wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 02:21 pm GMT

PDB ID	:	5EPU
Title	:	X-ray structure uridine phosphorylase from Vibrio cholerae in complex with cytosine at 1.06A.
Authors	:	Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on	:	2015-11-12
Resolution	:	1.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

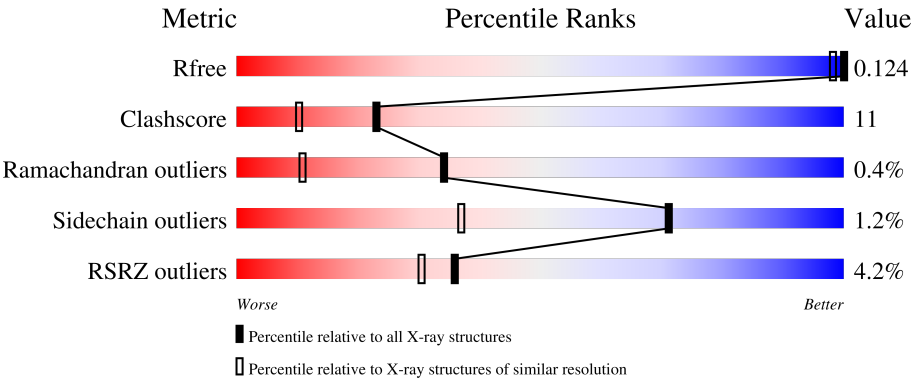
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.06 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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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	253	6% 85% 13%
1	B	253	6% 88% 11%
1	C	253	5% 86% 13%
1	D	253	6% 83% 16%
1	E	253	% 87% 12%

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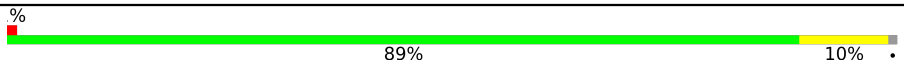
Mol	Chain	Length	Quality of chain
1	F	253	

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
2	CYT	A	301	-	-	X	-
2	CYT	D	302	-	-	X	-
7	TRS	B	305	-	-	X	-
7	TRS	F	306	-	-	X	-

2 Entry composition (i)

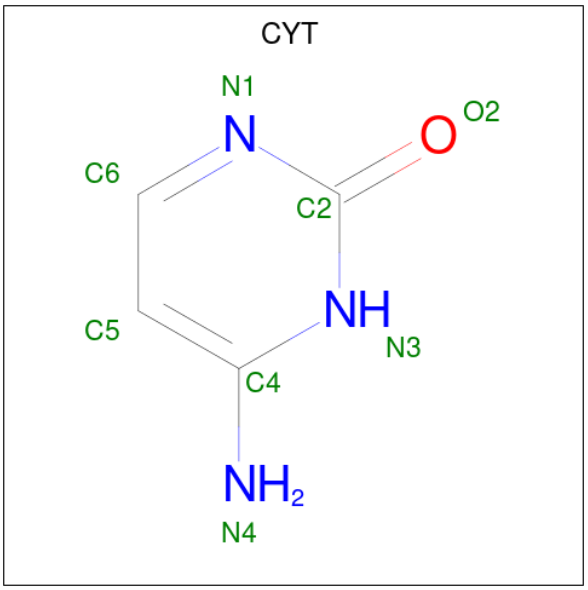
There are 9 unique types of molecules in this entry. The entry contains 28724 atoms, of which 13501 are hydrogens and 0 are deuteriums.

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.

