



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 12:28 PM JST

PDB ID : 7CED
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 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	:	2.20
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)	:	2.20

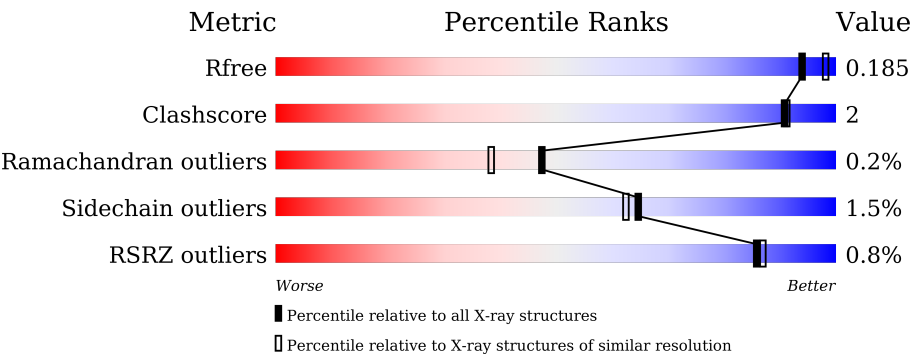
1 Overall quality at a glance i

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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	<div><div></div><div>94%6% .</div></div>
1	B	573	<div><div></div><div>94%5% .</div></div>
1	C	573	<div><div></div><div>93%6% .</div></div>
1	D	573	<div><div>%</div><div>94%5% .</div></div>
1	G	573	<div><div></div><div>94%6% .</div></div>
1	H	573	<div><div></div><div>93%6% .</div></div>

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Mol	Chain	Length	Quality of chain
1	M	573	<div><div></div><div>92%7%</div></div>
1	N	573	<div><div></div><div>92%7%.</div></div>
2	E	72	<div><div></div><div>%90%8%.</div></div>
2	F	72	<div><div></div><div>4%85%14%.</div></div>
2	I	72	<div><div></div><div>7%88%11%.</div></div>
2	J	72	<div><div></div><div>3%92%6%..</div></div>
2	K	72	<div><div></div><div>4%90%8%.</div></div>
2	L	72	<div><div></div><div>3%90%7%..</div></div>
2	O	72	<div><div></div><div>11%94%. .</div></div>
2	P	72	<div><div></div><div>7%90%7%..</div></div>

2 Entry composition

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
1	A	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	B	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	C	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	D	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	G	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	H	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	M	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	N	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			

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

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

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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			

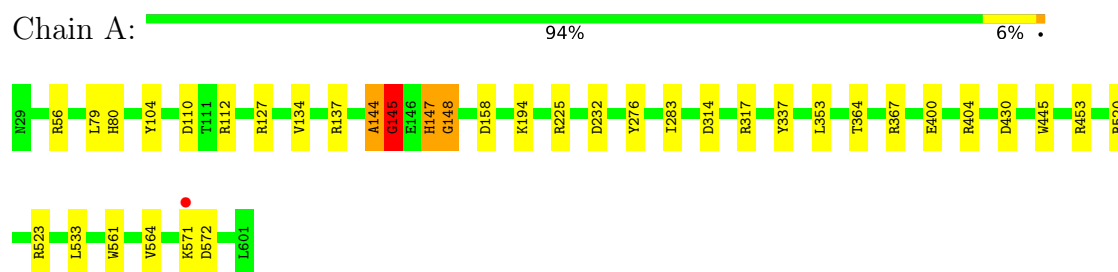
- Molecule 3 is water.

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		

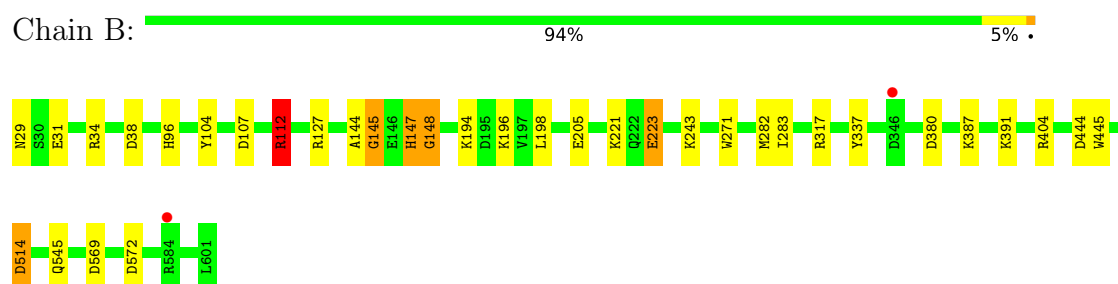
3 Residue-property plots

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.

