



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:08 pm BST

PDB ID : 1PDB
Title : Analysis of Three Crystal Structure Determinations of a 5-Methyl-6-N-Methylanilino Pyridopyrimidine Antifolate Complex with Human Dihydrofolate Reductase
Authors : Cody, V.; Luft, J.R.; Pangborn, W.; Gangjee, A.
Deposited on : 2003-05-19
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 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	:	2.11
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

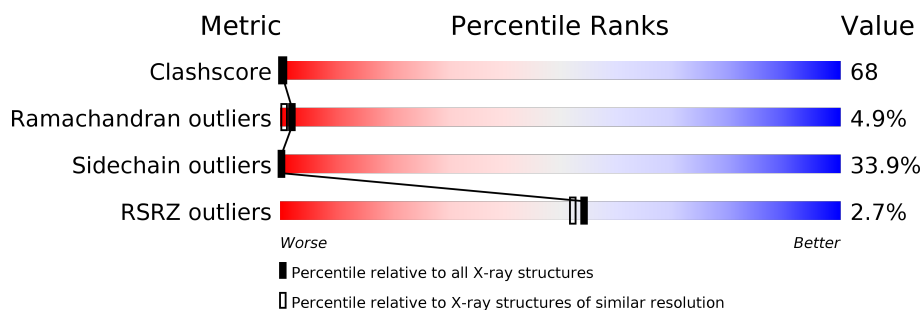
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
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 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	186	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1519 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	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

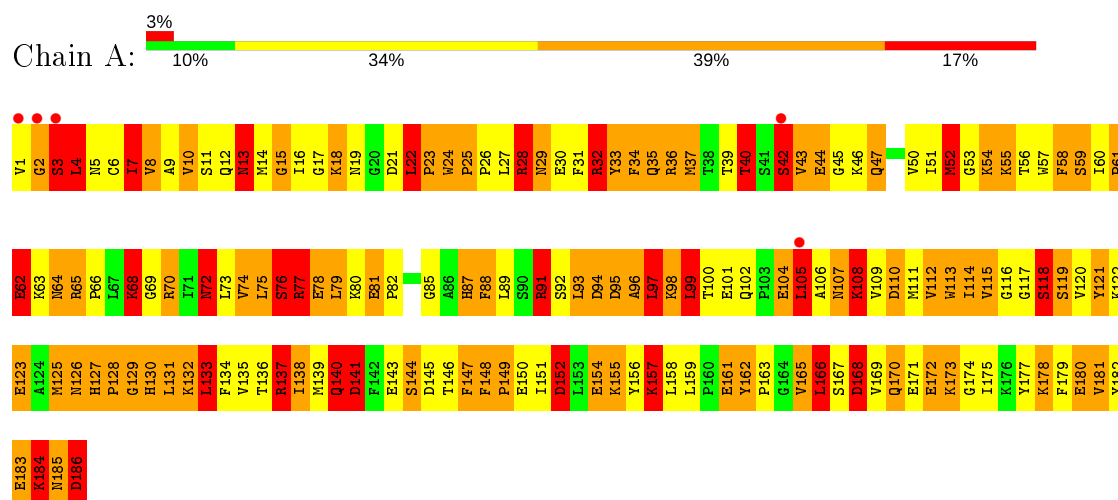
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		

3 Residue-property plots

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: Dihydrofolate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.93Å 62.93Å 95.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 52.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.5 (8.00-2.20) 80.8 (52.59-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.10Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.239 , 0.250 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1519	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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	1.40	4/1537 (0.3%)	3.23	189/2073 (9.1%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ARG	CZ-NH2	8.16	1.43	1.33
1	A	17	GLY	N-CA	7.30	1.57	1.46
1	A	180	GLU	CD-OE2	-5.38	1.19	1.25
1	A	168	ASP	CG-OD2	5.05	1.36	1.25

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	CD-NE-CZ	22.57	155.19	123.60
1	A	168	ASP	CB-CG-OD2	22.52	138.57	118.30
1	A	36	ARG	NE-CZ-NH2	-22.07	109.26	120.30
1	A	168	ASP	CB-CG-OD1	-21.66	98.81	118.30
1	A	32	ARG	NE-CZ-NH1	20.62	130.61	120.30
1	A	137	ARG	NE-CZ-NH2	20.42	130.51	120.30
1	A	32	ARG	NE-CZ-NH2	-17.79	111.41	120.30
1	A	2	GLY	C-N-CA	15.97	161.63	121.70
1	A	140	GLN	CA-CB-CG	15.61	147.75	113.40
1	A	137	ARG	NE-CZ-NH1	-15.09	112.76	120.30
1	A	132	LYS	CD-CE-NZ	14.65	145.39	111.70
1	A	72	ASN	CA-CB-CG	13.32	142.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LEU	CA-CB-CG	13.30	145.88	115.30
1	A	99	LEU	CA-CB-CG	12.60	144.29	115.30
1	A	150	GLU	CA-CB-CG	12.34	140.54	113.40