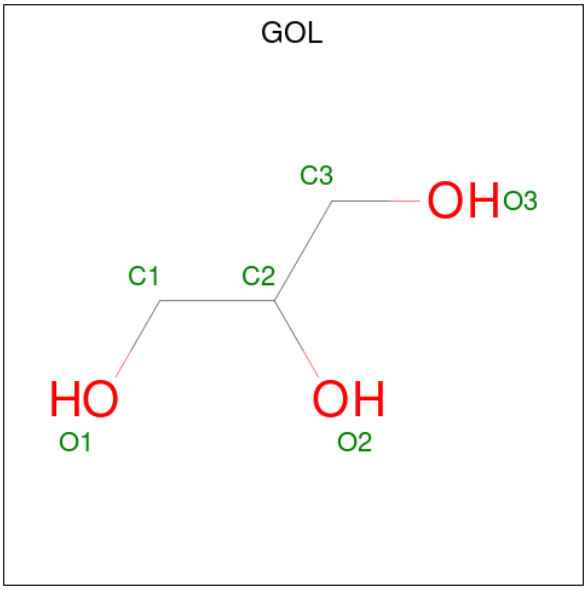
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	252	Total	C	H	N	O	S	56	52	0
			4528	1403	2310	383	413	19			
1	B	252	Total	C	H	N	O	S	52	32	0
			4211	1321	2125	360	387	18			
1	C	251	Total	C	H	N	O	S	49	39	0
			4316	1350	2195	364	388	19			
1	D	252	Total	C	H	N	O	S	56	50	0
			4463	1392	2263	380	409	19			
1	E	251	Total	C	H	N	O	S	49	39	0
			4369	1354	2238	369	390	18			
1	F	251	Total	C	H	N	O	S	51	35	0
			4291	1332	2196	359	386	18			

- Molecule 2 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula: $C_4H_5N_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			13	4	5	3	1		
2	B	1	Total	C	H	N	O	0	0
			13	4	5	3	1		
2	C	1	Total	C	H	N	O	0	0
			13	4	5	3	1		
2	D	1	Total	C	H	N	O	0	0
			13	4	5	3	1		
2	E	1	Total	C	H	N	O	0	0
			13	4	5	3	1		
2	F	1	Total	C	H	N	O	0	0
			13	4	5	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	4	1
			28	6	16	6		
3	B	1	Total	C	H	O	4	1
			28	6	16	6		
3	D	1	Total	C	H	O	4	1
			28	6	16	6		
3	E	1	Total	C	H	O	6	1
			42	9	24	9		
3	F	1	Total	C	H	O	4	1
			28	6	16	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	1	Total Mg 1 1	0	0
4	E	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

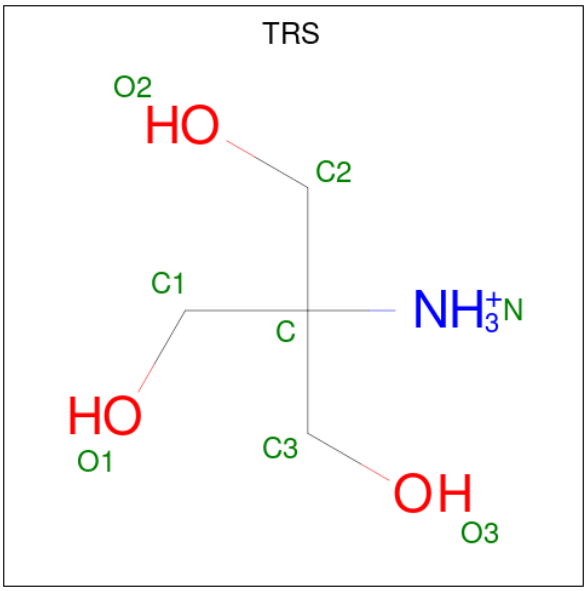
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

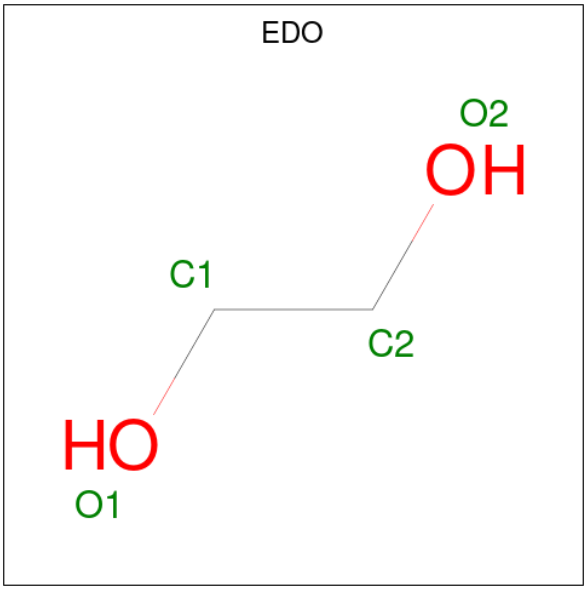
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	2	0
			20	4	12	1	3		
7	F	1	Total	C	H	N	O	2	0
			20	4	12	1	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	O		2	1
			20	4	12	4			
8	E	1	Total	C	H	O		1	0
			10	2	6	2			

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

- Molecule 9 is water.