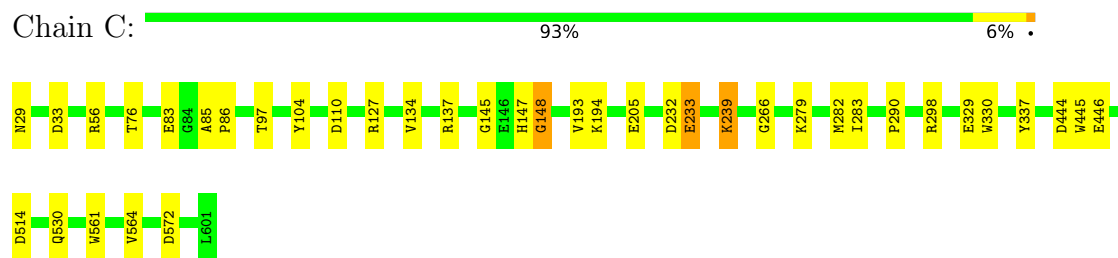
- Molecule 1: Methanol dehydrogenase protein, large subunit



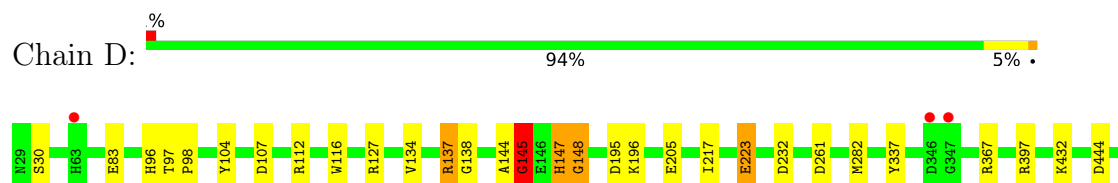
- Molecule 1: Methanol dehydrogenase protein, large subunit



- Molecule 1: Methanol dehydrogenase protein, large subunit



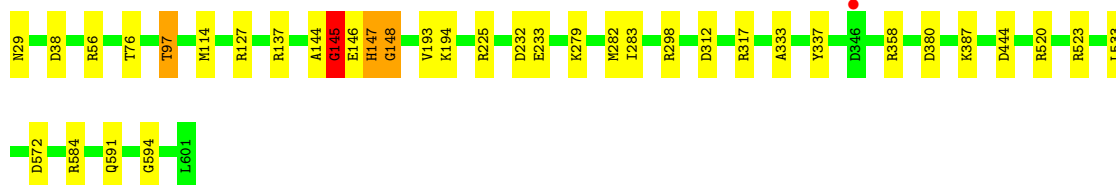
- Molecule 1: Methanol dehydrogenase protein, large subunit





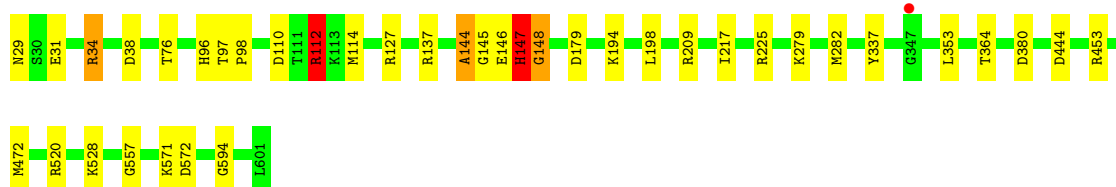
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G: 94% 6% •



