



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:33 PM BST

PDB ID : 6BUM  
Title : Crystal structures of cyanuric acid hydrolase from *Moorella thermoacetica*  
Authors : Shi, K.; Cho, S.; Seffernick, J.L.; Bera, A.; Wackett, L.P.; Aihara, H.  
Deposited on : 2017-12-11  
Resolution : 1.51 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.

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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 : 2.13  
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) : 2.13

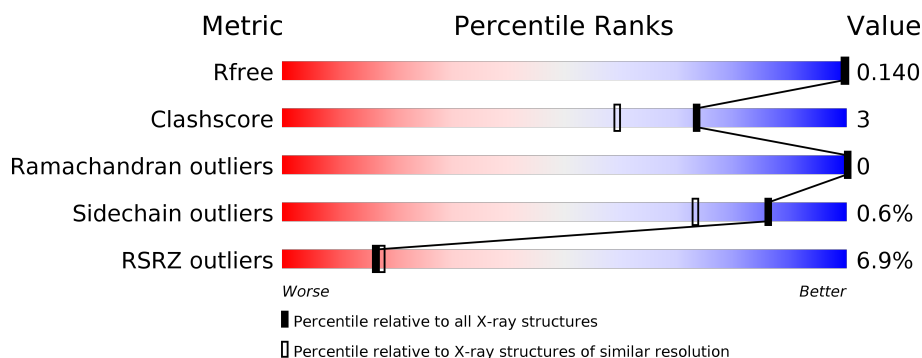
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 on 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	363	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
1	B	363	<div> <div>2%</div> <div>98%</div> <div></div> </div>
1	C	363	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
1	D	363	<div> <div>18%</div> <div>92%</div> <div>7%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PDO	A	410	-	-	X	-
4	PDO	C	405	-	-	X	-
4	PDO	C	409	-	-	X	-
4	PDO	D	405	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23325 atoms, of which 11152 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 Cyanuric acid amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	S	0	6	0
			5468	1681	2749	489	533	16			
1	B	363	Total	C	H	N	O	S	3	6	0
			5469	1682	2750	489	533	15			
1	C	363	Total	C	H	N	O	S	0	5	0
			5456	1680	2741	485	533	17			
1	D	362	Total	C	H	N	O	S	0	3	0
			5409	1669	2712	481	531	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q2RGM7
A	103	ALA	GLN	engineered mutation	UNP Q2RGM7
A	104	ALA	GLU	engineered mutation	UNP Q2RGM7
A	107	ALA	LYS	engineered mutation	UNP Q2RGM7
A	279	ILE	LEU	engineered mutation	UNP Q2RGM7
A	280	ARG	LYS	engineered mutation	UNP Q2RGM7
A	281	SER	PHE	engineered mutation	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	ALA	deletion	UNP Q2RGM7
A	283	ASP	GLU	engineered mutation	UNP Q2RGM7
A	290	MET	LEU	engineered mutation	UNP Q2RGM7
A	291	ASP	ALA	engineered mutation	UNP Q2RGM7
A	292	ARG	LYS	engineered mutation	UNP Q2RGM7
B	0	HIS	-	expression tag	UNP Q2RGM7
B	103	ALA	GLN	engineered mutation	UNP Q2RGM7
B	104	ALA	GLU	engineered mutation	UNP Q2RGM7
B	107	ALA	LYS	engineered mutation	UNP Q2RGM7
B	279	ILE	LEU	engineered mutation	UNP Q2RGM7

