



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 03:08 PM EDT

PDB ID : 6BUQ  
Title : Crystal structures of cyanuric acid hydrolase from *Moorella thermoacetica* complexed with barbituric acid  
Authors : Shi, K.; Aihara, H.  
Deposited on : 2017-12-11  
Resolution : 1.88 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 : 2.35.1  
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

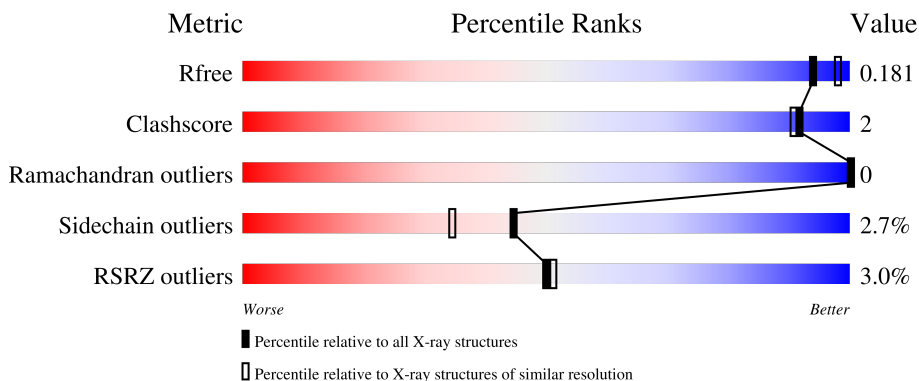
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	363	 95% 5%
1	B	363	 95% 5%
1	C	363	 96% .
1	D	363	 10% 94% 5% .

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
6	CL	A	406	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22601 atoms, of which 10936 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
			Total	C	H	N	O	S			
1	A	362	5430	1673	2724	482	536	15	0	5	0
1	B	363	5450	1680	2733	485	537	15	0	5	0
1	C	362	5371	1659	2690	479	529	14	0	0	0
1	D	360	5364	1653	2693	477	527	14	0	0	0

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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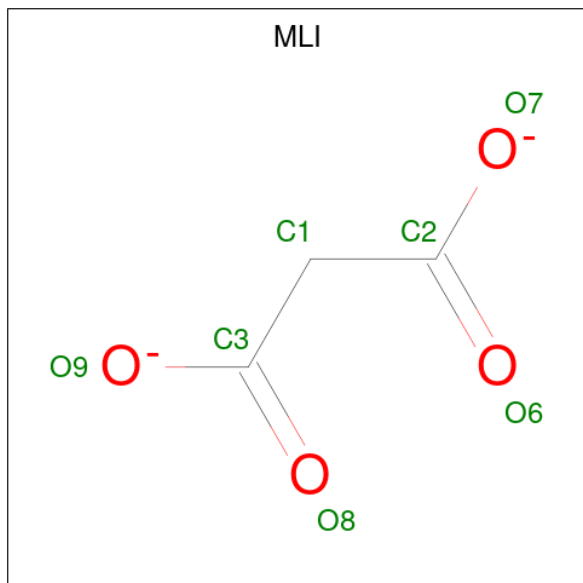
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ARG	LYS	engineered mutation	UNP Q2RGM7
B	281	SER	PHE	engineered mutation	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	ALA	deletion	UNP Q2RGM7
B	283	ASP	GLU	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
			Total	C	H	O		
2	A	1	9	3	2	4	0	0