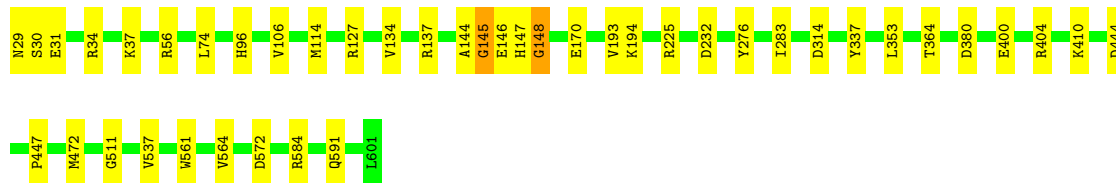
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H: 93% 6% •



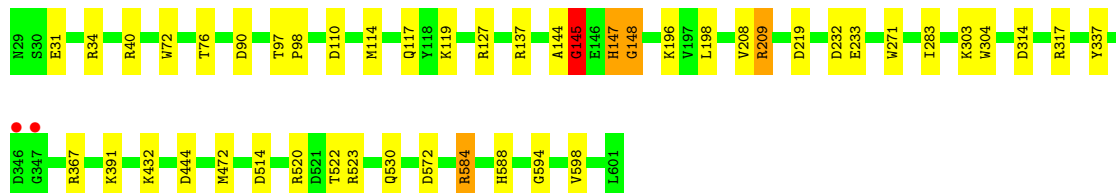
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain M: 92% 7% •



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain N: 92% 7% •

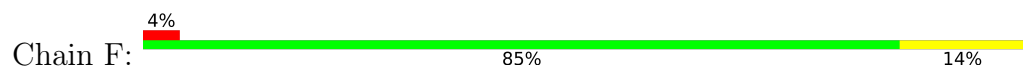


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

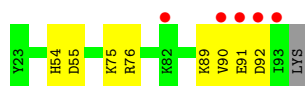
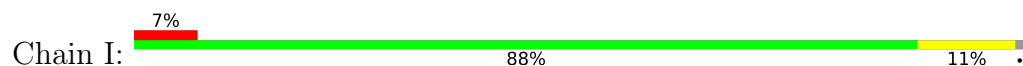
Chain E: 90% 8% •



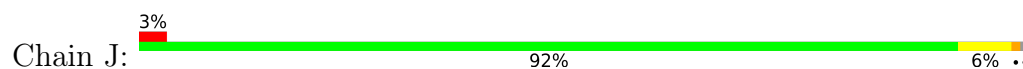
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



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



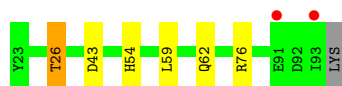
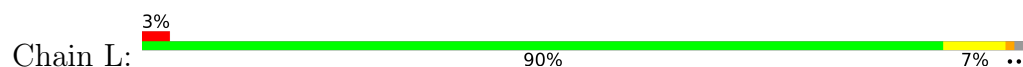
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



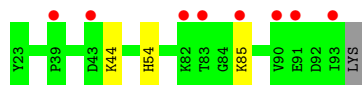
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



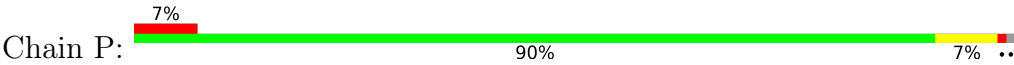
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- 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 29.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.00-1.90) 99.9 (29.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.140 , 0.180 0.146 , 0.185	Depositor DCC
R_{free} test set	24064 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

