73	111.36
1	A	49	SER	CA-C-O	-9.55	108.53	119.79
1	A	150	SER	CA-CB-OG	-9.37	92.37	111.10
1	A	11	ASP	O-C-N	9.31	131.50	122.00
1	A	95	GLY	N-CA-C	9.05	134.63	113.18
1	A	71	ARG	CD-NE-CZ	9.04	137.05	124.40
1	A	129	GLU	CA-C-O	8.97	127.84	119.59
1	A	125	PHE	N-CA-C	-8.95	97.95	110.29
1	A	57	ARG	CA-C-O	-8.93	110.99	120.99
1	A	22	TRP	N-CA-CB	-8.82	96.78	110.46
1	A	14	ILE	CB-CA-C	8.78	118.79	111.06
1	A	146	GLN	N-CA-C	8.74	124.07	113.41
1	A	146	GLN	OE1-CD-NE2	8.52	131.12	122.60
1	A	65	GLN	CB-CA-C	8.47	125.46	110.47
1	A	47	TRP	O-C-N	-8.45	113.04	122.08
1	A	22	TRP	CB-CA-C	8.44	125.06	110.45
1	A	149	HIS	CA-CB-CG	-8.44	105.36	113.80
1	A	145	ALA	CB-CA-C	8.39	124.23	110.81
1	A	104	LEU	CA-C-O	8.37	126.31	118.44
1	A	68	THR	N-CA-CB	-8.37	99.94	111.65
1	A	72	VAL	N-CA-CB	-8.29	103.17	112.45
1	A	96	GLY	CA-C-N	-8.28	105.18	121.41
1	A	96	GLY	C-N-CA	-8.28	105.18	121.41
1	A	157	GLU	CA-C-N	8.27	133.15	121.24
1	A	157	GLU	C-N-CA	8.27	133.15	121.24
1	A	51	GLY	CA-C-O	-8.26	111.02	119.20
1	A	90	GLU	N-CA-C	8.20	123.00	109.06
1	A	36	LEU	CA-C-O	-8.09	111.69	120.92
1	A	73	THR	CA-CB-CG2	8.05	124.18	110.50
1	A	121	GLY	O-C-N	7.89	130.90	123.57
1	A	82	ILE	CA-C-N	7.88	131.17	120.38
1	A	82	ILE	C-N-CA	7.88	131.17	120.38
1	A	54	LEU	N-CA-C	-7.86	99.75	109.65
1	A	145	ALA	N-CA-C	-7.86	101.68	111.11
1	A	112	LEU	O-C-N	7.84	133.42	123.23
1	A	36	LEU	CB-CA-C	7.81	122.08	109.90
1	A	59	ASN	CA-C-N	-7.70	112.28	122.99
1	A	59	ASN	C-N-CA	-7.70	112.28	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	TRP	O-C-N	7.66	131.92	123.27
1	A	159	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	A	70	ASP	O-C-N	7.56	132.80	122.37
1	A	59	ASN	CA-CB-CG	-7.54	105.06	112.60
1	A	125	PHE	CB-CA-C	7.53	119.70	108.86
1	A	59	ASN	CA-C-O	-7.51	112.02	120.43
1	A	9	ALA	N-CA-C	-7.36	98.45	109.86
1	A	123	THR	N-CA-C	7.21	121.77	110.17
1	A	150	SER	N-CA-C	-7.19	100.84	110.55
1	A	96	GLY	CA-C-O	-7.12	108.19	120.57
1	A	112	LEU	CA-C-O	-7.07	113.06	120.70
1	A	116	ASP	CB-CA-C	7.05	123.04	111.41
1	A	133	TRP	O-C-N	7.05	132.35	123.19
1	A	103	PHE	N-CA-C	-7.02	104.87	113.50
1	A	97	GLY	N-CA-C	-6.99	96.61	113.18
1	A	71	ARG	NH1-CZ-NH2	6.95	128.34	119.30
1	A	74	TRP	CA-C-O	-6.93	112.87	120.43
1	A	84	ALA	CA-C-N	6.92	132.41	120.58
1	A	84	ALA	C-N-CA	6.92	132.41	120.58
1	A	59	ASN	O-C-N	6.90	131.06	123.13
1	A	158	ARG	CA-CB-CG	6.89	127.89	114.10
1	A	114	HIS	N-CA-CB	6.87	121.71	110.37
1	A	46	THR	CA-C-O	-6.83	113.31	120.55
1	A	8	LEU	CA-C-O	-6.80	113.01	120.36
1	A	154	GLU	CB-CG-CD	6.74	124.05	112.60
