



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 01:58 PM EDT

PDB ID : 4FIO  
Title : Crystal Structure of Methenyltetrahydromethanopterin Cyclohydrolase from Methanobrevibacter ruminantium  
Authors : Carbone, V.; Schofield, L.R.; Beattie, A.K.; Sutherland-Smith, A.J.; Ronimus, R.S.  
Deposited on : 2012-06-10  
Resolution : 1.37 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

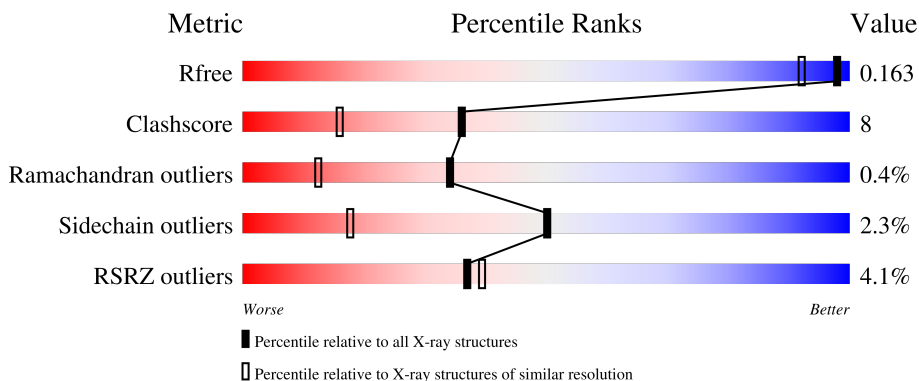
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.37 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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  $\geq 3$ , 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	354	 3% 82% 8% • 9%
1	B	354	 4% 79% 11% 10%
1	C	354	 4% 78% 10% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EEE	A	401	-	-	X	-
2	EEE	B	401	-	X	X	-
3	IPA	A	402	-	-	X	-
3	IPA	B	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8472 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 Methenyltetrahydromethanopterin cyclohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	Total 2471	C 1601	N 377	O 484	S 9	0	17	0
1	B	320	Total 2466	C 1595	N 374	O 489	S 8	0	19	0
1	C	319	Total 2440	C 1581	N 376	O 475	S 8	0	17	0

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP D3E4S5
A	-31	HIS	-	expression tag	UNP D3E4S5
A	-30	HIS	-	expression tag	UNP D3E4S5
A	-29	HIS	-	expression tag	UNP D3E4S5
A	-28	HIS	-	expression tag	UNP D3E4S5
A	-27	HIS	-	expression tag	UNP D3E4S5
A	-26	HIS	-	expression tag	UNP D3E4S5
A	-25	GLY	-	expression tag	UNP D3E4S5
A	-24	LYS	-	expression tag	UNP D3E4S5
A	-23	PRO	-	expression tag	UNP D3E4S5
A	-22	ILE	-	expression tag	UNP D3E4S5
A	-21	PRO	-	expression tag	UNP D3E4S5
A	-20	ASN	-	expression tag	UNP D3E4S5
A	-19	PRO	-	expression tag	UNP D3E4S5
A	-18	LEU	-	expression tag	UNP D3E4S5
A	-17	LEU	-	expression tag	UNP D3E4S5
A	-16	GLY	-	expression tag	UNP D3E4S5
A	-15	LEU	-	expression tag	UNP D3E4S5
A	-14	ASP	-	expression tag	UNP D3E4S5
A	-13	SER	-	expression tag	UNP D3E4S5
A	-12	THR	-	expression tag	UNP D3E4S5
A	-11	GLU	-	expression tag	UNP D3E4S5
A	-10	ASN	-	expression tag	UNP D3E4S5

