



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:22 PM UTC

PDB ID : 1PDB / pdb_00001pdb
Title : Analysis of Three Crystal Structure Determinations of a 5-Methyl-6-N-Methyl-5,6,7,8-tetrahydro-2H-pyrido[4,3-b]pyrimidin-2-one Antifolate Complex with Human Dihydrofolate Reductase
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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 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

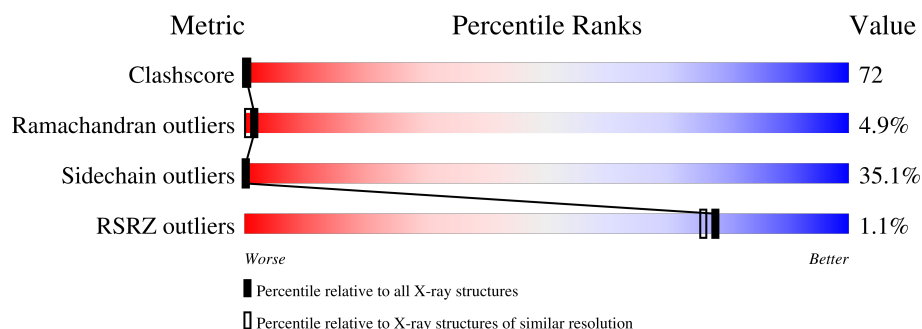
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	186	6% 25% 48% 21%

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			

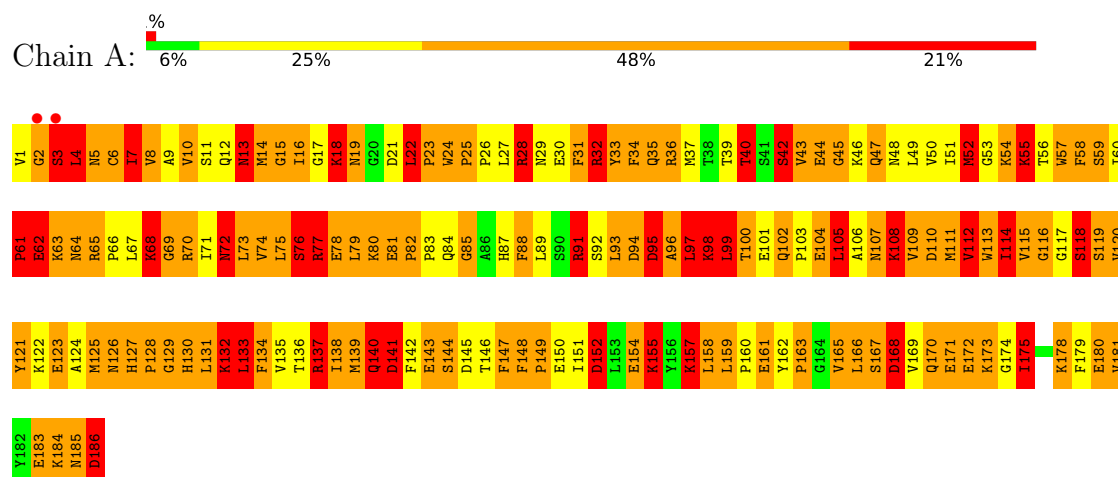
- Molecule 2 is water.

