



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:16 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

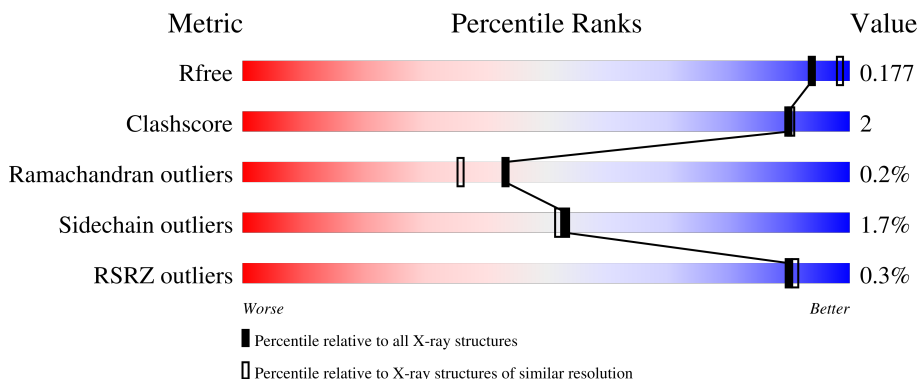
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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			

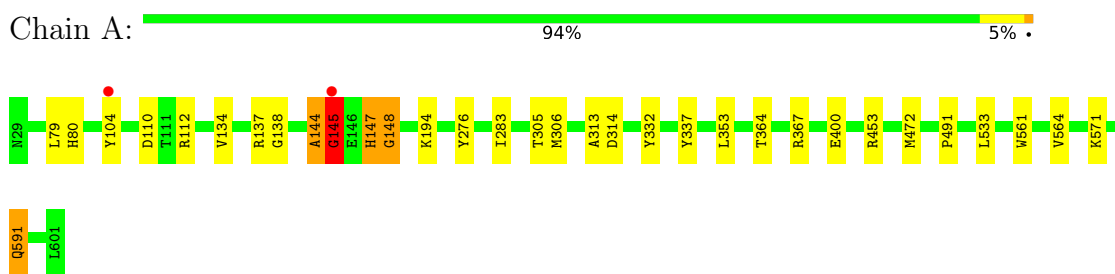
- Molecule 3 is water.

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		

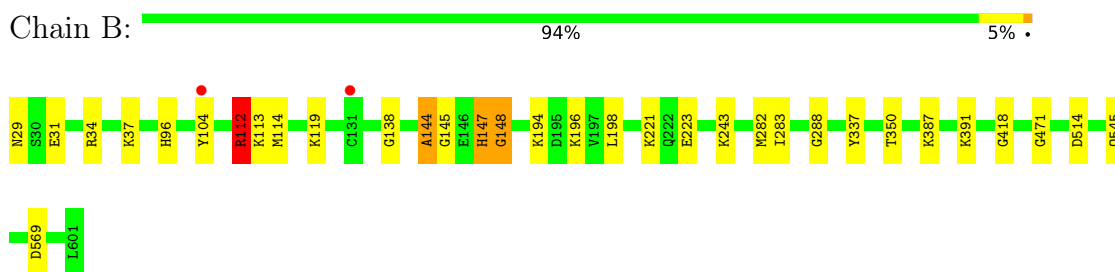
3 Residue-property plots [i](#)

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.

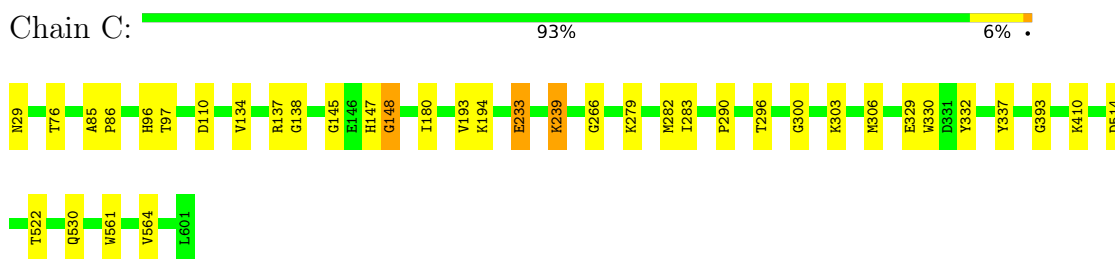
- Molecule 1: Methanol dehydrogenase protein, large subunit