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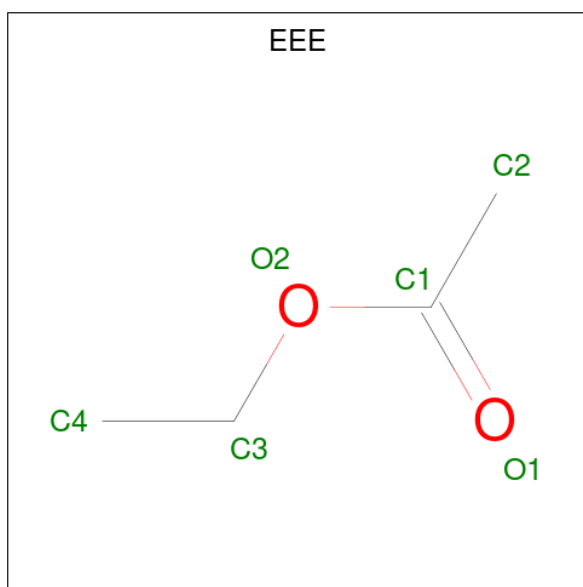
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	LEU	-	expression tag	UNP D3E4S5
A	-8	TYR	-	expression tag	UNP D3E4S5
A	-7	PHE	-	expression tag	UNP D3E4S5
A	-6	GLN	-	expression tag	UNP D3E4S5
A	-5	GLY	-	expression tag	UNP D3E4S5
A	-4	ILE	-	expression tag	UNP D3E4S5
A	-3	ASP	-	expression tag	UNP D3E4S5
A	-2	PRO	-	expression tag	UNP D3E4S5
A	-1	PHE	-	expression tag	UNP D3E4S5
A	0	THR	-	expression tag	UNP D3E4S5
B	-32	MET	-	initiating methionine	UNP D3E4S5
B	-31	HIS	-	expression tag	UNP D3E4S5
B	-30	HIS	-	expression tag	UNP D3E4S5
B	-29	HIS	-	expression tag	UNP D3E4S5
B	-28	HIS	-	expression tag	UNP D3E4S5
B	-27	HIS	-	expression tag	UNP D3E4S5
B	-26	HIS	-	expression tag	UNP D3E4S5
B	-25	GLY	-	expression tag	UNP D3E4S5
B	-24	LYS	-	expression tag	UNP D3E4S5
B	-23	PRO	-	expression tag	UNP D3E4S5
B	-22	ILE	-	expression tag	UNP D3E4S5
B	-21	PRO	-	expression tag	UNP D3E4S5
B	-20	ASN	-	expression tag	UNP D3E4S5
B	-19	PRO	-	expression tag	UNP D3E4S5
B	-18	LEU	-	expression tag	UNP D3E4S5
B	-17	LEU	-	expression tag	UNP D3E4S5
B	-16	GLY	-	expression tag	UNP D3E4S5
B	-15	LEU	-	expression tag	UNP D3E4S5
B	-14	ASP	-	expression tag	UNP D3E4S5
B	-13	SER	-	expression tag	UNP D3E4S5
B	-12	THR	-	expression tag	UNP D3E4S5
B	-11	GLU	-	expression tag	UNP D3E4S5
B	-10	ASN	-	expression tag	UNP D3E4S5
B	-9	LEU	-	expression tag	UNP D3E4S5
B	-8	TYR	-	expression tag	UNP D3E4S5
B	-7	PHE	-	expression tag	UNP D3E4S5
B	-6	GLN	-	expression tag	UNP D3E4S5
B	-5	GLY	-	expression tag	UNP D3E4S5
B	-4	ILE	-	expression tag	UNP D3E4S5
B	-3	ASP	-	expression tag	UNP D3E4S5
B	-2	PRO	-	expression tag	UNP D3E4S5
B	-1	PHE	-	expression tag	UNP D3E4S5