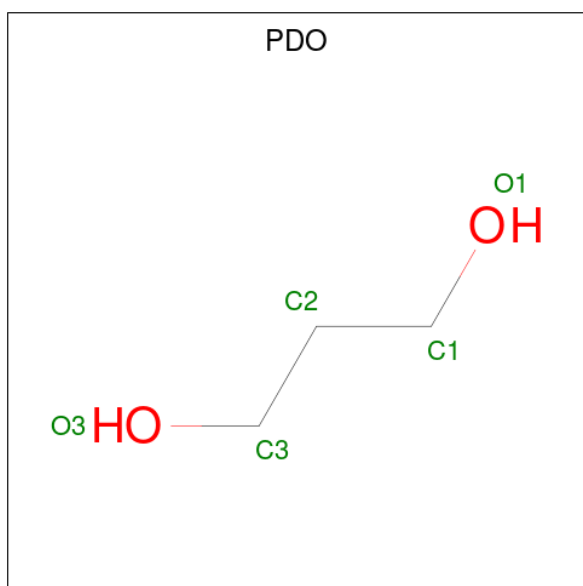
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0

- Molecule 5 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).

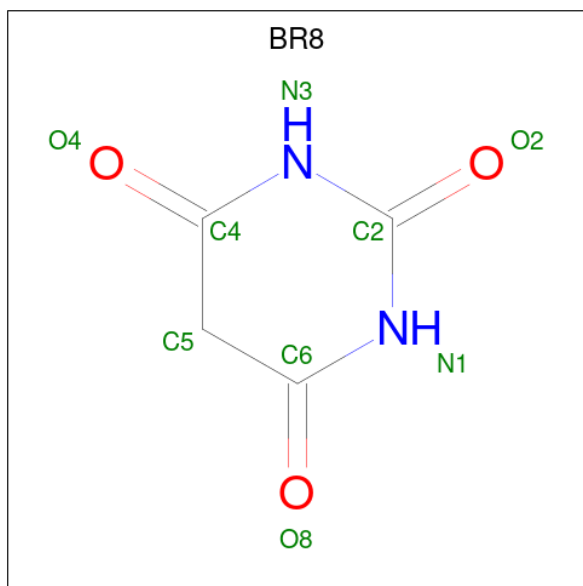


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			13	3	8	2		
5	A	1	Total	C	H	O	0	0
			13	3	8	2		
5	B	1	Total	C	H	O	0	0
			13	3	8	2		
5	B	1	Total	C	H	O	0	0
			13	3	8	2		
5	C	1	Total	C	H	O	0	0
			13	3	8	2		
5	C	1	Total	C	H	O	0	0
			13	3	8	2		
5	C	1	Total	C	H	O	0	0
			13	3	8	2		
5	D	1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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

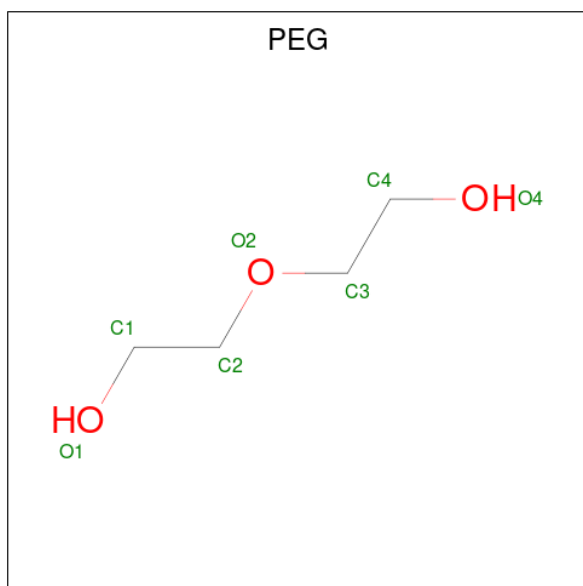
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is BARBITURIC ACID (three-letter code: BR8) (formula:  $C_4H_4N_2O_3$ ).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	245	Total	O	0	0
			245	245		
9	B	263	Total	O	0	0
			263	263		
9	C	181	Total	O	0	0
			181	181		
9	D	108	Total	O	0	0
			108	108		

### 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.

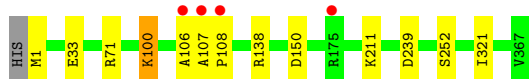
- Molecule 1: Cyanuric acid amidohydrolase



