



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 05:45 am GMT

PDB ID : 5M2T  
Title : X-ray structure of uridine phosphorylase from *Vibrio cholerae* in complex with uridine at 1.03 Å resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2016-10-13  
Resolution : 1.03 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

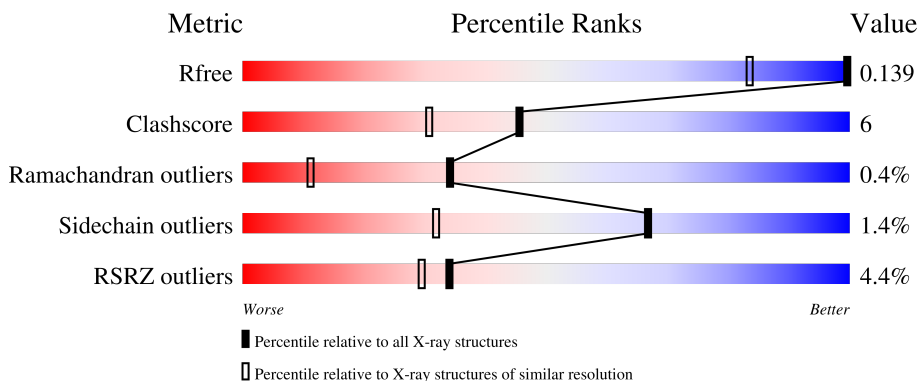
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.03 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.



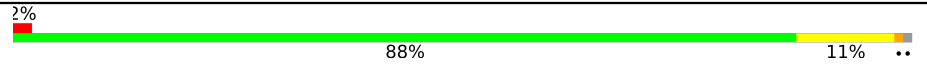
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)
RSRZ outliers	127900	1557 (1.10-0.98)

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	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	

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Mol	Chain	Length	Quality of chain
1	F	253	

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
4	CL	D	303	-	-	X	-
6	EDO	E	303	-	-	X	-

## 2 Entry composition [i](#)

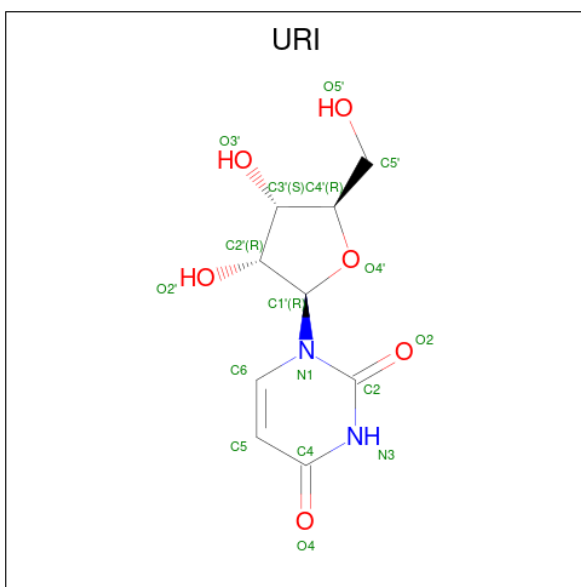
There are 7 unique types of molecules in this entry. The entry contains 28257 atoms, of which 13402 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	251	Total 4312	C 1328	H 2186	N 376	O 405	S 17	0	49	0
1	B	252	Total 4322	C 1336	H 2190	N 377	O 401	S 18	0	51	0
1	C	251	Total 4415	C 1359	H 2228	N 389	O 420	S 19	0	62	0
1	D	252	Total 4377	C 1348	H 2214	N 384	O 413	S 18	0	55	0
1	E	252	Total 4491	C 1381	H 2279	N 398	O 415	S 18	0	59	0
1	F	251	Total 4384	C 1346	H 2227	N 388	O 406	S 17	0	50	0

- Molecule 2 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	0	0
			29	9	12	2	6		
2	B	1	Total	C	H	N	O	0	0
			29	9	12	2	6		
2	C	1	Total	C	H	N	O	0	0
			29	9	12	2	6		
2	D	1	Total	C	H	N	O	0	0
			29	9	12	2	6		
2	E	1	Total	C	H	N	O	0	0
			29	9	12	2	6		
2	F	1	Total	C	H	N	O	0	0
			29	9	12	2	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	E	1	10	2	6	2	0	0

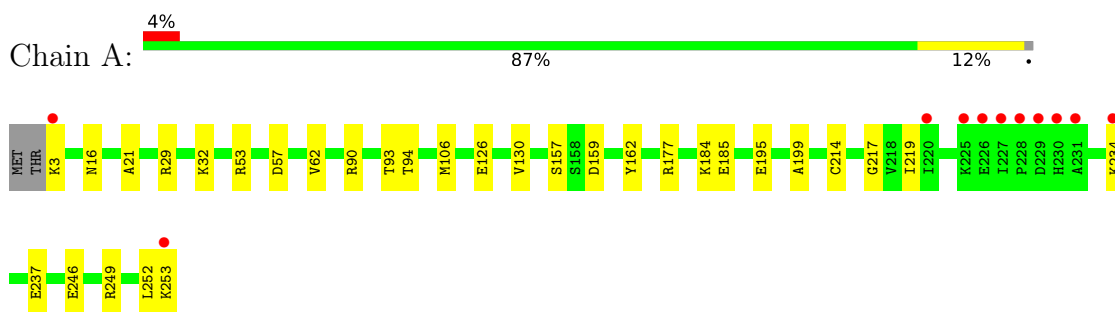
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	327	Total	O	0	3
			330	330		
7	B	301	Total	O	0	0
			301	301		
7	C	235	Total	O	0	3
			238	238		
7	D	290	Total	O	0	3
			293	293		
7	E	268	Total	O	0	2
			270	270		
7	F	328	Total	O	0	2
			330	330		