1	A	5	ILE	O-C-N	-6.69	115.94	123.10
1	A	127	ASP	CA-C-O	-6.59	112.85	120.49
1	A	138	SER	CB-CA-C	-6.55	98.66	109.80
1	A	1	MET	N-CA-CB	-6.55	99.36	110.50
1	A	90	GLU	CG-CD-OE1	6.50	133.35	118.40
1	A	127	ASP	O-C-N	6.50	131.01	123.02
1	A	116	ASP	CA-C-N	-6.42	110.72	121.64
1	A	116	ASP	C-N-CA	-6.42	110.72	121.64
1	A	138	SER	N-CA-CB	-6.42	100.06	110.71
1	A	99	VAL	N-CA-CB	-6.41	102.36	110.57
1	A	116	ASP	CA-CB-CG	-6.41	106.19	112.60
1	A	141	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	83	ALA	N-CA-CB	-6.33	100.56	110.06
1	A	151	TYR	CA-C-O	-6.33	114.68	121.45
1	A	37	ASP	N-CA-C	6.29	120.26	112.58
1	A	153	PHE	O-C-N	6.29	130.38	123.22
1	A	24	LEU	CA-C-O	6.28	128.76	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	O-C-N	-6.22	115.11	122.20
1	A	49	SER	N-CA-C	-6.21	104.40	112.23
1	A	133	TRP	CA-C-N	-6.13	114.34	122.99
1	A	133	TRP	C-N-CA	-6.13	114.34	122.99
1	A	47	TRP	CA-C-O	6.10	127.78	121.07
1	A	34	ASN	CA-C-O	-6.07	112.17	119.27
1	A	39	PRO	CA-C-N	6.05	131.57	122.98
1	A	39	PRO	C-N-CA	6.05	131.57	122.98
1	A	149	HIS	CA-C-O	-6.04	114.58	121.40
1	A	50	ILE	CA-C-N	6.00	131.22	122.28
1	A	50	ILE	C-N-CA	6.00	131.22	122.28
1	A	31	PHE	CA-C-N	5.99	129.12	120.79
1	A	31	PHE	C-N-CA	5.99	129.12	120.79
1	A	129	GLU	CA-C-N	5.99	127.33	119.84
1	A	129	GLU	C-N-CA	5.99	127.33	119.84
1	A	65	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	A	65	GLN	N-CA-CB	5.94	116.21	109.49
1	A	112	LEU	CA-C-N	-5.93	114.75	123.05
1	A	112	LEU	C-N-CA	-5.93	114.75	123.05
1	A	80	GLU	CG-CD-OE1	5.92	132.00	118.40
1	A	79	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	13	VAL	CA-C-N	-5.89	115.18	121.84
1	A	13	VAL	C-N-CA	-5.89	115.18	121.84
1	A	148	SER	CA-C-O	-5.89	112.36	119.49
1	A	134	GLU	CA-C-N	5.87	130.73	121.99
1	A	134	GLU	C-N-CA	5.87	130.73	121.99
1	A	133	TRP	CA-CB-CG	-5.85	102.49	113.60
1	A	40	VAL	O-C-N	5.79	129.21	123.18
1	A	60	ILE	CA-C-O	-5.79	114.22	120.36
1	A	135	SER	N-CA-CB	5.79	119.21	109.94
1	A	142	ASP	CA-C-O	-5.77	115.00	121.81
1	A	57	ARG	CA-C-N	-5.76	113.56	122.09
1	A	57	ARG	C-N-CA	-5.76	113.56	122.09
1	A	115	ILE	N-CA-CB	-5.72	104.13	110.99
1	A	30	TRP	CA-CB-CG	5.71	124.44	113.60
1	A	58	LYS	CA-C-N	5.69	129.98	122.30
1	A	58	LYS	C-N-CA	5.69	129.98	122.30
1	A	13	VAL	N-CA-CB	-5.67	104.36	110.53
1	A	117	ALA	CB-CA-C	5.66	119.45	109.89
1	A	147	ASN	N-CA-CB	-5.66	101.67	110.55
1	A	70	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	124	HIS	CA-CB-CG	-5.64	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PRO	O-C-N	5.61	129.81	122.86