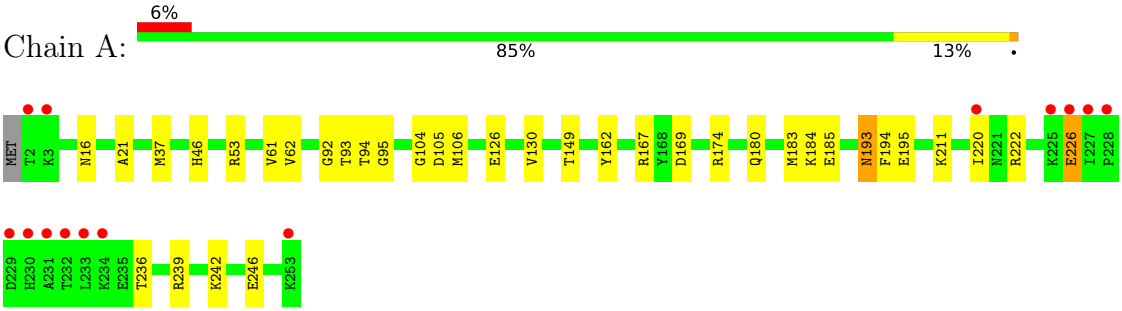
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	357	Total O 370 370	0	13
9	B	326	Total O 336 336	0	11
9	C	318	Total O 343 343	0	25
9	D	351	Total O 362 362	0	14
9	E	376	Total O 394 394	0	20
9	F	391	Total O 403 403	0	16

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.

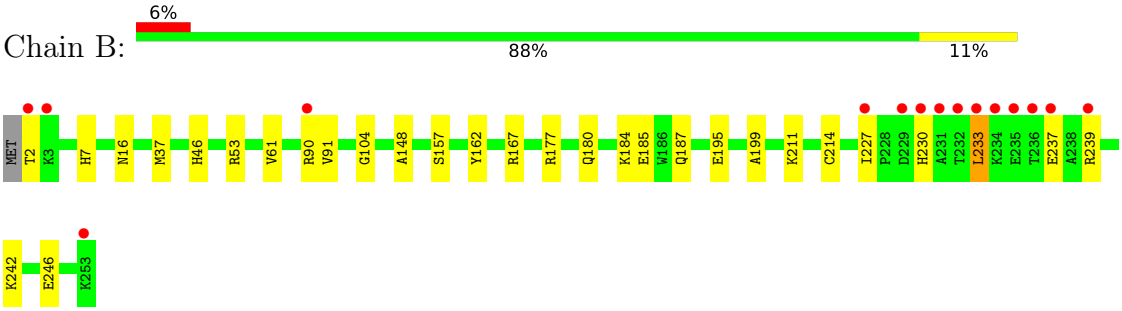
• Molecule 1: Uridine phosphorylase

Chain A:



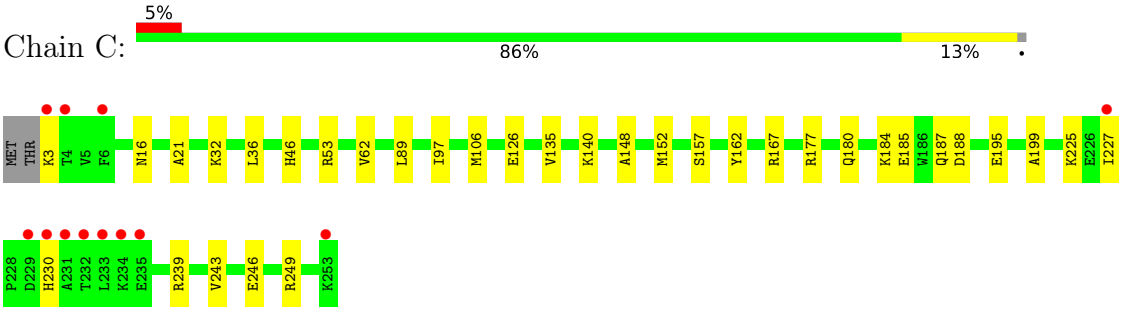
• Molecule 1: Uridine phosphorylase

Chain B:



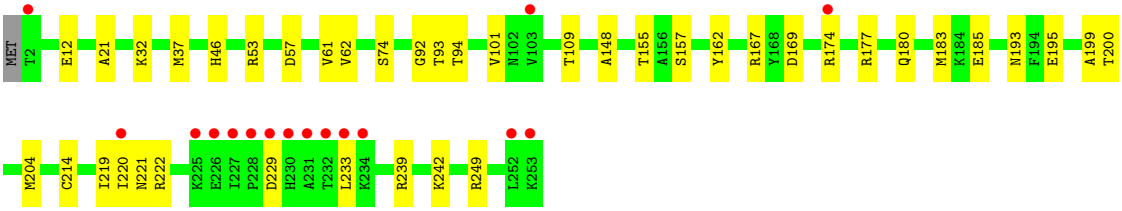
• Molecule 1: Uridine phosphorylase

Chain C:



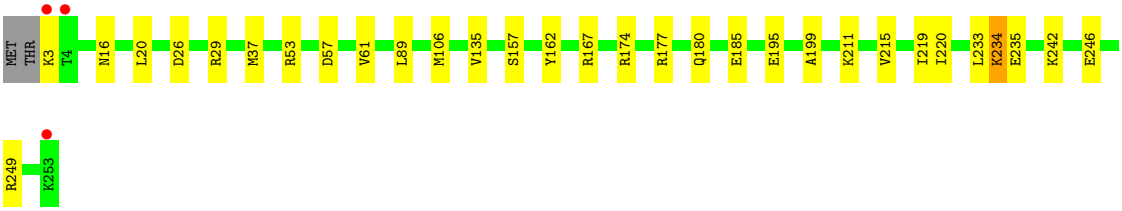
• Molecule 1: Uridine phosphorylase

Chain D:



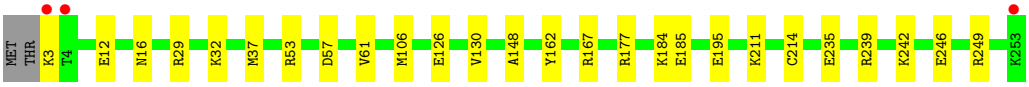
• Molecule 1: Uridine phosphorylase

Chain E:



• Molecule 1: Uridine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.85Å 96.72Å 92.89Å 90.00° 119.96° 90.00°	Depositor
Resolution (Å)	46.46 – 1.06 46.46 – 1.06	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.46-1.06) 95.7 (46.46-1.06)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.06Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.105 , 0.122 0.108 , 0.124	Depositor DCC
R_{free} test set	30490 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	6.6	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.117 for -h-l,k,h 0.117 for l,k,-h-l 0.016 for h,-k,-h-l 0.017 for -h-l,-k,l 0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: CYT, EDO, GOL, NA, TRS, MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/2364	0.71	0/3190
1	B	0.42	0/2202	0.72	0/2972
1	C	0.46	0/2268	0.72	0/3059
1	D	0.42	0/2337	0.70	0/3154
1	E	0.48	0/2268	0.73	0/3058
1	F	0.47	0/2235	0.72	0/3015
All	All	0.45	0/13674	0.72	0/18448

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	2218	2310	2344	62	0
1	B	2086	2125	2190	39	0
1	C	2121	2195	2249	51	0
1	D	2200	2263	2321	47	0
1	E	2131	2238	2259	38	0
1	F	2095	2196	2221	38	0
2	A	8	5	4	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	5	4	1	0
2	C	8	5	4	1	0
2	D	8	5	4	7	0
2	E	8	5	4	2	0
2	F	8	5	2	1	0
3	A	18	24	24	2	0
3	B	12	16	16	2	0
3	D	12	16	16	1	0
3	E	18	24	24	0	0
3	F	12	16	16	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	8	12	12	14	0
7	F	8	12	12	8	0
8	C	8	12	12	1	0
8	E	4	6	6	3	0
8	F	4	6	6	1	0
9	A	370	0	0	43	0
9	B	336	0	0	39	0
9	C	343	0	0	33	0
9	D	362	0	0	30	0
9	E	394	0	0	24	0
9	F	403	0	0	36	0
All	All	15223	13501	13750	305	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 11.

