



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:33 am BST

PDB ID : 6OE8  
Title : The crystal structure of hyper-thermostable AgUricase mutant K12C/E286C  
Authors : Shi, Y.; Wang, T.; Zhou, X.E.; Liu, Q.; Jiang, Y.; Xu, H.E.  
Deposited on : 2019-03-27  
Resolution : 1.99 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 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 : 2.11  
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) : 2.11

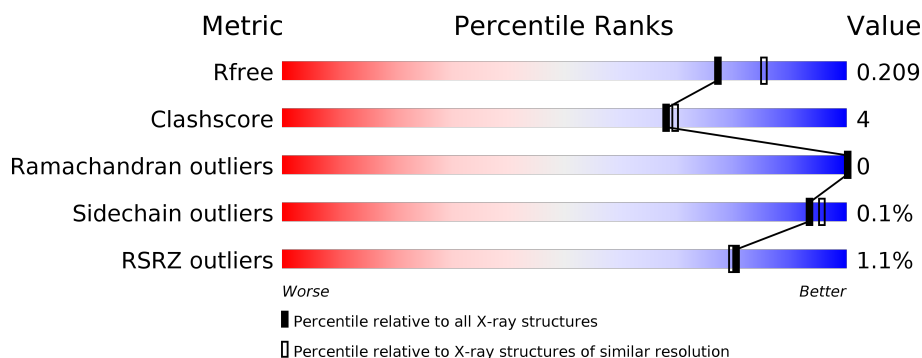
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 82%, green 82%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>8%</span> <span>10%</span> </div> </div>
1	B	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 80%, green 80%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>80%</span> <span>9%</span> <span>10%</span> </div> </div>
1	C	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 83%, green 83%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>7%</span> <span>10%</span> </div> </div>
1	D	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 81%, green 81%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>8%</span> <span>10%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10716 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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2322	1459	414	443	6			
1	B	292	Total	C	N	O	S	0	0	0
			2322	1459	414	443	6			
1	C	292	Total	C	N	O	S	0	0	0
			2322	1459	414	443	6			
1	D	292	Total	C	N	O	S	0	0	0
			2322	1459	414	443	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP D0VWQ1
A	-22	ALA	-	expression tag	UNP D0VWQ1
A	-21	SER	-	expression tag	UNP D0VWQ1
A	-20	MET	-	expression tag	UNP D0VWQ1
A	-19	THR	-	expression tag	UNP D0VWQ1
A	-18	GLY	-	expression tag	UNP D0VWQ1
A	-17	GLY	-	expression tag	UNP D0VWQ1
A	-16	GLN	-	expression tag	UNP D0VWQ1
A	-15	GLN	-	expression tag	UNP D0VWQ1
A	-14	MET	-	expression tag	UNP D0VWQ1
A	-13	GLY	-	expression tag	UNP D0VWQ1
A	-12	ARG	-	expression tag	UNP D0VWQ1
