Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2025 – 02:51 AM EDT

PDB ID	:	6OE8 / pdb_00006oe8
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

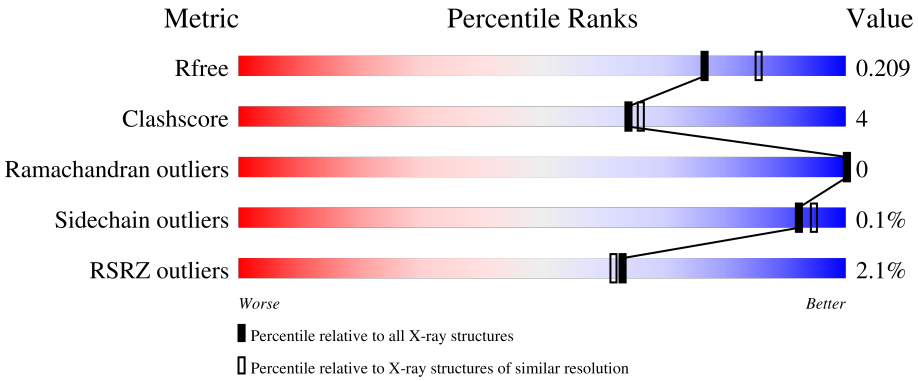
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 82% 8% 10%
1	B	326	2% 80% 9% 10%
1	C	326	2% 83% 7% 10%
1	D	326	2% 81% 8% 10%

2 Entry composition (i)

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

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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

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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

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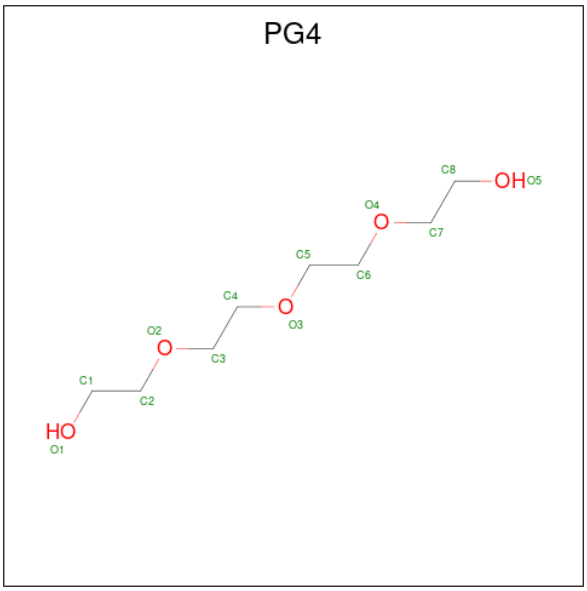
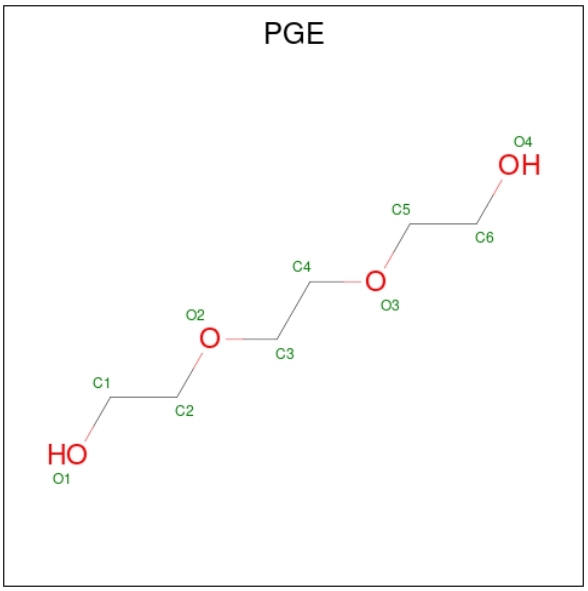
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	HIS	-	expression tag	UNP D0VWQ1
D	12	CYS	LYS	engineered mutation	UNP D0VWQ1
D	286	CYS	GLU	engineered mutation	UNP D0VWQ1

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



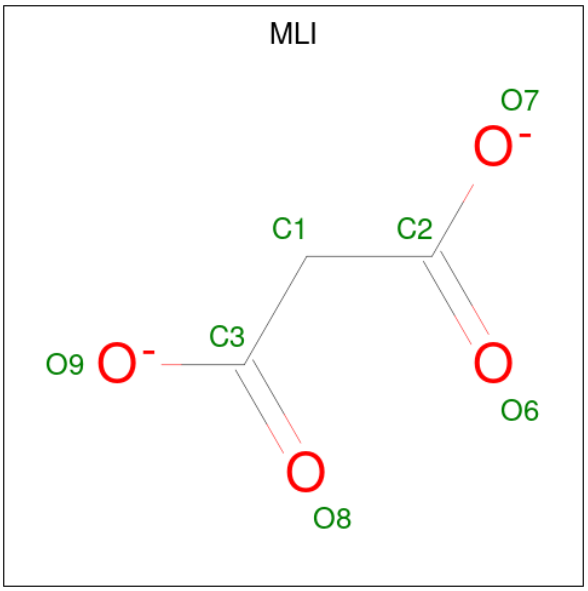
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	A	1	Total C O 13 8 5	0	0
2	B	1	Total C O 13 8 5	0	0
2	C	1	Total C O 13 8 5	0	0
2	D	1	Total C O 13 8 5	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 4 is MALONATE ION (CCD ID: 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.