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, 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: 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 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	80.5 (8.00-2.20) 82.5 (8.00-2.20)	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)	0.24 , 79.9	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	0.89	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

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	1.79	17/1537 (1.1%)	3.85	335/2073 (16.2%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLY	N-CA	11.01	1.57	1.45
1	A	180	GLU	N-CA	7.93	1.55	1.45
1	A	32	ARG	CZ-NH2	7.85	1.43	1.33
1	A	4	LEU	N-CA	6.59	1.54	1.46
1	A	21	ASP	N-CA	6.31	1.54	1.46
1	A	168	ASP	CG-OD2	6.12	1.36	1.25
1	A	171	GLU	N-CA	-5.98	1.38	1.46
1	A	140	GLN	N-CA	5.80	1.53	1.46
1	A	64	ASN	N-CA	5.76	1.53	1.45
1	A	114	ILE	CA-CB	5.72	1.60	1.54
1	A	11	SER	N-CA	5.69	1.52	1.45
1	A	35	GLN	N-CA	-5.44	1.39	1.46
1	A	22	LEU	CA-CB	-5.39	1.45	1.53
1	A	24	TRP	NE1-CE2	5.26	1.43	1.37
1	A	170	GLN	C-O	-5.13	1.17	1.23
1	A	169	VAL	C-N	-5.12	1.25	1.33
1	A	113	TRP	C-O	5.01	1.29	1.24

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASN	CA-CB-CG	30.10	142.70	112.60
1	A	28	ARG	CD-NE-CZ	22.00	155.19	124.40
1	A	2	GLY	CA-C-N	20.99	161.63	121.54
1	A	2	GLY	C-N-CA	20.99	161.63	121.54
1	A	130	HIS	CA-CB-CG	-17.41	96.39	113.80
1	A	140	GLN	CA-CB-CG	16.82	147.75	114.10
1	A	127	HIS	CA-CB-CG	16.25	130.05	113.80
1	A	149	PRO	CA-C-N	15.49	142.63	120.95
1	A	149	PRO	C-N-CA	15.49	142.63	120.95
1	A	168	ASP	CA-CB-CG	15.30	127.90	112.60
1	A	42	SER	N-CA-C	14.31	130.50	113.18
1	A	108	LYS	CA-C-N	13.50	140.40	120.69
1	A	108	LYS	C-N-CA	13.50	140.40	120.69
1	A	170	GLN	O-C-N	13.26	138.01	123.03
1	A	150	GLU	CA-CB-CG	13.22	140.54	114.10
1	A	44	GLU	CB-CG-CD	12.94	134.60	112.60
1	A	137	ARG	NE-CZ-NH2	12.57	130.51	119.20
1	A	9	ALA	CA-C-O	-11.90	107.50	120.36
1	A	74	VAL	O-C-N	-11.74	111.17	123.14
1	A	128	PRO	CA-C-O	11.73	135.17	121.56
1	A	25	PRO	CB-CA-C	11.67	125.16	110.92
1	A	21	ASP	CA-CB-CG	11.67	124.27	112.60
1	A	81	GLU	N-CA-C	11.26	134.70	109.81
1	A	165	VAL	CB-CA-C	11.20	127.51	110.83
1	A	74	VAL	CA-C-O	11.16	133.44	120.72
1	A	36	ARG	NE-CZ-NH2	-11.04	109.26	119.20
1	A	144	SER	CA-C-O	-10.99	108.58	121.44
1	A	72	ASN	CA-C-N	10.98	138.86	122.93
1	A	72	ASN	C-N-CA	10.98	138.86	122.93
1	A	68	LYS	CA-C-O	10.77	133.72	121.87
1	A	103	PRO	N-CA-C	-10.74	100.43	113.86
1	A	64	ASN	CA-CB-CG	-10.69	101.91	112.60
1	A	170	GLN	CA-C-O	-10.67	108.64	121.66
1	A	14	MET	CA-C-O	-10.66	108.37	119.78
1	A	18	LYS	N-CA-CB	10.64	125.91	110.37
1	A	110	ASP	CA-CB-CG	10.59	123.19	112.60
1	A	95	ASP	N-CA-C	-10.57	99.78	112.89
1	A	62	GLU	CA-CB-CG	10.49	135.08	114.10
1	A	132	LYS	CD-CE-NZ	10.47	145.39	111.90
1	A	4	LEU	CA-C-N	10.40	137.67	123.00
1	A	4	LEU	C-N-CA	10.40	137.67	123.00
1	A	34	PHE	CA-C-N	10.01	134.05	120.54
1	A	34	PHE	C-N-CA	10.01	134.05	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	VAL	CB-CA-C	-10.00	92.81	110.71