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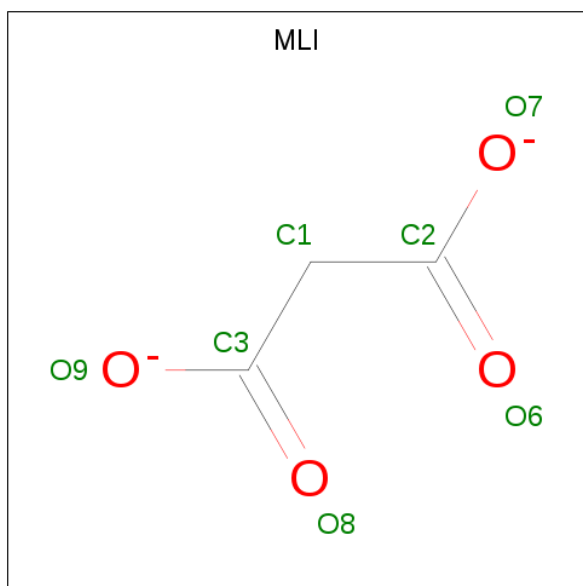
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ARG	LYS	engineered mutation	UNP Q2RGM7
B	281	SER	PHE	engineered mutation	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	ALA	deletion	UNP Q2RGM7
B	283	ASP	GLU	engineered mutation	UNP Q2RGM7
B	290	MET	LEU	engineered mutation	UNP Q2RGM7
B	291	ASP	ALA	engineered mutation	UNP Q2RGM7
B	292	ARG	LYS	engineered mutation	UNP Q2RGM7
C	0	HIS	-	expression tag	UNP Q2RGM7
C	103	ALA	GLN	engineered mutation	UNP Q2RGM7
C	104	ALA	GLU	engineered mutation	UNP Q2RGM7
C	107	ALA	LYS	engineered mutation	UNP Q2RGM7
C	279	ILE	LEU	engineered mutation	UNP Q2RGM7
C	280	ARG	LYS	engineered mutation	UNP Q2RGM7
C	281	SER	PHE	engineered mutation	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	ALA	deletion	UNP Q2RGM7
C	283	ASP	GLU	engineered mutation	UNP Q2RGM7
C	290	MET	LEU	engineered mutation	UNP Q2RGM7
C	291	ASP	ALA	engineered mutation	UNP Q2RGM7
C	292	ARG	LYS	engineered mutation	UNP Q2RGM7
D	0	HIS	-	expression tag	UNP Q2RGM7
D	103	ALA	GLN	engineered mutation	UNP Q2RGM7
D	104	ALA	GLU	engineered mutation	UNP Q2RGM7
D	107	ALA	LYS	engineered mutation	UNP Q2RGM7
D	279	ILE	LEU	engineered mutation	UNP Q2RGM7
D	280	ARG	LYS	engineered mutation	UNP Q2RGM7
D	281	SER	PHE	engineered mutation	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	ALA	deletion	UNP Q2RGM7
D	283	ASP	GLU	engineered mutation	UNP Q2RGM7
D	290	MET	LEU	engineered mutation	UNP Q2RGM7
D	291	ASP	ALA	engineered mutation	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	292	ARG	LYS	engineered mutation	UNP Q2RGM7

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).

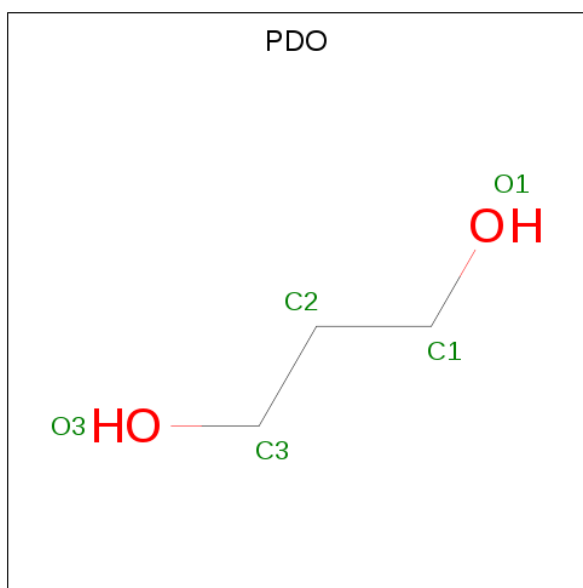


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	2	4		
2	B	1	Total	C	H	O	0	0
			9	3	2	4		
2	C	1	Total	C	H	O	0	0
			9	3	2	4		
2	D	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,3-PROPANDIOL (three-letter code: PDO) (formula:  $C_3H_8O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	A	1	Total	C	H	O	0	0
			13	3	8	2		
4	B	1	Total	C	H	O	0	0
			13	3	8	2		
4	B	1	Total	C	H	O	0	0
			13	3	8	2		
4	B	1	Total	C	H	O	0	0
			13	3	8	2		
4	B	1	Total	C	H	O	0	0
			13	3	8	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	C	1	Total	C	H	O	0	0
			13	3	8	2		
4	D	1	Total	C	H	O	0	0
			13	3	8	2		
4	D	1	Total	C	H	O	0	0
			13	3	8	2		
4	D	1	Total	C	H	O	0	0
			13	3	8	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