1	A	183	GLU	OE1-CD-OE2	12.26	138.01	123.30
1	A	22	LEU	CA-CB-CG	11.87	142.60	115.30
1	A	10	VAL	CG1-CB-CG2	-11.27	92.86	110.90
1	A	161	GLU	OE1-CD-OE2	11.00	136.50	123.30
1	A	65	ARG	NE-CZ-NH2	10.99	125.79	120.30
1	A	131	LEU	CA-CB-CG	10.94	140.46	115.30
1	A	145	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	130	HIS	CA-CB-CG	-10.12	96.39	113.60
1	A	62	GLU	CA-CB-CG	9.86	135.08	113.40
1	A	8	VAL	CB-CA-C	-9.78	92.81	111.40
1	A	182	TYR	CB-CG-CD2	-9.74	115.16	121.00
1	A	127	HIS	CA-CB-CG	9.68	130.05	113.60
1	A	170	GLN	O-C-N	9.57	138.01	122.70
1	A	91	ARG	CA-CB-CG	9.22	133.68	113.40
1	A	185	ASN	N-CA-CB	9.19	127.14	110.60
1	A	141	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	A	165	VAL	CA-CB-CG1	8.89	124.24	110.90
1	A	186	ASP	CA-C-O	-8.88	101.46	120.10
1	A	8	VAL	CG1-CB-CG2	8.79	124.96	110.90
1	A	81	GLU	N-CA-C	8.78	134.70	111.00
1	A	120	VAL	CA-CB-CG1	8.62	123.83	110.90
1	A	18	LYS	N-CA-CB	8.51	125.91	110.60
1	A	165	VAL	CB-CA-C	8.48	127.51	111.40
1	A	149	PRO	C-N-CA	8.37	142.63	121.70
1	A	168	ASP	N-CA-CB	-8.33	95.61	110.60
1	A	21	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	145	ASP	CB-CG-OD2	-8.28	110.84	118.30
1	A	177	TYR	CB-CG-CD1	8.12	125.87	121.00
1	A	70	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	170	GLN	N-CA-CB	8.09	125.16	110.60
1	A	172	GLU	CA-CB-CG	8.05	131.12	113.40
1	A	129	GLY	CA-C-N	-8.05	99.49	117.20
1	A	180	GLU	OE1-CD-OE2	8.01	132.91	123.30
1	A	129	GLY	CA-C-O	7.95	134.92	120.60
1	A	28	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	A	15	GLY	O-C-N	7.90	135.34	122.70
1	A	161	GLU	CG-CD-OE2	-7.82	102.66	118.30
1	A	184	LYS	N-CA-CB	7.68	124.43	110.60
1	A	28	ARG	CB-CG-CD	7.62	131.41	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	TYR	CB-CG-CD1	7.59	125.55	121.00
1	A	36	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	44	GLU	CB-CG-CD	7.56	134.60	114.20
1	A	91	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	32	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	113	TRP	O-C-N	7.51	134.71	122.70
1	A	108	LYS	C-N-CA	7.48	140.40	121.70
1	A	52	MET	CA-CB-CG	7.46	125.99	113.30
1	A	9	ALA	O-C-N	7.42	134.57	122.70
1	A	183	GLU	CG-CD-OE2	-7.40	103.50	118.30
1	A	178	LYS	CA-CB-CG	7.28	129.42	113.40
1	A	157	LYS	N-CA-CB	7.23	123.61	110.60
1	A	42	SER	N-CA-C	7.22	130.50	111.00
1	A	74	VAL	O-C-N	-7.21	111.17	122.70
1	A	101	GLU	OE1-CD-OE2	7.02	131.73	123.30
1	A	33	TYR	CA-CB-CG	7.00	126.70	113.40
1	A	24	TRP	CE3-CZ3-CH2	-6.98	113.53	121.20
1	A	96	ALA	CB-CA-C	6.96	120.53	110.10
1	A	65	ARG	CD-NE-CZ	6.95	133.33	123.60
1	A	23	PRO	N-CD-CG	-6.93	92.80	103.20