1	A	143	GLU	CA-C-O	-9.99	108.99	120.58
1	A	91	ARG	CA-CB-CG	9.79	133.68	114.10
1	A	113	TRP	O-C-N	9.74	134.71	123.31
1	A	94	ASP	CA-CB-CG	-9.55	103.05	112.60
1	A	9	ALA	O-C-N	9.47	134.57	123.30
1	A	170	GLN	N-CA-CB	9.36	125.16	110.56
1	A	8	VAL	CA-C-O	-9.35	111.37	121.28
1	A	78	GLU	N-CA-C	9.32	124.20	113.02
1	A	32	ARG	NE-CZ-NH1	9.11	130.61	121.50
1	A	15	GLY	CA-C-O	-9.04	110.20	122.31
1	A	17	GLY	CA-C-N	9.02	135.12	121.40
1	A	17	GLY	C-N-CA	9.02	135.12	121.40
1	A	158	LEU	CA-C-O	-9.00	110.05	120.49
1	A	105	LEU	CA-C-N	8.94	132.06	120.44
1	A	105	LEU	C-N-CA	8.94	132.06	120.44
1	A	149	PRO	O-C-N	-8.91	111.81	122.86
1	A	148	PHE	N-CA-C	-8.90	96.72	109.62
1	A	51	ILE	O-C-N	8.88	132.61	123.20
1	A	21	ASP	N-CA-C	-8.83	96.41	108.86
1	A	168	ASP	N-CA-CB	-8.80	95.61	110.49
1	A	168	ASP	CB-CG-OD2	8.77	138.57	118.40
1	A	179	PHE	CA-C-O	-8.76	110.99	120.36
1	A	28	ARG	CB-CG-CD	8.74	131.41	111.30
1	A	137	ARG	NE-CZ-NH1	-8.74	112.76	121.50
1	A	142	PHE	CA-CB-CG	8.69	122.49	113.80
1	A	32	ARG	NE-CZ-NH2	-8.66	111.41	119.20
1	A	98	LYS	CA-C-O	-8.64	110.03	119.97
1	A	31	PHE	CA-CB-CG	8.63	122.43	113.80
1	A	13	ASN	CA-C-O	8.62	130.04	119.78
1	A	105	LEU	N-CA-CB	-8.62	97.19	111.49
1	A	15	GLY	O-C-N	8.54	135.34	122.69
1	A	118	SER	CA-CB-OG	-8.54	94.02	111.10
1	A	185	ASN	N-CA-CB	8.53	127.14	111.11
1	A	154	GLU	N-CA-C	-8.53	102.66	113.23
1	A	168	ASP	CB-CG-OD1	-8.52	98.81	118.40
1	A	172	GLU	CA-CB-CG	8.51	131.12	114.10
1	A	133	LEU	CA-CB-CG	8.45	145.88	116.30
1	A	3	SER	CA-C-N	-8.40	109.48	121.99
1	A	3	SER	C-N-CA	-8.40	109.48	121.99
1	A	27	LEU	CA-C-O	-8.29	110.92	121.11
1	A	113	TRP	CA-C-O	-8.29	111.12	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLU	CA-C-O	-8.26	109.44	119.43
1	A	129	GLY	CA-C-O	8.25	134.92	120.57
1	A	169	VAL	O-C-N	-8.24	113.69	122.67
1	A	19	ASN	CA-CB-CG	8.23	120.83	112.60
1	A	4	LEU	O-C-N	-8.20	112.16	122.82
1	A	140	GLN	N-CA-C	-8.18	93.38	110.80
1	A	72	ASN	CB-CA-C	8.17	123.21	110.14
1	A	10	VAL	CG1-CB-CG2	-8.15	92.86	110.80
1	A	165	VAL	CA-CB-CG1	8.14	124.24	110.40
1	A	116	GLY	N-CA-C	8.13	120.29	112.08
1	A	139	MET	N-CA-C	8.11	123.27	110.70
1	A	24	TRP	O-C-N	8.08	132.19	120.96
1	A	95	ASP	CA-CB-CG	8.05	120.65	112.60
1	A	136	THR	CA-CB-OG1	-8.04	97.55	109.60
1	A	99	LEU	CA-CB-CG	8.00	144.29	116.30
1	A	36	ARG	CA-C-O	7.91	129.13	120.82
1	A	120	VAL	CA-CB-CG1	7.90	123.83	110.40
1	A	135	VAL	N-CA-C	7.87	119.12	108.11
1	A	145	ASP	CB-CA-C	7.84	122.73	109.55
1	A	25	PRO	N-CA-C	-7.78	101.20	110.70
1	A	121	TYR	N-CA-CB	7.76	121.32	110.07
1	A	136	THR	OG1-CB-CG2	7.74	124.79	109.30
1	A	13	ASN	CB-CA-C	7.73	123.70	110.94
1	A	137	ARG	CA-C-O	-7.66	113.56	122.37
1	A	178	LYS	CA-CB-CG	7.66	129.42	114.10
1	A	3	SER	CA-C-O	-7.65	109.56	120.51
1	A	22	LEU	CA-CB-CG	7.51	142.60	116.30
1	A	124	ALA	CA-C-N	7.49	130.64	120.38
1	A	124	ALA	C-N-CA	7.49	130.64	120.38
1	A	75	LEU	N-CA-C	-7.45	97.11	108.96
1	A	55	LYS	CA-C-O	7.38	129.19	121.07
1	A	5	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	157	LYS	N-CA-CB	7.34	123.61	110.83