The worst 5 of 305 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)
7:B:305:TRS:H22	9:B:404:HOH:O	1.22	1.35
1:A:184[C]:LYS:HE2	9:A:445:HOH:O	1.28	1.34
1:B:227[B]:ILE:CD1	9:B:635:HOH:O	1.75	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93[B]:THR:HG23	9:D:410:HOH:O	1.21	1.28
7:B:305:TRS:C2	9:B:404:HOH:O	1.74	1.26

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	306/253 (121%)	301 (98%)	4 (1%)	1 (0%)	41	14
1	B	284/253 (112%)	281 (99%)	2 (1%)	1 (0%)	34	11
1	C	290/253 (115%)	287 (99%)	2 (1%)	1 (0%)	41	14
1	D	303/253 (120%)	299 (99%)	3 (1%)	1 (0%)	41	14
1	E	291/253 (115%)	286 (98%)	4 (1%)	1 (0%)	41	14
1	F	287/253 (113%)	281 (98%)	5 (2%)	1 (0%)	41	14
All	All	1761/1518 (116%)	1735 (98%)	20 (1%)	6 (0%)	34	14

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	TYR
1	D	162	TYR
1	E	162	TYR
1	F	162	TYR
1	A	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	253/203 (125%)	250 (99%)	3 (1%)	71	37
1	B	236/203 (116%)	232 (98%)	4 (2%)	60	23
1	C	242/203 (119%)	240 (99%)	2 (1%)	81	52
1	D	250/203 (123%)	248 (99%)	2 (1%)	81	52
1	E	242/203 (119%)	238 (98%)	4 (2%)	60	23
1	F	239/203 (118%)	238 (100%)	1 (0%)	91	73
All	All	1462/1218 (120%)	1446 (99%)	16 (1%)	71	40

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	234[B]	LYS
1	E	234[A]	LYS
1	C	195	GLU
1	E	195	GLU
1	C	3	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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	CYT	E	304	-	7,8,8	1.01	0	8,10,10	7.55	3 (37%)
7	TRS	B	305	-	7,7,7	0.63	0	9,9,9	1.65	2 (22%)
2	CYT	B	304	-	7,8,8	0.77	0	8,10,10	7.24	4 (50%)
3	GOL	D	301[B]	-	5,5,5	0.30	0	5,5,5	0.38	0
8	EDO	C	303[A]	-	3,3,3	0.48	0	2,2,2	0.22	0
7	TRS	F	306	-	7,7,7	0.43	0	9,9,9	0.79	0
3	GOL	B	301[A]	-	5,5,5	0.24	0	5,5,5	0.71	0
8	EDO	C	303[B]	-	3,3,3	0.35	0	2,2,2	0.40	0
3	GOL	E	302[A]	-	5,5,5	0.13	0	5,5,5	0.82	0
3	GOL	F	301[A]	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	A	303[A]	-	5,5,5	0.33	0	5,5,5	1.18	1 (20%)
3	GOL	B	301[B]	-	5,5,5	0.20	0	5,5,5	0.54	0
3	GOL	E	302[C]	-	5,5,5	0.44	0	5,5,5	0.73	0
3	GOL	A	302	-	5,5,5	0.21	0	5,5,5	0.25	0
3	GOL	A	303[C]	-	5,5,5	0.32	0	5,5,5	0.61	0
2	CYT	D	302	-	7,8,8	0.86	0	8,10,10	7.87	4 (50%)
3	GOL	E	302[B]	-	5,5,5	0.31	0	5,5,5	0.20	0
3	GOL	F	301[B]	-	5,5,5	0.18	0	5,5,5	0.44	0
8	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.27	0
3	GOL	D	301[A]	-	5,5,5	0.37	0	5,5,5	0.26	0
8	EDO	E	305	-	3,3,3	0.47	0	2,2,2	0.17	0
2	CYT	A	301	-	7,8,8	0.97	0	8,10,10	6.21	4 (50%)
2	CYT	C	302	-	7,8,8	0.87	0	8,10,10	7.48	4 (50%)
2	CYT	F	304	-	7,8,8	1.15	1 (14%)	8,10,10	5.85	3 (37%)