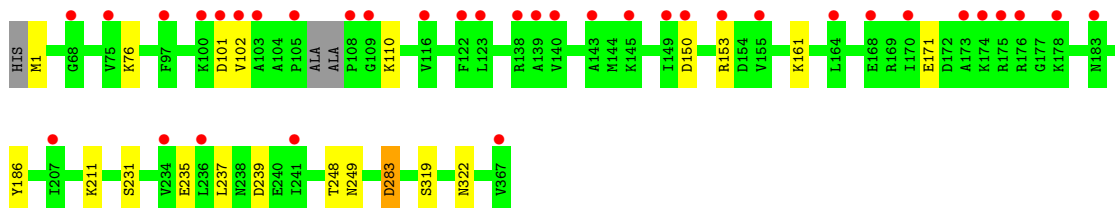
- Molecule 1: Cyanuric acid amidohydrolase



- 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, $\alpha$ , $\beta$ , $\gamma$	81.05Å 89.77Å 198.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.71 – 1.88 81.81 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.71-1.88) 99.5 (81.81-1.88)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.88Å)	Xtrriage
Refinement program	PHENIX (1.13rc2_2981: ???)	Depositor
R, $R_{free}$	0.156 , 0.182 0.153 , 0.181	Depositor DCC
$R_{free}$ test set	2019 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.248	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	22601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: MLI, PEG, CL, CA, NA, PDO, BR8

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	0.43	0/2758	0.58	0/3733
1	B	0.43	0/2772	0.58	0/3751
1	C	0.39	0/2713	0.56	0/3672
1	D	0.33	0/2702	0.50	0/3654
All	All	0.40	0/10945	0.56	0/14810