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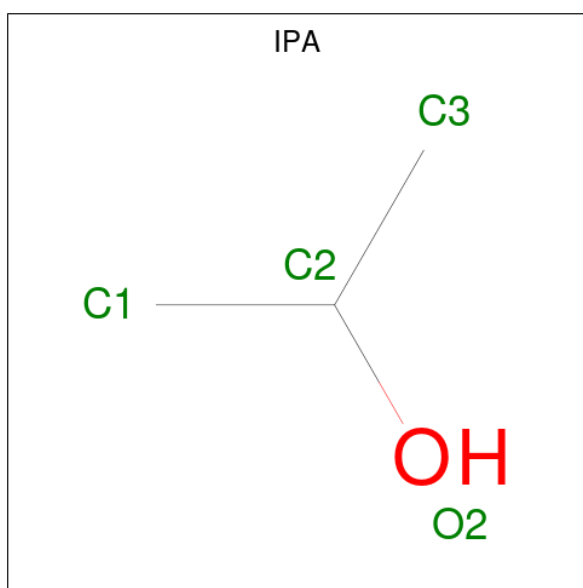
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP D3E4S5
C	-32	MET	-	expression tag	UNP D3E4S5
C	-31	HIS	-	expression tag	UNP D3E4S5
C	-30	HIS	-	expression tag	UNP D3E4S5
C	-29	HIS	-	expression tag	UNP D3E4S5
C	-28	HIS	-	expression tag	UNP D3E4S5
C	-27	HIS	-	expression tag	UNP D3E4S5
C	-26	HIS	-	expression tag	UNP D3E4S5
C	-25	GLY	-	expression tag	UNP D3E4S5
C	-24	LYS	-	expression tag	UNP D3E4S5
C	-23	PRO	-	expression tag	UNP D3E4S5
C	-22	ILE	-	expression tag	UNP D3E4S5
C	-21	PRO	-	expression tag	UNP D3E4S5
C	-20	ASN	-	expression tag	UNP D3E4S5
C	-19	PRO	-	expression tag	UNP D3E4S5
C	-18	LEU	-	expression tag	UNP D3E4S5
C	-17	LEU	-	expression tag	UNP D3E4S5
C	-16	GLY	-	expression tag	UNP D3E4S5
C	-15	LEU	-	expression tag	UNP D3E4S5
C	-14	ASP	-	expression tag	UNP D3E4S5
C	-13	SER	-	expression tag	UNP D3E4S5
C	-12	THR	-	expression tag	UNP D3E4S5
C	-11	GLU	-	expression tag	UNP D3E4S5
C	-10	ASN	-	expression tag	UNP D3E4S5
C	-9	LEU	-	expression tag	UNP D3E4S5
C	-8	TYR	-	expression tag	UNP D3E4S5
C	-7	PHE	-	expression tag	UNP D3E4S5
C	-6	GLN	-	expression tag	UNP D3E4S5
C	-5	GLY	-	expression tag	UNP D3E4S5
C	-4	ILE	-	expression tag	UNP D3E4S5
C	-3	ASP	-	expression tag	UNP D3E4S5
C	-2	PRO	-	expression tag	UNP D3E4S5
C	-1	PHE	-	expression tag	UNP D3E4S5
C	0	THR	-	expression tag	UNP D3E4S5

- Molecule 2 is ETHYL ACETATE (three-letter code: EEE) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	B	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

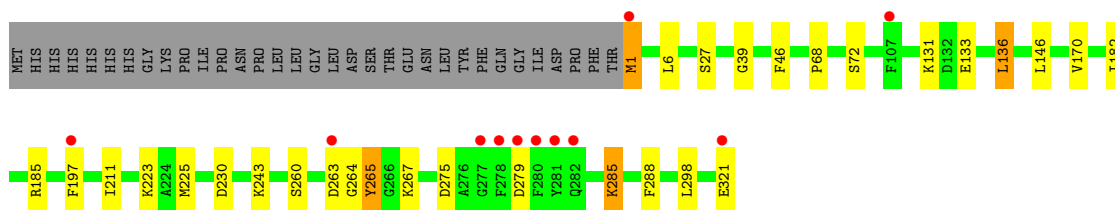
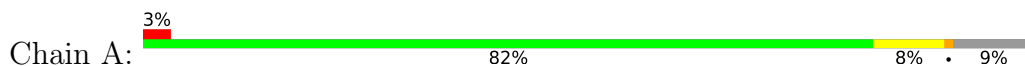
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	386	Total	O	0	0
			386	386		
4	B	354	Total	O	0	0
			354	354		
4	C	331	Total	O	0	0
			331	331		