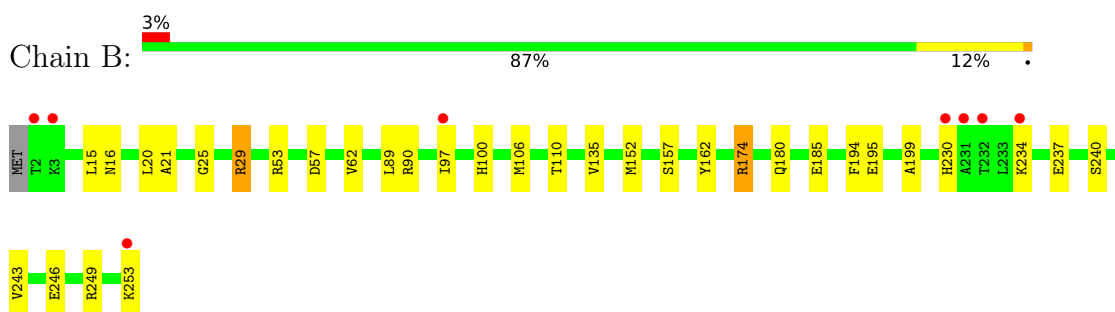
### 3 Residue-property plots [i](#)

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.

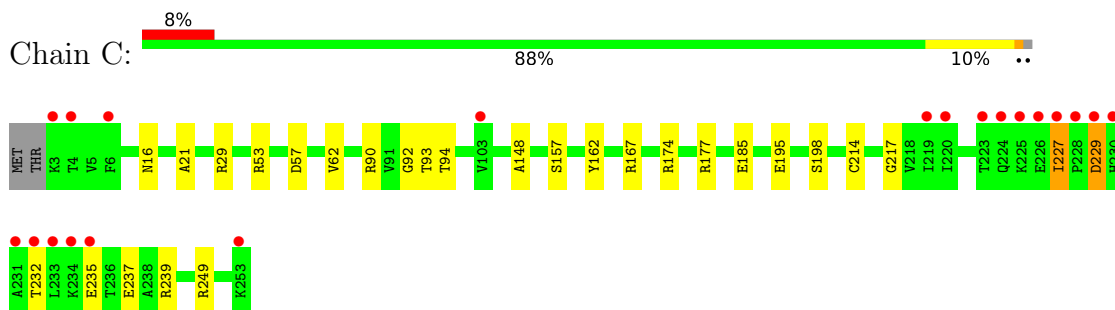
- Molecule 1: Uridine phosphorylase



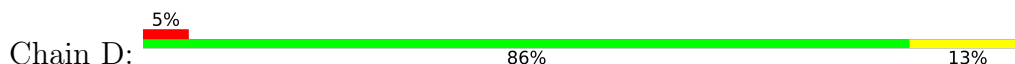
- Molecule 1: Uridine phosphorylase

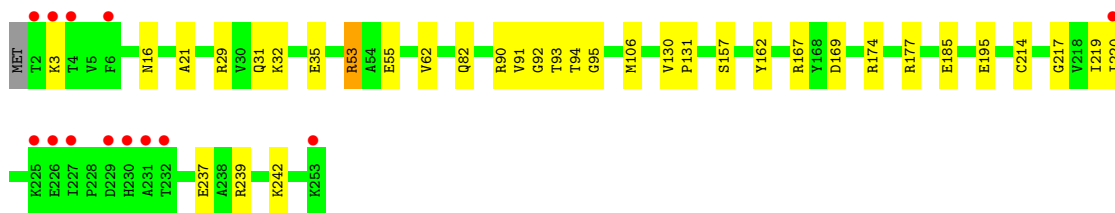


- Molecule 1: Uridine phosphorylase

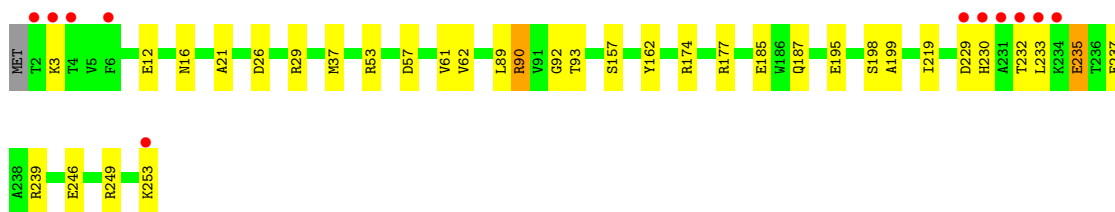
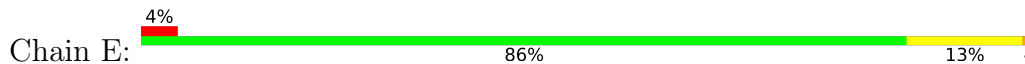