1	A	115	VAL	CA-CB-CG2	6.88	121.22	110.90
1	A	72	ASN	C-N-CA	6.86	138.86	121.70
1	A	172	GLU	OE1-CD-OE2	-6.84	115.09	123.30
1	A	149	PRO	O-C-N	-6.81	111.81	122.70
1	A	135	VAL	CA-CB-CG2	-6.74	100.79	110.90
1	A	128	PRO	CA-C-N	-6.67	102.86	116.20
1	A	13	ASN	CB-CA-C	6.65	123.70	110.40
1	A	4	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	7	ILE	CG1-CB-CG2	6.63	125.99	111.40
1	A	105	LEU	N-CA-CB	-6.61	97.19	110.40
1	A	4	LEU	O-C-N	-6.59	112.16	122.70
1	A	168	ASP	CA-CB-CG	6.59	127.90	113.40
1	A	36	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	A	121	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	126	ASN	CB-CG-OD1	-6.55	108.50	121.60
1	A	140	GLN	N-CA-C	-6.53	93.38	111.00
1	A	68	LYS	CA-C-O	6.48	133.72	120.10
1	A	154	GLU	CG-CD-OE1	6.46	131.22	118.30
1	A	136	THR	OG1-CB-CG2	6.43	124.79	110.00
1	A	70	ARG	CD-NE-CZ	6.42	132.58	123.60
1	A	72	ASN	CB-CA-C	6.41	123.21	110.40
1	A	30	GLU	CG-CD-OE1	6.40	131.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	C-N-CA	6.39	137.67	121.70
1	A	78	GLU	CG-CD-OE2	-6.38	105.54	118.30
1	A	118	SER	CA-CB-OG	-6.37	94.02	111.20
1	A	184	LYS	CB-CG-CD	6.36	128.13	111.60
1	A	74	VAL	CA-C-O	6.35	133.44	120.10
1	A	77	ARG	CA-CB-CG	6.34	127.35	113.40
1	A	173	LYS	CA-CB-CG	6.27	127.19	113.40
1	A	128	PRO	CA-C-O	6.24	135.17	120.20
1	A	137	ARG	CA-CB-CG	-6.21	99.74	113.40
1	A	51	ILE	O-C-N	6.19	132.61	122.70
1	A	145	ASP	CB-CA-C	6.17	122.73	110.40
1	A	10	VAL	CA-CB-CG1	6.13	120.10	110.90
1	A	138	ILE	CA-CB-CG2	-6.09	98.72	110.90
1	A	172	GLU	CG-CD-OE1	6.08	130.47	118.30
1	A	162	TYR	CZ-CE2-CD2	6.08	125.27	119.80
1	A	14	MET	CB-CG-SD	-6.05	94.23	112.40
1	A	76	SER	O-C-N	6.05	132.39	122.70
1	A	9	ALA	CA-C-O	-6.00	107.50	120.10
1	A	97	LEU	CB-CA-C	5.99	121.58	110.20
1	A	186	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	121	TYR	N-CA-CB	5.96	121.32	110.60
1	A	184	LYS	CA-CB-CG	5.95	126.50	113.40
1	A	120	VAL	N-CA-CB	5.95	124.59	111.50
1	A	157	LYS	CB-CA-C	-5.95	98.51	110.40
1	A	27	LEU	CA-CB-CG	5.93	128.93	115.30
1	A	21	ASP	CB-CA-C	5.92	122.25	110.40
1	A	30	GLU	CG-CD-OE2	-5.92	106.47	118.30
1	A	4	LEU	N-CA-CB	-5.90	98.59	110.40
1	A	11	SER	CB-CA-C	5.90	121.32	110.10
1	A	94	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	36	ARG	CD-NE-CZ	-5.88	115.37	123.60
1	A	81	GLU	CA-CB-CG	5.87	126.31	113.40
1	A	24	TRP	O-C-N	5.84	132.19	121.10
1	A	115	VAL	CA-CB-CG1	-5.79	102.21	110.90
1	A	15	GLY	CA-C-O	-5.78	110.20	120.60
1	A	139	MET	CA-CB-CG	-5.73	103.55	113.30
1	A	110	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	4	LEU	CB-CA-C	5.70	121.03	110.20