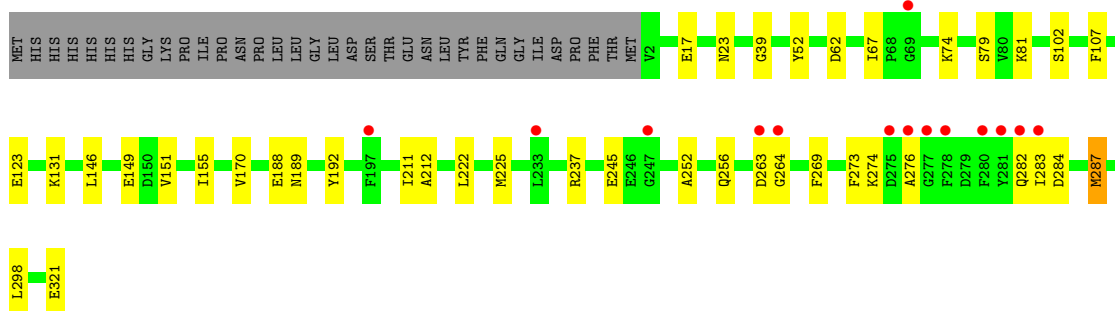
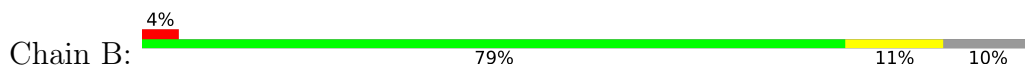
### 3 Residue-property plots [i](#)

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.

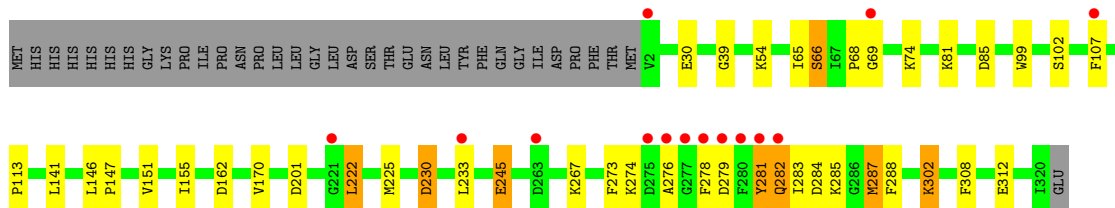
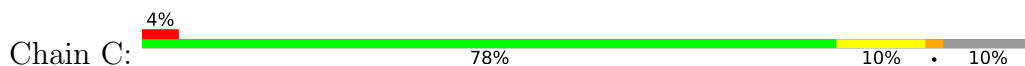
- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase



- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase



- Molecule 1: Methenyltetrahydromethanopterin cyclohydrolase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.37Å 74.86Å 74.82Å 120.06° 100.01° 98.28°	Depositor
Resolution (Å)	19.88 – 1.37 19.88 – 1.37	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.88-1.37) 93.8 (19.88-1.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 1.37Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.130 , 0.175 0.124 , 0.163	Depositor DCC
$R_{free}$ test set	9299 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: EEE, IPA

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	1.09	3/2571 (0.1%)	1.13	4/3482 (0.1%)
1	B	1.07	1/2577 (0.0%)	1.07	3/3488 (0.1%)
1	C	1.04	3/2549 (0.1%)	1.13	8/3451 (0.2%)
All	All	1.06	7/7697 (0.1%)	1.11	15/10421 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	GLU	CB-CG	-5.57	1.41	1.52
1	C	66	SER	CB-OG	-5.46	1.35	1.42
1	A	27	SER	CB-OG	5.15	1.49	1.42
1	B	52	TYR	CE1-CZ	-5.14	1.31	1.38
1	C	99	TRP	CG-CD1	5.10	1.43	1.36
1	A	265	TYR	CE2-CZ	5.04	1.45	1.38
1	A	46	PHE	CG-CD2	5.02	1.46	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	LEU	CB-CG-CD2	5.71	120.71	111.00
1	B	62	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	223	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	C	230	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	65[A]	ILE	CA-CB-CG1	-5.51	100.53	111.00
1	C	65[B]	ILE	CA-CB-CG1	-5.51	100.53	111.00
1	A	230	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	237	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	298	LEU	CB-CG-CD2	5.37	120.13	111.00
1	C	85	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	65[A]	ILE	CG1-CB-CG2	-5.31	99.72	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65[B]	ILE	CG1-CB-CG2	-5.31	99.72	111.40
1	C	201	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	287	MET	CG-SD-CE	-5.28	91.75	100.20
1	A	279	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2471	0	2512	41	0
1	B	2466	0	2486	38	0
1	C	2440	0	2483	33	0
2	A	6	0	8	9	0
2	B	6	0	8	7	0
3	A	4	0	8	6	0
3	B	8	0	15	5	0
4	A	386	0	0	17	0
4	B	354	0	0	15	0
4	C	331	0	0	10	0
All	All	8472	0	7520	120	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 8.