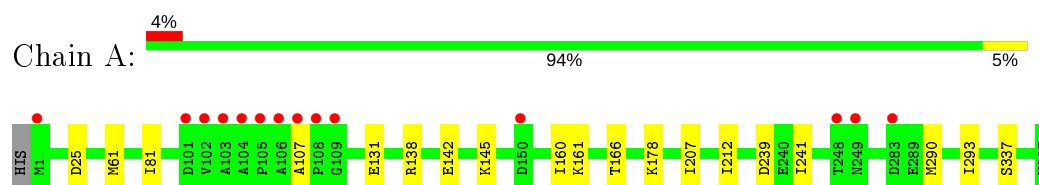
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	332	Total	O	0	0
			332	332		
6	B	329	Total	O	0	0
			329	329		
6	C	314	Total	O	0	2
			316	316		
6	D	192	Total	O	0	1
			193	193		



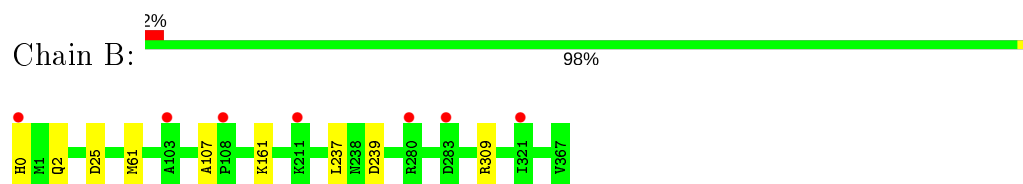
### 3 Residue-property plots

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.

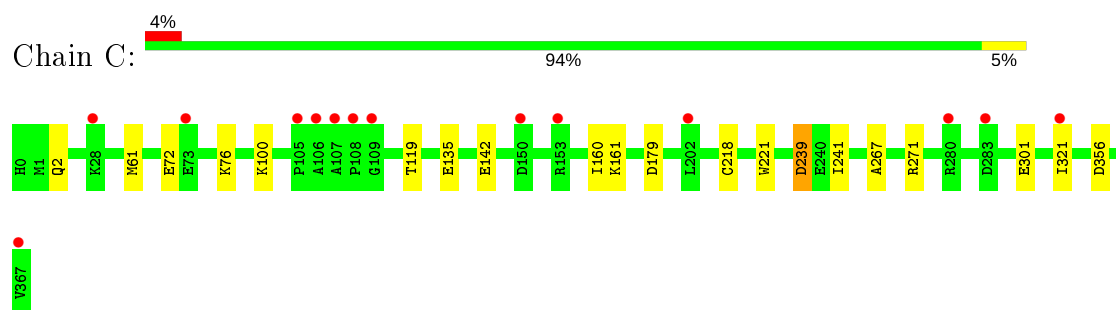
- Molecule 1: Cyanuric acid amidohydrolase



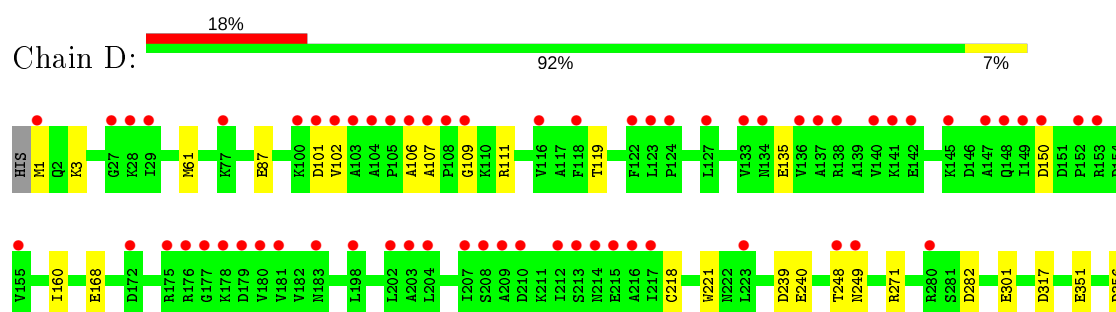
- Molecule 1: Cyanuric acid amidohydrolase