1	A	65	ARG	NE-CZ-NH2	7.33	125.79	119.20
1	A	181	VAL	CB-CA-C	7.32	121.53	110.62
1	A	184	LYS	CB-CG-CD	7.32	128.13	111.30
1	A	120	VAL	N-CA-C	-7.29	101.67	111.44
1	A	159	LEU	CA-C-N	7.28	126.96	119.82
1	A	159	LEU	C-N-CA	7.28	126.96	119.82
1	A	120	VAL	N-CA-CB	7.22	124.59	110.95
1	A	179	PHE	CA-CB-CG	-7.21	106.59	113.80
1	A	161	GLU	O-C-N	7.19	130.02	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	CA-CB-CG	-7.18	99.74	114.10
1	A	102	GLN	OE1-CD-NE2	7.16	129.76	122.60
1	A	27	LEU	CA-C-N	7.12	132.09	120.63
1	A	27	LEU	C-N-CA	7.12	132.09	120.63
1	A	33	TYR	CA-CB-CG	7.11	126.70	113.90
1	A	4	LEU	N-CA-CB	-7.09	98.59	109.94
1	A	140	GLN	CA-C-O	-7.09	110.37	120.51
1	A	69	GLY	N-CA-C	-7.09	103.98	114.90
1	A	64	ASN	O-C-N	7.00	130.96	122.35
1	A	32	ARG	CD-NE-CZ	6.94	134.11	124.40
1	A	23	PRO	N-CD-CG	-6.93	92.80	103.20
1	A	184	LYS	N-CA-CB	6.93	124.43	111.53
1	A	76	SER	O-C-N	6.93	132.39	123.24
1	A	138	ILE	CA-CB-CG2	-6.93	98.72	110.50
1	A	81	GLU	CB-CG-CD	6.93	124.38	112.60
1	A	75	LEU	CA-C-O	-6.91	112.69	120.43
1	A	3	SER	N-CA-C	6.91	125.52	110.80
1	A	131	LEU	CA-CB-CG	6.90	140.46	116.30
1	A	67	LEU	CA-C-N	6.88	132.50	120.87
1	A	67	LEU	C-N-CA	6.88	132.50	120.87
1	A	54	LYS	CG-CD-CE	6.88	127.12	111.30
1	A	161	GLU	CG-CD-OE2	-6.84	102.66	118.40
1	A	9	ALA	N-CA-C	-6.78	97.84	108.90
1	A	58	PHE	CB-CA-C	6.64	121.31	110.88
1	A	61	PRO	CA-C-O	6.63	128.23	121.27
1	A	54	LYS	CA-C-O	-6.63	113.86	120.82
1	A	77	ARG	CA-CB-CG	6.62	127.35	114.10
1	A	138	ILE	N-CA-CB	6.61	118.16	110.82
1	A	121	TYR	CB-CA-C	-6.58	100.50	110.90
1	A	173	LYS	CA-CB-CG	6.54	127.19	114.10
1	A	14	MET	CA-C-N	-6.54	113.14	120.53
1	A	14	MET	C-N-CA	-6.54	113.14	120.53
1	A	68	LYS	CB-CG-CD	6.53	126.31	111.30
1	A	3	SER	O-C-N	6.52	131.26	122.59
1	A	186	ASP	CA-C-O	-6.51	101.46	121.00
1	A	183	GLU	CG-CD-OE2	-6.48	103.50	118.40
1	A	36	ARG	CD-NE-CZ	-6.45	115.37	124.40
1	A	128	PRO	N-CA-CB	6.44	108.95	103.35
1	A	8	VAL	CG1-CB-CG2	6.43	124.96	110.80
1	A	65	ARG	CD-NE-CZ	6.38	133.33	124.40
1	A	58	PHE	N-CA-C	-6.37	104.26	111.07
1	A	115	VAL	CA-CB-CG2	6.36	121.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LEU	CA-C-O	-6.34	114.11	119.76
1	A	68	LYS	O-C-N	-6.34	115.34	122.75
1	A	75	LEU	CB-CA-C	6.33	120.79	110.22
1	A	131	LEU	CA-C-N	6.32	131.68	122.77
1	A	131	LEU	C-N-CA	6.32	131.68	122.77
1	A	13	ASN	O-C-N	-6.32	114.58	122.35
1	A	4	LEU	N-CA-C	6.31	118.45	108.67
1	A	61	PRO	CB-CA-C	6.30	119.90	111.71
1	A	144	SER	O-C-N	6.30	131.34	123.15
1	A	183	GLU	OE1-CD-OE2	6.29	138.01	122.90
1	A	36	ARG	CB-CG-CD	6.29	125.77	111.30
1	A	33	TYR	O-C-N	6.21	128.47	122.07
1	A	134	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	184	LYS	CA-CB-CG	6.20	126.50	114.10
1	A	49	LEU	CA-C-O	-6.17	113.95	120.80
1	A	100	THR	O-C-N	6.17	128.42	122.07
1	A	14	MET	CB-CG-SD	-6.16	94.23	112.70
1	A	126	ASN	CB-CG-OD1	-6.15	108.50	120.80
1	A	170	GLN	CB-CG-CD	-6.15	102.14	112.60
1	A	4	LEU	CB-CA-C	6.14	121.03	110.77
1	A	101	GLU	CA-C-O	6.14	126.97	119.11