All (120) 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)
3:A:402:IPA:H12	4:A:603:HOH:O	1.27	1.32
1:B:17:GLU:HG2	4:B:636:HOH:O	1.35	1.22
1:A:285:LYS:O	1:A:285:LYS:HD2	1.40	1.20
1:A:285:LYS:HG2	2:A:401:EEE:H41	1.21	1.18
1:A:285:LYS:HG2	2:A:401:EEE:C4	1.75	1.14
3:A:402:IPA:H2	4:A:665:HOH:O	1.52	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:HB	4:B:586:HOH:O	1.68	0.93
1:A:285:LYS:CG	2:A:401:EEE:H41	2.02	0.89
1:B:225:MET:CE	4:B:638:HOH:O	2.22	0.87
1:C:273:PHE:HD1	1:C:283:ILE:HD11	1.40	0.85
1:A:225:MET:CE	4:A:666:HOH:O	2.23	0.84
1:B:74:LYS:HD2	4:C:500:HOH:O	1.78	0.82
1:A:68:PRO:HB3	4:A:669:HOH:O	1.78	0.82
1:A:285:LYS:CG	2:A:401:EEE:C4	2.56	0.81
1:A:285:LYS:HD3	1:A:288:PHE:HD2	1.44	0.81
1:A:131:LYS:HE2	1:A:133[B]:GLU:OE2	1.80	0.81
1:A:6:LEU:HD23	1:A:136[A]:LEU:HD11	1.65	0.78
1:B:79:SER:HB3	1:B:211[B]:ILE:HD11	1.66	0.78
1:C:308:PHE:CZ	4:C:552:HOH:O	2.38	0.77
1:A:285:LYS:HD3	1:A:288:PHE:CD2	2.20	0.76
1:A:225:MET:HE1	4:A:666:HOH:O	1.83	0.76
1:C:146:LEU:HD23	1:C:170[B]:VAL:HG21	1.69	0.75
1:A:285:LYS:HG2	2:A:401:EEE:H42	1.67	0.75
2:B:401:EEE:H43	3:B:402:IPA:C3	2.17	0.74
1:B:225:MET:HE1	4:B:638:HOH:O	1.85	0.73
1:B:146:LEU:HD23	1:B:170[B]:VAL:HG11	1.70	0.72
1:C:308:PHE:CE1	4:C:552:HOH:O	2.41	0.71
3:A:402:IPA:C2	4:A:665:HOH:O	2.23	0.70
1:B:321[B]:GLU:HG3	4:B:789:HOH:O	1.90	0.70
1:B:276:ALA:HB1	1:B:282:GLN:HB3	1.74	0.69
1:A:267[B]:LYS:HD3	4:A:668:HOH:O	1.91	0.69
1:C:66:SER:O	1:C:68:PRO:HD3	1.94	0.68
1:C:274:LYS:HG3	1:C:278:PHE:CZ	2.30	0.67
1:A:146:LEU:HD23	1:A:170[B]:VAL:HG11	1.78	0.66
1:A:285:LYS:O	1:A:285:LYS:CD	2.30	0.66
1:C:81[B]:LYS:HE2	4:C:667:HOH:O	1.94	0.66
1:A:6:LEU:HD23	1:A:136[B]:LEU:HD21	1.77	0.66
1:C:141:LEU:HB2	1:C:170[B]:VAL:HG12	1.78	0.66
1:B:146:LEU:CD2	1:B:170[B]:VAL:HG11	2.26	0.65
1:A:285:LYS:NZ	2:A:401:EEE:O1	2.29	0.65
1:B:264:GLY:N	4:B:830:HOH:O	2.28	0.64
1:C:146:LEU:CD2	1:C:170[B]:VAL:HG21	2.28	0.63
1:B:192:TYR:CG	2:B:401:EEE:H31	2.34	0.62
1:C:276:ALA:HB1	1:C:282:GLN:HB3	1.80	0.62
3:A:402:IPA:C1	4:A:665:HOH:O	2.45	0.61
1:B:79:SER:CB	1:B:211[B]:ILE:HD11	2.30	0.61
1:C:233[B]:LEU:HD11	1:C:288:PHE:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LYS:HD3	2:A:401:EEE:H42	1.82	0.61
1:C:30:GLU:HG3	4:C:521:HOH:O	2.00	0.61
1:C:273:PHE:CD1	1:C:283:ILE:HD11	2.29	0.61
1:A:146:LEU:CD2	1:A:170[B]:VAL:HG11	2.31	0.60
1:A:225:MET:HE2	4:A:666:HOH:O	1.95	0.60
1:C:54[A]:LYS:NZ	4:C:543:HOH:O	2.34	0.60