- Molecule 1: Cyanuric acid amidohydrolase



- Molecule 1: Cyanuric acid amidohydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 88.69Å 204.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 1.51 44.34 – 1.51	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.99-1.51) 95.7 (44.34-1.51)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.51Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2975: ???)	Depositor
R, $R_{free}$	0.126 , 0.141 0.125 , 0.140	Depositor DCC
$R_{free}$ test set	11226 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	23325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: PDO, CA, MLI, CL

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	0.31	0/2769	0.58	0/3745
1	B	0.30	0/2782	0.56	0/3763
1	C	0.29	0/2769	0.55	0/3746
1	D	0.28	0/2742	0.53	0/3710
All	All	0.30	0/11062	0.56	0/14964

There are no bond length outliers.

There are no bond angle outliers.

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	2719	2749	2733	20	0
1	B	2719	2750	2728	8	0
1	C	2715	2741	2718	17	0
1	D	2697	2712	2713	21	0
2	A	7	2	2	0	0
2	B	7	2	2	0	0
2	C	7	2	2	0	0
2	D	7	2	2	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	40	64	64	10	0
4	B	30	48	48	3	0
4	C	35	56	56	10	0
4	D	15	24	24	7	0
5	B	1	0	0	1	0
6	A	332	0	0	14	2
6	B	329	0	0	6	2
6	C	316	0	0	3	0
6	D	193	0	0	6	0
All	All	12173	11152	11092	73	2