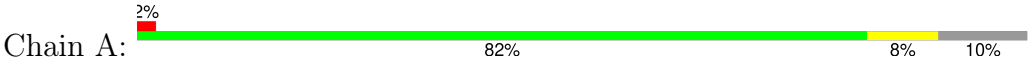
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	323	Total O 323 323	0	0
5	B	275	Total O 275 275	0	0
5	C	327	Total O 327 327	0	0
5	D	302	Total O 302 302	0	0

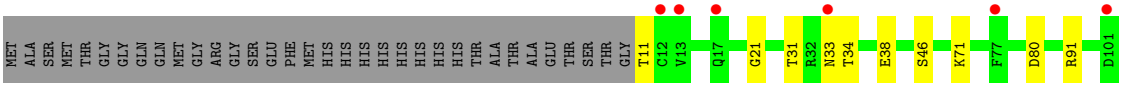
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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: Uricase

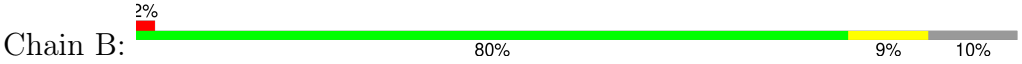
Chain A:

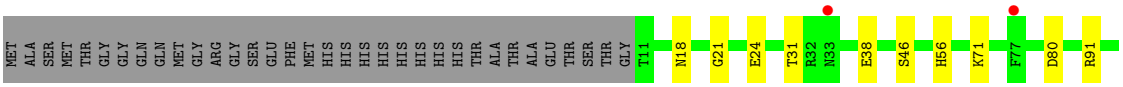


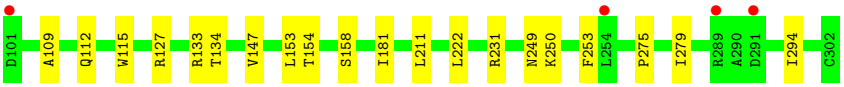


• Molecule 1: Uricase

Chain B:

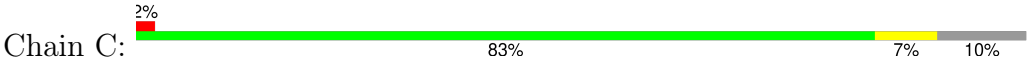


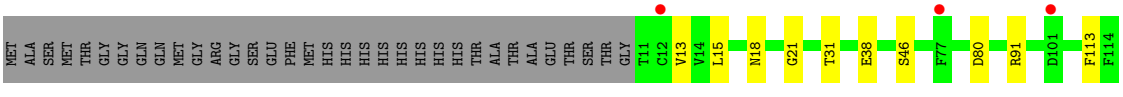




• Molecule 1: Uricase

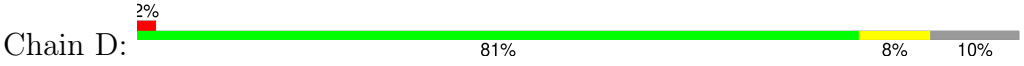
Chain C:

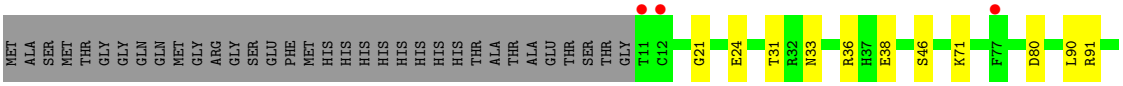


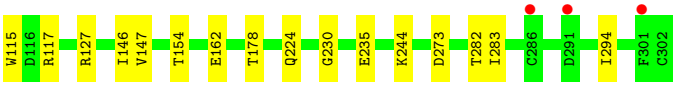


• Molecule 1: Uricase

Chain D:






W115
D116
R117
R127
I146
V147
T154
E162
T178
Q224
G230
E235
K244
D273
T282
I283
C286
D291
I294
F301
C302

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.93Å 149.10Å 84.96Å 90.00° 118.57° 90.00°	Depositor
Resolution (Å)	37.28 – 1.99 37.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.28-1.99) 97.6 (37.28-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.60 (at 1.98Å)	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	95578 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PG4, MLI