- Molecule 1: Uridine phosphorylase

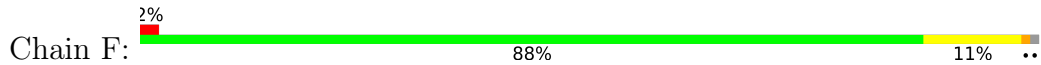




● Molecule 1: Uridine phosphorylase



● Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.32Å 72.04Å 89.19Å 110.56° 107.53° 85.83°	Depositor
Resolution (Å)	44.46 – 1.03 46.21 – 1.03	Depositor EDS
% Data completeness (in resolution range)	93.2 (44.46-1.03) 93.2 (46.21-1.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.03Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.118 , 0.137 0.119 , 0.139	Depositor DCC
$R_{free}$ test set	6560 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.5	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 56.4	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	0.98	EDS
Total number of atoms	28257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: CL, EDO, MG, NA, URI

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	0.65	0/2309	0.80	3/3121 (0.1%)
1	B	0.65	0/2343	0.92	4/3172 (0.1%)
1	C	0.63	2/2436 (0.1%)	0.88	4/3297 (0.1%)
1	D	0.68	2/2374 (0.1%)	0.86	8/3208 (0.2%)
1	E	0.62	0/2432	0.78	1/3283 (0.0%)
1	F	0.62	1/2371 (0.0%)	0.81	1/3204 (0.0%)
All	All	0.64	5/14265 (0.0%)	0.84	21/19285 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	90	ARG	CG-CD	-6.73	1.35	1.51
1	D	90[A]	ARG	CG-CD	-5.58	1.38	1.51
1	D	90[B]	ARG	CG-CD	-5.58	1.38	1.51
1	C	90[A]	ARG	CG-CD	-5.51	1.38	1.51
1	C	90[B]	ARG	CG-CD	-5.51	1.38	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174[A]	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	C	174[B]	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	B	90[A]	ARG	NE-CZ-NH1	-12.76	113.92	120.30
1	B	90[B]	ARG	NE-CZ-NH1	-12.76	113.92	120.30
1	C	174[A]	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	C	174[B]	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	174[A]	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	174[B]	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	167	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	D	53[A]	ARG	NE-CZ-NH1	5.75	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53[B]	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	90[A]	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	90[B]	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	159	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	89	LEU	CB-CG-CD1	5.53	120.41	111.00
1	D	177	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	169	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	90[A]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	D	90[B]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	F	89	LEU	CB-CG-CD1	5.15	119.76	111.00
1	D	167	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2126	2186	2025	29	0
1	B	2132	2190	2020	28	0
1	C	2187	2228	2003	23	0
1	D	2163	2214	2024	29	0
1	E	2212	2279	2101	33	0
1	F	2157	2227	2063	27	0
2	A	17	12	12	0	0
2	B	17	12	12	1	0
2	C	17	12	12	0	0
2	D	17	12	12	0	0
2	E	17	12	12	2	0
2	F	17	12	12	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	B	1	0	0	1	0
4	C	2	0	0	1	0
4	D	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
5	D	1	0	0	0	0
6	E	4	6	6	7	0
7	A	330	0	0	16	0
7	B	301	0	0	11	0
7	C	238	0	0	12	0
7	D	293	0	0	17	0
7	E	270	0	0	14	0
7	F	330	0	0	16	0
All	All	14855	13402	12314	170	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 6.