1	A	47	GLN	O-C-N	6.12	130.24	123.33
1	A	81	GLU	CA-CB-CG	6.11	126.31	114.10
1	A	96	ALA	CB-CA-C	6.10	120.53	110.90
1	A	152	ASP	CA-CB-CG	-6.08	106.52	112.60
1	A	105	LEU	N-CA-C	6.07	120.56	112.30
1	A	140	GLN	O-C-N	6.07	130.66	122.59
1	A	99	LEU	N-CA-C	-6.06	105.60	112.87
1	A	13	ASN	N-CA-C	-6.04	105.83	112.72
1	A	88	PHE	CB-CA-C	-6.03	100.31	110.43
1	A	16	ILE	N-CA-C	-6.00	107.41	113.47
1	A	14	MET	O-C-N	5.97	130.40	122.04
1	A	145	ASP	N-CA-C	-5.97	105.96	113.72
1	A	64	ASN	OD1-CG-ND2	5.96	128.56	122.60
1	A	65	ARG	O-C-N	5.96	127.27	121.66
1	A	158	LEU	CB-CA-C	5.96	120.07	110.29
1	A	170	GLN	N-CA-C	-5.95	101.19	110.42
1	A	175	ILE	CA-C-O	5.95	126.58	120.39
1	A	52	MET	CA-CB-CG	5.95	125.99	114.10
1	A	185	ASN	CA-C-N	-5.93	111.02	121.70
1	A	185	ASN	C-N-CA	-5.93	111.02	121.70
1	A	77	ARG	CA-C-O	5.92	126.70	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	O-C-N	5.92	130.46	122.59
1	A	150	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	83	PRO	O-C-N	5.91	130.62	122.64
1	A	132	LYS	CA-CB-CG	-5.88	102.34	114.10
1	A	70	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	134	PHE	N-CA-C	-5.84	98.89	108.41
1	A	30	GLU	N-CA-C	-5.83	104.52	111.69
1	A	24	TRP	CE3-CZ3-CH2	-5.83	113.53	121.10
1	A	98	LYS	O-C-N	5.77	129.37	122.27
1	A	171	GLU	CA-C-N	5.77	132.29	122.37
1	A	171	GLU	C-N-CA	5.77	132.29	122.37
1	A	31	PHE	CA-C-N	5.76	128.47	120.29
1	A	31	PHE	C-N-CA	5.76	128.47	120.29
1	A	172	GLU	CA-C-O	5.74	127.49	120.60
1	A	186	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	160	PRO	CA-C-O	5.72	127.53	118.89
1	A	10	VAL	CA-CB-CG1	5.71	120.10	110.40
1	A	17	GLY	O-C-N	-5.71	118.25	123.56
1	A	155	LYS	CA-C-O	-5.70	112.86	119.64
1	A	76	SER	CA-C-N	5.69	128.37	120.29
1	A	76	SER	C-N-CA	5.69	128.37	120.29
1	A	157	LYS	CB-CA-C	-5.69	98.51	109.37
1	A	111	MET	CA-C-O	-5.68	114.50	120.80
1	A	135	VAL	N-CA-CB	-5.67	103.59	111.41
1	A	161	GLU	OE1-CD-OE2	5.67	136.50	122.90
1	A	119	SER	CA-C-N	5.66	130.02	120.29
1	A	119	SER	C-N-CA	5.66	130.02	120.29
1	A	135	VAL	CA-CB-CG2	-5.65	100.79	110.40
1	A	36	ARG	NH1-CZ-NH2	5.65	126.65	119.30
1	A	95	ASP	N-CA-CB	5.63	119.58	110.40
1	A	65	ARG	CB-CA-C	5.63	117.32	108.88
1	A	28	ARG	NE-CZ-NH2	5.63	124.26	119.20
1	A	109	VAL	O-C-N	-5.62	117.33	122.79
1	A	47	GLN	CA-CB-CG	5.62	125.34	114.10
1	A	107	ASN	CA-C-O	-5.61	112.69	119.59
1	A	163	PRO	CA-C-N	5.61	132.19	122.05
1	A	163	PRO	C-N-CA	5.61	132.19	122.05
1	A	78	GLU	CG-CD-OE2	-5.59	105.54	118.40
1	A	94	ASP	CB-CA-C	5.59	120.96	110.63
1	A	84	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	154	GLU	CG-CD-OE1	5.57	131.22	118.40
1	A	170	GLN	OE1-CD-NE2	5.57	128.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	GLU	N-CA-CB	-5.57	102.39	111.24
1	A	150	GLU	N-CA-C	5.56	118.30	109.96
1	A	61	PRO	CA-C-N	5.56	129.16	120.82
1	A	61	PRO	C-N-CA	5.56	129.16	120.82
1	A	7	ILE	CB-CA-C	5.56	118.66	110.77
1	A	93	LEU	CB-CA-C	5.55	120.12	110.68
1	A	97	LEU	CB-CA-C	5.54	121.58	109.99
1	A	13	ASN	CA-C-N	5.54	133.11	123.91
1	A	13	ASN	C-N-CA	5.54	133.11	123.91