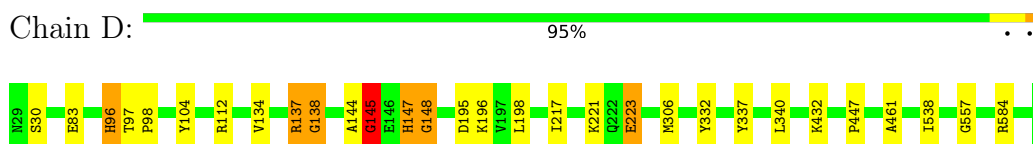
- Molecule 1: Methanol dehydrogenase protein, large subunit



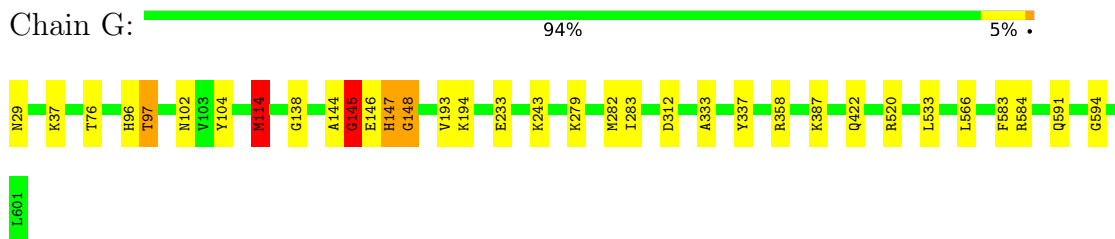
- Molecule 1: Methanol dehydrogenase protein, large subunit



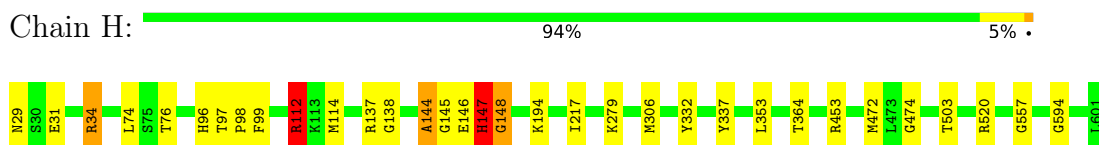
- Molecule 1: Methanol dehydrogenase protein, large subunit



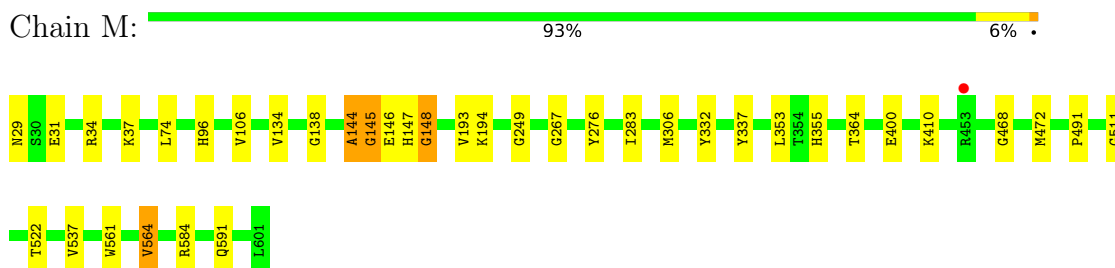
- Molecule 1: Methanol dehydrogenase protein, large subunit