1	A	68	LYS	CB-CG-CD	5.66	126.31	111.60
1	A	169	VAL	O-C-N	-5.63	113.69	122.70
1	A	21	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	14	MET	CA-C-O	-5.59	108.37	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LEU	CB-CA-C	5.57	120.79	110.20
1	A	34	PHE	CB-CG-CD2	5.54	124.68	120.80
1	A	162	TYR	CG-CD2-CE2	-5.51	116.89	121.30
1	A	144	SER	CA-C-O	-5.48	108.58	120.10
1	A	170	GLN	CA-C-O	-5.46	108.64	120.10
1	A	136	THR	CA-CB-OG1	-5.46	97.55	109.00
1	A	58	PHE	CB-CA-C	5.45	121.31	110.40
1	A	36	ARG	CB-CG-CD	5.45	125.77	111.60
1	A	47	GLN	CA-CB-CG	5.43	125.34	113.40
1	A	21	ASP	N-CA-C	-5.40	96.41	111.00
1	A	123	GLU	CG-CD-OE2	-5.40	107.49	118.30
1	A	144	SER	O-C-N	5.40	131.34	122.70
1	A	3	SER	N-CA-C	5.38	125.52	111.00
1	A	17	GLY	C-N-CA	5.37	135.12	121.70
1	A	177	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	3	SER	O-C-N	5.35	131.26	122.70
1	A	181	VAL	CB-CA-C	5.33	121.53	111.40
1	A	119	SER	N-CA-CB	-5.33	102.51	110.50
1	A	35	GLN	CA-CB-CG	5.30	125.06	113.40
1	A	143	GLU	CA-C-O	-5.29	108.99	120.10
1	A	148	PHE	N-CA-C	-5.29	96.72	111.00
1	A	76	SER	N-CA-CB	5.29	118.43	110.50
1	A	94	ASP	CB-CA-C	5.28	120.96	110.40
1	A	101	GLU	CA-CB-CG	5.28	125.02	113.40
1	A	154	GLU	CA-CB-CG	5.28	125.01	113.40
1	A	25	PRO	CB-CA-C	5.26	125.16	112.00
1	A	154	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	A	64	ASN	CA-CB-CG	-5.22	101.91	113.40
1	A	93	LEU	CB-CA-C	5.22	120.12	110.20
1	A	158	LEU	CB-CA-C	5.19	120.07	110.20
1	A	156	TYR	CG-CD2-CE2	5.18	125.44	121.30
1	A	64	ASN	O-C-N	5.16	130.96	122.70
1	A	166	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	28	ARG	CG-CD-NE	5.15	122.61	111.80
1	A	75	LEU	N-CA-C	-5.14	97.11	111.00
1	A	78	GLU	CG-CD-OE1	5.13	128.57	118.30
1	A	22	LEU	O-C-N	5.13	130.84	121.10
1	A	74	VAL	CA-CB-CG2	5.12	118.57	110.90
1	A	147	PHE	CD1-CE1-CZ	5.09	126.21	120.10
1	A	37	MET	CG-SD-CE	5.09	108.35	100.20
1	A	140	GLN	CB-CA-C	5.08	120.56	110.40
1	A	13	ASN	O-C-N	-5.08	114.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLU	CA-C-O	-5.08	109.44	120.10
1	A	54	LYS	CG-CD-CE	5.07	127.12	111.90
1	A	78	GLU	CA-C-N	5.07	128.36	117.20
1	A	88	PHE	CB-CA-C	-5.05	100.31	110.40
1	A	179	PHE	CA-C-N	5.03	128.26	117.20
1	A	132	LYS	CA-CB-CG	-5.03	102.34	113.40
1	A	152	ASP	N-CA-CB	-5.02	101.56	110.60
1	A	3	SER	CA-C-O	-5.02	109.56	120.10
1	A	147	PHE	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	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	1502	0	1508	206	0
2	A	17	0	0	6	0
All	All	1519	0	1508	206	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 68.