A	-11	GLY	-	expression tag	UNP D0VWQ1
A	-10	SER	-	expression tag	UNP D0VWQ1
A	-9	GLU	-	expression tag	UNP D0VWQ1
A	-8	PHE	-	expression tag	UNP D0VWQ1
A	-7	MET	-	expression tag	UNP D0VWQ1
A	-6	HIS	-	expression tag	UNP D0VWQ1
A	-5	HIS	-	expression tag	UNP D0VWQ1
A	-4	HIS	-	expression tag	UNP D0VWQ1
A	-3	HIS	-	expression tag	UNP D0VWQ1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	expression tag	UNP D0VWQ1
A	-1	HIS	-	expression tag	UNP D0VWQ1
A	0	HIS	-	expression tag	UNP D0VWQ1
A	1	HIS	-	expression tag	UNP D0VWQ1
A	12	CYS	LYS	engineered mutation	UNP D0VWQ1
A	286	CYS	GLU	engineered mutation	UNP D0VWQ1
B	-23	MET	-	initiating methionine	UNP D0VWQ1
B	-22	ALA	-	expression tag	UNP D0VWQ1
B	-21	SER	-	expression tag	UNP D0VWQ1
B	-20	MET	-	expression tag	UNP D0VWQ1
B	-19	THR	-	expression tag	UNP D0VWQ1
B	-18	GLY	-	expression tag	UNP D0VWQ1
B	-17	GLY	-	expression tag	UNP D0VWQ1
B	-16	GLN	-	expression tag	UNP D0VWQ1
B	-15	GLN	-	expression tag	UNP D0VWQ1
B	-14	MET	-	expression tag	UNP D0VWQ1
B	-13	GLY	-	expression tag	UNP D0VWQ1
B	-12	ARG	-	expression tag	UNP D0VWQ1
B	-11	GLY	-	expression tag	UNP D0VWQ1
B	-10	SER	-	expression tag	UNP D0VWQ1
B	-9	GLU	-	expression tag	UNP D0VWQ1
B	-8	PHE	-	expression tag	UNP D0VWQ1
B	-7	MET	-	expression tag	UNP D0VWQ1
B	-6	HIS	-	expression tag	UNP D0VWQ1
B	-5	HIS	-	expression tag	UNP D0VWQ1
B	-4	HIS	-	expression tag	UNP D0VWQ1
B	-3	HIS	-	expression tag	UNP D0VWQ1
B	-2	HIS	-	expression tag	UNP D0VWQ1
B	-1	HIS	-	expression tag	UNP D0VWQ1
B	0	HIS	-	expression tag	UNP D0VWQ1
B	1	HIS	-	expression tag	UNP D0VWQ1
B	12	CYS	LYS	engineered mutation	UNP D0VWQ1
B	286	CYS	GLU	engineered mutation	UNP D0VWQ1
C	-23	MET	-	initiating methionine	UNP D0VWQ1
C	-22	ALA	-	expression tag	UNP D0VWQ1
C	-21	SER	-	expression tag	UNP D0VWQ1
C	-20	MET	-	expression tag	UNP D0VWQ1
C	-19	THR	-	expression tag	UNP D0VWQ1
C	-18	GLY	-	expression tag	UNP D0VWQ1
C	-17	GLY	-	expression tag	UNP D0VWQ1
C	-16	GLN	-	expression tag	UNP D0VWQ1
C	-15	GLN	-	expression tag	UNP D0VWQ1