1:A:72:SER:HB3	1:C:74:LYS:HD2	1.84	0.59
1:B:263:ASP:HA	4:B:830:HOH:O	2.02	0.59
1:A:131:LYS:CE	1:A:133[B]:GLU:OE2	2.51	0.58
1:B:225:MET:HE2	4:B:638:HOH:O	1.92	0.58
2:B:401:EEE:H43	3:B:402:IPA:H32	1.84	0.58
1:A:285:LYS:CD	2:A:401:EEE:H42	2.33	0.57
1:C:312:GLU:HG2	4:C:537:HOH:O	2.03	0.57
1:A:185:ARG:HB2	3:A:402:IPA:H31	1.87	0.56
2:B:401:EEE:H43	3:B:402:IPA:H33	1.87	0.56
1:C:222:LEU:HD12	1:C:225[A]:MET:HE1	1.87	0.56
1:B:102[B]:SER:HB3	1:B:107:PHE:HD1	1.71	0.56
1:A:285:LYS:CG	2:A:401:EEE:H42	2.30	0.55
1:C:81[B]:LYS:CE	4:C:667:HOH:O	2.53	0.54
1:A:68:PRO:CB	4:A:669:HOH:O	2.46	0.53
1:C:273:PHE:HD1	1:C:283:ILE:CD1	2.15	0.53
1:A:264:GLY:N	4:A:630:HOH:O	2.22	0.51
1:C:274:LYS:HG3	1:C:278:PHE:HZ	1.75	0.51
1:B:192:TYR:CD2	2:B:401:EEE:H31	2.46	0.50
1:B:252:ALA:O	1:B:256[A]:GLN:HG3	2.10	0.50
1:A:197[A]:PHE:CZ	1:A:285:LYS:HB3	2.47	0.50
1:C:147:PRO:HD3	1:C:170[B]:VAL:HG11	1.93	0.50
1:B:225:MET:HE3	1:B:269:PHE:HE2	1.77	0.50
1:B:225:MET:CE	1:B:269:PHE:HE2	2.25	0.49
1:C:284:ASP:O	1:C:287:MET:HG2	2.12	0.49
1:C:146:LEU:HD23	1:C:170[B]:VAL:CG2	2.40	0.49
1:A:285:LYS:HD2	1:A:285:LYS:C	2.17	0.48
1:A:267[B]:LYS:HE2	1:A:275[B]:ASP:OD2	2.14	0.48
1:A:6:LEU:HD23	1:A:136[A]:LEU:CD1	2.39	0.47
1:B:245:GLU:OE2	4:B:627:HOH:O	2.20	0.47
1:A:211:ILE:HD12	4:B:586:HOH:O	2.14	0.47
1:C:146:LEU:CD2	1:C:170[B]:VAL:CG2	2.92	0.47
1:A:68:PRO:CA	4:A:669:HOH:O	2.63	0.47
1:C:279:ASP:OD2	1:C:281:TYR:HB2	2.14	0.47
1:A:1:MET:HG3	4:A:672:HOH:O	2.14	0.46
1:C:66:SER:C	1:C:68:PRO:HD3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ILE:CA	4:B:586:HOH:O	2.64	0.46
1:C:273:PHE:CD1	1:C:283:ILE:CD1	2.95	0.46
1:B:189:ASN:HD21	3:B:403:IPA:H2	1.81	0.46
1:A:68:PRO:HB3	4:A:870:HOH:O	2.16	0.45
1:B:146:LEU:CD2	1:B:170[B]:VAL:CG1	2.95	0.45
1:B:192:TYR:CB	2:B:401:EEE:H31	2.46	0.45
1:A:182:ILE:HG23	3:A:402:IPA:H32	1.97	0.45
1:A:275[B]:ASP:OD1	4:A:800:HOH:O	2.21	0.44
1:B:284:ASP:O	1:B:287[B]:MET:HG2	2.17	0.44
1:B:67:ILE:CB	4:B:586:HOH:O	2.43	0.44
1:B:151:VAL:O	1:B:155[B]:ILE:HG12	2.18	0.43
1:B:79:SER:HB3	1:B:211[B]:ILE:CD1	2.45	0.43
1:A:260:SER:HA	1:A:265:TYR:CG	2.54	0.43
1:C:102[A]:SER:HB3	1:C:107:PHE:HD1	1.83	0.43
1:B:146:LEU:HD23	1:B:170[B]:VAL:CG1	2.45	0.42
1:B:81:LYS:HD3	4:C:695:HOH:O	2.20	0.42
1:B:123:GLU:HB2	4:B:718:HOH:O	2.19	0.42
1:B:23:ASN:ND2	4:B:614:HOH:O	2.52	0.42
1:C:230:ASP:HA	1:C:233[A]:LEU:HG	2.02	0.42
3:B:402:IPA:H12	3:B:403:IPA:H11	2.02	0.41