All (170) 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:E:174[C]:ARG:NH2	7:E:401:HOH:O	1.65	1.23
1:C:177[A]:ARG:NH2	7:C:402:HOH:O	1.77	1.16
1:A:177[A]:ARG:NH2	7:A:401:HOH:O	1.78	1.15
1:C:185[B]:GLU:OE1	7:C:401:HOH:O	1.72	1.07
1:D:55[A]:GLU:OE1	7:D:401:HOH:O	1.75	1.04
1:F:122:PHE:O	7:F:401:HOH:O	1.77	1.01
1:D:185[A]:GLU:OE1	7:D:402:HOH:O	1.77	1.00
1:E:177[A]:ARG:NH2	7:E:403:HOH:O	1.97	0.98
1:F:185[B]:GLU:OE1	7:F:402:HOH:O	1.84	0.95
1:A:185[A]:GLU:OE2	7:A:402:HOH:O	1.86	0.94
1:A:53[A]:ARG:NH1	7:A:403:HOH:O	1.98	0.94
1:B:97[B]:ILE:HD11	1:B:194:PHE:CD2	2.03	0.94
1:E:185[B]:GLU:OE1	7:E:402:HOH:O	1.88	0.92
1:D:239[A]:ARG:NH1	7:D:405:HOH:O	2.04	0.89
1:D:55[A]:GLU:OE1	7:D:403:HOH:O	1.92	0.88
1:E:90[B]:ARG:NH1	7:E:404:HOH:O	2.05	0.88
1:E:174[C]:ARG:NH1	7:F:401:HOH:O	1.89	0.85
1:B:29[B]:ARG:NH2	1:B:237:GLU:OE2	2.09	0.85
7:A:601:HOH:O	4:B:302:CL:CL	2.30	0.85
1:B:185[B]:GLU:OE2	7:B:401:HOH:O	1.93	0.85
7:C:402:HOH:O	1:E:185[A]:GLU:OE1	1.97	0.82
7:A:401:HOH:O	1:C:185[A]:GLU:OE1	1.97	0.81
1:A:106[A]:MET:SD	7:A:595:HOH:O	2.38	0.81
1:F:126[B]:GLU:OE1	7:F:403:HOH:O	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:GLU:OE2	1:C:239[B]:ARG:NH2	2.15	0.79
1:D:92[A]:GLY:O	7:D:404:HOH:O	2.02	0.78
1:D:106[A]:MET:SD	7:D:431:HOH:O	2.42	0.76
1:A:130[B]:VAL:HG11	1:F:130[B]:VAL:HG12	1.69	0.75
4:D:303:CL:CL	7:D:509:HOH:O	2.42	0.75
1:A:130[B]:VAL:HG12	1:F:130[B]:VAL:HG11	1.70	0.74
1:B:97[B]:ILE:HD11	1:B:194:PHE:CE2	2.22	0.73
1:D:93[A]:THR:HG23	7:D:404:HOH:O	1.87	0.73
7:A:401:HOH:O	1:C:185[A]:GLU:CD	2.28	0.72
1:A:126[A]:GLU:OE2	7:A:405:HOH:O	2.08	0.72
1:A:246[B]:GLU:OE1	7:A:404:HOH:O	2.08	0.71
1:E:12:GLU:OE2	7:E:405:HOH:O	2.09	0.71
1:F:177[A]:ARG:NH2	7:F:404:HOH:O	2.20	0.71
1:D:185[A]:GLU:OE2	7:D:406:HOH:O	2.09	0.70
1:A:130[B]:VAL:CG1	1:F:130[B]:VAL:CG1	2.70	0.70
1:D:93[A]:THR:HB	1:D:219:ILE:HG23	1.74	0.70
1:F:106[A]:MET:SD	7:F:642:HOH:O	2.50	0.69
4:C:302:CL:CL	7:C:471:HOH:O	2.48	0.69
1:B:185[B]:GLU:OE1	7:B:402:HOH:O	2.10	0.68
1:E:198[B]:SER:OG	7:E:406:HOH:O	2.11	0.68
1:C:227:ILE:HD12	1:C:227:ILE:N	2.10	0.67
1:A:3:LYS:N	7:A:408:HOH:O	2.27	0.67
1:C:214[B]:CYS:SG	7:C:529:HOH:O	2.53	0.66
1:A:130[B]:VAL:CG1	1:F:130[B]:VAL:HG11	2.26	0.65
1:A:130[B]:VAL:HG11	1:F:130[B]:VAL:CG1	2.25	0.65
1:B:246[A]:GLU:OE1	7:B:403:HOH:O	2.13	0.65
1:D:93[A]:THR:HB	1:D:219:ILE:CG2	2.27	0.65
1:E:230[A]:HIS:O	1:E:233[A]:LEU:HB2	1.98	0.63
1:D:237[B]:GLU:HG3	7:D:448:HOH:O	1.99	0.63
1:D:214[B]:CYS:SG	7:D:601:HOH:O	2.55	0.62
1:C:93[B]:THR:HG22	7:C:403:HOH:O	1.99	0.61
1:E:187[A]:GLN:NE2	7:E:414:HOH:O	2.33	0.61
1:E:235[A]:GLU:O	7:E:407:HOH:O	2.16	0.60
1:C:94[B]:THR:N	1:C:217[B]:GLY:O	2.32	0.58
1:A:185[B]:GLU:CD	7:E:403:HOH:O	2.43	0.56