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	0.95	4/4622 (0.1%)	1.01	22/6281 (0.4%)
1	B	1.01	10/4621 (0.2%)	1.10	23/6281 (0.4%)
1	C	0.97	6/4622 (0.1%)	0.98	15/6281 (0.2%)
1	D	0.97	7/4621 (0.2%)	1.02	20/6281 (0.3%)
1	G	0.97	4/4622 (0.1%)	1.03	28/6281 (0.4%)
1	H	0.93	3/4621 (0.1%)	1.05	28/6281 (0.4%)
1	M	0.95	4/4622 (0.1%)	0.98	17/6281 (0.3%)
1	N	1.00	6/4621 (0.1%)	1.07	30/6281 (0.5%)
2	E	0.95	0/583	0.91	2/785 (0.3%)
2	F	0.89	0/583	0.96	2/785 (0.3%)
2	I	0.92	0/583	0.98	3/785 (0.4%)
2	J	0.88	0/583	0.85	0/785
2	K	1.01	1/583 (0.2%)	0.95	4/785 (0.5%)
2	L	1.03	1/583 (0.2%)	1.01	3/785 (0.4%)
2	O	0.83	0/583	0.86	0/785
2	P	0.95	0/583	0.99	2/785 (0.3%)
All	All	0.96	46/41636 (0.1%)	1.02	199/56528 (0.4%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	112	ARG	CD-NE	-9.96	1.29	1.46
1	B	112	ARG	CD-NE	-9.93	1.29	1.46
1	N	148	GLY	N-CA	-9.61	1.31	1.46
1	D	145	GLY	N-CA	-9.49	1.31	1.46
1	A	148	GLY	N-CA	-9.34	1.32	1.46
1	N	145	GLY	N-CA	-9.10	1.32	1.46
1	G	148	GLY	N-CA	-8.87	1.32	1.46
1	G	145	GLY	N-CA	-8.82	1.32	1.46
1	A	145	GLY	N-CA	-8.45	1.33	1.46
1	B	223	GLU	CD-OE1	-8.24	1.16	1.25
1	B	148	GLY	N-CA	-8.19	1.33	1.46
1	C	148	GLY	N-CA	-7.86	1.34	1.46
1	N	145	GLY	C-O	-7.54	1.11	1.23
1	C	233	GLU	CG-CD	6.99	1.62	1.51
1	D	223	GLU	CD-OE2	6.97	1.33	1.25
1	B	104	TYR	CB-CG	-6.96	1.41	1.51
1	B	104	TYR	CE1-CZ	6.93	1.47	1.38
1	N	233	GLU	CD-OE1	6.85	1.33	1.25
1	H	96	HIS	C-N	6.76	1.49	1.34
1	H	148	GLY	N-CA	-6.76	1.35	1.46
1	A	104	TYR	CB-CG	-6.63	1.41	1.51
1	D	148	GLY	N-CA	-6.32	1.36	1.46
1	C	446	GLU	CD-OE2	6.21	1.32	1.25
1	C	104	TYR	CE1-CZ	6.17	1.46	1.38
1	M	148	GLY	N-CA	-6.11	1.36	1.46
1	D	30	SER	CB-OG	-5.99	1.34	1.42
1	N	584	ARG	CZ-NH1	5.91	1.40	1.33
1	N	271	TRP	CE3-CZ3	5.81	1.48	1.38
1	G	148	GLY	C-O	-5.78	1.14	1.23
1	D	116	TRP	CB-CG	5.78	1.60	1.50
2	K	80	TYR	CE1-CZ	5.73	1.46	1.38
2	L	26	THR	CB-CG2	-5.66	1.33	1.52
1	B	96	HIS	C-N	5.66	1.47	1.34
1	M	96	HIS	C-N	5.62	1.47	1.34
1	G	233	GLU	CG-CD	5.53	1.60	1.51
1	B	148	GLY	C-O	-5.50	1.14	1.23
1	D	205	GLU	CD-OE2	5.34	1.31	1.25
1	B	205	GLU	CD-OE2	5.29	1.31	1.25
1	M	170	GLU	CD-OE1	5.25	1.31	1.25
1	B	145	GLY	N-CA	-5.22	1.38	1.46
1	D	104	TYR	CB-CG	-5.21	1.43	1.51
1	C	83	GLU	CD-OE1	5.16	1.31	1.25
1	C	205	GLU	CD-OE2	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	TYR	CE2-CZ	5.10	1.45	1.38
1	M	30	SER	CB-OG	-5.09	1.35	1.42
1	B	271	TRP	CE3-CZ3	5.07	1.47	1.38