*Continued on next page...*

*Continued from previous page...*

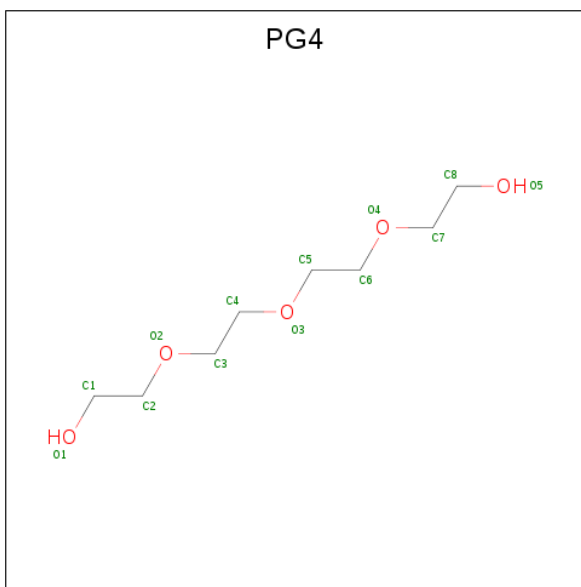
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	MET	-	expression tag	UNP D0VWQ1
C	-13	GLY	-	expression tag	UNP D0VWQ1
C	-12	ARG	-	expression tag	UNP D0VWQ1
C	-11	GLY	-	expression tag	UNP D0VWQ1
C	-10	SER	-	expression tag	UNP D0VWQ1
C	-9	GLU	-	expression tag	UNP D0VWQ1
C	-8	PHE	-	expression tag	UNP D0VWQ1
C	-7	MET	-	expression tag	UNP D0VWQ1
C	-6	HIS	-	expression tag	UNP D0VWQ1
C	-5	HIS	-	expression tag	UNP D0VWQ1
C	-4	HIS	-	expression tag	UNP D0VWQ1
C	-3	HIS	-	expression tag	UNP D0VWQ1
C	-2	HIS	-	expression tag	UNP D0VWQ1
C	-1	HIS	-	expression tag	UNP D0VWQ1
C	0	HIS	-	expression tag	UNP D0VWQ1
C	1	HIS	-	expression tag	UNP D0VWQ1
C	12	CYS	LYS	engineered mutation	UNP D0VWQ1
C	286	CYS	GLU	engineered mutation	UNP D0VWQ1
D	-23	MET	-	initiating methionine	UNP D0VWQ1
D	-22	ALA	-	expression tag	UNP D0VWQ1
D	-21	SER	-	expression tag	UNP D0VWQ1
D	-20	MET	-	expression tag	UNP D0VWQ1
D	-19	THR	-	expression tag	UNP D0VWQ1
D	-18	GLY	-	expression tag	UNP D0VWQ1
D	-17	GLY	-	expression tag	UNP D0VWQ1
D	-16	GLN	-	expression tag	UNP D0VWQ1
D	-15	GLN	-	expression tag	UNP D0VWQ1
D	-14	MET	-	expression tag	UNP D0VWQ1
D	-13	GLY	-	expression tag	UNP D0VWQ1
D	-12	ARG	-	expression tag	UNP D0VWQ1
D	-11	GLY	-	expression tag	UNP D0VWQ1
D	-10	SER	-	expression tag	UNP D0VWQ1
D	-9	GLU	-	expression tag	UNP D0VWQ1
D	-8	PHE	-	expression tag	UNP D0VWQ1
D	-7	MET	-	expression tag	UNP D0VWQ1
D	-6	HIS	-	expression tag	UNP D0VWQ1
D	-5	HIS	-	expression tag	UNP D0VWQ1
D	-4	HIS	-	expression tag	UNP D0VWQ1
D	-3	HIS	-	expression tag	UNP D0VWQ1
D	-2	HIS	-	expression tag	UNP D0VWQ1
D	-1	HIS	-	expression tag	UNP D0VWQ1
D	0	HIS	-	expression tag	UNP D0VWQ1

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	HIS	-	expression tag	UNP D0VWQ1
D	12	CYS	LYS	engineered mutation	UNP D0VWQ1
D	286	CYS	GLU	engineered mutation	UNP D0VWQ1

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



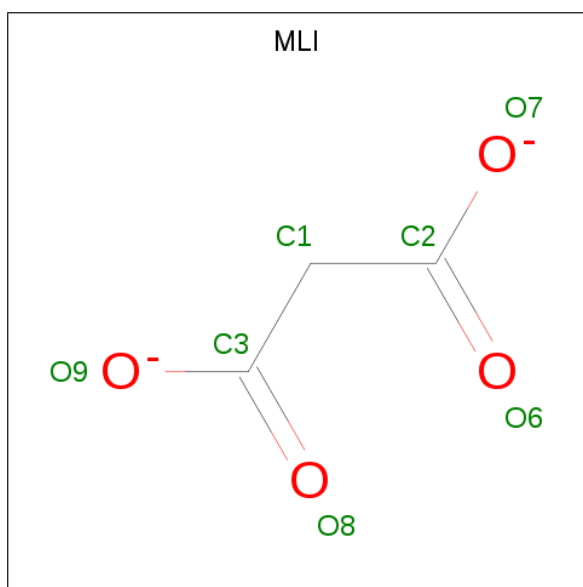
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0

- Molecule 5 is water.

