



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:19 AM UTC

PDB ID : 7CED / pdb_00007ced
Title : Apo-methanol dehydrogenase (MDH) from *Methylococcus capsulatus* (Bath)
Authors : Chuankhayan, P.; Chan, S.I.; Nareddy, P.K.R.; Tsai, I.K.; Tsai, Y.F.; Chen, K.H.-C.; Yu, S.S.-F.; Chen, C.J.
Deposited on : 2020-06-22
Resolution : 1.90 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
Xtrriage (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

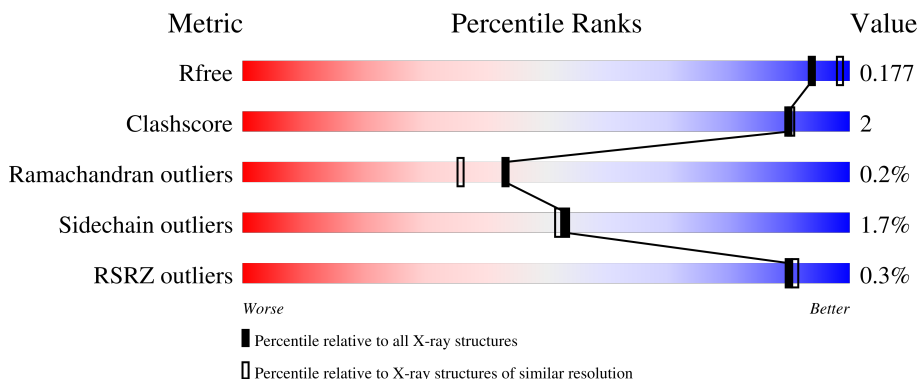
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	573	94% 5% .
1	B	573	94% 5% .
1	C	573	93% 6% .
1	D	573	95% . .
1	G	573	94% 5% .

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Mol	Chain	Length	Quality of chain
1	H	573	 94% 5% .
1	M	573	 93% 6% .
1	N	573	 92% 7% .
2	E	72	 94% . .
2	F	72	 4% 86% 12% .
2	I	72	 8% 90% 7% ..
2	J	72	 89% 8% ..
2	K	72	 94% . .
2	L	72	 90% 7% ..
2	O	72	 % 90% 8% .
2	P	72	 3% 89% 7% ...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45177 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 Methanol dehydrogenase protein, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	573	4491	2871	765	832	23	0	0	0
1	B	573	4490	2871	765	831	23	0	0	0
1	C	573	4491	2871	765	832	23	0	0	0
1	D	573	4490	2871	765	831	23	0	0	0
1	G	573	4491	2871	765	832	23	0	0	0
1	H	573	4490	2871	765	831	23	0	0	0
1	M	573	4491	2871	765	832	23	0	0	0
1	N	573	4490	2871	765	831	23	0	0	0

- Molecule 2 is a protein called Methanol dehydrogenase [cytochrome c] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	71	568	356	100	109	3	0	0	0
2	F	71	568	356	100	109	3	0	0	0
2	I	71	568	356	100	109	3	0	0	0
2	J	71	568	356	100	109	3	0	0	0
2	K	71	568	356	100	109	3	0	0	0
2	L	71	568	356	100	109	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	P	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			

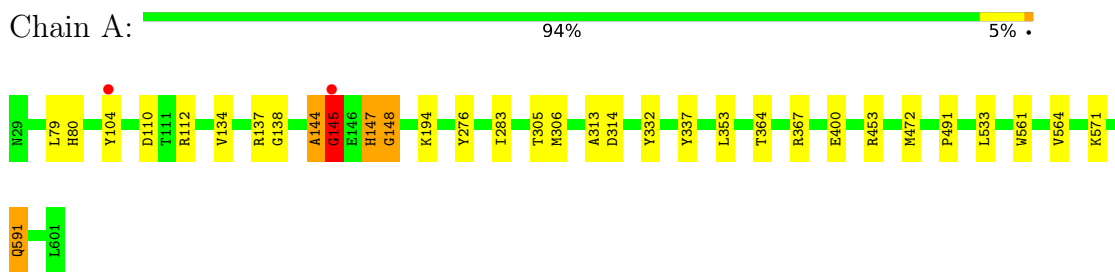
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	548	Total	O	0	0
			548	548		
3	B	491	Total	O	0	0
			491	491		
3	C	500	Total	O	0	0
			500	500		
3	D	511	Total	O	0	0
			511	511		
3	E	114	Total	O	0	0
			114	114		
3	F	77	Total	O	0	0
			77	77		
3	G	529	Total	O	0	0
			529	529		
3	H	481	Total	O	0	0
			481	481		
3	I	84	Total	O	0	0
			84	84		
3	J	79	Total	O	0	0
			79	79		
3	K	81	Total	O	0	0
			81	81		
3	L	97	Total	O	0	0
			97	97		
3	M	453	Total	O	0	0
			453	453		
3	N	505	Total	O	0	0
			505	505		
3	O	61	Total	O	0	0
			61	61		
3	P	98	Total	O	0	0
			98	98		

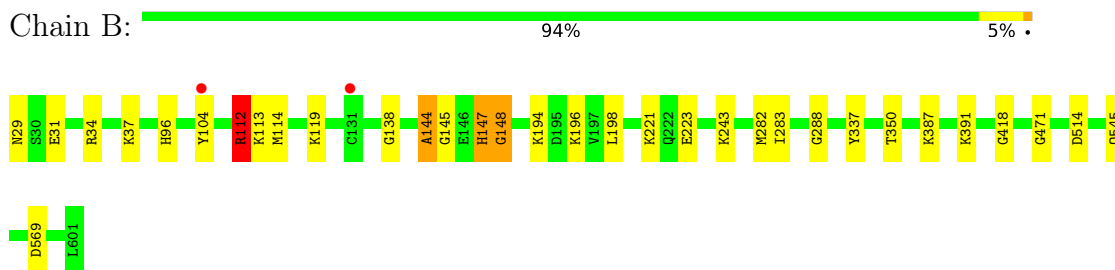
3 Residue-property plots [i](#)

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.