1:D:3:LYS:HE3	1:D:82:GLN:OE1	2.05	0.56
1:C:227:ILE:HD12	1:C:227:ILE:H	1.68	0.56
1:B:106[A]:MET:SD	1:B:243:VAL:HG21	2.47	0.55
1:D:93[A]:THR:CG2	7:D:404:HOH:O	2.48	0.55
1:A:93[B]:THR:HB	1:A:219:ILE:CG2	2.36	0.55
1:C:167[B]:ARG:NH2	7:C:409:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:URI:H2'	2:B:301:URI:O2	2.05	0.54
1:A:184[B]:LYS:HE3	7:A:672:HOH:O	2.07	0.54
1:B:174[B]:ARG:HD2	7:F:564:HOH:O	2.08	0.54
1:A:57:ASP:OD2	1:A:249[B]:ARG:HG3	2.08	0.53
1:A:246[B]:GLU:CD	7:A:404:HOH:O	2.46	0.53
1:B:29[B]:ARG:CZ	1:B:237:GLU:OE2	2.55	0.53
1:F:235[A]:GLU:HG2	7:F:508:HOH:O	2.08	0.52
1:A:214[B]:CYS:SG	7:A:611:HOH:O	2.59	0.52
1:B:15[A]:LEU:HG	1:B:62[A]:VAL:CG2	2.39	0.52
1:B:29[A]:ARG:CZ	1:B:237:GLU:HB3	2.39	0.52
1:C:229[A]:ASP:OD2	1:C:232:THR:OG1	2.27	0.52
1:D:94[A]:THR:N	1:D:217:GLY:O	2.43	0.52
1:C:92[B]:GLY:O	7:C:403:HOH:O	2.19	0.52
1:D:130[B]:VAL:HG13	1:D:131:PRO:HD2	1.92	0.51
1:E:93:THR:OG1	6:E:303:EDO:H12	2.11	0.51
1:B:230[A]:HIS:NE2	7:B:405:HOH:O	2.16	0.51
1:C:148:ALA:HB2	1:C:239[A]:ARG:HD2	1.92	0.51
1:C:229[A]:ASP:OD1	1:C:229[A]:ASP:N	2.35	0.51
1:F:16[B]:ASN:ND2	7:F:428[B]:HOH:O	2.40	0.51
1:B:20:LEU:HD21	1:B:89[B]:LEU:HD23	1.92	0.51
1:F:230:HIS:NE2	1:F:234:LYS:HE2	2.26	0.51
1:E:16[A]:ASN:HB2	1:E:53[A]:ARG:HD2	1.93	0.50
1:C:53[A]:ARG:NH2	7:C:407:HOH:O	2.30	0.50
1:E:229[B]:ASP:O	1:E:232[B]:THR:HB	2.11	0.50
1:F:207:SER:OG	7:F:401:HOH:O	2.19	0.50
7:D:564:HOH:O	1:F:174[B]:ARG:HD2	2.11	0.50
1:A:16:ASN:HB2	1:A:53[A]:ARG:HD2	1.94	0.50
1:F:148:ALA:HB2	1:F:239[B]:ARG:HD3	1.93	0.49
1:E:93:THR:H	6:E:303:EDO:H12	1.76	0.49
1:B:174[A]:ARG:NH1	7:B:411:HOH:O	2.46	0.49
1:F:239[A]:ARG:HG3	1:F:242[A]:LYS:HZ1	1.77	0.49
1:A:93[B]:THR:HB	1:A:219:ILE:HG21	1.94	0.49
1:E:26:ASP:HB3	1:E:29[A]:ARG:HG2	1.95	0.49
1:B:110:THR:HG22	1:B:152[B]:MET:HE2	1.94	0.48
1:D:31[B]:GLN:NE2	1:D:35[B]:GLU:OE2	2.47	0.48
1:F:253:LYS:HE3	7:F:479:HOH:O	2.14	0.48
1:F:29[A]:ARG:NH1	1:F:237:GLU:OE2	2.46	0.48
1:D:16:ASN:HB2	1:D:53[A]:ARG:HD2	1.97	0.47
1:A:21:ALA:HA	1:A:62[B]:VAL:O	2.14	0.47
1:B:29[B]:ARG:NH1	1:B:240[B]:SER:OG	2.48	0.47
1:C:57:ASP:OD2	1:C:249[B]:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:URI:H2'	2:E:301:URI:O2	2.14	0.47
1:F:239[B]:ARG:HD2	7:F:642:HOH:O	2.13	0.47
1:B:16[B]:ASN:HB3	1:B:53[B]:ARG:HD2	1.97	0.47
1:E:233[A]:LEU:O	1:E:237[A]:GLU:HG3	2.15	0.46
1:F:47[B]:ARG:NH1	7:F:418:HOH:O	2.48	0.46
1:A:3:LYS:HA	7:A:626:HOH:O	2.16	0.46
1:C:93[B]:THR:CG2	7:C:403:HOH:O	2.62	0.46
7:C:402:HOH:O	1:E:185[A]:GLU:CD	2.48	0.46
1:A:252:LEU:O	1:A:253:LYS:HB2	2.15	0.46
1:F:3:LYS:N	7:F:417:HOH:O	2.48	0.46
1:D:29[C]:ARG:NH2	4:D:303:CL:CL	2.86	0.46
1:E:185[B]:GLU:OE2	7:E:408:HOH:O	2.21	0.46
1:A:237[A]:GLU:HG2	7:A:560:HOH:O	2.15	0.45