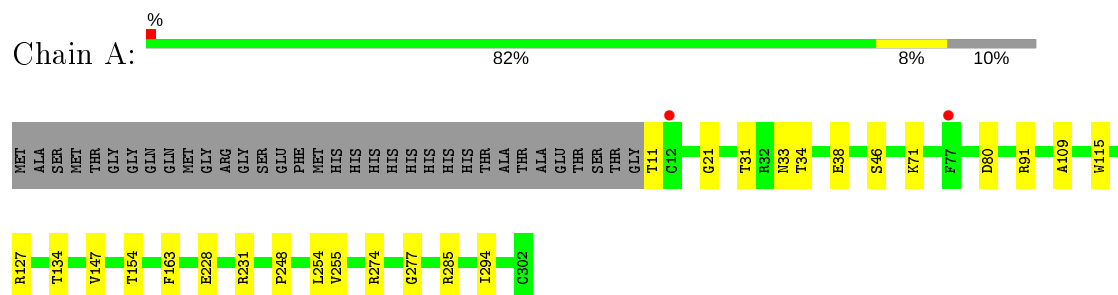
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	323	Total O 323 323	0	0
5	B	275	Total O 275 275	0	0
5	C	327	Total O 327 327	0	0
5	D	302	Total O 302 302	0	0



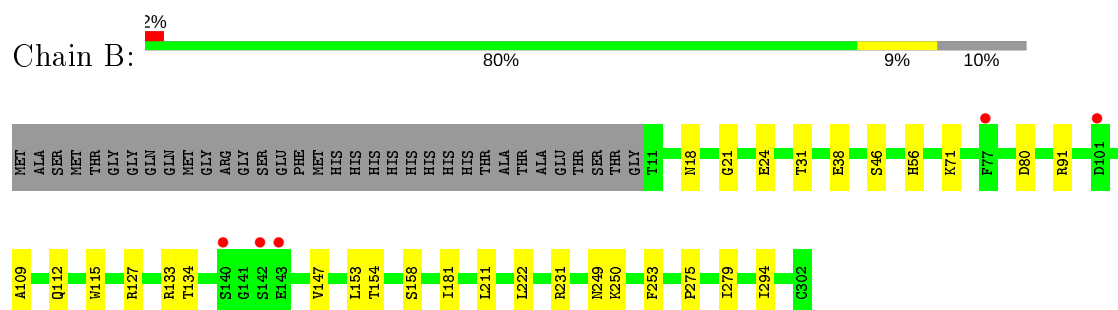
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

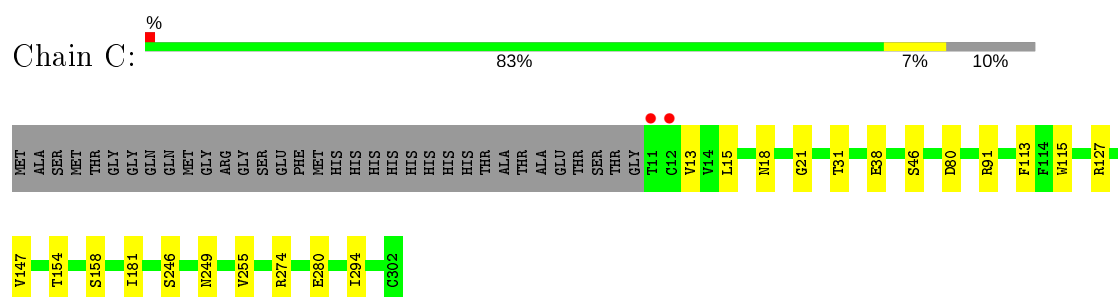
- Molecule 1: Uricase



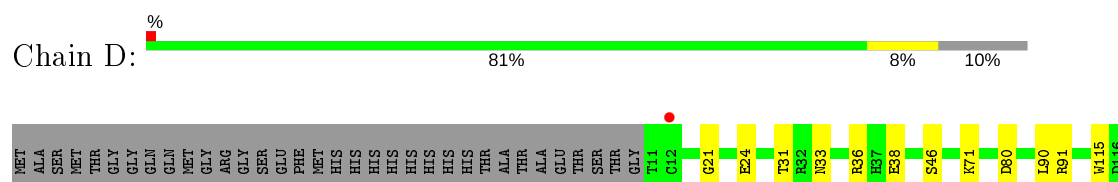
- Molecule 1: Uricase



- Molecule 1: Uricase



- Molecule 1: Uricase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.93 Å   149.10 Å   84.96 Å 90.00°   118.57°   90.00°	Depositor
Resolution (Å)	37.28 – 1.99 48.19 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.28-1.99) 97.6 (48.19-1.99)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.60 (at 1.98 Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.180   ,   0.206 0.185   ,   0.209	Depositor DCC
$R_{free}$ test set	2000 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: PG4, MLI, PGE