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	-24.88	107.86	120.30
1	H	112	ARG	NE-CZ-NH2	-22.07	109.27	120.30
1	B	112	ARG	NE-CZ-NH1	18.30	129.45	120.30
1	H	112	ARG	NE-CZ-NH1	17.21	128.91	120.30
1	N	584	ARG	NE-CZ-NH1	13.27	126.93	120.30
1	N	584	ARG	NE-CZ-NH2	-12.23	114.18	120.30
1	D	147	HIS	CA-C-N	11.93	140.07	116.20
1	N	147	HIS	CA-C-N	11.73	139.66	116.20
1	C	147	HIS	CA-C-N	11.55	139.31	116.20
1	A	147	HIS	CA-C-N	11.32	138.83	116.20
1	B	147	HIS	CA-C-N	11.28	138.77	116.20
1	C	147	HIS	C-N-CA	10.94	145.26	122.30
1	D	147	HIS	C-N-CA	10.93	145.25	122.30
1	N	147	HIS	C-N-CA	10.58	144.51	122.30
1	N	110	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	B	147	HIS	C-N-CA	10.32	143.98	122.30
1	B	147	HIS	O-C-N	-10.19	105.87	123.20
1	M	147	HIS	CA-C-N	10.10	136.40	116.20
1	H	147	HIS	CA-C-N	10.04	136.28	116.20
1	G	147	HIS	CA-C-N	10.00	136.20	116.20
1	C	127	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	N	147	HIS	O-C-N	-9.89	106.38	123.20
1	D	147	HIS	O-C-N	-9.88	106.41	123.20
1	A	147	HIS	C-N-CA	9.80	142.88	122.30
1	C	147	HIS	O-C-N	-9.73	106.65	123.20
1	H	147	HIS	C-N-CA	9.13	141.47	122.30
1	A	147	HIS	O-C-N	-9.04	107.83	123.20
1	G	147	HIS	O-C-N	-8.83	108.19	123.20
1	N	572	ASP	CB-CG-OD1	8.79	126.21	118.30
1	G	147	HIS	C-N-CA	8.59	140.33	122.30
1	H	147	HIS	O-C-N	-8.45	108.83	123.20
1	M	147	HIS	C-N-CA	8.39	139.92	122.30
1	H	127	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	A	367	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	G	520	ARG	NE-CZ-NH1	-8.26	116.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	520	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	G	114	MET	CG-SD-CE	-8.20	87.08	100.20
1	G	232	ASP	CB-CG-OD1	8.14	125.63	118.30
1	B	282	MET	CG-SD-CE	-8.14	87.18	100.20
1	G	520	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	M	147	HIS	O-C-N	-8.02	109.57	123.20
1	D	107	ASP	CB-CG-OD1	8.01	125.51	118.30
1	C	232	ASP	CB-CG-OD1	8.00	125.50	118.30
1	D	137	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	C	282	MET	CG-SD-CE	-7.61	88.03	100.20
1	D	127	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	56	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	N	367	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	317	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	N	127	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	127	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	H	110	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	C	127	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	G	137	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	D	127	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	K	76	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	G	282	MET	CG-SD-CE	-7.04	88.93	100.20
1	N	444	ASP	CB-CG-OD1	7.02	124.62	118.30
1	G	144	ALA	O-C-N	-7.00	111.31	123.20
1	B	545	GLN	CA-CB-CG	6.99	128.78	113.40
1	G	38	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	127	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	N	317	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	144	ALA	CA-C-N	6.92	130.05	116.20
1	N	572	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	572	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	514	ASP	CB-CG-OD1	6.77	124.39	118.30
1	G	144	ALA	CA-C-N	6.75	129.70	116.20
1	B	444	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	232	ASP	CB-CG-OD1	6.66	124.30	118.30
1	G	572	ASP	CB-CG-OD1	6.66	124.30	118.30
1	N	144	ALA	O-C-N	-6.57	112.03	123.20
1	D	444	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	317	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	I	76	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	H	127	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	G	523	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	232	ASP	CB-CG-OD1	6.37	124.03	118.30
1	M	114	MET	CG-SD-CE	-6.37	90.02	100.20
1	N	522	THR	O-C-N	-6.35	112.54	122.70
1	D	147	HIS	N-CA-C	6.32	128.07	111.00
1	H	148	GLY	N-CA-C	6.32	128.90	113.10
1	N	144	ALA	CA-C-N	6.32	128.83	116.20
1	B	38	ASP	CB-CG-OD1	6.31	123.98	118.30
1	M	147	HIS	N-CA-C	6.29	127.98	111.00
1	M	572	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	127	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	N	514	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	404	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	144	ALA	O-C-N	-6.18	112.69	123.20
2	F	76	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	158	ASP	CB-CG-OD1	6.14	123.82	118.30
1	C	232	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	H	380	ASP	CB-CG-OD1	6.10	123.79	118.30
1	C	56	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	M	572	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	514	ASP	CB-CG-OD1	6.03	123.73	118.30
1	C	444	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	225	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	H	520	ARG	NE-CZ-NH1	-6.00	117.30	120.30
2	K	72	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	H	198	LEU	CA-CB-CG	5.99	129.07	115.30
1	N	444	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	N	110	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	572	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	E	24	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	N	40	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	N	145	GLY	CA-C-N	5.91	130.21	117.20
1	D	137	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	M	232	ASP	CB-CG-OD1	5.85	123.56	118.30
2	P	26	THR	OG1-CB-CG2	5.85	123.45	110.00
2	P	26	THR	N-CA-CB	-5.83	99.21	110.30
1	A	572	ASP	CB-CG-OD2	-5.83	113.05	118.30
2	K	76	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	H	444	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	D	144	ALA	CA-C-N	5.77	127.75	116.20
1	A	137	ARG	CG-CD-NE	-5.77	99.69	111.80
1	M	137	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	M	56	ARG	NE-CZ-NH1	5.73	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	523	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	H	38	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	520	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	B	107	ASP	CB-CG-OD1	5.67	123.41	118.30
2	F	51	ASP	CB-CG-OD1	5.67	123.41	118.30
2	E	76	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	B	127	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	33	ASP	CB-CG-OD1	5.61	123.35	118.30
1	G	127	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	M	127	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	514	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	H	137	ARG	CG-CD-NE	-5.58	100.07	111.80
2	L	76	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	430	ASP	CB-CG-OD1	5.58	123.32	118.30
1	H	144	ALA	CA-C-N	5.57	127.35	116.20
1	H	147	HIS	N-CA-C	5.57	126.03	111.00
1	B	380	ASP	CB-CG-OD1	5.56	123.30	118.30
1	H	444	ASP	CB-CG-OD1	5.54	123.29	118.30
1	G	298	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	M	225	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	380	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	H	572	ASP	CB-CG-OD1	5.52	123.27	118.30
1	N	520	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	N	145	GLY	CA-C-O	-5.50	110.69	120.60
1	N	209	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	N	219	ASP	CB-CG-OD1	5.48	123.23	118.30
2	I	55	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	147	HIS	N-CA-C	5.44	125.69	111.00
1	H	225	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	M	314	ASP	CB-CG-OD1	5.44	123.19	118.30
1	G	144	ALA	C-N-CA	5.43	133.71	122.30
1	H	282	MET	CG-SD-CE	-5.43	91.52	100.20
1	G	148	GLY	CA-C-O	-5.42	110.85	120.60
1	N	314	ASP	CB-CG-OD1	5.41	123.17	118.30
1	N	367	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	B	572	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	225	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	G	127	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	137	ARG	CG-CD-NE	-5.37	100.53	111.80
1	G	317	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	G	444	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	367	ARG	NE-CZ-NH1	-5.35	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	104	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	N	127	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	N	147	HIS	N-CA-C	5.34	125.41	111.00
1	H	209	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	572	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	G	147	HIS	N-CA-C	5.31	125.34	111.00
2	L	26	THR	CA-CB-CG2	5.30	119.83	112.40
2	K	72	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	404	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	282	MET	CG-SD-CE	-5.28	91.75	100.20
1	G	380	ASP	CB-CG-OD1	5.25	123.02	118.30
1	G	56	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	34	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	312	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	M	404	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	261	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	145	GLY	CA-C-O	-5.21	111.23	120.60
1	A	144	ALA	C-N-CA	5.18	133.19	122.30
1	H	34	ARG	CG-CD-NE	-5.18	100.92	111.80
1	D	232	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	317	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	M	444	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	147	HIS	N-CA-C	5.16	124.92	111.00
1	G	572	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	H	110	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	317	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	147	HIS	N-CA-C	5.09	124.76	111.00
1	D	144	ALA	O-C-N	-5.08	114.57	123.20
1	N	137	ARG	CG-CD-NE	-5.06	101.17	111.80
1	H	179	ASP	CB-CG-OD1	5.06	122.85	118.30
1	H	528	LYS	CD-CE-NZ	-5.06	100.07	111.70
1	M	472	MET	CG-SD-CE	5.04	108.26	100.20
2	I	76	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	D	397	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	L	62	GLN	CB-CA-C	-5.01	100.37	110.40
1	C	298	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	M	380	ASP	CB-CG-OD1	5.00	122.80	118.30
1	B	104	TYR	CB-CG-CD2	-5.00	118.00	121.00