1:B:234[B]:LYS:HD2	7:B:546:HOH:O	2.16	0.45
2:E:301:URI:H4'	6:E:303:EDO:H11	1.99	0.45
1:C:29:ARG:NH1	1:C:237:GLU:HG2	2.32	0.45
1:E:246[B]:GLU:HG2	7:E:417:HOH:O	2.16	0.44
1:E:229[A]:ASP:OD2	1:E:232[A]:THR:HG23	2.18	0.44
1:F:21:ALA:HA	1:F:62[B]:VAL:O	2.17	0.44
1:B:185[B]:GLU:OE1	7:B:406:HOH:O	2.21	0.44
1:D:53[A]:ARG:NE	7:D:401:HOH:O	2.49	0.44
1:D:95[A]:GLY:HA2	1:D:220:ILE:O	2.17	0.44
1:F:169[B]:ASP:OD2	7:F:406:HOH:O	2.21	0.44
7:B:542:HOH:O	1:D:174[B]:ARG:HD2	2.18	0.44
1:E:239[A]:ARG:NH2	7:E:422:HOH:O	2.50	0.44
1:B:185[B]:GLU:CD	7:B:406:HOH:O	2.56	0.44
1:C:21:ALA:HA	1:C:62[B]:VAL:O	2.18	0.44
1:E:253:LYS:HE3	7:E:628:HOH:O	2.17	0.44
1:E:53[B]:ARG:NH1	7:E:424:HOH:O	2.51	0.43
1:F:148:ALA:HB2	1:F:239[A]:ARG:HD3	2.00	0.43
1:A:29:ARG:NH2	1:A:32[B]:LYS:HD3	2.33	0.43
1:B:25:GLY:HA3	7:B:422:HOH:O	2.17	0.43
1:D:91:VAL:HG22	1:D:92[A]:GLY:N	2.34	0.43
1:D:239[B]:ARG:NE	7:D:412:HOH:O	2.40	0.43
1:E:92:GLY:HA3	6:E:303:EDO:H21	1.99	0.43
1:D:242[A]:LYS:HE3	7:D:563:HOH:O	2.18	0.43
1:A:246[B]:GLU:HG2	7:A:407:HOH:O	2.19	0.43
1:C:16:ASN:HB2	1:C:53[B]:ARG:HD2	2.00	0.43
1:D:21:ALA:HA	1:D:62[B]:VAL:O	2.18	0.43
1:E:37:MET:SD	1:E:61[B]:VAL:HG21	2.59	0.43
1:C:198[B]:SER:OG	7:C:405:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180[A]:GLN:NE2	7:B:404:HOH:O	2.17	0.43
1:E:21:ALA:HA	1:E:62[B]:VAL:O	2.19	0.43
1:B:89[B]:LEU:HD12	1:B:135:VAL:HG13	2.00	0.42
1:B:110:THR:CG2	1:B:152[B]:MET:HE2	2.49	0.42
1:E:157:SER:HB3	1:E:199:ALA:HB2	2.01	0.42
1:B:57:ASP:OD2	1:B:249[A]:ARG:HG3	2.19	0.42
1:B:21:ALA:HA	1:B:62[B]:VAL:O	2.19	0.42
1:A:29:ARG:HD2	1:A:32[B]:LYS:HD2	2.02	0.41
1:F:57:ASP:OD2	1:F:249[A]:ARG:HG3	2.19	0.41
1:D:29[A]:ARG:NH1	1:D:92[A]:GLY:HA2	2.35	0.41
1:E:90[B]:ARG:HH12	6:E:303:EDO:C2	2.33	0.41
1:A:94[B]:THR:N	1:A:217:GLY:O	2.53	0.41
1:B:157:SER:HB3	1:B:199:ALA:HB2	2.02	0.41
1:D:53[B]:ARG:NH2	7:D:422:HOH:O	2.53	0.41
1:E:57:ASP:OD2	1:E:249[A]:ARG:HG3	2.21	0.41
1:A:157:SER:HB3	1:A:199:ALA:HB2	2.03	0.40
1:E:219:ILE:HD12	1:E:233[B]:LEU:HD11	2.02	0.40
1:E:90[A]:ARG:HH21	6:E:303:EDO:H22	1.86	0.40
1:E:90[A]:ARG:NH2	6:E:303:EDO:H22	2.36	0.40
1:F:242[B]:LYS:HG3	7:F:539:HOH:O	2.21	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	299/253 (118%)	296 (99%)	2 (1%)	1 (0%)	41	14
1	B	303/253 (120%)	300 (99%)	2 (1%)	1 (0%)	41	14
1	C	315/253 (124%)	309 (98%)	5 (2%)	1 (0%)	41	14
1	D	307/253 (121%)	303 (99%)	3 (1%)	1 (0%)	41	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	312/253 (123%)	309 (99%)	2 (1%)	1 (0%)	41	14
1	F	304/253 (120%)	301 (99%)	2 (1%)	1 (0%)	41	14
All	All	1840/1518 (121%)	1818 (99%)	16 (1%)	6 (0%)	34	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	162	TYR
1	A	162	TYR
1	B	162	TYR
1	C	162	TYR
1	D	162	TYR
1	F	162	TYR