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	0.34	0/2375	0.57	0/3222
1	B	0.33	0/2375	0.56	0/3222
1	C	0.34	0/2375	0.58	0/3222
1	D	0.34	0/2375	0.59	0/3222
All	All	0.34	0/9500	0.57	0/12888

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	2322	0	2221	20	0
1	B	2322	0	2221	25	0
1	C	2322	0	2221	15	0
1	D	2322	0	2221	18	0
2	A	26	0	36	2	0
2	B	13	0	18	1	0
2	C	13	0	18	0	0
2	D	13	0	18	1	0
3	A	20	0	28	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	28	7	0
3	C	30	0	42	5	0
3	D	10	0	14	0	0
4	A	7	0	2	0	0
4	B	7	0	2	1	0
4	C	21	0	6	2	0
4	D	21	0	6	1	0
5	A	323	0	0	1	0
5	B	275	0	0	2	0
5	C	327	0	0	0	0
5	D	302	0	0	1	0
All	All	10716	0	9102	71	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 4.

All (71) 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:71:LYS:HD2	3:A:402:PGE:H22	1.52	0.91
1:B:250:LYS:HE3	2:B:401:PG4:H51	1.63	0.81
1:C:255:VAL:HG13	3:C:407:PGE:H42	1.66	0.77
1:B:71:LYS:NZ	3:B:402:PGE:H52	2.08	0.69
1:A:109:ALA:HB1	3:A:403:PGE:H52	1.73	0.69
1:B:109:ALA:HB1	3:B:403:PGE:H52	1.80	0.63
1:B:134:THR:HB	3:B:403:PGE:H62	1.85	0.59
1:A:254:LEU:CD2	2:A:404:PG4:H22	2.32	0.59
1:A:285:ARG:HD2	5:A:668:HOH:O	2.02	0.58
1:A:255:VAL:HG13	3:B:402:PGE:H62	1.86	0.56
1:D:80:ASP:HB2	1:D:91:ARG:HH12	1.69	0.56
1:C:113:PHE:CZ	4:C:401:MLI:H11	2.42	0.55
1:B:71:LYS:HZ3	3:B:402:PGE:H52	1.72	0.54
1:B:80:ASP:HB2	1:B:91:ARG:HH12	1.72	0.54
1:A:134:THR:HB	3:A:403:PGE:H62	1.90	0.54
1:C:80:ASP:HB2	1:C:91:ARG:HH12	1.73	0.53
3:C:407:PGE:H32	1:D:71:LYS:NZ	2.23	0.53
1:B:71:LYS:NZ	5:B:504:HOH:O	2.39	0.52
1:B:249:ASN:ND2	4:C:402:MLI:O6	2.42	0.52
1:B:71:LYS:HZ2	3:B:402:PGE:H52	1.75	0.51
1:B:18:ASN:HD22	1:B:56:HIS:CE1	2.30	0.50
1:B:31:THR:HB	1:B:38:GLU:HB2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLU:HG2	1:D:178:THR:O	2.13	0.49
1:A:31:THR:HB	1:A:38:GLU:HB2	1.95	0.48
1:B:275:PRO:HG2	3:C:404:PGE:H1	1.95	0.48
1:D:244:LYS:NZ	1:D:282:THR:OG1	2.43	0.47
1:B:71:LYS:HD2	3:B:402:PGE:H42	1.97	0.47
1:B:158:SER:HA	1:B:181:ILE:HG12	1.97	0.47
1:C:31:THR:HB	1:C:38:GLU:HB2	1.96	0.46
1:D:224:GLN:HG3	5:D:621:HOH:O	2.15	0.46
3:A:402:PGE:H5	5:B:663:HOH:O	2.16	0.46
1:A:80:ASP:HB2	1:A:91:ARG:HH12	1.81	0.45
1:B:24:GLU:HB3	1:C:274:ARG:HD2	1.99	0.45
1:A:127:ARG:HB2	1:B:154:THR:HB	1.99	0.45
1:D:147:VAL:HG23	1:D:294:ILE:HD13	1.98	0.44
1:A:274:ARG:HD2	1:D:24:GLU:HB3	1.99	0.44