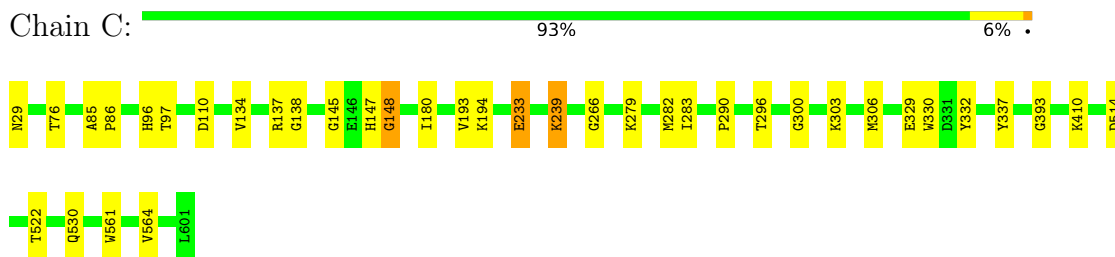
- Molecule 1: Methanol dehydrogenase protein, large subunit



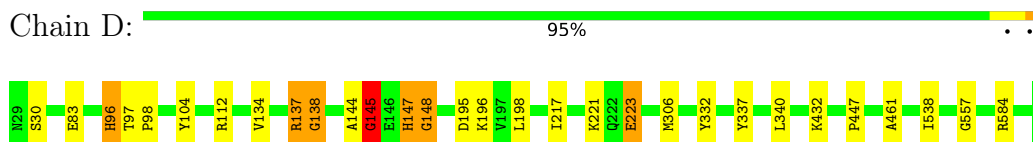
- Molecule 1: Methanol dehydrogenase protein, large subunit



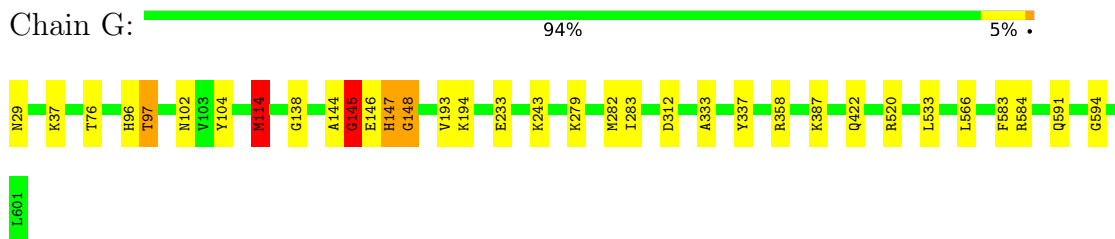
- Molecule 1: Methanol dehydrogenase protein, large subunit



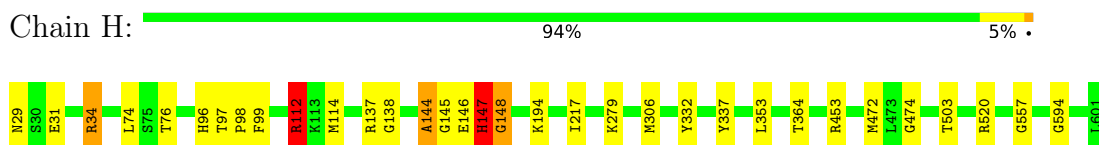
- Molecule 1: Methanol dehydrogenase protein, large subunit



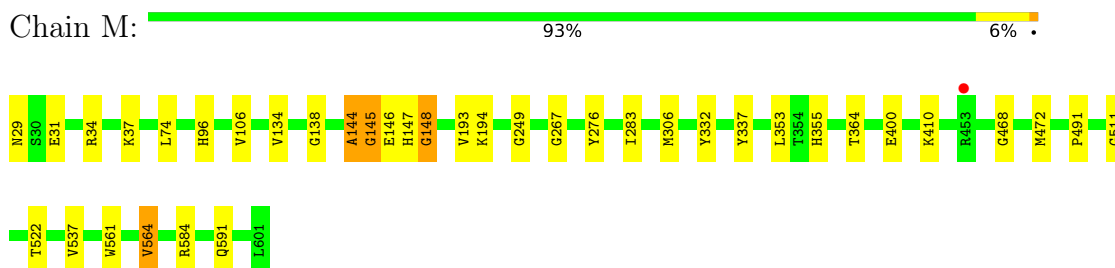
- Molecule 1: Methanol dehydrogenase protein, large subunit



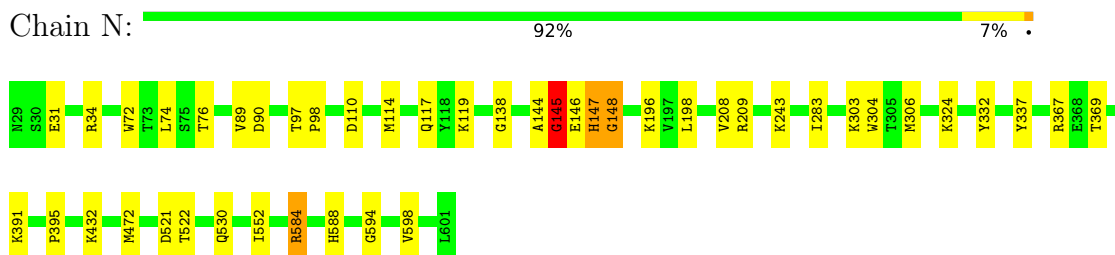
- Molecule 1: Methanol dehydrogenase protein, large subunit



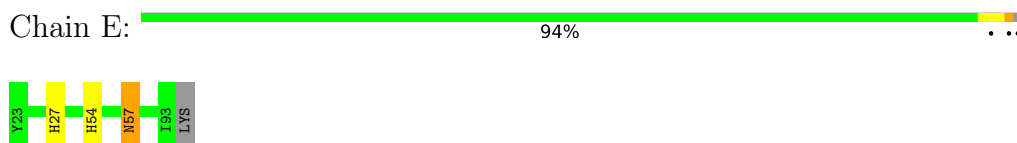
- Molecule 1: Methanol dehydrogenase protein, large subunit



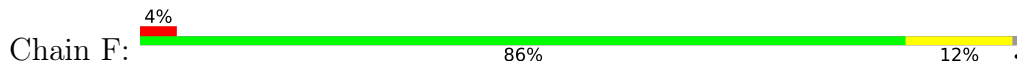
- Molecule 1: Methanol dehydrogenase protein, large subunit