### 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	245/203 (121%)	243 (99%)	2 (1%)	81	52
1	B	247/203 (122%)	243 (98%)	4 (2%)	62	27
1	C	258/203 (127%)	254 (98%)	4 (2%)	62	27
1	D	250/203 (123%)	247 (99%)	3 (1%)	71	38
1	E	259/203 (128%)	253 (98%)	6 (2%)	50	15
1	F	253/203 (125%)	248 (98%)	5 (2%)	55	19
All	All	1512/1218 (124%)	1488 (98%)	24 (2%)	67	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	234	LYS
1	B	29[A]	ARG
1	B	29[B]	ARG

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Mol	Chain	Res	Type
1	B	195	GLU
1	B	253	LYS
1	C	195	GLU
1	C	227	ILE
1	C	229[A]	ASP
1	C	229[B]	ASP
1	D	32[A]	LYS
1	D	32[B]	LYS
1	D	195	GLU
1	E	3	LYS
1	E	90[A]	ARG
1	E	90[B]	ARG
1	E	195	GLU
1	E	235[A]	GLU
1	E	235[B]	GLU
1	F	29[A]	ARG
1	F	29[B]	ARG
1	F	29[C]	ARG
1	F	195	GLU
1	F	253	LYS

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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
2	URI	A	301	-	18,18,18	0.96	1 (5%)	26,26,26	1.34	3 (11%)
2	URI	F	301	-	18,18,18	0.72	1 (5%)	26,26,26	1.49	6 (23%)
6	EDO	E	303	-	3,3,3	0.27	0	2,2,2	0.21	0
2	URI	E	301	-	18,18,18	0.83	0	26,26,26	1.60	5 (19%)
2	URI	C	301	-	18,18,18	0.87	1 (5%)	26,26,26	1.37	3 (11%)
2	URI	D	301	-	18,18,18	1.27	1 (5%)	26,26,26	1.41	4 (15%)
2	URI	B	301	-	18,18,18	0.78	0	26,26,26	1.72	6 (23%)

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	URI	A	301	-	-	4/6/22/22	0/2/2/2
2	URI	F	301	-	-	4/6/22/22	0/2/2/2
6	EDO	E	303	-	-	1/1/1/1	-
2	URI	E	301	-	-	4/6/22/22	0/2/2/2
2	URI	C	301	-	-	4/6/22/22	0/2/2/2
2	URI	D	301	-	-	4/6/22/22	0/2/2/2
2	URI	B	301	-	-	2/6/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	URI	O2-C2	-4.84	1.14	1.23
2	A	301	URI	O2-C2	-3.22	1.17	1.23
2	C	301	URI	O2-C2	-3.00	1.17	1.23
2	F	301	URI	O2-C2	-2.19	1.19	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	URI	C1'-N1-C2	4.61	125.92	117.57
2	E	301	URI	C1'-N1-C2	4.13	125.05	117.57
2	B	301	URI	O4'-C1'-N1	-3.90	99.44	108.36
2	F	301	URI	C1'-N1-C2	3.88	124.59	117.57
2	D	301	URI	C1'-N1-C2	3.43	123.79	117.57
2	E	301	URI	C2'-C1'-N1	3.41	122.88	113.22
2	A	301	URI	C1'-N1-C2	3.21	123.39	117.57
2	C	301	URI	C2'-C1'-N1	3.15	122.13	113.22
2	A	301	URI	C2'-C1'-N1	2.95	121.57	113.22
2	E	301	URI	O4'-C1'-N1	-2.94	101.64	108.36
2	F	301	URI	C2'-C1'-N1	2.78	121.10	113.22
2	C	301	URI	C1'-N1-C2	2.75	122.55	117.57
2	F	301	URI	O4'-C1'-N1	-2.73	102.13	108.36
2	D	301	URI	C2'-C1'-N1	2.71	120.90	113.22
2	D	301	URI	O4'-C1'-N1	-2.65	102.31	108.36
2	A	301	URI	O4'-C1'-N1	-2.63	102.36	108.36
2	B	301	URI	C2'-C1'-N1	2.60	120.57	113.22
2	C	301	URI	O4'-C1'-N1	-2.60	102.43	108.36
2	B	301	URI	C1'-N1-C6	-2.52	115.36	120.84
2	E	301	URI	C1'-N1-C6	-2.38	115.65	120.84
2	F	301	URI	C1'-N1-C6	-2.35	115.71	120.84
2	E	301	URI	C6-N1-C2	-2.25	118.11	120.99
2	F	301	URI	C6-N1-C2	-2.24	118.12	120.99
2	B	301	URI	C4-N3-C2	2.12	129.39	126.58
2	B	301	URI	C6-N1-C2	-2.11	118.30	120.99
2	F	301	URI	N3-C2-N1	2.10	117.67	114.89
2	D	301	URI	C1'-N1-C6	-2.00	116.48	120.84