1:A:147:VAL:HG23	1:A:294:ILE:HD13	2.00	0.44
1:A:254:LEU:HD23	2:A:404:PG4:H22	2.00	0.44
1:C:154:THR:HB	1:D:127:ARG:HB2	2.00	0.44
1:D:115:TRP:CH2	1:D:127:ARG:HG2	2.52	0.43
1:C:21:GLY:HA3	1:C:46:SER:O	2.17	0.43
1:A:154:THR:HB	1:B:127:ARG:HB2	2.00	0.43
1:C:15:LEU:HD11	1:C:18:ASN:ND2	2.33	0.43
1:C:158:SER:HA	1:C:181:ILE:HG12	2.00	0.43
1:B:115:TRP:CH2	1:B:127:ARG:HG2	2.53	0.43
1:B:153:LEU:HD21	1:B:211:LEU:HD21	2.00	0.43
1:C:127:ARG:HB2	1:D:154:THR:HB	2.01	0.43
1:A:163:PHE:CE2	4:D:402:MLI:H11	2.53	0.43
1:D:21:GLY:HA3	1:D:46:SER:O	2.19	0.42
1:C:246:SER:HA	1:C:280:GLU:HG2	2.00	0.42
4:B:404:MLI:O6	1:C:249:ASN:ND2	2.52	0.42
1:B:231:ARG:HG3	1:C:13:VAL:HG21	2.02	0.42
3:C:407:PGE:H32	1:D:71:LYS:HZ3	1.84	0.42
1:D:36:ARG:NH2	1:D:117:ARG:NE	2.67	0.42
1:D:31:THR:HB	1:D:38:GLU:HB2	2.00	0.42
1:C:147:VAL:HG23	1:C:294:ILE:HD13	2.01	0.42
1:A:11:THR:HB	1:D:235:GLU:HG2	2.02	0.42
1:A:115:TRP:CH2	1:A:127:ARG:HG2	2.55	0.42
1:B:147:VAL:HG23	1:B:294:ILE:HD13	2.01	0.42
1:A:248:PRO:HA	1:A:277:GLY:O	2.20	0.41
1:D:90:LEU:HD21	1:D:146:ILE:HD11	2.02	0.41
1:B:112:GLN:HB3	1:B:133:ARG:HB3	2.02	0.41
1:A:228:GLU:OE1	1:A:231:ARG:NH2	2.42	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:GLY:HA3	1:D:283:ILE:HG13	2.02	0.41
1:B:21:GLY:HA3	1:B:46:SER:O	2.21	0.41
1:A:33:ASN:OD1	1:A:34:THR:N	2.54	0.41
1:C:115:TRP:CH2	1:C:127:ARG:HG2	2.56	0.41
1:D:273:ASP:O	2:D:403:PG4:H51	2.20	0.40
1:B:222:LEU:HD23	1:B:279:ILE:HG13	2.02	0.40
1:A:21:GLY:HA3	1:A:46:SER:O	2.22	0.40
1:B:253:PHE:CZ	3:C:404:PGE:H22	2.56	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	290/326 (89%)	289 (100%)	1 (0%)	0	100	100
1	B	290/326 (89%)	289 (100%)	1 (0%)	0	100	100
1	C	290/326 (89%)	289 (100%)	1 (0%)	0	100	100
1	D	290/326 (89%)	290 (100%)	0	0	100	100
All	All	1160/1304 (89%)	1157 (100%)	3 (0%)	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	243/269 (90%)	243 (100%)	0	100	100
1	B	243/269 (90%)	243 (100%)	0	100	100
1	C	243/269 (90%)	243 (100%)	0	100	100
1	D	243/269 (90%)	242 (100%)	1 (0%)	91	93
All	All	972/1076 (90%)	971 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 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
4	MLI	C	406	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PGE	B	402	-	9,9,9	0.43	0	8,8,8	0.48	0
4	MLI	C	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PGE	C	405	-	9,9,9	0.49	0	8,8,8	0.42	0