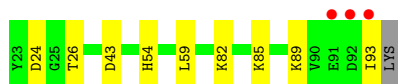


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

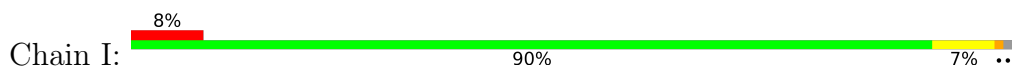


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

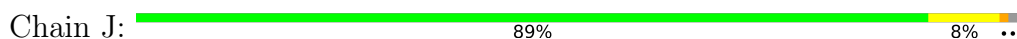




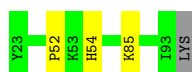
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



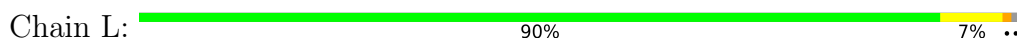
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



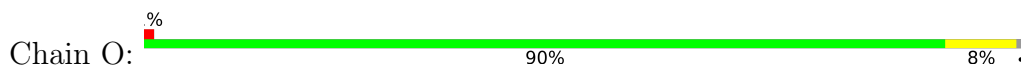
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



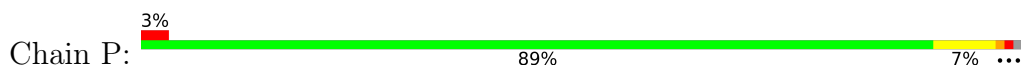
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.70Å 211.85Å 223.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.00 – 1.90 153.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.00-1.90) 99.9 (153.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.140 , 0.180 (Not available) , 0.177	Depositor DCC
R_{free} test set	24064 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45177	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	1.18	4/4622 (0.1%)	1.09	17/6281 (0.3%)
1	B	1.20	6/4621 (0.1%)	1.12	15/6281 (0.2%)
1	C	1.19	6/4622 (0.1%)	1.07	12/6281 (0.2%)
1	D	1.16	6/4621 (0.1%)	1.09	9/6281 (0.1%)
1	G	1.18	5/4622 (0.1%)	1.09	16/6281 (0.3%)
1	H	1.17	5/4621 (0.1%)	1.09	16/6281 (0.3%)
1	M	1.20	6/4622 (0.1%)	1.07	14/6281 (0.2%)
1	N	1.20	10/4621 (0.2%)	1.11	15/6281 (0.2%)
2	E	1.18	0/583	1.06	1/785 (0.1%)
2	F	1.08	0/583	1.08	0/785
2	I	1.16	0/583	1.07	0/785
2	J	1.16	0/583	1.09	1/785 (0.1%)
2	K	1.17	0/583	1.11	0/785
2	L	1.20	1/583 (0.2%)	1.22	5/785 (0.6%)
2	O	1.12	1/583 (0.2%)	1.12	2/785 (0.3%)
2	P	1.26	0/583	1.17	3/785 (0.4%)
All	All	1.18	50/41636 (0.1%)	1.09	126/56528 (0.2%)

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	2
1	B	0	1
1	D	0	1
1	G	0	2
1	H	0	2
1	M	0	2
All	All	0	10

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	112	ARG	CD-NE	-11.95	1.29	1.46
1	B	112	ARG	CD-NE	-11.91	1.29	1.46
1	N	148	GLY	N-CA	-8.69	1.31	1.45
1	D	145	GLY	N-CA	-8.58	1.31	1.45
1	A	148	GLY	N-CA	-8.44	1.32	1.45
1	A	145	GLY	N-CA	-8.28	1.33	1.45
1	N	145	GLY	N-CA	-8.22	1.32	1.45
1	N	522	THR	C-N	-8.05	1.23	1.33
1	G	148	GLY	N-CA	-8.00	1.32	1.45
1	G	145	GLY	N-CA	-7.96	1.32	1.45
1	H	96	HIS	C-N	7.75	1.49	1.33
1	B	148	GLY	N-CA	-7.36	1.33	1.45
1	C	148	GLY	N-CA	-7.06	1.34	1.45
1	B	147	HIS	CA-C	6.90	1.62	1.52
1	B	96	HIS	C-N	6.53	1.47	1.33
1	M	96	HIS	C-N	6.49	1.47	1.33
1	A	147	HIS	CA-C	6.25	1.61	1.52
1	H	148	GLY	N-CA	-6.02	1.35	1.45
1	N	145	GLY	C-O	-5.98	1.11	1.23
1	C	300	GLY	N-CA	5.95	1.50	1.45
1	A	144	ALA	C-O	-5.95	1.15	1.23
1	D	340	LEU	C-O	5.92	1.31	1.23
1	C	303	LYS	CA-CB	5.84	1.63	1.53
2	L	26	THR	CB-CG2	-5.72	1.33	1.52
1	N	584	ARG	CZ-NH1	5.70	1.40	1.32
1	M	355	HIS	N-CA	-5.66	1.41	1.46
1	N	146	GLU	N-CA	5.66	1.53	1.46
1	C	522	THR	C-O	-5.61	1.16	1.24
1	G	102	ASN	C-N	-5.61	1.25	1.33
1	D	148	GLY	N-CA	-5.61	1.36	1.45
1	N	395	PRO	CA-C	5.61	1.57	1.52
1	M	147	HIS	CA-C	5.58	1.62	1.52
1	B	350	THR	CA-C	5.57	1.57	1.52
1	H	503	THR	N-CA	5.54	1.53	1.45
1	D	96	HIS	C-N	5.46	1.44	1.33
1	N	521	ASP	C-N	-5.45	1.26	1.33
1	M	148	GLY	N-CA	-5.41	1.36	1.45
1	C	96	HIS	C-N	5.40	1.44	1.33
1	M	522	THR	C-O	-5.34	1.17	1.24
2	O	71	ALA	N-CA	5.32	1.52	1.46
1	G	312	ASP	C-O	5.28	1.30	1.23
1	N	369	THR	N-CA	5.25	1.53	1.46
1	D	147	HIS	CA-C	5.25	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	96	HIS	C-N	5.22	1.44	1.33
1	H	474	GLY	CA-C	-5.21	1.47	1.52
1	D	223	GLU	CA-C	-5.20	1.46	1.52
1	C	393	GLY	CA-C	5.17	1.58	1.51
1	B	418	GLY	C-O	5.12	1.30	1.23
1	M	267	GLY	CA-C	-5.02	1.47	1.52
1	N	110	ASP	CG-OD1	5.00	1.34	1.25