1	A	99	VAL	CA-C-N	5.60	127.78	120.28
1	A	99	VAL	C-N-CA	5.60	127.78	120.28
1	A	46	THR	O-C-N	5.59	128.04	122.12
1	A	50	ILE	CA-CB-CG2	5.58	120.00	110.50
1	A	52	ARG	N-CA-CB	5.58	119.12	111.25
1	A	37	ASP	N-CA-CB	-5.58	103.99	112.47
1	A	48	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	A	58	LYS	CA-C-O	-5.54	114.55	120.92
1	A	77	SER	N-CA-C	5.54	117.22	108.96
1	A	83	ALA	CA-C-N	5.54	129.98	120.72
1	A	83	ALA	C-N-CA	5.54	129.98	120.72
1	A	4	LEU	CA-C-N	-5.54	115.25	122.94
1	A	4	LEU	C-N-CA	-5.54	115.25	122.94
1	A	5	ILE	CB-CA-C	5.48	118.93	110.50
1	A	126	PRO	CA-C-O	5.47	127.91	121.56
1	A	101	GLU	CA-CB-CG	5.44	124.98	114.10
1	A	21	PRO	CA-C-N	-5.43	113.28	122.67
1	A	21	PRO	C-N-CA	-5.43	113.28	122.67
1	A	27	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	77	SER	CA-C-O	5.42	127.25	121.45
1	A	91	ILE	CA-C-O	-5.42	114.74	120.48
1	A	53	PRO	CB-CA-C	5.40	118.42	111.56
1	A	111	TYR	CA-C-O	-5.37	114.53	120.33
1	A	103	PHE	CB-CA-C	5.36	119.04	109.29
1	A	72	VAL	N-CA-C	5.35	115.35	108.82
1	A	46	THR	N-CA-C	-5.33	105.47	111.28
1	A	1	MET	CG-SD-CE	-5.30	89.24	100.90
1	A	131	ASP	CB-CA-C	5.28	120.75	110.57
1	A	12	ARG	N-CA-C	-5.25	104.65	111.74
1	A	104	LEU	CA-C-N	5.24	124.95	119.82
1	A	104	LEU	C-N-CA	5.24	124.95	119.82
1	A	35	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	153	PHE	CA-C-O	-5.21	114.65	120.54
1	A	38	LYS	CB-CA-C	-5.20	101.91	109.97
1	A	123	THR	CA-C-N	5.20	131.54	122.81
1	A	123	THR	C-N-CA	5.20	131.54	122.81
1	A	89	PRO	CB-CA-C	5.18	119.68	112.11
1	A	80	GLU	N-CA-C	-5.16	105.73	111.36
1	A	91	ILE	O-C-N	5.15	128.59	123.18
1	A	22	TRP	CA-C-O	-5.15	115.35	121.89
1	A	152	CYS	CA-C-O	-5.15	114.42	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	CA-C-O	-5.14	115.07	121.50
1	A	70	ASP	CB-CG-OD1	5.13	130.21	118.40
1	A	68	THR	O-C-N	5.12	128.34	121.99
1	A	134	GLU	CA-C-O	-5.11	114.84	120.36
1	A	118	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	154	GLU	CA-C-N	5.05	129.76	123.14
1	A	154	GLU	C-N-CA	5.05	129.76	123.14
1	A	146	GLN	O-C-N	-5.05	115.19	122.36
1	A	93	VAL	CB-CA-C	5.04	118.36	111.31
1	A	49	SER	N-CA-CB	5.03	118.05	110.30
1	A	138	SER	CA-C-O	-5.02	113.43	120.21
1	A	4	LEU	O-C-N	5.02	129.75	123.23
1	A	38	LYS	CA-C-O	-5.00	115.74	120.34
1	A	136	VAL	N-CA-C	-5.00	107.98	113.43

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
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	1179	93	0
2	A	3	0	0	2	0
3	A	120	0	0	16	0
All	All	1343	0	1179	94	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 39.