1	A	127	HIS	O-C-N	5.53	127.63	121.43
1	A	30	GLU	CG-CD-OE1	5.53	131.11	118.40
1	A	85	GLY	N-CA-C	-5.53	107.41	114.37
1	A	6	CYS	CB-CA-C	5.52	118.86	109.75
1	A	134	PHE	O-C-N	5.48	129.63	123.27
1	A	91	ARG	N-CA-CB	5.48	119.33	110.40
1	A	35	GLN	CA-CB-CG	5.48	125.06	114.10
1	A	71	ILE	N-CA-C	-5.46	101.78	109.21
1	A	101	GLU	CA-CB-CG	5.46	125.02	114.10
1	A	126	ASN	CB-CG-ND2	5.45	124.58	116.40
1	A	154	GLU	CA-CB-CG	5.45	125.01	114.10
1	A	73	LEU	CA-C-N	5.44	130.12	123.10
1	A	73	LEU	C-N-CA	5.44	130.12	123.10
1	A	109	VAL	CA-C-N	5.42	131.90	121.54
1	A	109	VAL	C-N-CA	5.42	131.90	121.54
1	A	148	PHE	N-CA-CB	5.41	118.23	109.90
1	A	82	PRO	N-CA-C	-5.40	104.12	110.70
1	A	15	GLY	N-CA-C	-5.39	105.64	112.54
1	A	47	GLN	CB-CG-CD	-5.38	103.45	112.60
1	A	172	GLU	CA-C-N	5.33	131.71	121.54
1	A	172	GLU	C-N-CA	5.33	131.71	121.54
1	A	33	TYR	CB-CA-C	-5.33	102.52	110.88
1	A	148	PHE	O-C-N	5.32	130.31	121.59
1	A	94	ASP	N-CA-C	5.29	117.80	111.71
1	A	157	LYS	CA-C-O	-5.29	114.98	120.70
1	A	100	THR	N-CA-CB	5.29	117.68	110.01
1	A	22	LEU	N-CA-C	-5.29	103.52	110.39
1	A	152	ASP	N-CA-CB	-5.29	101.56	110.49
1	A	31	PHE	CA-C-O	-5.28	114.95	120.55
1	A	85	GLY	O-C-N	5.28	128.26	122.56
1	A	139	MET	CA-CB-CG	-5.27	103.55	114.10
1	A	181	VAL	CA-C-O	5.27	126.84	120.67
1	A	8	VAL	O-C-N	5.27	129.00	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	VAL	CA-C-O	5.26	126.06	120.48
1	A	123	GLU	CB-CG-CD	-5.26	103.66	112.60
1	A	136	THR	CA-C-N	5.25	130.04	122.16
1	A	136	THR	C-N-CA	5.25	130.04	122.16
1	A	157	LYS	O-C-N	5.25	130.06	123.23
1	A	172	GLU	CG-CD-OE1	5.25	130.47	118.40
1	A	84	GLN	N-CA-CB	5.24	117.79	109.51
1	A	45	GLY	N-CA-C	5.24	125.59	113.18
1	A	141	ASP	O-C-N	5.22	128.91	123.06
1	A	111	MET	N-CA-C	5.21	118.30	109.76
1	A	2	GLY	N-CA-C	5.21	125.52	113.18
1	A	48	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	74	VAL	N-CA-C	-5.20	100.99	108.53
1	A	30	GLU	CG-CD-OE2	-5.19	106.47	118.40
1	A	147	PHE	CB-CA-C	5.18	120.40	109.79
1	A	18	LYS	O-C-N	5.17	129.56	123.36
1	A	116	GLY	CA-C-O	-5.15	118.61	122.37
1	A	57	TRP	N-CA-CB	-5.14	102.55	110.01
1	A	73	LEU	O-C-N	5.13	129.73	123.21
1	A	4	LEU	CA-C-O	5.12	126.39	120.60
1	A	63	LYS	CA-CB-CG	-5.12	103.86	114.10
1	A	63	LYS	CA-C-N	-5.12	114.12	122.26
1	A	63	LYS	C-N-CA	-5.12	114.12	122.26
1	A	161	GLU	CA-C-O	-5.12	115.53	121.26
1	A	103	PRO	CA-C-O	5.11	126.16	119.00
1	A	30	GLU	CA-CB-CG	-5.11	103.88	114.10
1	A	127	HIS	N-CA-C	5.11	116.32	109.83
1	A	18	LYS	CB-CA-C	-5.11	104.41	110.94
1	A	80	LYS	CB-CG-CD	5.10	123.03	111.30
1	A	7	ILE	CG1-CB-CG2	5.10	125.99	110.70
1	A	88	PHE	N-CA-C	5.10	116.27	108.42
1	A	140	GLN	CB-CA-C	5.09	120.56	110.42
1	A	167	SER	N-CA-C	-5.08	104.72	112.04
1	A	96	ALA	N-CA-C	-5.07	105.67	111.14
1	A	119	SER	N-CA-CB	-5.06	102.51	110.30
1	A	76	SER	N-CA-CB	5.04	118.43	110.71
1	A	75	LEU	O-C-N	5.04	128.93	123.13
1	A	19	ASN	N-CA-CB	-5.02	104.36	111.84
1	A	7	ILE	CA-CB-CG1	-5.02	101.87	110.40
1	A	22	LEU	CB-CA-C	5.01	116.28	108.61

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	1510	218	0