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

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

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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

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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:31:THR:HB	1:D:38:GLU:HB2	2.00	0.42
1:D:36:ARG:NH2	1:D:117:ARG:NE	2.67	0.42
1:A:11:THR:HB	1:D:235:GLU:HG2	2.02	0.42
1:C:147:VAL:HG23	1:C:294:ILE:HD13	2.01	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

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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%)	89 92
All	All	972/1076 (90%)	971 (100%)	1 (0%)	92 95

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

Mol	Chain	Res	Type
1	D	33	ASN

Sometimes 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 oligosaccharides 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	$\#\|Z\|>2$
2	PG4	A	401	-	12,12,12	0.52	0	11,11,11	0.27	0
4	MLI	A	405	-	6,6,6	1.35	0	7,7,7	1.17	0
4	MLI	D	402	-	6,6,6	1.15	0	7,7,7	1.14	0
2	PG4	D	403	-	12,12,12	0.49	0	11,11,11	0.37	0
3	PGE	C	407	-	9,9,9	0.41	0	8,8,8	0.43	0
4	MLI	C	401	-	6,6,6	1.35	0	7,7,7	1.13	0
3	PGE	C	405	-	9,9,9	0.50	0	8,8,8	0.41	0
4	MLI	C	406	-	6,6,6	1.30	0	7,7,7	1.16	0
2	PG4	B	401	-	12,12,12	0.47	0	11,11,11	0.38	0
4	MLI	B	404	-	6,6,6	1.20	0	7,7,7	1.13	0
3	PGE	C	404	-	9,9,9	0.48	0	8,8,8	0.24	0
3	PGE	A	402	-	9,9,9	0.45	0	8,8,8	0.44	0
4	MLI	D	401	-	6,6,6	1.43	0	7,7,7	1.35	1 (14%)
3	PGE	B	403	-	9,9,9	0.47	0	8,8,8	0.30	0
3	PGE	D	404	-	9,9,9	0.48	0	8,8,8	0.50	0
3	PGE	A	403	-	9,9,9	0.48	0	8,8,8	0.33	0
4	MLI	C	402	-	6,6,6	1.38	0	7,7,7	0.95	0
2	PG4	C	403	-	12,12,12	0.51	0	11,11,11	0.27	0
3	PGE	B	402	-	9,9,9	0.44	0	8,8,8	0.48	0
2	PG4	A	404	-	12,12,12	0.49	0	11,11,11	0.46	0
4	MLI	D	405	-	6,6,6	1.32	0	7,7,7	1.19	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
2	PG4	A	401	-	-	0/10/10/10	-
4	MLI	A	405	-	-	4/4/4/4	-
4	MLI	D	402	-	-	2/4/4/4	-
2	PG4	D	403	-	-	0/10/10/10	-
3	PGE	C	407	-	-	6/7/7/7	-
4	MLI	C	401	-	-	2/4/4/4	-
3	PGE	C	405	-	-	1/7/7/7	-
4	MLI	C	406	-	-	2/4/4/4	-
2	PG4	B	401	-	-	3/10/10/10	-
4	MLI	B	404	-	-	0/4/4/4	-
3	PGE	C	404	-	-	5/7/7/7	-
3	PGE	A	402	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	D	401	-	-	2/4/4/4	-
3	PGE	B	403	-	-	2/7/7/7	-
3	PGE	D	404	-	-	4/7/7/7	-
3	PGE	A	403	-	-	1/7/7/7	-
4	MLI	C	402	-	-	4/4/4/4	-
2	PG4	C	403	-	-	0/10/10/10	-
3	PGE	B	402	-	-	6/7/7/7	-
2	PG4	A	404	-	-	3/10/10/10	-
4	MLI	D	405	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	MLI	O9-C3-C1	2.11	121.05	114.51

There are no chirality outliers.