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	10	0
1	B	4490	0	4320	11	0
1	C	4491	0	4320	11	0
1	D	4490	0	4320	17	0
1	G	4491	0	4320	14	0
1	H	4490	0	4320	12	0
1	M	4491	0	4320	13	0
1	N	4490	0	4319	20	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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
3	O	61	0	0	1	0
3	P	98	0	0	1	0
All	All	45177	0	38919	131	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 (131) 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: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
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
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
1:B:112:ARG:HD3	1:B:112:ARG:C	2.17	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:193:VAL:HG21	1:G:283:ILE:HD11	1.88	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:M:591:GLN:HG2	1:N:114:MET:HE1	1.90	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
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
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
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
3:C:1031:HOH:O	2:K:54:HIS:HE1	1.96	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: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:G:29:ASN:N	1:G:194:LYS:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:196:LYS:CD	1:D:223:GLU:HG3	2.46	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
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
1:G:591:GLN:HE21	1:H:114:MET:CE	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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%)	47 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	571/573 (100%)	542 (95%)	29 (5%)	0	100	100
1	C	571/573 (100%)	544 (95%)	26 (5%)	1 (0%)	47	38
1	D	571/573 (100%)	543 (95%)	25 (4%)	3 (0%)	29	18
1	G	571/573 (100%)	539 (94%)	30 (5%)	2 (0%)	34	24
1	H	571/573 (100%)	539 (94%)	30 (5%)	2 (0%)	34	24
1	M	571/573 (100%)	541 (95%)	29 (5%)	1 (0%)	47	38
1	N	571/573 (100%)	545 (95%)	24 (4%)	2 (0%)	34	24
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%)	47	38