2	A	17	0	0	6	0
All	All	1519	0	1510	218	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 72.

All (218) 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
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:55:LYS:C	1:A:55:LYS:HE2	1.91	0.96
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:ARG:HA	1:A:66:PRO:C	2.08	0.77
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: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
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: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:100:THR:HG23	1:A:109:VAL:HG11	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:139:MET:HE1	1:A:178:LYS:HB2	1.78	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:CA	1:A:55:LYS:CE	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:46:LYS:NZ	1:A:107:ASN:C	2.58	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:13:ASN:HD22	1:A:13:ASN:C	2.08	0.60
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:29:ASN:HB2	1:A:172:GLU:CD	2.27	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
1:A:58:PHE:CD2	1:A:65:ARG:NH1	2.71	0.58
1:A:39:THR:O	1:A:40:THR:C	2.47	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:134:PHE:C	2:A:196:HOH:O	2.46	0.57
1:A:78:GLU:O	1:A:78:GLU:HG2	2.05	0.57
1:A:148:PHE:CD1	1:A:149:PRO:HD2	2.40	0.57
1:A:1:VAL:HG12	1:A:109:VAL:CG1	2.34	0.57
1:A:13:ASN:C	1:A:13:ASN:ND2	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:LEU:C	1:A:102:GLN:HB2	2.30	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:46:LYS:HZ2	1:A:107:ASN:C	2.13	0.55
1:A:55:LYS:HE2	1:A:55:LYS:HA	1.89	0.55
1:A:114:ILE:HD12	1:A:114:ILE:N	2.21	0.55
1:A:58:PHE:HA	1:A:65:ARG:NH2	2.21	0.55
1:A:102:GLN:C	1:A:104:GLU:N	2.62	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:18:LYS:HE3	1:A:19:ASN:CG	2.33	0.54
1:A:107:ASN:HD22	1:A:107:ASN:C	2.11	0.54
1:A:33:TYR:CE2	1:A:37:MET:HE3	2.44	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:13:ASN:HB3	1:A:141:ASP:CB	2.39	0.52
1:A:55:LYS:C	1:A:55:LYS:CE	2.76	0.52
1:A:99:LEU:O	1:A:102:GLN:HB2	2.08	0.52
1:A:107:ASN:O	1:A:107:ASN:CG	2.52	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:168:ASP:O	1:A:170:GLN:NE2	2.41	0.52
1:A:114:ILE:N	1:A:114:ILE:CD1	2.73	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:3:SER:O	1:A:112:VAL:O	2.29	0.50
1:A:78:GLU:O	1:A:78:GLU:CG	2.59	0.49
1:A:93:LEU:HG	1:A:97:LEU:CD2	2.42	0.49
1:A:93:LEU:O	1:A:96:ALA:N	2.46	0.49
1:A:129:GLY:O	1:A:184:LYS:HD2	2.13	0.49
1:A:174:GLY:C	1:A:175:ILE:HG13	2.37	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:24:TRP:C	1:A:25:PRO:O	2.53	0.48
1:A:81:GLU:HG2	1:A:82:PRO:O	2.14	0.48
1:A:61:PRO:HB2	1:A:64:ASN:ND2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:HB2	1:A:181:VAL:HG11	1.95	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:125:MET:HE1	1:A:148:PHE:CZ	2.50	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:HD22	1:A:97:LEU:H	1.80	0.47
1:A:97:LEU:HD22	1:A:97:LEU:N	2.30	0.46