All (206) 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:89:LEU:HD22	1:A:91:ARG:HH12	1.14	1.10
1:A:28:ARG:HB3	1:A:32:ARG:HH21	1.15	1.09
1:A:89:LEU:HD22	1:A:91:ARG:NH1	1.67	1.08
1:A:89:LEU:CD2	1:A:91:ARG:NH1	2.18	1.07
1:A:95:ASP:HA	1:A:98:LYS:CD	1.87	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:NZ	1:A:107:ASN:HD22	1.58	1.01
1:A:46:LYS:HZ1	1:A:107:ASN:HD22	1.02	0.99
1:A:58:PHE:O	1:A:65:ARG:NH2	1.97	0.97
1:A:99:LEU:HA	1:A:102:GLN:HG3	1.48	0.95
1:A:102:GLN:HB3	1:A:104:GLU:HB2	1.48	0.95
1:A:61:PRO:O	1:A:64:ASN:N	1.98	0.95
1:A:95:ASP:HA	1:A:98:LYS:CG	1.95	0.95
1:A:55:LYS:HE2	1:A:55:LYS:O	1.67	0.94
1:A:46:LYS:HZ1	1:A:107:ASN:ND2	1.65	0.92
1:A:55:LYS:C	1:A:55:LYS:HE2	1.91	0.91
1:A:122:LYS:HG3	1:A:149:PRO:HG3	1.53	0.91
1:A:28:ARG:HB3	1:A:32:ARG:NH2	1.85	0.90
1:A:50:VAL:CG2	1:A:72:ASN:HB3	2.00	0.90
1:A:107:ASN:ND2	1:A:107:ASN:O	2.08	0.87
1:A:1:VAL:HB	1:A:100:THR:CG2	2.06	0.85
1:A:76:SER:O	1:A:89:LEU:HD21	1.78	0.84
1:A:4:LEU:HD12	1:A:112:VAL:CG2	2.07	0.83
1:A:134:PHE:HB3	2:A:196:HOH:O	1.78	0.82
1:A:94:ASP:O	1:A:98:LYS:HG2	1.80	0.82
1:A:46:LYS:NZ	1:A:107:ASN:ND2	2.25	0.80
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.49	0.78
1:A:93:LEU:O	1:A:96:ALA:HB3	1.82	0.78
1:A:95:ASP:HB3	1:A:98:LYS:HD2	1.64	0.78
1:A:77:ARG:HG3	1:A:77:ARG:NH1	1.99	0.77
1:A:122:LYS:HE3	1:A:149:PRO:HB3	1.65	0.77
1:A:31:PHE:O	1:A:34:PHE:HB3	1.85	0.77
1:A:54:LYS:HA	1:A:74:VAL:CG1	2.15	0.76
1:A:54:LYS:HA	1:A:74:VAL:HG11	1.68	0.76
1:A:99:LEU:O	1:A:105:LEU:HB3	1.86	0.76
1:A:99:LEU:HA	1:A:102:GLN:CG	2.16	0.75
1:A:1:VAL:HA	1:A:109:VAL:HG13	1.67	0.75
1:A:95:ASP:HA	1:A:98:LYS:HD2	1.67	0.75
1:A:61:PRO:HB2	1:A:64:ASN:HD22	1.52	0.74
1:A:65:ARG:HA	1:A:66:PRO:C	2.08	0.74
1:A:46:LYS:HB3	1:A:108:LYS:O	1.88	0.73
1:A:93:LEU:O	1:A:97:LEU:HD22	1.88	0.73
1:A:184:LYS:HD3	1:A:186:ASP:OD2	1.90	0.72
1:A:95:ASP:HA	1:A:98:LYS:HG2	1.72	0.72
1:A:55:LYS:HE2	1:A:55:LYS:CA	2.20	0.71
1:A:89:LEU:HD21	1:A:91:ARG:NH1	2.06	0.71
1:A:152:ASP:OD1	1:A:155:LYS:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:HIS:HB2	1:A:185:ASN:OD1	1.92	0.69
1:A:47:GLN:O	1:A:109:VAL:HA	1.91	0.69
1:A:77:ARG:HA	1:A:91:ARG:HG3	1.72	0.69
1:A:28:ARG:O	1:A:32:ARG:HG3	1.92	0.69
1:A:93:LEU:HG	1:A:97:LEU:HD21	1.75	0.69
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.73	0.68
1:A:100:THR:O	1:A:106:ALA:HA	1.92	0.68
1:A:100:THR:HG23	1:A:109:VAL:HG11	1.76	0.67
1:A:50:VAL:HG22	1:A:72:ASN:HB3	1.75	0.67
1:A:95:ASP:HA	1:A:98:LYS:CE	2.24	0.67
1:A:1:VAL:HB	1:A:100:THR:HG22	1.76	0.66
1:A:66:PRO:HD3	1:A:85:GLY:CA	2.26	0.66