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 ⓘ

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%)	458 (99%)	6 (1%)	69	68
1	B	464/464 (100%)	456 (98%)	8 (2%)	60	57
1	C	464/464 (100%)	458 (99%)	6 (1%)	69	68
1	D	464/464 (100%)	462 (100%)	2 (0%)	91	91
1	G	464/464 (100%)	460 (99%)	4 (1%)	78	79
1	H	464/464 (100%)	458 (99%)	6 (1%)	69	68
1	M	464/464 (100%)	458 (99%)	6 (1%)	69	68
1	N	464/464 (100%)	459 (99%)	5 (1%)	73	73
2	E	60/61 (98%)	58 (97%)	2 (3%)	38	29
2	F	60/61 (98%)	57 (95%)	3 (5%)	24	15
2	I	60/61 (98%)	57 (95%)	3 (5%)	24	15
2	J	60/61 (98%)	57 (95%)	3 (5%)	24	15
2	K	60/61 (98%)	59 (98%)	1 (2%)	60	57
2	L	60/61 (98%)	57 (95%)	3 (5%)	24	15
2	O	60/61 (98%)	59 (98%)	1 (2%)	60	57
2	P	60/61 (98%)	57 (95%)	3 (5%)	24	15
All	All	4192/4200 (100%)	4130 (98%)	62 (2%)	65	62

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	TYR
1	A	400	GLU
1	A	445	TRP
1	A	453	ARG
1	A	523	ARG
1	A	571	LYS
1	B	112	ARG
1	B	221	LYS

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Mol	Chain	Res	Type
1	B	243	LYS
1	B	337	TYR
1	B	387	LYS
1	B	391	LYS
1	B	445	TRP
1	B	569	ASP
1	C	233	GLU
1	C	239	LYS
1	C	279	LYS
1	C	337	TYR
1	C	445	TRP
1	C	530	GLN
1	D	337	TYR
1	D	584	ARG
2	E	57	ASN
2	E	80	TYR
2	F	43	ASP
2	F	59	LEU
2	F	93	ILE
1	G	146	GLU
1	G	279	LYS
1	G	337	TYR
1	G	387	LYS
1	H	112	ARG
1	H	146	GLU
1	H	279	LYS
1	H	337	TYR
1	H	472	MET
1	H	571	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	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