1:A:4:LEU:HD11	1:A:97:LEU:HD11	1.97	0.46
1:A:134:PHE:CB	2:A:196:HOH:O	2.50	0.46
1:A:61:PRO:O	1:A:62:GLU:C	2.57	0.46
1:A:94:ASP:O	1:A:98:LYS:HE2	2.15	0.46
1:A:98:LYS:C	1:A:100:THR:N	2.71	0.46
1:A:166:LEU:HB3	1:A:168:ASP:OD1	2.16	0.46
1:A:54:LYS:CA	1:A:74:VAL:HG11	2.42	0.46
1:A:68:LYS:HD3	1:A:68:LYS:H	1.80	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:117:GLY:O	1:A:118:SER:C	2.60	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:13:ASN:C	1:A:14:MET:HG2	2.41	0.44
1:A:77:ARG:NH1	1:A:91:ARG:HG3	2.32	0.44
1:A:140:GLN:HE21	1:A:140:GLN:HB3	1.57	0.44
1:A:111:MET:HE3	1:A:113:TRP:HE1	1.83	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:18:LYS:HB3	1:A:18:LYS:HE2	1.47	0.43
1:A:81:GLU:O	1:A:82:PRO:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:CB	1:A:115:VAL:HG23	2.49	0.43
1:A:33:TYR:O	1:A:37:MET:HB2	2.17	0.43
1:A:53:GLY:N	1:A:116:GLY:O	2.52	0.43
1:A:13:ASN:CG	1:A:141:ASP:HB2	2.44	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:16:ILE:HD12	1:A:121:TYR:HE1	1.84	0.42
1:A:105:LEU:HG	1:A:108:LYS:HE2	2.01	0.42
1:A:157:LYS:HD2	1:A:157:LYS:HA	1.72	0.42
1:A:79:LEU:C	1:A:81:GLU:N	2.78	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:31:PHE:O	1:A:35:GLN:HG2	2.20	0.41
1:A:42:SER:N	1:A:110:ASP:OD1	2.53	0.41
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.62	0.41
1:A:162:TYR:N	2:A:197:HOH:O	2.37	0.41
1:A:162:TYR:HA	1:A:163:PRO:HD2	1.87	0.41
1:A:58:PHE:C	1:A:65:ARG:NH2	2.73	0.41
1:A:14:MET:HB3	1:A:14:MET:HE3	1.58	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:79:LEU:C	1:A:81:GLU:H	2.28	0.41
1:A:123:GLU:O	1:A:126:ASN:HB2	2.21	0.40
1:A:98:LYS:C	1:A:100:THR:H	2.28	0.40
1:A:102:GLN:C	1:A:104:GLU:H	2.21	0.40
1:A:119:SER:HA	1:A:122:LYS:HB2	2.02	0.40
1:A:36:ARG:HH21	1:A:36:ARG:HD3	1.28	0.40
1:A:108:LYS:HB3	1:A:108:LYS:HE3	1.71	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%)	1 0

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%)	109 (65%)	59 (35%)	0 0

All (59) 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	18	LYS
1	A	22	LEU
1	A	28	ARG
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	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	108	LYS
1	A	112	VAL
1	A	114	ILE
1	A	118	SER
1	A	120	VAL
1	A	125	MET
1	A	131	LEU
1	A	132	LYS
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	143	GLU
1	A	146	THR
1	A	154	GLU
1	A	155	LYS
1	A	157	LYS
1	A	158	LEU
1	A	161	GLU
1	A	165	VAL
1	A	166	LEU
1	A	167	SER
1	A	168	ASP
1	A	175	ILE
1	A	180	GLU
1	A	186	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	13	ASN
1	A	64	ASN
1	A	107	ASN
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 oligosaccharides 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 [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%)	-0.01	2 (1%) 78 76	4, 20, 41, 46	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLY	4.3
1	A	3	SER	2.8

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 oligosaccharides 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.