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 3.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLN:OE1	6:B:501:HOH:O	1.73	1.06
5:B:403:CL:CL	6:B:597:HOH:O	2.15	0.98
1:D:168:GLU:OE1	6:D:501:HOH:O	1.89	0.90
1:A:142:GLU:OE2	6:A:501:HOH:O	1.89	0.90
1:A:138[B]:ARG:NH1	6:A:505:HOH:O	2.11	0.83
1:B:0:HIS:N	6:B:503:HOH:O	2.09	0.81
4:A:409:PDO:O3	6:A:502:HOH:O	1.99	0.80
1:C:356:ASP:HA	4:C:405:PDO:H11	1.65	0.78
1:A:25:ASP:OD1	6:A:503:HOH:O	2.02	0.77
4:D:404:PDO:O1	6:D:502:HOH:O	2.05	0.74
1:B:25:ASP:OD1	6:B:502:HOH:O	2.06	0.72
1:D:1:MET:CE	1:D:106:ALA:HB2	2.19	0.72
1:C:2:GLN:OE1	6:C:501:HOH:O	2.07	0.72
1:D:248:THR:O	6:D:503:HOH:O	2.11	0.68
1:D:356:ASP:HA	4:D:405:PDO:H32	1.75	0.68
1:D:109:GLY:O	6:D:503:HOH:O	2.13	0.67
4:D:405:PDO:O1	6:D:504:HOH:O	2.12	0.66
1:A:107:ALA:O	6:A:506:HOH:O	2.14	0.66
1:C:142:GLU:OE1	6:C:502:HOH:O	2.14	0.63
1:C:271:ARG:NH2	4:C:409:PDO:O3	2.34	0.61
1:D:1:MET:SD	1:D:106:ALA:HB2	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ASP:OD1	4:D:403:PDO:O1	2.10	0.59
1:A:61[A]:MET:SD	1:B:61[A]:MET:SD	3.00	0.59
1:A:138[A]:ARG:NE	6:A:511:HOH:O	2.36	0.57
1:D:249:ASN:ND2	1:D:249:ASN:O	2.38	0.57
1:A:178:LYS:NZ	6:A:513:HOH:O	2.38	0.56
1:A:178:LYS:NZ	6:A:515:HOH:O	2.39	0.56
1:A:138[A]:ARG:NH2	6:A:514:HOH:O	2.38	0.56
1:C:267:ALA:CB	4:C:409:PDO:H11	2.36	0.55
1:B:237:LEU:HD13	4:B:409:PDO:H12	1.90	0.53
1:C:321:ILE:HG21	4:C:404:PDO:H32	1.90	0.52
4:A:410:PDO:H11	6:A:648:HOH:O	2.10	0.51
1:C:301:GLU:OE2	4:C:405:PDO:H22	2.10	0.51
4:A:406:PDO:HO1	4:A:409:PDO:HO1	1.59	0.50
4:A:410:PDO:C1	6:A:504:HOH:O	2.57	0.49
1:A:290[A]:MET:HG3	1:A:293:ILE:HD12	1.95	0.48
1:D:107:ALA:HB3	1:D:111:ARG:HG3	1.96	0.48
1:A:145:LYS:NZ	6:A:522:HOH:O	2.46	0.47
1:B:309:ARG:O	4:B:408:PDO:H22	2.13	0.47
1:C:160:ILE:HG12	1:C:241:ILE:HG13	1.96	0.47
1:C:221:TRP:CZ3	4:C:405:PDO:H21	2.50	0.47
1:A:337:SER:O	4:C:409:PDO:C3	2.63	0.46
1:D:1:MET:HE3	1:D:106:ALA:HB2	1.97	0.46
1:D:221:TRP:CZ3	4:D:405:PDO:H22	2.51	0.46
1:D:271:ARG:NH1	6:D:508:HOH:O	2.44	0.46
1:C:61[A]:MET:SD	1:D:61[A]:MET:SD	3.14	0.46
4:B:407:PDO:H21	1:D:87:GLU:HB3	1.99	0.45
1:D:351:GLU:HA	4:D:405:PDO:C2	2.47	0.45
1:C:72:GLU:O	1:C:76:LYS:HG2	2.17	0.45
1:D:301:GLU:OE2	4:D:405:PDO:H21	2.17	0.44
4:A:410:PDO:H22	1:D:317:ASP:OD2	2.17	0.44
1:A:138[B]:ARG:HD2	6:A:505:HOH:O	2.18	0.43
1:D:119:THR:HB	1:D:135:GLU:HG3	2.00	0.43
1:C:271:ARG:HH22	4:C:409:PDO:C3	2.32	0.43
1:C:119:THR:HB	1:C:135:GLU:HG3	2.00	0.43
1:D:3:LYS:HD3	1:D:102:VAL:HG21	2.00	0.43
1:B:107:ALA:O	6:B:504:HOH:O	2.21	0.43
1:A:160:ILE:HG12	1:A:241:ILE:HG13	2.00	0.42
1:D:218:CYS:HA	1:D:221:TRP:CH2	2.54	0.42
1:A:207:ILE:CD1	1:A:212:ILE:HD11	2.49	0.42
1:C:218:CYS:HA	1:C:221:TRP:CH2	2.55	0.42
1:C:161:LYS:O	1:C:239:ASP:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:THR:CG2	4:A:410:PDO:H21	2.50	0.42
1:C:221:TRP:CH2	4:C:405:PDO:H21	2.55	0.41
1:C:271:ARG:NH1	6:C:509:HOH:O	2.46	0.41
4:A:406:PDO:H21	6:A:505:HOH:O	2.20	0.41
1:B:161:LYS:O	1:B:239:ASP:HA	2.20	0.41
1:A:337:SER:O	4:C:409:PDO:H31	2.21	0.41
4:A:410:PDO:C3	6:B:582:HOH:O	2.69	0.41
1:A:81:ILE:HG23	1:A:161:LYS:HB2	2.03	0.41
1:A:166:THR:HG21	4:A:410:PDO:C2	2.51	0.41
1:D:160:ILE:HA	1:D:240:GLU:O	2.20	0.40
1:A:131:GLU:HA	4:A:409:PDO:H21	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:525:HOH:O	6:B:505:HOH:O[3_645]	1.90	0.30
6:A:794:HOH:O	6:B:573:HOH:O[1_455]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	366/363 (101%)	357 (98%)	9 (2%)	0	100	100
1	B	367/363 (101%)	359 (98%)	8 (2%)	0	100	100
1	C	366/363 (101%)	357 (98%)	9 (2%)	0	100	100
1	D	363/363 (100%)	354 (98%)	9 (2%)	0	100	100
All	All	1462/1452 (101%)	1427 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	290/286 (101%)	289 (100%)	1 (0%)	92	84
1	B	292/286 (102%)	292 (100%)	0	100	100
1	C	291/286 (102%)	288 (99%)	3 (1%)	76	56
1	D	288/286 (101%)	285 (99%)	3 (1%)	76	56
All	All	1161/1144 (102%)	1154 (99%)	7 (1%)	86	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ASP
1	C	100	LYS
1	C	179	ASP
1	C	239	ASP
1	D	101	ASP
1	D	150	ASP
1	D	239	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	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](#)