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	2706	2724	2705	10	0
1	B	2717	2733	2715	12	0
1	C	2681	2690	2705	5	0
1	D	2671	2693	2695	7	0
2	A	7	2	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	10	16	16	2	0
5	B	10	16	16	0	0
5	C	20	32	32	1	0
5	D	5	8	8	0	0
6	A	1	0	0	2	0
6	B	1	0	0	0	0
7	B	9	4	4	0	0
7	C	9	4	4	0	0
7	D	9	4	4	0	0
8	D	7	10	10	0	0
9	A	245	0	0	4	0
9	B	263	0	0	5	0
9	C	181	0	0	1	0
9	D	108	0	0	3	0
All	All	11665	10936	10916	35	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 (35) 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:A:25:ASP:OD1	9:A:501:HOH:O	1.97	0.83
1:B:235[A]:GLU:O	9:B:501:HOH:O	1.96	0.83
1:B:235[A]:GLU:OE2	9:B:502:HOH:O	1.99	0.79
1:B:2:GLN:OE1	9:B:503:HOH:O	2.04	0.75
1:C:106:ALA:HB1	1:C:107:ALA:HA	1.70	0.73
1:D:102:VAL:O	9:D:501:HOH:O	2.07	0.72
1:D:283:ASP:OD2	9:D:502:HOH:O	2.08	0.72
1:D:186:TYR:OH	1:D:322:ASN:OD1	2.01	0.71
1:A:171:GLU:OE1	1:A:174:LYS:NZ	2.26	0.69
1:A:25:ASP:OD2	9:A:502:HOH:O	2.13	0.64
1:B:178:LYS:NZ	9:B:506:HOH:O	2.34	0.60
1:A:50:PHE:HA	6:A:406:CL:CL	2.39	0.60
1:B:280:ARG:NH2	1:B:289:GLU:OE2	2.34	0.59
1:C:1:MET:N	9:C:502:HOH:O	2.35	0.59
1:B:275:LYS:NZ	9:B:508:HOH:O	2.37	0.57
1:B:1:MET:HE3	1:B:250:SER:HA	1.85	0.57
1:D:235:GLU:HG3	9:D:522:HOH:O	2.09	0.53
1:A:271:ARG:NH1	9:A:504:HOH:O	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:405:PDO:H31	9:A:607:HOH:O	2.10	0.50
1:B:1:MET:HE3	1:B:250:SER:CA	2.41	0.50
1:D:161:LYS:HD2	1:D:231:SER:O	2.14	0.47
1:A:49:ASP:O	6:A:406:CL:CL	2.69	0.47
5:A:405:PDO:H32	1:D:319:SER:HA	1.98	0.46
1:A:107:ALA:N	1:A:108:PRO:CD	2.79	0.46
1:A:81:ILE:HG23	1:A:161:LYS:HB2	2.00	0.43
1:D:283:ASP:OD1	1:D:283:ASP:N	2.52	0.43
1:A:291:ASP:OD1	1:A:291:ASP:N	2.53	0.42
1:B:1:MET:CE	1:B:250:SER:CA	2.98	0.42
1:C:33:GLU:OE1	1:C:100:LYS:HE3	2.20	0.42
1:C:106:ALA:HA	1:C:108:PRO:HD3	2.02	0.42
1:B:107:ALA:HB3	1:B:111:ARG:HG3	2.03	0.41
1:B:64:ALA:HB1	1:B:69:ILE:O	2.20	0.40
1:A:135[B]:GLU:OE1	1:A:138:ARG:NH1	2.53	0.40
1:C:321:ILE:HD13	5:C:405:PDO:H11	2.03	0.40
1:B:1:MET:HE2	1:B:106:ALA:HA	2.03	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	365/363 (101%)	356 (98%)	9 (2%)	0	100	100
1	B	366/363 (101%)	357 (98%)	9 (2%)	0	100	100
1	C	360/363 (99%)	347 (96%)	13 (4%)	0	100	100
1	D	356/363 (98%)	345 (97%)	11 (3%)	0	100	100
All	All	1447/1452 (100%)	1405 (97%)	42 (3%)	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%)	283 (98%)	7 (2%)	49	39
1	B	291/286 (102%)	286 (98%)	5 (2%)	60	54
1	C	285/286 (100%)	278 (98%)	7 (2%)	47	37
1	D	285/286 (100%)	272 (95%)	13 (5%)	27	15
All	All	1151/1144 (101%)	1119 (97%)	32 (3%)	44	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	73	GLU
1	A	101	ASP
1	A	135[A]	GLU
1	A	135[B]	GLU
1	A	239	ASP
1	A	280	ARG
1	B	0	HIS
1	B	153	ARG
1	B	236	LEU
1	B	239	ASP
1	B	290	MET
1	C	71	ARG
1	C	100	LYS
1	C	138	ARG
1	C	150	ASP
1	C	211	LYS
1	C	239	ASP
1	C	252	SER
1	D	1	MET
1	D	76	LYS
1	D	101	ASP
1	D	110	LYS
1	D	150	ASP

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Mol	Chain	Res	Type
1	D	153	ARG
1	D	171	GLU
1	D	211	LYS
1	D	237	LEU
1	D	239	ASP
1	D	248	THR
1	D	249	ASN
1	D	283	ASP