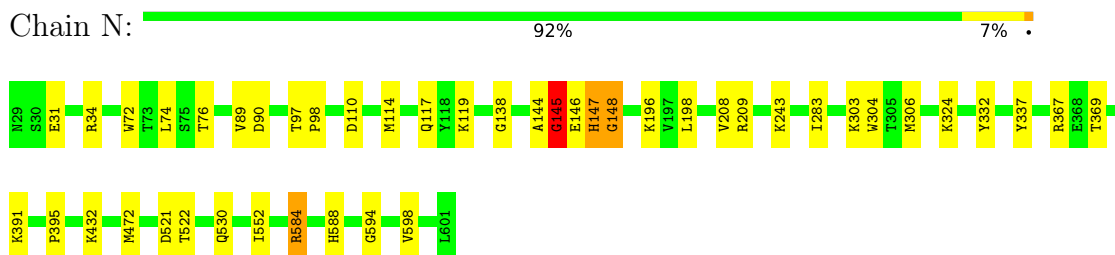
- Molecule 1: Methanol dehydrogenase protein, large subunit



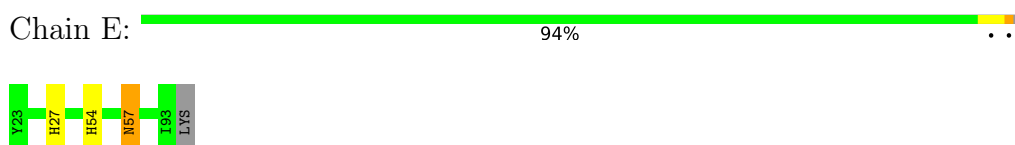
- Molecule 1: Methanol dehydrogenase protein, large subunit



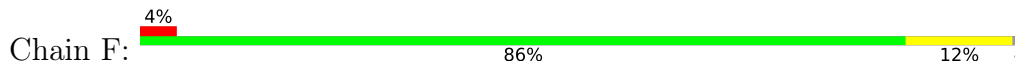
- Molecule 1: Methanol dehydrogenase protein, large subunit

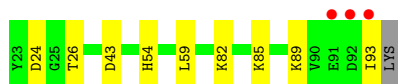


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

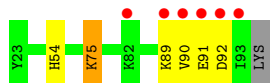
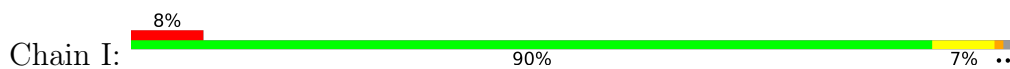


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

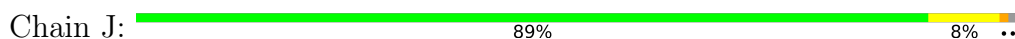




- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



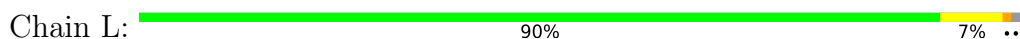
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



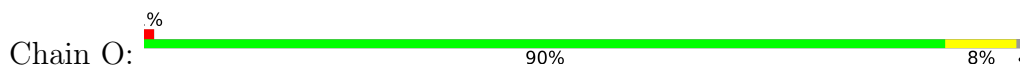
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



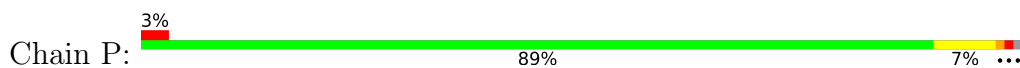
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- 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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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	97	THR	Mainchain

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
1	M	4491	0	4320	16	0
1	N	4490	0	4320	23	0
2	E	568	0	545	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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
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

5 of 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

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
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

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	410	LYS
1	N	74	LEU
1	N	552	ILE
2	F	43	ASP
2	E	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	408	ASN
1	N	408	ASN
1	H	588	HIS
1	N	250	GLN
2	O	79	ASN

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 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 [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	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

The worst 5 of 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

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.