Of 33 ligands modelled in this entry, 5 are monoatomic - leaving 28 for Mogul analysis.

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	$\# Z  > 2$
4	PDO	C	406	-	4,4,4	0.37	0	3,3,3	0.31	0
4	PDO	B	406	-	4,4,4	0.34	0	3,3,3	0.49	0
2	MLI	B	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	PDO	D	404	-	4,4,4	0.36	0	3,3,3	0.36	0
2	MLI	A	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	PDO	C	403	-	4,4,4	0.36	0	3,3,3	0.26	0
4	PDO	A	410	-	4,4,4	0.31	0	3,3,3	0.60	0
4	PDO	B	408	-	4,4,4	0.38	0	3,3,3	0.46	0
4	PDO	D	403	-	4,4,4	0.35	0	3,3,3	0.46	0
2	MLI	D	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	PDO	A	404	-	4,4,4	0.35	0	3,3,3	0.48	0
4	PDO	C	408	-	4,4,4	0.36	0	3,3,3	0.40	0
4	PDO	D	405	3	4,4,4	0.39	0	3,3,3	0.39	0
4	PDO	B	407	-	4,4,4	0.40	0	3,3,3	0.31	0
4	PDO	A	405	-	4,4,4	0.41	0	3,3,3	0.35	0
4	PDO	B	404	-	4,4,4	0.37	0	3,3,3	0.24	0
4	PDO	B	405	-	4,4,4	0.34	0	3,3,3	0.48	0
4	PDO	A	403	-	4,4,4	0.37	0	3,3,3	0.28	0
4	PDO	C	407	-	4,4,4	0.37	0	3,3,3	0.37	0
2	MLI	C	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	PDO	A	407	-	4,4,4	0.35	0	3,3,3	0.45	0
4	PDO	A	406	-	4,4,4	0.35	0	3,3,3	0.40	0
4	PDO	C	405	3	4,4,4	0.44	0	3,3,3	0.57	0
4	PDO	A	409	-	4,4,4	0.38	0	3,3,3	0.37	0
4	PDO	B	409	-	4,4,4	0.35	0	3,3,3	0.49	0
4	PDO	C	409	-	4,4,4	0.36	0	3,3,3	0.27	0
4	PDO	C	404	-	4,4,4	0.45	0	3,3,3	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PDO	A	408	-	4,4,4	0.36	0	3,3,3	0.29	0