1:A:57:TRP:O	1:A:65:ARG:CD	2.43	0.66
1:A:66:PRO:HD3	1:A:85:GLY:HA3	1.77	0.66
1:A:52:MET:HA	1:A:116:GLY:O	1.95	0.65
1:A:56:THR:O	1:A:59:SER:HB2	1.97	0.65
1:A:95:ASP:CA	1:A:98:LYS:CG	2.74	0.65
1:A:58:PHE:HD2	1:A:65:ARG:NH1	1.95	0.64
1:A:99:LEU:HA	1:A:102:GLN:HB2	1.79	0.64
1:A:6:CYS:HB2	1:A:133:LEU:HD12	1.79	0.64
1:A:76:SER:O	1:A:89:LEU:CD2	2.45	0.64
1:A:99:LEU:CA	1:A:102:GLN:HB2	2.27	0.64
1:A:171:GLU:HA	1:A:175:ILE:O	1.99	0.63
1:A:125:MET:HG3	1:A:133:LEU:HD11	1.81	0.63
1:A:55:LYS:CE	1:A:55:LYS:CA	2.77	0.62
1:A:88:PHE:CD1	1:A:99:LEU:HD11	2.34	0.62
1:A:99:LEU:HA	1:A:102:GLN:CB	2.30	0.62
1:A:122:LYS:HG3	1:A:149:PRO:CG	2.29	0.62
1:A:105:LEU:HA	1:A:108:LYS:HD3	1.82	0.62
1:A:54:LYS:O	1:A:57:TRP:HB3	2.00	0.62
1:A:23:PRO:HB2	1:A:24:TRP:CE3	2.35	0.61
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.81	0.61
1:A:55:LYS:CE	1:A:55:LYS:HA	2.30	0.61
1:A:77:ARG:HH11	1:A:77:ARG:CG	2.13	0.61
1:A:159:LEU:HD21	1:A:183:GLU:HB3	1.82	0.61
1:A:4:LEU:HD12	1:A:112:VAL:HG21	1.81	0.60
1:A:178:LYS:HD3	2:A:191:HOH:O	2.01	0.60
1:A:95:ASP:CA	1:A:98:LYS:HG2	2.33	0.59
1:A:118:SER:HB3	1:A:147:PHE:O	2.03	0.59
1:A:168:ASP:HB2	1:A:170:GLN:HE22	1.68	0.59
1:A:54:LYS:CA	1:A:74:VAL:CG1	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PHE:CD2	1:A:65:ARG:NH1	2.71	0.58
1:A:23:PRO:HD2	1:A:24:TRP:CZ3	2.39	0.57
1:A:99:LEU:HD12	1:A:105:LEU:HD13	1.86	0.57
1:A:76:SER:HB3	1:A:89:LEU:HD21	1.87	0.57
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.40	0.57
1:A:78:GLU:O	1:A:78:GLU:HG2	2.05	0.57
1:A:1:VAL:HG12	1:A:109:VAL:CG1	2.34	0.57
1:A:46:LYS:NZ	1:A:107:ASN:C	2.58	0.57
1:A:50:VAL:HG23	1:A:72:ASN:HB3	1.84	0.57
1:A:6:CYS:O	1:A:134:PHE:N	2.30	0.56
1:A:13:ASN:C	1:A:13:ASN:HD22	2.08	0.56
1:A:118:SER:HA	1:A:121:TYR:HD1	1.71	0.56
1:A:18:LYS:HE3	1:A:19:ASN:OD1	2.06	0.55
1:A:29:ASN:HB2	1:A:172:GLU:CD	2.27	0.55
1:A:55:LYS:HE2	1:A:55:LYS:HA	1.89	0.55
1:A:114:ILE:N	1:A:114:ILE:HD12	2.21	0.55
1:A:58:PHE:HA	1:A:65:ARG:NH2	2.21	0.55
1:A:125:MET:CE	1:A:151:ILE:HG12	2.37	0.55
1:A:52:MET:HB3	1:A:115:VAL:CG2	2.37	0.54
1:A:5:ASN:HA	1:A:132:LYS:O	2.08	0.54
1:A:66:PRO:O	1:A:68:LYS:HD3	2.07	0.54
1:A:89:LEU:HD21	1:A:91:ARG:HH11	1.73	0.54
1:A:39:THR:O	1:A:40:THR:C	2.47	0.53
1:A:134:PHE:C	2:A:196:HOH:O	2.46	0.53
1:A:52:MET:HB3	1:A:115:VAL:HG23	1.89	0.53
1:A:57:TRP:O	1:A:65:ARG:HD3	2.08	0.52
1:A:99:LEU:O	1:A:102:GLN:HB2	2.08	0.52
1:A:13:ASN:HB3	1:A:141:ASP:CB	2.39	0.52
1:A:102:GLN:O	1:A:106:ALA:HB2	2.08	0.52
1:A:127:HIS:O	1:A:184:LYS:NZ	2.37	0.52
1:A:13:ASN:ND2	1:A:13:ASN:C	2.63	0.52
1:A:168:ASP:O	1:A:170:GLN:NE2	2.41	0.52