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	HIS	CA-C-N	13.09	145.26	121.70
1	C	147	HIS	C-N-CA	13.09	145.26	121.70
1	D	147	HIS	CA-C-N	13.08	145.25	121.70
1	D	147	HIS	C-N-CA	13.08	145.25	121.70
1	N	147	HIS	CA-C-N	12.67	144.51	121.70
1	N	147	HIS	C-N-CA	12.67	144.51	121.70
1	D	147	HIS	N-CA-C	12.66	128.07	112.87
1	B	112	ARG	NE-CZ-NH2	-12.60	107.86	119.20
1	M	147	HIS	N-CA-C	12.43	127.98	113.19
1	B	147	HIS	CA-C-N	12.38	143.98	121.70
1	B	147	HIS	C-N-CA	12.38	143.98	121.70
1	D	147	HIS	O-C-N	-12.04	106.41	122.43
1	B	147	HIS	O-C-N	-12.02	105.87	122.46
1	C	147	HIS	O-C-N	-11.78	106.65	122.43
1	A	147	HIS	CA-C-N	11.77	142.88	121.70
1	A	147	HIS	C-N-CA	11.77	142.88	121.70
1	N	147	HIS	O-C-N	-11.65	106.38	122.46
1	A	147	HIS	O-C-N	-11.20	107.83	122.39
1	H	112	ARG	NE-CZ-NH2	-11.04	109.27	119.20
1	H	147	HIS	CA-C-N	10.98	141.47	121.70
1	H	147	HIS	C-N-CA	10.98	141.47	121.70
1	A	147	HIS	N-CA-C	10.91	125.69	112.38
1	G	147	HIS	O-C-N	-10.71	108.19	122.43
1	G	147	HIS	N-CA-C	10.39	125.34	112.87
1	G	147	HIS	CA-C-N	10.35	140.33	121.70
1	G	147	HIS	C-N-CA	10.35	140.33	121.70
1	H	147	HIS	O-C-N	-10.35	108.83	122.59
1	N	147	HIS	N-CA-C	10.34	125.41	113.01
1	C	147	HIS	N-CA-C	10.15	124.92	112.54
1	M	147	HIS	CA-C-N	10.12	139.92	121.70
1	M	147	HIS	C-N-CA	10.12	139.92	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	HIS	N-CA-C	9.79	124.76	113.01
1	G	148	GLY	CA-C-N	-9.54	111.05	120.21
1	G	148	GLY	C-N-CA	-9.54	111.05	120.21
1	G	144	ALA	O-C-N	-9.35	111.31	122.81
1	A	144	ALA	O-C-N	-8.86	112.69	122.79
1	N	144	ALA	O-C-N	-8.77	112.03	122.81
1	G	138	GLY	N-CA-C	8.16	123.44	111.76
1	M	147	HIS	O-C-N	-8.02	109.57	122.41
1	B	112	ARG	NE-CZ-NH1	7.95	129.45	121.50
2	E	57	ASN	N-CA-C	7.83	119.90	111.36
2	P	26	THR	N-CA-CB	-7.78	99.21	110.65
1	B	138	GLY	N-CA-C	7.49	122.47	111.76
1	H	112	ARG	NE-CZ-NH1	7.41	128.91	121.50
1	A	148	GLY	CA-C-N	-7.37	112.73	120.03
1	A	148	GLY	C-N-CA	-7.37	112.73	120.03
1	B	545	GLN	CA-CB-CG	7.34	128.78	114.10
1	N	522	THR	O-C-N	-7.19	112.54	122.46
1	H	147	HIS	N-CA-C	7.15	126.03	110.80
2	P	26	THR	OG1-CB-CG2	7.08	123.45	109.30
1	D	144	ALA	O-C-N	-6.75	114.57	122.87
1	H	144	ALA	O-C-N	-6.70	114.91	122.75
1	G	144	ALA	CA-C-N	6.67	133.71	121.70
1	G	144	ALA	C-N-CA	6.67	133.71	121.70
2	L	62	GLN	CB-CA-C	-6.53	100.37	110.81
2	O	62	GLN	CB-CA-C	-6.49	100.69	110.88
2	L	26	THR	N-CA-CB	-6.47	100.84	110.61
1	A	138	GLY	N-CA-C	6.41	119.54	111.85
1	M	138	GLY	N-CA-C	6.36	120.85	111.76
1	D	138	GLY	N-CA-C	6.29	119.40	111.85
1	G	114	MET	CG-SD-CE	-6.28	87.08	100.90
1	B	282	MET	CG-SD-CE	-6.24	87.18	100.90
1	C	138	GLY	N-CA-C	6.23	119.33	111.85
1	M	249	GLY	N-CA-C	-6.12	103.70	111.72
1	A	144	ALA	CA-C-N	6.01	133.19	121.41
1	A	144	ALA	C-N-CA	6.01	133.19	121.41
1	G	583	PHE	N-CA-C	5.99	119.55	112.72
1	M	468	GLY	CA-C-N	5.99	126.41	119.47
1	M	468	GLY	C-N-CA	5.99	126.41	119.47
1	H	138	GLY	N-CA-C	5.97	119.01	111.85
1	B	148	GLY	CA-C-N	-5.95	114.63	120.52
1	B	148	GLY	C-N-CA	-5.95	114.63	120.52
1	C	282	MET	CG-SD-CE	-5.85	88.03	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	M	148	GLY	CA-C-N	-5.81	114.28	120.03
1	M	148	GLY	C-N-CA	-5.81	114.28	120.03
1	H	520	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	L	26	THR	OG1-CB-CG2	5.78	120.85	109.30
1	G	520	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	B	144	ALA	O-C-N	-5.69	116.09	122.75
1	A	137	ARG	CG-CD-NE	-5.60	99.69	112.00
1	N	584	ARG	NE-CZ-NH2	-5.57	114.18	119.20
1	D	30	SER	N-CA-C	5.54	117.32	111.28
1	H	148	GLY	CA-C-N	-5.53	114.56	120.03
1	H	148	GLY	C-N-CA	-5.53	114.56	120.03
2	J	62	GLN	CB-CA-C	-5.52	102.22	110.88
1	B	104	TYR	N-CA-C	5.51	117.56	109.24
2	L	26	THR	CA-CB-CG2	5.49	119.83	110.50
1	B	471	GLY	N-CA-C	5.46	121.19	114.69
1	N	324	LYS	N-CA-C	5.45	117.30	111.36
1	G	282	MET	CG-SD-CE	-5.44	88.93	100.90
1	N	584	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	H	137	ARG	CG-CD-NE	-5.42	100.07	112.00
1	D	104	TYR	N-CA-C	5.40	117.39	109.24
1	N	138	GLY	N-CA-C	5.39	119.47	111.76
1	H	148	GLY	N-CA-C	5.38	128.90	113.30
1	A	104	TYR	N-CA-C	5.36	117.22	109.07
1	N	144	ALA	CA-C-N	5.35	131.34	121.70
1	N	144	ALA	C-N-CA	5.35	131.34	121.70
1	N	148	GLY	CA-C-N	-5.34	114.75	120.03
1	N	148	GLY	C-N-CA	-5.34	114.75	120.03
1	M	144	ALA	O-C-N	-5.34	116.71	122.79
1	G	520	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	N	367	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	591	GLN	O-C-N	-5.33	116.66	122.84
1	A	305	THR	N-CA-C	-5.30	103.53	110.53
1	A	313	ALA	N-CA-C	5.29	117.05	111.28
1	C	296	THR	N-CA-C	-5.29	106.33	112.89
1	C	148	GLY	CA-C-N	-5.26	114.82	120.03
1	C	148	GLY	C-N-CA	-5.26	114.82	120.03
1	M	564	VAL	CB-CA-C	-5.26	105.04	112.14
1	C	137	ARG	CG-CD-NE	-5.21	100.53	112.00
1	M	144	ALA	CA-C-N	5.20	131.61	121.41
1	M	144	ALA	C-N-CA	5.20	131.61	121.41
2	O	79	ASN	N-CA-C	5.16	116.90	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	62	GLN	N-CA-C	5.15	116.89	111.28
1	A	147	HIS	CA-C-O	-5.14	113.28	119.49
1	C	180	ILE	N-CA-C	5.13	117.47	111.05
1	G	422	GLN	N-CA-C	5.13	119.29	113.19
1	B	288	GLY	N-CA-C	5.12	120.44	112.31
1	D	137	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	C	233	GLU	CB-CG-CD	5.08	121.24	112.60
2	L	82	LYS	N-CA-C	5.08	116.89	111.36
1	H	144	ALA	CA-C-N	5.05	131.31	121.41
1	H	144	ALA	C-N-CA	5.05	131.31	121.41
1	H	34	ARG	CG-CD-NE	-5.04	100.92	112.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ALA	Peptide
1	A	145	GLY	Peptide
1	B	144	ALA	Peptide
1	D	137	ARG	Sidechain
1	G	145	GLY	Peptide
1	G	97	THR	Mainchain
1	H	144	ALA	Peptide
1	H	147	HIS	Peptide
1	M	144	ALA	Peptide
1	M	145	GLY	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4491	0	4320	13	0
1	B	4490	0	4320	13	0
1	C	4491	0	4320	12	0
1	D	4490	0	4320	18	0
1	G	4491	0	4320	16	0
1	H	4490	0	4320	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	4491	0	4320	16	0
1	N	4490	0	4320	23	0
2	E	568	0	545	3	0
2	F	568	0	545	5	0
2	I	568	0	545	3	0
2	J	568	0	545	6	0
2	K	568	0	545	3	0
2	L	568	0	545	2	0
2	O	568	0	545	3	0
2	P	568	0	545	8	0
3	A	548	0	0	3	0
3	B	491	0	0	3	0
3	C	500	0	0	4	0
3	D	511	0	0	3	0
3	E	114	0	0	1	0
3	F	77	0	0	2	0
3	G	529	0	0	2	0
3	H	481	0	0	3	0
3	I	84	0	0	0	0
3	J	79	0	0	1	0
3	K	81	0	0	0	0
3	L	97	0	0	0	0
3	M	453	0	0	4	0
3	N	505	0	0	7	0
3	O	61	0	0	1	0
3	P	98	0	0	1	0
All	All	45177	0	38920	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (146) 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)
2:J:74:GLN:HG2	3:J:166:HOH:O	1.64	0.98
1:H:112:ARG:HD3	1:H:112:ARG:O	1.67	0.94
1:G:591:GLN:HE21	1:H:114:MET:HE1	1.38	0.89
1:B:112:ARG:O	1:B:112:ARG:HD3	1.75	0.87
1:D:196:LYS:HE3	1:D:223:GLU:HG3	1.60	0.83
2:P:26:THR:HG23	3:P:167:HOH:O	1.80	0.79
1:N:209:ARG:H	2:P:62:GLN:HE22	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:OD1	3:A:701:HOH:O	2.01	0.78
1:D:145:GLY:HA3	1:D:148:GLY:O	1.84	0.77
1:D:196:LYS:CE	1:D:223:GLU:HG3	2.16	0.76