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
4	PDO	C	406	-	-	0/2/2/2	-
4	PDO	B	406	-	-	0/2/2/2	-
2	MLI	B	401	-	-	0/0/4/4	-
4	PDO	D	404	-	-	1/2/2/2	-
2	MLI	A	401	-	-	0/0/4/4	-
4	PDO	C	403	-	-	0/2/2/2	-
4	PDO	A	410	-	-	1/2/2/2	-
4	PDO	B	408	-	-	1/2/2/2	-
4	PDO	D	403	-	-	0/2/2/2	-
2	MLI	D	401	-	-	0/0/4/4	-
4	PDO	A	404	-	-	0/2/2/2	-
4	PDO	C	408	-	-	0/2/2/2	-
4	PDO	D	405	3	-	0/2/2/2	-
4	PDO	B	407	-	-	1/2/2/2	-
4	PDO	A	405	-	-	1/2/2/2	-
4	PDO	B	404	-	-	0/2/2/2	-
4	PDO	B	405	-	-	0/2/2/2	-
4	PDO	A	403	-	-	0/2/2/2	-
4	PDO	C	407	-	-	2/2/2/2	-
2	MLI	C	401	-	-	0/0/4/4	-
4	PDO	A	407	-	-	0/2/2/2	-
4	PDO	A	406	-	-	1/2/2/2	-
4	PDO	C	405	3	-	0/2/2/2	-
4	PDO	A	409	-	-	0/2/2/2	-
4	PDO	B	409	-	-	0/2/2/2	-
4	PDO	C	409	-	-	1/2/2/2	-
4	PDO	C	404	-	-	1/2/2/2	-
4	PDO	A	408	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	404	PDO	O1-C1-C2-C3
4	A	410	PDO	C1-C2-C3-O3
4	B	408	PDO	O1-C1-C2-C3
4	B	407	PDO	O1-C1-C2-C3
4	C	407	PDO	C1-C2-C3-O3
4	A	406	PDO	C1-C2-C3-O3
4	C	409	PDO	C1-C2-C3-O3
4	C	404	PDO	C1-C2-C3-O3
4	C	407	PDO	O1-C1-C2-C3
4	A	405	PDO	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	404	PDO	1	0
4	A	410	PDO	6	0
4	B	408	PDO	1	0
4	D	403	PDO	1	0
4	D	405	PDO	5	0
4	B	407	PDO	1	0
4	A	406	PDO	2	0
4	C	405	PDO	4	0
4	A	409	PDO	3	0
4	B	409	PDO	1	0
4	C	409	PDO	5	0
4	C	404	PDO	1	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	362/363 (99%)	0.09	14 (3%) 39 44	14, 19, 39, 83	0
1	B	363/363 (100%)	-0.19	7 (1%) 66 71	14, 20, 38, 59	1 (0%)
1	C	363/363 (100%)	0.11	14 (3%) 39 44	15, 23, 43, 80	0
1	D	362/363 (99%)	0.88	65 (17%) 1 1	16, 33, 61, 91	0
All	All	1450/1452 (99%)	0.22	100 (6%) 16 17	14, 22, 51, 91	1 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	16.6
1	C	107	ALA	10.8
1	A	103	ALA	9.8
1	D	105	PRO	9.8
1	D	103	ALA	9.3
1	D	104	ALA	8.8
1	C	108	PRO	8.6
1	D	109	GLY	8.0
1	D	102	VAL	8.0
1	A	108	PRO	7.9
1	D	106	ALA	7.6
1	C	106	ALA	6.9
1	A	107	ALA	6.7
1	D	1	MET	6.6
1	A	105	PRO	6.4
1	D	108	PRO	6.0
1	D	207	ILE	5.9
1	D	123	LEU	5.7
1	D	212	ILE	5.7
1	D	249	ASN	5.1
1	D	202	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	209	ALA	4.9
1	D	149	ILE	4.8
1	A	102	VAL	4.4
1	D	179	ASP	4.3
1	A	104	ALA	4.3
1	D	210	ASP	4.3
1	D	140	VAL	4.2
1	C	105	PRO	4.0
1	D	150	ASP	4.0
1	D	248	THR	4.0
1	D	107	ALA	3.9
1	C	280	ARG	3.8
1	A	249	ASN	3.8
1	C	109	GLY	3.8
1	D	77	LYS	3.7
1	A	1	MET	3.6
1	B	103	ALA	3.6
1	D	153	ARG	3.5
1	D	181	VAL	3.4
1	D	175	ARG	3.3
1	D	148	GLN	3.2
1	D	208	SER	3.2