2	PG4	D	403	-	12,12,12	0.48	0	11,11,11	0.37	0
4	MLI	D	401	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	404	-	0,6,6	0.00	-	0,7,7	0.00	-
2	PG4	A	401	-	12,12,12	0.51	0	11,11,11	0.27	0
3	PGE	D	404	-	9,9,9	0.47	0	8,8,8	0.50	0
4	MLI	D	405	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PGE	C	407	-	9,9,9	0.40	0	8,8,8	0.43	0
4	MLI	C	401	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PGE	B	403	-	9,9,9	0.46	0	8,8,8	0.31	0
2	PG4	A	404	-	12,12,12	0.48	0	11,11,11	0.46	0
3	PGE	C	404	-	9,9,9	0.47	0	8,8,8	0.25	0
4	MLI	A	405	-	0,6,6	0.00	-	0,7,7	0.00	-
3	PGE	A	403	-	9,9,9	0.46	0	8,8,8	0.33	0
2	PG4	C	403	-	12,12,12	0.50	0	11,11,11	0.27	0
2	PG4	B	401	-	12,12,12	0.46	0	11,11,11	0.39	0
3	PGE	A	402	-	9,9,9	0.44	0	8,8,8	0.45	0
4	MLI	D	402	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLI	C	406	-	-	0/0/4/4	-
3	PGE	B	402	-	-	6/7/7/7	-
4	MLI	C	402	-	-	0/0/4/4	-
3	PGE	C	405	-	-	1/7/7/7	-
2	PG4	D	403	-	-	0/10/10/10	-
4	MLI	D	401	-	-	0/0/4/4	-
4	MLI	B	404	-	-	0/0/4/4	-
2	PG4	A	401	-	-	0/10/10/10	-
3	PGE	D	404	-	-	4/7/7/7	-
4	MLI	D	405	-	-	0/0/4/4	-
3	PGE	C	407	-	-	6/7/7/7	-
4	MLI	C	401	-	-	0/0/4/4	-
3	PGE	B	403	-	-	2/7/7/7	-
2	PG4	A	404	-	-	3/10/10/10	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	C	404	-	-	5/7/7/7	-
4	MLI	A	405	-	-	0/0/4/4	-
3	PGE	A	403	-	-	1/7/7/7	-
2	PG4	C	403	-	-	0/10/10/10	-
2	PG4	B	401	-	-	3/10/10/10	-
3	PGE	A	402	-	-	3/7/7/7	-
4	MLI	D	402	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PGE	O2-C3-C4-O3
3	B	402	PGE	O2-C3-C4-O3
3	C	407	PGE	O3-C5-C6-O4
3	C	407	PGE	O2-C3-C4-O3
3	C	405	PGE	O1-C1-C2-O2
2	A	404	PG4	O1-C1-C2-O2
3	C	404	PGE	O2-C3-C4-O3
3	B	402	PGE	C4-C3-O2-C2
3	C	407	PGE	C1-C2-O2-C3
3	B	402	PGE	C3-C4-O3-C5
3	A	402	PGE	C1-C2-O2-C3
3	B	402	PGE	C6-C5-O3-C4
2	A	404	PG4	C6-C5-O3-C4
3	C	404	PGE	C4-C3-O2-C2
2	B	401	PG4	C5-C6-O4-C7
3	B	402	PGE	O3-C5-C6-O4
2	B	401	PG4	O4-C7-C8-O5
3	B	403	PGE	C4-C3-O2-C2
2	A	404	PG4	C1-C2-O2-C3
3	D	404	PGE	C4-C3-O2-C2
3	D	404	PGE	O1-C1-C2-O2
3	B	403	PGE	O2-C3-C4-O3
3	A	403	PGE	O2-C3-C4-O3
3	C	404	PGE	C3-C4-O3-C5
3	C	407	PGE	O1-C1-C2-O2
3	C	407	PGE	C3-C4-O3-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	404	PGE	C1-C2-O2-C3
3	B	402	PGE	O1-C1-C2-O2
2	B	401	PG4	C4-C3-O2-C2
3	D	404	PGE	C3-C4-O3-C5
3	A	402	PGE	C4-C3-O2-C2
3	D	404	PGE	O2-C3-C4-O3
3	C	404	PGE	O1-C1-C2-O2
3	C	407	PGE	C6-C5-O3-C4