1:N:145:GLY:HA3	1:N:148:GLY:O	1.87	0.75
1:B:112:ARG:O	1:B:112:ARG:CD	2.37	0.73
1:N:432:LYS:HE3	3:N:847:HOH:O	1.89	0.73
1:G:145:GLY:HA2	1:G:147:HIS:CD2	2.26	0.69
1:H:112:ARG:O	1:H:112:ARG:CD	2.41	0.68
3:M:1002:HOH:O	2:O:54:HIS:HD2	1.77	0.68
3:H:1031:HOH:O	2:J:54:HIS:HD2	1.78	0.67
1:B:198:LEU:HD11	1:B:283:ILE:HD13	1.77	0.65
1:G:145:GLY:HA3	1:G:148:GLY:O	1.96	0.65
1:B:112:ARG:HD3	1:B:112:ARG:C	2.17	0.64
3:D:965:HOH:O	2:L:54:HIS:HD2	1.80	0.63
1:N:209:ARG:H	2:P:62:GLN:NE2	1.95	0.62
1:C:145:GLY:O	1:C:148:GLY:HA2	2.00	0.61
3:G:942:HOH:O	2:I:54:HIS:HD2	1.85	0.59
1:G:193:VAL:HG21	1:G:283:ILE:CD1	2.33	0.59
3:D:1028:HOH:O	2:L:54:HIS:HE1	1.86	0.58
1:M:145:GLY:O	1:M:148:GLY:HA2	2.04	0.58
3:M:1017:HOH:O	2:O:54:HIS:HE1	1.88	0.57
1:A:591:GLN:HE21	1:B:114:MET:HE1	1.71	0.56
1:N:306:MET:HE1	1:N:332:TYR:C	2.30	0.56
1:G:193:VAL:HG21	1:G:283:ILE:HD11	1.88	0.55
1:M:472:MET:HE2	1:M:491:PRO:HB3	1.89	0.55
1:G:145:GLY:O	1:G:148:GLY:HA2	2.05	0.55
3:G:1046:HOH:O	2:I:54:HIS:HE1	1.89	0.55
1:H:31:GLU:OE1	1:H:34:ARG:NH1	2.40	0.55
1:H:453:ARG:HG3	3:H:1028:HOH:O	2.07	0.55
3:N:1031:HOH:O	2:P:54:HIS:HE1	1.89	0.54
1:B:145:GLY:O	1:B:148:GLY:HA2	2.08	0.54
3:A:976:HOH:O	2:E:54:HIS:HD2	1.90	0.54
1:D:196:LYS:HE3	1:D:223:GLU:CG	2.35	0.54
1:M:306:MET:HE1	1:M:332:TYR:C	2.33	0.54
3:B:1053:HOH:O	2:F:54:HIS:HE1	1.91	0.53
3:C:897:HOH:O	2:K:54:HIS:HD2	1.91	0.53
1:N:31:GLU:OE1	1:N:34:ARG:NH1	2.42	0.53
1:N:145:GLY:O	1:N:148:GLY:HA2	2.09	0.53
1:H:145:GLY:O	1:H:148:GLY:HA2	2.09	0.53
1:A:145:GLY:O	1:A:148:GLY:HA2	2.10	0.52
1:M:31:GLU:OE2	1:M:34:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:THR:HB	1:H:98:PRO:HD2	1.91	0.52
2:P:24:ASP:OD1	2:P:26:THR:HB	2.11	0.51
3:B:952:HOH:O	2:F:54:HIS:HD2	1.93	0.51
2:J:53:LYS:HA	2:J:53:LYS:CE	2.41	0.50
2:I:75:LYS:HD3	2:I:90:VAL:HB	1.93	0.50
2:F:89:LYS:HG2	3:F:147:HOH:O	2.10	0.50
1:N:76:THR:HB	1:N:97:THR:HG22	1.94	0.50
1:N:243:LYS:NZ	3:N:701:HOH:O	2.42	0.50
3:N:989:HOH:O	2:P:54:HIS:HD2	1.94	0.49
2:O:44:LYS:NZ	3:O:101:HOH:O	2.44	0.49
3:A:1059:HOH:O	2:E:54:HIS:HE1	1.96	0.49
1:C:514:ASP:O	1:D:112:ARG:HD3	2.12	0.48
1:G:333:ALA:O	1:G:358:ARG:HG3	2.13	0.48
1:N:198:LEU:HD11	1:N:283:ILE:HD13	1.95	0.48
1:A:306:MET:HE1	1:A:332:TYR:C	2.38	0.48
3:C:1031:HOH:O	2:K:54:HIS:HE1	1.96	0.48
1:G:104:TYR:CD1	1:G:114:MET:HE3	2.48	0.48
1:M:37:LYS:HE2	3:M:1082:HOH:O	2.14	0.48
2:E:27:HIS:HE1	3:E:130:HOH:O	1.97	0.48
1:A:145:GLY:HA2	1:A:147:HIS:CD2	2.49	0.47
3:H:994:HOH:O	2:J:54:HIS:HE1	1.97	0.47
1:A:472:MET:HE2	1:A:491:PRO:HB3	1.97	0.47
1:M:561:TRP:O	1:M:564:VAL:HG22	2.15	0.47
1:H:147:HIS:CD2	1:H:217:ILE:HD11	2.50	0.46
1:M:276:TYR:HD1	1:M:283:ILE:HD13	1.79	0.46
1:M:591:GLN:HG2	1:N:114:MET:HE1	1.96	0.46
1:B:37:LYS:NZ	3:B:707:HOH:O	2.48	0.46
1:G:29:ASN:N	1:G:194:LYS:H	2.13	0.46
1:G:533:LEU:O	1:H:112:ARG:NH2	2.45	0.46
1:M:193:VAL:HG11	1:M:283:ILE:HD11	1.97	0.46
1:C:193:VAL:HG21	1:C:283:ILE:CD1	2.46	0.46
1:C:239:LYS:HD3	3:C:1077:HOH:O	2.15	0.46
1:N:209:ARG:N	2:P:62:GLN:HE22	2.06	0.46
1:D:145:GLY:O	1:D:148:GLY:HA2	2.16	0.46
2:F:24:ASP:OD1	2:F:26:THR:OG1	2.25	0.46
1:M:591:GLN:HE21	1:N:114:MET:HE1	1.80	0.45
1:D:196:LYS:CD	1:D:223:GLU:HG3	2.46	0.45
1:D:306:MET:HE1	1:D:332:TYR:C	2.42	0.45
1:G:145:GLY:HA2	1:G:147:HIS:NE2	2.31	0.45
1:D:147:HIS:CD2	1:D:217:ILE:HD11	2.51	0.45
1:M:276:TYR:CD1	1:M:283:ILE:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:OD1	3:C:701:HOH:O	2.21	0.45
1:D:432:LYS:HE3	3:D:719:HOH:O	2.16	0.45
1:G:584:ARG:CZ	1:G:584:ARG:HB3	2.46	0.45
1:G:193:VAL:HG21	1:G:283:ILE:HD12	1.99	0.44
1:G:193:VAL:HG11	1:G:283:ILE:HD11	1.99	0.44
3:M:1038:HOH:O	1:N:588:HIS:HD2	1.99	0.44
1:A:353:LEU:O	1:A:364:THR:HA	2.17	0.44
1:N:145:GLY:HA2	1:N:147:HIS:CD2	2.52	0.44
1:B:196:LYS:CE	1:B:223:GLU:HG2	2.48	0.44
1:D:145:GLY:CA	1:D:148:GLY:O	2.62	0.44
1:H:306:MET:HE1	1:H:332:TYR:C	2.43	0.43
1:C:306:MET:HE1	1:C:332:TYR:C	2.43	0.43
1:D:195:ASP:OD1	1:D:196:LYS:NZ	2.51	0.43
2:J:53:LYS:HA	2:J:53:LYS:HE2	1.99	0.43
1:N:117:GLN:NE2	1:N:119:LYS:HD2	2.33	0.43
1:D:97:THR:HB	1:D:98:PRO:HD2	2.01	0.43
1:N:72:TRP:CZ2	1:N:598:VAL:HG21	2.54	0.43
1:N:97:THR:HB	1:N:98:PRO:HD2	1.99	0.43
1:A:194:LYS:NZ	1:A:314:ASP:OD1	2.45	0.43
1:A:561:TRP:O	1:A:564:VAL:HG22	2.19	0.43
1:A:533:LEU:O	1:B:112:ARG:NH2	2.51	0.43
1:D:145:GLY:HA2	1:D:147:HIS:CD2	2.54	0.43
1:D:196:LYS:HD2	1:D:223:GLU:HG3	2.01	0.43
1:A:112:ARG:HD3	1:B:514:ASP:O	2.19	0.43
1:C:561:TRP:O	1:C:564:VAL:HG22	2.19	0.42
1:H:76:THR:HB	1:H:97:THR:HG22	2.02	0.42
1:N:90:ASP:HB3	3:N:726:HOH:O	2.19	0.42
1:C:29:ASN:N	1:C:194:LYS:H	2.18	0.42
1:C:85:ALA:HB1	1:C:86:PRO:CD	2.49	0.42
1:B:29:ASN:N	1:B:194:LYS:H	2.18	0.42
1:G:76:THR:HB	1:G:97:THR:HG22	2.02	0.42
1:M:74:LEU:HD11	1:M:106:VAL:HG21	2.02	0.41
1:D:83:GLU:HG3	1:D:538:ILE:HD12	2.02	0.41
1:N:208:VAL:HA	2:P:62:GLN:HE22	1.85	0.41
1:C:76:THR:HB	1:C:97:THR:HG22	2.02	0.41
1:H:98:PRO:O	1:H:99:PHE:C	2.63	0.41
1:H:353:LEU:O	1:H:364:THR:HA	2.20	0.41
1:A:79:LEU:O	1:A:80:HIS:HB2	2.21	0.41
1:B:145:GLY:HA3	1:B:147:HIS:CD2	2.55	0.41
1:M:353:LEU:O	1:M:364:THR:HA	2.20	0.41
2:J:53:LYS:HE2	2:J:53:LYS:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:145:GLY:HA3	1:M:148:GLY:O	2.21	0.41
1:N:196:LYS:HE2	3:N:704:HOH:O	2.19	0.41
1:C:329:GLU:HB2	1:C:330:TRP:CE2	2.56	0.41
1:M:29:ASN:N	1:M:194:LYS:H	2.18	0.41
1:B:31:GLU:OE1	1:B:34:ARG:NH1	2.54	0.41
1:D:447:PRO:HA	1:D:461:ALA:HA	2.02	0.41
1:H:29:ASN:N	1:H:194:LYS:H	2.19	0.41
1:N:303:LYS:HA	1:N:304:TRP:HA	1.86	0.41
1:A:276:TYR:HD1	1:A:283:ILE:HD13	1.85	0.41
2:F:85:LYS:NZ	3:F:102:HOH:O	2.52	0.40
2:K:52:PRO:HB2	2:K:54:HIS:CE1	2.57	0.40
1:M:511:GLY:HA3	1:M:537:VAL:HG11	2.04	0.40
1:C:266:GLY:O	1:C:290:PRO:HA	2.21	0.40
1:D:96:HIS:CE1	1:D:138:GLY:HA2	2.57	0.40
1:N:584:ARG:HD3	3:N:1065:HOH:O	2.20	0.40
1:G:566:LEU:C	1:G:566:LEU:HD12	2.45	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	571/573 (100%)	543 (95%)	27 (5%)	1 (0%)	43 36
1	B	571/573 (100%)	542 (95%)	29 (5%)	0	100 100
1	C	571/573 (100%)	544 (95%)	26 (5%)	1 (0%)	43 36
1	D	571/573 (100%)	543 (95%)	25 (4%)	3 (0%)	24 16
1	G	571/573 (100%)	539 (94%)	30 (5%)	2 (0%)	30 22
1	H	571/573 (100%)	539 (94%)	30 (5%)	2 (0%)	30 22
1	M	571/573 (100%)	541 (95%)	29 (5%)	1 (0%)	43 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	571/573 (100%)	545 (95%)	24 (4%)	2 (0%)	30	22
2	E	69/72 (96%)	69 (100%)	0	0	100	100
2	F	69/72 (96%)	69 (100%)	0	0	100	100
2	I	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	J	69/72 (96%)	69 (100%)	0	0	100	100
2	K	69/72 (96%)	69 (100%)	0	0	100	100
2	L	69/72 (96%)	69 (100%)	0	0	100	100
2	O	69/72 (96%)	69 (100%)	0	0	100	100
2	P	69/72 (96%)	69 (100%)	0	0	100	100
All	All	5120/5160 (99%)	4887 (95%)	221 (4%)	12 (0%)	43	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	145	GLY
1	N	145	GLY
1	H	557	GLY
1	A	134	VAL
1	C	134	VAL
1	G	145	GLY
1	G	594	GLY
1	M	134	VAL
1	N	594	GLY
1	D	134	VAL
1	D	557	GLY
1	H	594	GLY