All (94) 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:HH21	1:A:12:ARG:CB	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: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
1:A:65:GLN:HB2	3:A:389:HOH:O	1.91	0.70
1:A:159:ARG:OXT	1:A:159:ARG:HG3	1.89	0.69
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:60:ILE:C	1:A:61:ILE:HD13	2.21	0.66
1:A:24:LEU:C	3:A:426:HOH:O	2.39	0.65
1:A:67:GLY:C	1:A:68:THR:HG23	2.22	0.64
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:61:ILE:HD13	1:A:61:ILE:N	2.21	0.55
2:A:501:CL:CL	3:A:338:HOH:O	2.55	0.55
1:A:22:TRP:C	3:A:344:HOH:O	2.51	0.54
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:130:PRO:C	1:A:132:ASP:H	2.15	0.53
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:HG23	1:A:40:VAL:O	2.10	0.50
1:A:23:ASN:C	1:A:25:PRO:HD3	2.36	0.50
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.94	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
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:59:ASN:N	1:A:59:ASN:ND2	2.63	0.47
1:A:115:ILE:HG22	1:A:117:ALA:HB3	1.96	0.47
1:A:65:GLN:N	3:A:348:HOH:O	2.47	0.47
1:A:130:PRO:C	1:A:132:ASP:N	2.72	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:12:ARG:NH2	1:A:12:ARG:HG3	2.31	0.45
1:A:129:GLU:HA	1:A:130:PRO:HD2	1.44	0.45
1:A:128:TYR:CD1	1:A:128:TYR:N	2.79	0.44
1:A:67:GLY:C	1:A:68:THR:CG2	2.90	0.44
1:A:10:VAL:O	1:A:11:ASP:CB	2.55	0.44
1:A:116:ASP:O	1:A:117:ALA:HB2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PRO:N	3:A:366:HOH:O	2.52	0.43
1:A:67:GLY:HA3	1:A:74:TRP:CD2	2.54	0.42
1:A:159:ARG:OXT	1:A:159:ARG:CG	2.62	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:HH21	1:A:12:ARG:HG3	1.85	0.42
1:A:21:PRO:C	3:A:344:HOH:O	2.62	0.41
1:A:65:GLN:CB	1:A:66:PRO:HD3	2.50	0.41
1:A:32:LYS:O	1:A:36:LEU:HB2	2.21	0.41
1:A:112:LEU:HD12	1:A:156:LEU:CD1	2.51	0.41
1:A:12:ARG:CB	1:A:12:ARG:NH2	2.73	0.41
1:A:24:LEU:O	1:A:25:PRO:C	2.59	0.40
1:A:103:PHE:O	1:A:104:LEU:C	2.62	0.40
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 [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	129/136 (95%)	107 (83%)	22 (17%)	2 2

All (22) 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	102	GLN
1	A	119	VAL
1	A	123	THR
1	A	128	TYR
1	A	129	GLU
1	A	131	ASP
1	A	138	SER
1	A	142	ASP

Sometimes 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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.