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

Mol	Chain	Res	Type
1	A	249	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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
5	PDO	B	404	-	4,4,4	0.39	0	3,3,3	0.47	0
7	BR8	B	401	-	9,9,9	2.72	4 (44%)	12,12,12	2.31	5 (41%)
8	PEG	D	404	-	6,6,6	0.53	0	5,5,5	0.59	0
5	PDO	C	406	-	4,4,4	0.37	0	3,3,3	0.33	0
7	BR8	D	401	-	9,9,9	2.81	4 (44%)	12,12,12	2.61	6 (50%)
5	PDO	A	405	-	4,4,4	0.41	0	3,3,3	0.36	0
5	PDO	C	405	-	4,4,4	0.52	0	3,3,3	0.58	0
5	PDO	B	403	-	4,4,4	0.39	0	3,3,3	0.37	0
5	PDO	C	404	-	4,4,4	0.39	0	3,3,3	0.40	0
7	BR8	C	401	-	9,9,9	2.57	4 (44%)	12,12,12	2.34	5 (41%)
5	PDO	A	404	-	4,4,4	0.39	0	3,3,3	0.44	0
5	PDO	C	403	-	4,4,4	0.36	0	3,3,3	0.35	0
2	MLI	A	401	-	6,6,6	1.17	1 (16%)	7,7,7	0.77	0
5	PDO	D	403	-	4,4,4	0.39	0	3,3,3	0.51	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
5	PDO	B	404	-	-	1/2/2/2	-
8	PEG	D	404	-	-	2/4/4/4	-
7	BR8	B	401	-	-	-	0/1/1/1
5	PDO	C	406	-	-	0/2/2/2	-
7	BR8	D	401	-	-	-	0/1/1/1
5	PDO	A	405	-	-	2/2/2/2	-
5	PDO	C	405	-	-	1/2/2/2	-
5	PDO	B	403	-	-	1/2/2/2	-
5	PDO	C	404	-	-	0/2/2/2	-
7	BR8	C	401	-	-	-	0/1/1/1
5	PDO	A	404	-	-	1/2/2/2	-
5	PDO	C	403	-	-	1/2/2/2	-
2	MLI	A	401	-	-	2/4/4/4	-
5	PDO	D	403	-	-	0/2/2/2	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	401	BR8	C2-N3	4.61	1.45	1.37
7	D	401	BR8	C2-N1	4.54	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	BR8	C4-N3	4.54	1.45	1.37
7	C	401	BR8	C2-N1	4.15	1.44	1.37
7	B	401	BR8	C2-N1	4.10	1.44	1.37
7	B	401	BR8	C2-N3	4.05	1.44	1.37
7	D	401	BR8	C4-N3	4.02	1.44	1.37
7	C	401	BR8	C2-N3	3.89	1.44	1.37
7	C	401	BR8	C4-N3	3.79	1.44	1.37
7	D	401	BR8	O8-C6	-2.42	1.18	1.23
7	B	401	BR8	O2-C2	-2.42	1.18	1.23
7	C	401	BR8	O4-C4	-2.26	1.18	1.23
2	A	401	MLI	C1-C2	-2.09	1.47	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	BR8	C4-N3-C2	-5.58	121.25	125.73
7	C	401	BR8	C4-N3-C2	-5.48	121.33	125.73
7	B	401	BR8	C4-N3-C2	-4.89	121.80	125.73
7	D	401	BR8	C5-C6-N1	3.94	120.57	116.82
7	D	401	BR8	C6-N1-C2	-3.79	122.68	125.73
7	B	401	BR8	C6-N1-C2	-3.26	123.10	125.73
7	C	401	BR8	C5-C4-N3	3.03	119.70	116.82
7	C	401	BR8	C5-C6-N1	3.02	119.69	116.82
7	B	401	BR8	O8-C6-C5	-2.83	118.24	122.85
7	D	401	BR8	C5-C4-N3	2.58	119.28	116.82
7	B	401	BR8	C5-C6-N1	2.57	119.27	116.82
7	D	401	BR8	O8-C6-C5	-2.52	118.75	122.85
7	C	401	BR8	C6-N1-C2	-2.26	123.91	125.73
7	D	401	BR8	N3-C2-N1	2.23	119.39	115.80
7	C	401	BR8	O8-C6-C5	-2.18	119.30	122.85