All (52) 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
4	A	405	MLI	C2-C1-C3-O9
2	A	404	PG4	O1-C1-C2-O2
3	C	405	PGE	O1-C1-C2-O2
3	C	407	PGE	O2-C3-C4-O3
3	C	404	PGE	O2-C3-C4-O3
4	A	405	MLI	C3-C1-C2-O7
4	D	405	MLI	C2-C1-C3-O8
4	C	402	MLI	C2-C1-C3-O9
4	D	405	MLI	C2-C1-C3-O9
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	B	402	PGE	C6-C5-O3-C4
3	A	402	PGE	C1-C2-O2-C3
2	B	401	PG4	O4-C7-C8-O5
3	B	402	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	C	404	PGE	C4-C3-O2-C2
2	A	404	PG4	C6-C5-O3-C4
2	B	401	PG4	C5-C6-O4-C7
4	A	405	MLI	C3-C1-C2-O6
4	C	402	MLI	C2-C1-C3-O8
4	A	405	MLI	C2-C1-C3-O8
3	D	404	PGE	C4-C3-O2-C2
4	C	406	MLI	C2-C1-C3-O9
4	D	401	MLI	C3-C1-C2-O7
3	B	403	PGE	C4-C3-O2-C2
2	A	404	PG4	C1-C2-O2-C3
3	D	404	PGE	O1-C1-C2-O2
4	D	402	MLI	C3-C1-C2-O6
3	B	403	PGE	O2-C3-C4-O3
4	C	402	MLI	C3-C1-C2-O6
4	D	401	MLI	C3-C1-C2-O6
3	A	403	PGE	O2-C3-C4-O3
4	C	406	MLI	C2-C1-C3-O8
3	C	407	PGE	O1-C1-C2-O2
3	C	404	PGE	C3-C4-O3-C5
4	C	401	MLI	C3-C1-C2-O6
4	C	402	MLI	C3-C1-C2-O7
4	D	402	MLI	C3-C1-C2-O7
3	C	407	PGE	C3-C4-O3-C5
4	C	401	MLI	C3-C1-C2-O7
3	C	404	PGE	C1-C2-O2-C3
3	B	402	PGE	O1-C1-C2-O2
3	C	404	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	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
4	D	402	MLI	1	0
2	D	403	PG4	1	0
3	C	407	PGE	3	0
4	C	401	MLI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PG4	1	0
4	B	404	MLI	1	0
3	C	404	PGE	2	0
3	A	402	PGE	2	0
3	B	403	PGE	2	0
3	A	403	PGE	2	0
4	C	402	MLI	1	0
3	B	402	PGE	5	0
2	A	404	PG4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	292/326 (89%)	0.12	7 (2%)	59	58	14, 20, 30, 41	0
1	B	292/326 (89%)	0.25	6 (2%)	63	62	13, 23, 34, 48	0
1	C	292/326 (89%)	0.09	5 (1%)	69	67	13, 20, 29, 45	0
1	D	292/326 (89%)	0.09	6 (2%)	63	62	12, 19, 30, 42	0
All	All	1168/1304 (89%)	0.14	24 (2%)	63	62	12, 20, 31, 48	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	291	ASP	3.6
1	B	77	PHE	3.4
1	A	33	ASN	3.3
1	A	77	PHE	2.8
1	C	77	PHE	2.8
1	A	291	ASP	2.6
1	C	121	HIS	2.4
1	A	13	VAL	2.4
1	D	12	CYS	2.4
1	B	101	ASP	2.4
1	C	101	ASP	2.4
1	B	291	ASP	2.3
1	B	254	LEU	2.3
1	A	12	CYS	2.3
1	C	12	CYS	2.3
1	D	286	CYS	2.2
1	B	33	ASN	2.2
1	D	77	PHE	2.2
1	A	101	ASP	2.1
1	C	291	ASP	2.1
1	B	289	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	301	PHE	2.1
1	D	11	THR	2.1
1	A	17	GLN	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^{th} 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^2)	Q<0.9
3	PGE	C	404	10/10	0.73	0.16	29,34,38,40	0
3	PGE	C	407	10/10	0.73	0.18	28,32,36,38	0
4	MLI	A	405	7/7	0.81	0.15	25,27,33,36	0
2	PG4	A	404	13/13	0.82	0.14	28,35,42,46	0
3	PGE	B	402	10/10	0.83	0.15	29,32,37,37	0
3	PGE	A	403	10/10	0.84	0.11	20,24,29,30	0
4	MLI	D	402	7/7	0.84	0.14	20,23,32,33	0
2	PG4	B	401	13/13	0.85	0.11	26,32,41,45	0
4	MLI	B	404	7/7	0.85	0.15	21,23,31,32	0
4	MLI	D	401	7/7	0.85	0.18	25,27,31,34	0
3	PGE	A	402	10/10	0.85	0.13	31,33,39,39	0
4	MLI	C	401	7/7	0.86	0.15	25,26,32,40	0
3	PGE	C	405	10/10	0.88	0.10	19,25,30,33	0
4	MLI	C	402	7/7	0.89	0.17	27,28,33,34	0
3	PGE	D	404	10/10	0.89	0.10	21,25,31,36	0
3	PGE	B	403	10/10	0.89	0.10	21,25,30,34	0
2	PG4	A	401	13/13	0.90	0.09	22,26,38,40	0
2	PG4	D	403	13/13	0.90	0.09	21,28,32,41	0
4	MLI	D	405	7/7	0.90	0.12	24,26,32,33	0
4	MLI	C	406	7/7	0.91	0.09	25,28,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PG4	C	403	13/13	0.93	0.07	22,24,35,42	0

6.5 Other polymers (i)

There are no such residues in this entry.