1:A:107:ASN:C	1:A:107:ASN:HD22	2.11	0.52
1:A:111:MET:HE3	1:A:113:TRP:HE1	1.75	0.52
1:A:114:ILE:N	1:A:114:ILE:CD1	2.73	0.51
1:A:99:LEU:C	1:A:102:GLN:HB2	2.30	0.51
1:A:87:HIS:O	1:A:88:PHE:CD2	2.64	0.51
1:A:118:SER:HB2	1:A:122:LYS:NZ	2.26	0.51
1:A:46:LYS:HZ2	1:A:107:ASN:C	2.13	0.51
1:A:3:SER:O	1:A:112:VAL:O	2.29	0.50
1:A:102:GLN:C	1:A:104:GLU:N	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:CG	1:A:78:GLU:O	2.59	0.49
1:A:18:LYS:HE3	1:A:19:ASN:CG	2.33	0.49
1:A:93:LEU:HG	1:A:97:LEU:CD2	2.42	0.49
1:A:129:GLY:O	1:A:184:LYS:HD2	2.13	0.49
1:A:93:LEU:O	1:A:96:ALA:N	2.46	0.49
1:A:16:ILE:HG21	1:A:148:PHE:HB2	1.95	0.48
1:A:29:ASN:HB2	1:A:172:GLU:OE1	2.13	0.48
1:A:81:GLU:HG2	1:A:82:PRO:O	2.14	0.48
1:A:162:TYR:HB2	1:A:181:VAL:HG11	1.95	0.48
1:A:61:PRO:HB2	1:A:64:ASN:ND2	2.26	0.48
1:A:107:ASN:O	1:A:107:ASN:CG	2.52	0.48
1:A:69:GLY:O	1:A:70:ARG:HG3	2.14	0.48
1:A:95:ASP:CB	1:A:98:LYS:HD2	2.39	0.47
1:A:12:GLN:HE21	1:A:12:GLN:HB3	1.45	0.47
1:A:88:PHE:CD1	1:A:99:LEU:CD1	2.97	0.47
1:A:93:LEU:O	1:A:96:ALA:CB	2.57	0.47
1:A:1:VAL:HB	1:A:100:THR:HG21	1.93	0.47
1:A:130:HIS:CB	1:A:185:ASN:OD1	2.62	0.47
1:A:95:ASP:O	1:A:98:LYS:HG3	2.15	0.47
1:A:97:LEU:H	1:A:97:LEU:HD22	1.80	0.47
1:A:97:LEU:N	1:A:97:LEU:HD22	2.30	0.46
1:A:134:PHE:CB	2:A:196:HOH:O	2.50	0.46
1:A:4:LEU:HD11	1:A:97:LEU:HD11	1.97	0.46
1:A:94:ASP:O	1:A:98:LYS:HE2	2.15	0.46
1:A:166:LEU:HB3	1:A:168:ASP:OD1	2.16	0.46
1:A:68:LYS:H	1:A:68:LYS:HD3	1.80	0.46
1:A:54:LYS:CA	1:A:74:VAL:HG11	2.42	0.46
1:A:55:LYS:CE	1:A:55:LYS:C	2.76	0.46
1:A:178:LYS:CD	2:A:191:HOH:O	2.61	0.45
1:A:1:VAL:N	1:A:109:VAL:O	2.34	0.45
1:A:3:SER:OG	1:A:111:MET:HG2	2.17	0.45
1:A:15:GLY:HA3	1:A:144:SER:CB	2.46	0.45
1:A:88:PHE:CE1	1:A:99:LEU:CD1	2.99	0.45
1:A:26:PRO:O	1:A:173:LYS:NZ	2.49	0.44
1:A:1:VAL:CA	1:A:109:VAL:HG13	2.41	0.44
1:A:76:SER:O	1:A:91:ARG:NH1	2.50	0.44
1:A:140:GLN:HB3	1:A:140:GLN:HE21	1.57	0.44
1:A:77:ARG:NH1	1:A:91:ARG:HG3	2.32	0.44
1:A:16:ILE:CG2	1:A:148:PHE:HB2	2.46	0.44
1:A:28:ARG:NE	1:A:173:LYS:NZ	2.65	0.44
1:A:98:LYS:C	1:A:100:THR:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:C	1:A:175:ILE:HG13	2.37	0.43
1:A:18:LYS:HE2	1:A:18:LYS:HB3	1.47	0.43
1:A:127:HIS:HA	1:A:128:PRO:HD3	1.93	0.43
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.44	0.43
1:A:54:LYS:HD3	1:A:79:LEU:HD11	1.99	0.43
1:A:46:LYS:HZ3	1:A:107:ASN:ND2	2.15	0.43
1:A:24:TRP:C	1:A:25:PRO:O	2.53	0.43
1:A:52:MET:CB	1:A:115:VAL:HG23	2.49	0.43
1:A:53:GLY:N	1:A:116:GLY:O	2.52	0.43
1:A:33:TYR:O	1:A:37:MET:HB2	2.17	0.43
1:A:15:GLY:HA2	1:A:147:PHE:CD2	2.54	0.43