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Mol	Chain	Res	Type
1	M	410	LYS
1	M	447	PRO
1	M	584	ARG
1	N	337	TYR
1	N	391	LYS
1	N	472	MET
1	N	523	ARG
1	N	530	GLN
2	O	85	LYS
2	P	26	THR
2	P	59	LEU
2	P	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	GLN
1	B	117	GLN
1	B	216	ASN
1	C	270	ASN
1	D	156	GLN
1	D	216	ASN
1	D	270	ASN
2	E	54	HIS
2	F	54	HIS
1	G	591	GLN
1	H	545	GLN
1	H	588	HIS
1	H	591	GLN
2	I	54	HIS
2	J	54	HIS
2	K	54	HIS
2	L	54	HIS
1	M	591	GLN
1	N	117	GLN
1	N	156	GLN
1	N	464	ASN
1	N	588	HIS
2	O	54	HIS
2	P	54	HIS
2	P	62	GLN

5.3.3 RNA [i](#)

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 monosaccharides 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%)	-0.50	1 (0%) 95 95	12, 17, 29, 52	0
1	B	573/573 (100%)	-0.48	2 (0%) 94 94	12, 16, 29, 44	0
1	C	573/573 (100%)	-0.53	0 100 100	12, 16, 27, 43	0
1	D	573/573 (100%)	-0.49	3 (0%) 91 92	12, 17, 28, 49	0
1	G	573/573 (100%)	-0.53	1 (0%) 95 95	12, 17, 28, 41	0
1	H	573/573 (100%)	-0.45	1 (0%) 95 95	12, 19, 32, 49	0
1	M	573/573 (100%)	-0.39	0 100 100	13, 20, 34, 58	0
1	N	573/573 (100%)	-0.55	2 (0%) 94 94	12, 16, 28, 41	0
2	E	71/72 (98%)	-0.15	1 (1%) 75 77	17, 24, 41, 54	0
2	F	71/72 (98%)	-0.10	3 (4%) 36 39	14, 21, 46, 86	0
2	I	71/72 (98%)	0.14	5 (7%) 16 18	16, 23, 66, 100	0
2	J	71/72 (98%)	0.32	2 (2%) 53 56	22, 30, 49, 63	0
2	K	71/72 (98%)	-0.20	3 (4%) 36 39	15, 22, 36, 51	0
2	L	71/72 (98%)	-0.18	2 (2%) 53 56	16, 23, 38, 56	0
2	O	71/72 (98%)	0.44	8 (11%) 5 5	24, 34, 55, 64	0
2	P	71/72 (98%)	-0.04	5 (7%) 16 18	16, 21, 43, 60	0
All	All	5152/5160 (99%)	-0.43	39 (0%) 86 87	12, 18, 34, 100	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	93	ILE	9.2
2	F	93	ILE	7.0
2	F	92	ASP	5.8
2	I	92	ASP	5.6
2	F	91	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
2	I	91	GLU	4.3
2	I	90	VAL	3.9
2	O	82	LYS	3.9
2	J	91	GLU	3.7
2	E	93	ILE	3.3
2	O	90	VAL	3.0
2	O	85	LYS	3.0
2	O	91	GLU	2.9
2	P	91	GLU	2.8
1	A	571	LYS	2.7
2	K	91	GLU	2.7
2	O	93	ILE	2.7
2	L	91	GLU	2.7
1	H	347	GLY	2.6
1	B	584	ARG	2.6
2	P	89	LYS	2.6
2	P	81	ALA	2.5
2	O	83	THR	2.5
1	D	346	ASP	2.5
1	N	347	GLY	2.5
1	N	346	ASP	2.3
1	G	346	ASP	2.3
2	P	85	LYS	2.3
1	B	346	ASP	2.3
2	L	93	ILE	2.2
2	O	43	ASP	2.2
2	O	39	PRO	2.2
2	J	82	LYS	2.2
2	P	82	LYS	2.1
2	K	92	ASP	2.1
1	D	63	HIS	2.1
2	I	82	LYS	2.0
1	D	347	GLY	2.0
2	K	93	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.