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	URI	C2'-C1'-N1-C6
2	B	301	URI	C2'-C1'-N1-C2
2	E	301	URI	C2'-C1'-N1-C2
2	E	301	URI	C2'-C1'-N1-C6
2	F	301	URI	C2'-C1'-N1-C6
2	A	301	URI	C2'-C1'-N1-C6
2	C	301	URI	C2'-C1'-N1-C6
2	D	301	URI	C2'-C1'-N1-C6
6	E	303	EDO	O1-C1-C2-O2
2	A	301	URI	C2'-C1'-N1-C2
2	D	301	URI	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	F	301	URI	C2'-C1'-N1-C2
2	C	301	URI	C2'-C1'-N1-C2
2	C	301	URI	O4'-C1'-N1-C6
2	D	301	URI	O4'-C1'-N1-C6
2	C	301	URI	O4'-C1'-N1-C2
2	A	301	URI	O4'-C1'-N1-C6
2	A	301	URI	O4'-C1'-N1-C2
2	D	301	URI	O4'-C1'-N1-C2
2	E	301	URI	O4'-C1'-N1-C2
2	F	301	URI	O4'-C1'-N1-C2
2	F	301	URI	O4'-C1'-N1-C6
2	E	301	URI	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	303	EDO	7	0
2	E	301	URI	2	0
2	B	301	URI	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	251/253 (99%)	-0.18	11 (4%) 34 29	5, 10, 23, 44	2 (0%)
1	B	252/253 (99%)	-0.30	8 (3%) 47 41	6, 10, 19, 40	5 (1%)
1	C	251/253 (99%)	0.13	20 (7%) 12 14	6, 14, 43, 67	1 (0%)
1	D	252/253 (99%)	-0.08	13 (5%) 27 24	6, 12, 28, 49	1 (0%)
1	E	252/253 (99%)	-0.19	11 (4%) 34 29	6, 11, 26, 45	2 (0%)
1	F	251/253 (99%)	-0.28	4 (1%) 72 64	5, 11, 23, 42	2 (0%)
All	All	1509/1518 (99%)	-0.15	67 (4%) 34 29	5, 11, 27, 67	13 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	THR	11.2
1	C	227	ILE	10.8
1	D	2	THR	8.9
1	B	2	THR	7.0
1	C	231	ALA	6.8
1	C	229[A]	ASP	6.5
1	D	227	ILE	6.4
1	F	253	LYS	6.2
1	A	227[A]	ILE	6.1
1	C	225	LYS	5.7
1	C	226	GLU	5.5
1	C	230[A]	HIS	5.4
1	C	3	LYS	5.4
1	C	253	LYS	5.1
1	D	253	LYS	5.1
1	C	228	PRO	5.0
1	B	253	LYS	4.8
1	A	253	LYS	4.8
1	D	3	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	219[A]	ILE	4.6
1	E	231[A]	ALA	4.5
1	B	3	LYS	4.3
1	D	226	GLU	3.8
1	C	224	GLN	3.6
1	B	234[A]	LYS	3.6
1	C	232	THR	3.5
1	E	253	LYS	3.5
1	A	231	ALA	3.5
1	D	225	LYS	3.5
1	A	229	ASP	3.4
1	C	220[A]	ILE	3.3
1	D	4	THR	3.3
1	E	3	LYS	3.3
1	A	230	HIS	3.2
1	C	234	LYS	3.1
1	D	229	ASP	3.1
1	E	232[A]	THR	3.1
1	E	233[A]	LEU	3.0
1	B	231[A]	ALA	3.0
1	C	103	VAL	2.9
1	F	230	HIS	2.9
1	D	220	ILE	2.9
1	D	6	PHE	2.9
1	A	228	PRO	2.8
1	E	230[A]	HIS	2.7
1	E	229[A]	ASP	2.6
1	D	231	ALA	2.6
1	D	232	THR	2.6
1	C	233	LEU	2.6
1	C	4	THR	2.5
1	C	223	THR	2.5
1	E	6	PHE	2.5
1	B	230[A]	HIS	2.5
1	B	97[A]	ILE	2.5
1	C	235	GLU	2.5
1	C	6	PHE	2.5
1	A	226[A]	GLU	2.5
1	F	229	ASP	2.5
1	A	220[A]	ILE	2.4
1	A	225	LYS	2.3
1	F	3	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	232	THR	2.3
1	A	3	LYS	2.1
1	D	230	HIS	2.1
1	E	4	THR	2.1
1	A	234	LYS	2.1
1	E	234[A]	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	E	303	4/4	0.86	0.14	31,37,38,39	10
2	URI	D	301	17/17	0.96	0.08	9,13,16,18	29
5	MG	D	304	1/1	0.96	0.14	16,16,16,16	1
2	URI	C	301	17/17	0.96	0.07	11,14,17,20	29
4	CL	B	302	1/1	0.97	0.09	35,35,35,35	0
2	URI	A	301	17/17	0.97	0.07	8,11,15,17	29
2	URI	B	301	17/17	0.97	0.07	7,10,18,21	2
4	CL	D	302	1/1	0.98	0.05	19,19,19,19	1
4	CL	D	303	1/1	0.98	0.04	32,32,32,32	1
2	URI	F	301	17/17	0.98	0.05	9,13,18,19	4
4	CL	C	302	1/1	0.98	0.05	28,28,28,28	1
4	CL	C	303	1/1	0.99	0.04	19,19,19,19	1
3	NA	C	304	1/1	0.99	0.07	15,15,15,15	1
3	NA	E	302	1/1	0.99	0.11	13,13,13,13	1
2	URI	E	301	17/17	0.99	0.04	7,10,15,16	7
3	NA	A	302	1/1	0.99	0.10	10,10,10,10	1
4	CL	F	302	1/1	1.00	0.03	21,21,21,21	1



## 6.5 Other polymers [i](#)

There are no such residues in this entry.