1	D	138	ARG	3.2
1	D	122	PHE	3.2
1	D	133	VAL	3.1
1	D	101	ASP	3.1
1	D	215	GLU	3.1
1	D	155	VAL	3.1
1	C	150	ASP	3.0
1	D	27	GLY	3.0
1	D	141	LYS	3.0
1	D	177	GLY	2.9
1	A	283	ASP	2.9
1	A	101	ASP	2.9
1	C	367	VAL	2.9
1	D	213	SER	2.9
1	D	134	ASN	2.8
1	B	280	ARG	2.8
1	D	152	PRO	2.8
1	B	283	ASP	2.8
1	D	223	LEU	2.7
1	D	216	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	183	ASN	2.7
1	D	280	ARG	2.7
1	A	248	THR	2.6
1	D	214	ASN	2.6
1	A	150	ASP	2.6
1	D	172	ASP	2.6
1	B	0	HIS	2.5
1	D	124	PRO	2.5
1	D	180	VAL	2.5
1	D	147	ALA	2.5
1	B	211	LYS	2.5
1	D	145	LYS	2.5
1	A	109	GLY	2.4
1	D	137	ALA	2.4
1	D	100	LYS	2.4
1	D	142	GLU	2.3
1	B	321	ILE	2.3
1	D	367	VAL	2.3
1	D	28	LYS	2.3
1	D	127	LEU	2.3
1	C	283	ASP	2.3
1	D	176	ARG	2.3
1	D	217	ILE	2.3
1	D	178	LYS	2.3
1	C	153	ARG	2.2
1	C	321	ILE	2.2
1	D	204	LEU	2.2
1	D	203	ALA	2.2
1	D	116	VAL	2.1
1	D	198	LEU	2.1
1	D	136	VAL	2.1
1	D	118	PHE	2.1
1	D	29	ILE	2.1
1	C	73	GLU	2.1
1	C	28	LYS	2.0
1	C	202	LEU	2.0
1	B	108	PRO	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
4	PDO	A	408	5/5	0.29	0.33	59,71,74,74	0
4	PDO	A	409	5/5	0.46	0.38	72,86,90,91	0
4	PDO	C	406	5/5	0.47	0.36	51,62,66,66	0
4	PDO	B	408	5/5	0.65	0.18	53,63,64,65	0
4	PDO	A	406	5/5	0.65	0.33	81,97,100,101	0
4	PDO	D	403	5/5	0.69	0.27	76,92,93,94	0
4	PDO	D	405	5/5	0.75	0.13	48,57,59,63	0
4	PDO	C	405	5/5	0.76	0.19	37,44,49,52	0
4	PDO	C	404	5/5	0.77	0.33	27,39,45,47	0
4	PDO	B	407	5/5	0.79	0.23	27,40,46,48	0
4	PDO	A	405	5/5	0.80	0.14	30,41,46,49	0
4	PDO	C	407	5/5	0.82	0.24	38,49,58,58	0
4	PDO	B	409	5/5	0.83	0.20	43,52,61,63	0
4	PDO	C	409	5/5	0.84	0.43	45,55,56,60	0
4	PDO	A	410	5/5	0.85	0.36	37,49,58,61	0
4	PDO	B	405	5/5	0.89	0.21	60,72,74,75	0
4	PDO	A	407	5/5	0.90	0.12	62,74,79,79	0
4	PDO	C	408	5/5	0.90	0.10	60,72,75,75	0
5	CL	B	403	1/1	0.91	0.11	73,73,73,73	0
4	PDO	A	404	5/5	0.92	0.16	33,42,52,54	0
4	PDO	B	406	5/5	0.94	0.15	39,49,57,59	0
4	PDO	D	404	5/5	0.94	0.31	56,67,75,77	0
4	PDO	A	403	5/5	0.94	0.18	25,34,41,41	0
4	PDO	B	404	5/5	0.95	0.08	25,30,35,35	0
2	MLI	B	401	7/7	0.97	0.12	17,18,22,22	0
2	MLI	C	401	7/7	0.97	0.14	18,19,23,23	0
2	MLI	A	401	7/7	0.98	0.13	16,17,21,21	0
4	PDO	C	403	5/5	0.98	0.09	27,32,38,39	0
3	CA	B	402	1/1	0.99	0.09	18,18,18,18	1
2	MLI	D	401	7/7	0.99	0.10	20,21,25,25	0
3	CA	D	402	1/1	1.00	0.09	27,27,27,27	1
3	CA	A	402	1/1	1.00	0.12	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	C	402	1/1	1.00	0.13	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.