7	B	401	BR8	N3-C2-N1	2.11	119.19	115.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	PDO	O1-C1-C2-C3
5	B	403	PDO	O1-C1-C2-C3
5	B	404	PDO	O1-C1-C2-C3
5	C	405	PDO	O1-C1-C2-C3
8	D	404	PEG	O2-C3-C4-O4
2	A	401	MLI	C3-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
5	C	403	PDO	C1-C2-C3-O3
2	A	401	MLI	C3-C1-C2-O6
8	D	404	PEG	O1-C1-C2-O2
5	A	405	PDO	C1-C2-C3-O3
5	A	404	PDO	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	PDO	2	0
5	C	405	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%)	-0.11	3 (0%) 86 87	19, 27, 58, 116	0
1	B	363/363 (100%)	-0.18	1 (0%) 94 94	20, 30, 53, 92	0
1	C	362/363 (99%)	-0.11	4 (1%) 80 82	22, 37, 67, 128	0
1	D	360/363 (99%)	0.49	36 (10%) 7 7	25, 55, 98, 126	0
All	All	1447/1452 (99%)	0.02	44 (3%) 50 51	19, 34, 79, 128	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	ALA	9.0
1	D	175	ARG	6.3
1	A	107	ALA	5.5
1	C	107	ALA	4.7
1	D	150	ASP	4.2
1	D	102	VAL	4.2
1	A	106	ALA	4.1
1	A	108	PRO	4.0
1	D	108	PRO	3.8
1	D	123	LEU	3.4
1	D	173	ALA	3.2
1	D	105	PRO	3.2
1	D	143	ALA	3.1
1	C	108	PRO	3.1
1	D	140	VAL	3.0
1	D	176	ARG	2.9
1	D	170	ILE	2.9
1	D	241	ILE	2.8
1	D	122	PHE	2.8
1	D	101	ASP	2.8
1	D	174	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	367	VAL	2.7
1	D	103	ALA	2.7
1	D	75	VAL	2.7
1	D	236	LEU	2.7
1	D	100	LYS	2.5
1	D	116	VAL	2.5
1	D	178	LYS	2.5
1	D	139	ALA	2.5
1	D	234	VAL	2.5
1	D	155	VAL	2.4
1	D	164	LEU	2.4
1	D	153	ARG	2.3
1	D	97	PHE	2.3
1	D	145	LYS	2.3
1	D	68	GLY	2.2
1	D	168	GLU	2.2
1	D	109	GLY	2.1
1	D	183	ASN	2.1
1	C	175	ARG	2.1
1	D	149	ILE	2.1
1	D	207	ILE	2.1
1	B	153	ARG	2.0
1	D	138	ARG	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PDO	C	403	5/5	0.65	0.26	79,95,99,99	0
5	PDO	C	405	5/5	0.69	0.23	35,42,51,51	0
5	PDO	A	405	5/5	0.71	0.28	55,72,88,93	0
5	PDO	D	403	5/5	0.73	0.23	40,48,59,62	0
5	PDO	A	404	5/5	0.79	0.19	50,62,71,75	0
8	PEG	D	404	7/7	0.85	0.18	62,90,108,108	0
5	PDO	B	403	5/5	0.87	0.15	41,61,80,83	0
5	PDO	C	406	5/5	0.91	0.13	40,57,71,73	0
5	PDO	C	404	5/5	0.92	0.13	44,54,63,65	0
4	NA	A	403	1/1	0.93	0.24	30,30,30,30	0
5	PDO	B	404	5/5	0.93	0.17	35,46,66,75	0
3	CA	D	402	1/1	0.96	0.09	40,40,40,40	0
7	BR8	B	401	9/9	0.98	0.11	22,23,28,28	0
7	BR8	C	401	9/9	0.98	0.10	23,25,29,30	0
7	BR8	D	401	9/9	0.98	0.10	28,29,35,35	0
6	CL	B	405	1/1	0.98	0.07	62,62,62,62	0
3	CA	B	402	1/1	0.99	0.07	32,32,32,32	0
3	CA	C	402	1/1	0.99	0.13	30,30,30,30	0
2	MLI	A	401	7/7	0.99	0.10	23,24,29,29	0
6	CL	A	406	1/1	1.00	0.10	41,41,41,41	0
3	CA	A	402	1/1	1.00	0.25	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.