1:B:211[B]:ILE:HD13	1:B:212:ALA:N	2.34	0.41
1:B:149[B]:GLU:CD	4:B:782:HOH:O	2.59	0.41
1:B:188:GLU:OE2	2:B:401:EEE:H32	2.20	0.41
1:B:273:PHE:HD1	1:B:283:ILE:CD1	2.34	0.40
1:C:151:VAL:O	1:C:155[B]:ILE:HG12	2.21	0.40
1:C:147:PRO:CD	1:C:170[A]:VAL:HG21	2.51	0.40
1:C:162:ASP:HB3	4:C:491:HOH:O	2.22	0.40
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.79	0.40
1:A:68:PRO:HA	4:A:669: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	336/354 (95%)	332 (99%)	3 (1%)	1 (0%)	41	18
1	B	336/354 (95%)	330 (98%)	5 (2%)	1 (0%)	41	18
1	C	334/354 (94%)	327 (98%)	5 (2%)	2 (1%)	25	7
All	All	1006/1062 (95%)	989 (98%)	13 (1%)	4 (0%)	34	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLY
1	B	39	GLY
1	C	39	GLY
1	C	69	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	267/280 (95%)	259 (97%)	8 (3%)	41	10
1	B	268/280 (96%)	264 (98%)	4 (2%)	65	36
1	C	265/280 (95%)	256 (97%)	9 (3%)	37	8
All	All	800/840 (95%)	779 (97%)	21 (3%)	50	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	136[A]	LEU
1	A	136[B]	LEU
1	A	243	LYS
1	A	263[A]	ASP
1	A	263[B]	ASP
1	A	285	LYS
1	A	321	GLU
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	274	LYS
1	B	287[A]	MET
1	B	287[B]	MET
1	C	113	PRO
1	C	222	LEU
1	C	245	GLU
1	C	267	LYS
1	C	281	TYR
1	C	282	GLN
1	C	285	LYS
1	C	302[A]	LYS
1	C	302[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	B	23	ASN
1	B	282	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IPA	A	402	-	3,3,3	0.97	0	3,3,3	0.89	0
2	EEE	A	401	-	5,5,5	1.66	2 (40%)	5,5,5	1.41	1 (20%)
2	EEE	B	401	-	5,5,5	1.83	1 (20%)	5,5,5	3.04	4 (80%)
3	IPA	B	402	-	3,3,3	0.42	0	3,3,3	1.65	1 (33%)
3	IPA	B	403	-	3,3,3	0.33	0	3,3,3	2.09	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EEE	B	401	-	-	3/3/3/3	-
2	EEE	A	401	-	-	0/3/3/3	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	EEE	O2-C1	3.71	1.51	1.33
2	A	401	EEE	O1-C1	-2.49	1.11	1.20
2	A	401	EEE	O2-C1	2.48	1.45	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	EEE	C3-O2-C1	3.48	139.47	117.57
2	B	401	EEE	O2-C1-C2	3.42	127.29	112.38
2	B	401	EEE	O1-C1-C2	-3.40	112.43	124.81
2	B	401	EEE	O2-C3-C4	3.27	120.45	108.42
3	B	402	IPA	O2-C2-C3	2.79	129.03	110.36
3	B	403	IPA	O2-C2-C3	-2.59	93.05	110.36
2	A	401	EEE	C3-O2-C1	2.26	131.80	117.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	EEE	O1-C1-O2-C3
2	B	401	EEE	C4-C3-O2-C1
2	B	401	EEE	C2-C1-O2-C3