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	464/464 (100%)	460 (99%)	4 (1%)	70	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	464/464 (100%)	455 (98%)	9 (2%)	50	47
1	C	464/464 (100%)	458 (99%)	6 (1%)	61	61
1	D	464/464 (100%)	460 (99%)	4 (1%)	70	73
1	G	464/464 (100%)	456 (98%)	8 (2%)	53	52
1	H	464/464 (100%)	458 (99%)	6 (1%)	61	61
1	M	464/464 (100%)	459 (99%)	5 (1%)	65	67
1	N	464/464 (100%)	457 (98%)	7 (2%)	57	56
2	E	60/61 (98%)	59 (98%)	1 (2%)	53	52
2	F	60/61 (98%)	56 (93%)	4 (7%)	15	7
2	I	60/61 (98%)	56 (93%)	4 (7%)	15	7
2	J	60/61 (98%)	56 (93%)	4 (7%)	15	7
2	K	60/61 (98%)	59 (98%)	1 (2%)	53	52
2	L	60/61 (98%)	57 (95%)	3 (5%)	22	14
2	O	60/61 (98%)	59 (98%)	1 (2%)	53	52
2	P	60/61 (98%)	56 (93%)	4 (7%)	15	7
All	All	4192/4200 (100%)	4121 (98%)	71 (2%)	53	52