1:A:43:VAL:HG11	1:A:46:LYS:HG3	2.00	0.42
1:A:105:LEU:HG	1:A:108:LYS:HE2	2.01	0.42
1:A:157:LYS:HA	1:A:157:LYS:HD2	1.72	0.42
1:A:16:ILE:HD12	1:A:121:TYR:HE1	1.84	0.42
1:A:46:LYS:NZ	1:A:107:ASN:O	2.52	0.42
1:A:22:LEU:HA	1:A:23:PRO:HD3	1.69	0.42
1:A:23:PRO:HD2	1:A:24:TRP:CE3	2.54	0.42
1:A:50:VAL:HG23	1:A:72:ASN:CB	2.49	0.42
1:A:57:TRP:O	1:A:65:ARG:HD2	2.18	0.42
1:A:92:SER:N	1:A:95:ASP:OD2	2.50	0.42
1:A:2:GLY:HA3	1:A:110:ASP:O	2.20	0.42
1:A:42:SER:N	1:A:110:ASP:OD1	2.53	0.41
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.62	0.41
1:A:162:TYR:N	2:A:197:HOH:O	2.37	0.41
1:A:31:PHE:O	1:A:35:GLN:HG2	2.20	0.41
1:A:61:PRO:O	1:A:62:GLU:C	2.57	0.41
1:A:162:TYR:HA	1:A:163:PRO:HD2	1.87	0.41
1:A:105:LEU:CD1	1:A:108:LYS:HE2	2.49	0.41
1:A:7:ILE:HA	1:A:134:PHE:O	2.21	0.41
1:A:60:ILE:CG2	1:A:65:ARG:HB3	2.51	0.41
1:A:123:GLU:O	1:A:126:ASN:HB2	2.21	0.40
1:A:119:SER:HA	1:A:122:LYS:HB2	2.02	0.40
1:A:108:LYS:HE3	1:A:108:LYS:HB3	1.71	0.40
1:A:117:GLY:O	1:A:118:SER:C	2.60	0.40
1:A:36:ARG:HD3	1:A:36:ARG:HH21	1.28	0.40
1:A:54:LYS:HA	1:A:74:VAL:HG13	1.96	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	184/186 (99%)	161 (88%)	14 (8%)	9 (5%)	2 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	44	GLU
1	A	118	SER
1	A	152	ASP
1	A	168	ASP
1	A	45	GLY
1	A	140	GLN
1	A	59	SER
1	A	40	THR

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	168/168 (100%)	111 (66%)	57 (34%)	0 0

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	VAL
1	A	10	VAL
1	A	13	ASN
1	A	22	LEU
1	A	28	ARG
1	A	29	ASN
1	A	40	THR
1	A	42	SER
1	A	43	VAL
1	A	52	MET
1	A	55	LYS
1	A	61	PRO
1	A	62	GLU
1	A	63	LYS
1	A	68	LYS
1	A	72	ASN
1	A	73	LEU
1	A	75	LEU
1	A	76	SER
1	A	77	ARG
1	A	79	LEU
1	A	80	LYS
1	A	87	HIS
1	A	91	ARG
1	A	95	ASP
1	A	97	LEU
1	A	98	LYS
1	A	99	LEU
1	A	104	GLU
1	A	105	LEU
1	A	107	ASN
1	A	108	LYS
1	A	112	VAL
1	A	114	ILE
1	A	118	SER
1	A	125	MET
1	A	131	LEU
1	A	133	LEU
1	A	137	ARG
1	A	138	ILE
1	A	140	GLN

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	146	THR
1	A	154	GLU
1	A	155	LYS
1	A	157	LYS
1	A	161	GLU
1	A	165	VAL
1	A	166	LEU
1	A	167	SER
1	A	168	ASP
1	A	180	GLU
1	A	184	LYS
1	A	186	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	13	ASN
1	A	29	ASN
1	A	64	ASN
1	A	107	ASN
1	A	140	GLN
1	A	170	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	186/186 (100%)	-0.17	5 (2%) 54 52	4, 20, 41, 46	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLY	6.2
1	A	1	VAL	3.9
1	A	3	SER	3.1
1	A	42	SER	2.5
1	A	105	LEU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.