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	IPA	6	0
2	A	401	EEE	9	0
2	B	401	EEE	7	0
3	B	402	IPA	4	0
3	B	403	IPA	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/354 (90%)	0.02	11 (3%) 45 47	9, 13, 28, 45	13 (4%)
1	B	320/354 (90%)	0.01	14 (4%) 34 36	10, 15, 30, 42	17 (5%)
1	C	319/354 (90%)	0.10	14 (4%) 34 36	10, 16, 30, 47	15 (4%)
All	All	960/1062 (90%)	0.04	39 (4%) 37 39	9, 14, 30, 47	45 (4%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	TYR	10.7
1	C	281	TYR	8.2
1	B	281	TYR	7.2
1	C	280	PHE	5.5
1	A	280	PHE	5.3
1	B	69	GLY	5.1
1	B	280	PHE	4.7
1	A	1	MET	4.6
1	A	278	PHE	4.5
1	C	69	GLY	4.4
1	A	321	GLU	4.0
1	A	282	GLN	3.8
1	C	276	ALA	3.6
1	C	233[A]	LEU	3.6
1	C	277	GLY	3.5
1	B	197[A]	PHE	3.5
1	B	263	ASP	3.4
1	A	277	GLY	3.2
1	A	197[A]	PHE	3.0
1	C	278	PHE	3.0
1	B	282	GLN	3.0
1	B	276	ALA	2.8
1	C	2	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	275	ASP	2.7
1	C	282	GLN	2.7
1	B	283	ILE	2.6
1	C	107	PHE	2.6
1	B	247	GLY	2.5
1	B	278	PHE	2.5
1	B	264	GLY	2.5
1	B	233	LEU	2.5
1	A	263[A]	ASP	2.4
1	C	263	ASP	2.4
1	A	279	ASP	2.4
1	B	277	GLY	2.3
1	A	107	PHE	2.2
1	C	221	GLY	2.1
1	C	279	ASP	2.1
1	B	275	ASP	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	IPA	B	403	4/4	0.80	0.18	15,32,33,35	0
2	EEE	B	401	6/6	0.90	0.21	26,33,41,49	0
3	IPA	B	402	4/4	0.92	0.14	14,28,31,34	0
3	IPA	A	402	4/4	0.92	0.14	17,27,28,28	0
2	EEE	A	401	6/6	0.95	0.15	22,31,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.