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	PGE	5	0
4	C	402	MLI	1	0
2	D	403	PG4	1	0
4	B	404	MLI	1	0
3	C	407	PGE	3	0
4	C	401	MLI	1	0
3	B	403	PGE	2	0
2	A	404	PG4	2	0
3	C	404	PGE	2	0
3	A	403	PGE	2	0
2	B	401	PG4	1	0
3	A	402	PGE	2	0
4	D	402	MLI	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	292/326 (89%)	-0.09	2 (0%) 87 87	14, 20, 30, 41	0
1	B	292/326 (89%)	0.05	5 (1%) 70 68	13, 23, 34, 48	0
1	C	292/326 (89%)	-0.04	2 (0%) 87 87	13, 20, 29, 45	0
1	D	292/326 (89%)	-0.07	4 (1%) 75 74	12, 19, 30, 42	0
All	All	1168/1304 (89%)	-0.04	13 (1%) 80 79	12, 20, 31, 48	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	291	ASP	3.1
1	B	101	ASP	3.0
1	D	12	CYS	2.9
1	B	142	SER	2.8
1	D	287	GLY	2.6
1	C	11	THR	2.4
1	C	12	CYS	2.2
1	B	140	SER	2.2
1	B	77	PHE	2.2
1	A	77	PHE	2.1
1	A	12	CYS	2.1
1	D	261	GLY	2.1
1	B	143	GLU	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 carbohydrates 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
3	PGE	C	407	10/10	0.73	0.24	28,32,36,38	0
3	PGE	C	404	10/10	0.78	0.22	29,34,38,40	0
3	PGE	B	402	10/10	0.83	0.19	29,32,37,37	0
3	PGE	A	403	10/10	0.84	0.15	20,24,29,30	0
3	PGE	A	402	10/10	0.84	0.17	31,33,39,39	0
2	PG4	A	404	13/13	0.85	0.15	28,35,42,46	0
2	PG4	B	401	13/13	0.85	0.20	26,32,41,45	0
4	MLI	A	405	7/7	0.85	0.18	25,27,33,36	0
4	MLI	B	404	7/7	0.86	0.15	21,23,31,32	0
4	MLI	D	402	7/7	0.88	0.15	20,23,32,33	0
3	PGE	D	404	10/10	0.90	0.10	21,25,31,36	0
4	MLI	C	401	7/7	0.90	0.15	25,26,32,40	0
3	PGE	B	403	10/10	0.91	0.13	21,25,30,34	0
2	PG4	D	403	13/13	0.91	0.18	21,28,32,41	0
4	MLI	D	401	7/7	0.91	0.14	25,27,31,34	0
4	MLI	C	402	7/7	0.91	0.20	27,28,33,34	0
3	PGE	C	405	10/10	0.92	0.12	19,25,30,33	0
4	MLI	D	405	7/7	0.93	0.12	24,26,32,33	0
2	PG4	A	401	13/13	0.94	0.14	22,26,38,40	0
4	MLI	C	406	7/7	0.94	0.11	25,28,35,35	0
2	PG4	C	403	13/13	0.95	0.12	22,24,35,42	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.