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	TYR
1	A	400	GLU
1	A	453	ARG
1	A	571	LYS
1	B	112	ARG
1	B	113	LYS
1	B	119	LYS
1	B	221	LYS
1	B	243	LYS
1	B	337	TYR
1	B	387	LYS
1	B	391	LYS
1	B	569	ASP
1	C	233	GLU
1	C	239	LYS
1	C	279	LYS
1	C	337	TYR

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Mol	Chain	Res	Type
1	C	410	LYS
1	C	530	GLN
1	D	198	LEU
1	D	221	LYS
1	D	337	TYR
1	D	584	ARG
2	E	57	ASN
2	F	43	ASP
2	F	59	LEU
2	F	82	LYS
2	F	93	ILE
1	G	37	LYS
1	G	114	MET
1	G	146	GLU
1	G	233	GLU
1	G	243	LYS
1	G	279	LYS
1	G	337	TYR
1	G	387	LYS
1	H	74	LEU
1	H	112	ARG
1	H	146	GLU
1	H	279	LYS
1	H	337	TYR
1	H	472	MET
2	I	75	LYS
2	I	89	LYS
2	I	91	GLU
2	I	92	ASP
2	J	53	LYS
2	J	59	LEU
2	J	82	LYS
2	J	85	LYS
2	K	85	LYS
2	L	26	THR
2	L	43	ASP
2	L	59	LEU
1	M	146	GLU
1	M	337	TYR
1	M	400	GLU
1	M	410	LYS
1	M	584	ARG

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Mol	Chain	Res	Type
1	N	74	LEU
1	N	89	VAL
1	N	337	TYR
1	N	391	LYS
1	N	472	MET
1	N	530	GLN
1	N	552	ILE
2	O	85	LYS
2	P	26	THR
2	P	59	LEU
2	P	64	GLU
2	P	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	222	GLN
1	A	407	HIS
1	A	408	ASN
1	A	591	GLN
1	B	63	HIS
1	B	117	GLN
1	B	155	ASN
1	B	216	ASN
1	B	270	ASN
1	B	407	HIS
1	C	407	HIS
1	D	156	GLN
1	D	177	ASN
1	D	216	ASN
1	D	250	GLN
1	D	270	ASN
1	D	408	ASN
1	D	464	ASN
2	E	54	HIS
2	E	57	ASN
2	F	54	HIS
2	F	79	ASN
1	G	117	GLN
1	G	155	ASN
1	G	177	ASN

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Mol	Chain	Res	Type
1	G	250	GLN
1	G	270	ASN
1	G	408	ASN
1	G	591	GLN
1	H	63	HIS
1	H	117	GLN
1	H	216	ASN
1	H	408	ASN
1	H	475	GLN
1	H	588	HIS
1	H	591	GLN
2	I	27	HIS
2	I	54	HIS
2	J	54	HIS
2	J	79	ASN
2	K	54	HIS
2	L	54	HIS
1	M	155	ASN
1	M	156	GLN
1	M	177	ASN
1	M	216	ASN
1	M	530	GLN
1	M	588	HIS
1	M	591	GLN
1	N	63	HIS
1	N	117	GLN
1	N	156	GLN
1	N	216	ASN
1	N	250	GLN
1	N	408	ASN
1	N	464	ASN
1	N	588	HIS
2	O	54	HIS
2	O	79	ASN
2	P	54	HIS
2	P	62	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	573/573 (100%)	-0.58	2 (0%) 90 91	12, 17, 29, 52	0
1	B	573/573 (100%)	-0.62	2 (0%) 90 91	12, 16, 29, 44	0
1	C	573/573 (100%)	-0.63	0 100 100	12, 16, 27, 43	0
1	D	573/573 (100%)	-0.60	0 100 100	12, 17, 28, 49	0
1	G	573/573 (100%)	-0.61	0 100 100	12, 17, 28, 41	0
1	H	573/573 (100%)	-0.48	0 100 100	12, 19, 32, 49	0
1	M	573/573 (100%)	-0.41	1 (0%) 91 92	13, 20, 34, 58	0
1	N	573/573 (100%)	-0.59	0 100 100	12, 16, 28, 41	0
2	E	71/72 (98%)	-0.17	0 100 100	17, 24, 41, 54	0
2	F	71/72 (98%)	-0.03	3 (4%) 40 43	14, 21, 46, 86	0
2	I	71/72 (98%)	0.19	6 (8%) 16 17	16, 23, 66, 100	0
2	J	71/72 (98%)	0.24	0 100 100	22, 30, 49, 63	0
2	K	71/72 (98%)	-0.12	0 100 100	15, 22, 36, 51	0
2	L	71/72 (98%)	-0.22	0 100 100	16, 23, 38, 56	0
2	O	71/72 (98%)	0.41	1 (1%) 73 76	24, 34, 55, 64	0
2	P	71/72 (98%)	-0.04	2 (2%) 55 59	16, 21, 42, 60	0
All	All	5152/5160 (99%)	-0.50	17 (0%) 90 91	12, 18, 34, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	93	ILE	10.0
2	I	90	VAL	6.1
2	F	93	ILE	5.5
1	B	104	TYR	3.6
1	A	104	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	92	ASP	2.9
2	F	92	ASP	2.8
2	I	82	LYS	2.7
2	I	91	GLU	2.7
2	P	43	ASP	2.6
2	I	89	LYS	2.5
2	P	82	LYS	2.4
2	F	91	GLU	2.4
1	M	453	ARG	2.4
1	A	145	GLY	2.3
1	B	131	CYS	2.1
2	O	93	ILE	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 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.