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	CYT	E	304	-	-	-	0/1/1/1
7	TRS	B	305	-	-	6/9/9/9	-
3	GOL	D	301[B]	-	-	2/4/4/4	-
2	CYT	B	304	-	-	-	0/1/1/1
8	EDO	C	303[A]	-	-	0/1/1/1	-
7	TRS	F	306	-	-	3/9/9/9	-
3	GOL	B	301[A]	-	-	2/4/4/4	-
8	EDO	C	303[B]	-	-	1/1/1/1	-
3	GOL	E	302[A]	-	-	2/4/4/4	-
3	GOL	F	301[A]	-	-	2/4/4/4	-
3	GOL	A	303[A]	-	-	0/4/4/4	-
3	GOL	B	301[B]	-	-	2/4/4/4	-
3	GOL	E	302[C]	-	-	2/4/4/4	-
3	GOL	A	302	-	-	0/4/4/4	-
3	GOL	A	303[C]	-	-	4/4/4/4	-
2	CYT	D	302	-	-	-	0/1/1/1
3	GOL	E	302[B]	-	-	0/4/4/4	-
3	GOL	F	301[B]	-	-	0/4/4/4	-
8	EDO	F	305	-	-	0/1/1/1	-
3	GOL	D	301[A]	-	-	2/4/4/4	-
8	EDO	E	305	-	-	0/1/1/1	-
2	CYT	A	301	-	-	-	0/1/1/1
2	CYT	C	302	-	-	-	0/1/1/1
2	CYT	F	304	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	304	CYT	C4-N4	-2.02	1.29	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	302	CYT	C6-N1-C2	16.33	122.48	114.42
2	E	304	CYT	N3-C2-N1	-14.62	116.81	128.43
2	C	302	CYT	N3-C2-N1	-14.44	116.95	128.43
2	B	304	CYT	N3-C2-N1	-14.20	117.14	128.43
2	D	302	CYT	N3-C2-N1	-13.45	117.74	128.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303[C]	GOL	O1-C1-C2-C3
3	B	301[A]	GOL	C1-C2-C3-O3
3	B	301[B]	GOL	C1-C2-C3-O3
3	D	301[A]	GOL	O1-C1-C2-C3
3	D	301[B]	GOL	O1-C1-C2-C3

There are no ring outliers.

16 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	304	CYT	2	0
7	B	305	TRS	14	0
2	B	304	CYT	1	0
7	F	306	TRS	8	0
3	B	301[A]	GOL	1	0
8	C	303[B]	EDO	1	0
3	F	301[A]	GOL	1	0
3	B	301[B]	GOL	1	0
3	A	303[C]	GOL	2	0
2	D	302	CYT	7	0
8	F	305	EDO	1	0
3	D	301[A]	GOL	1	0
8	E	305	EDO	3	0
2	A	301	CYT	9	0
2	C	302	CYT	1	0
2	F	304	CYT	1	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	252/253 (99%)	-0.21	14 (5%)	24	22	4, 8, 24, 71	0
1	B	252/253 (99%)	-0.22	15 (5%)	21	21	4, 8, 22, 72	0
1	C	251/253 (99%)	-0.25	12 (4%)	30	27	4, 8, 25, 45	0
1	D	252/253 (99%)	-0.19	16 (6%)	20	19	4, 8, 28, 73	0
1	E	251/253 (99%)	-0.49	3 (1%)	79	74	4, 7, 15, 45	0
1	F	251/253 (99%)	-0.48	3 (1%)	79	74	4, 7, 15, 35	0
All	All	1509/1518 (99%)	-0.31	63 (4%)	36	30	4, 8, 21, 73	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	9.9
1	B	232	THR	9.0
1	A	227	ILE	8.7
1	C	231	ALA	8.1
1	A	2	THR	8.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (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	GOL	A	302	6/6	0.81	0.14	16,20,22,23	14
8	EDO	C	303[A]	4/4	0.83	0.23	8,11,12,12	10
8	EDO	C	303[B]	4/4	0.83	0.23	10,11,13,14	10
3	GOL	E	302[C]	6/6	0.84	0.19	7,15,19,20	14
3	GOL	E	302[A]	6/6	0.84	0.19	6,7,7,7	14
3	GOL	E	302[B]	6/6	0.84	0.19	8,12,15,15	14
7	TRS	B	305	8/8	0.85	0.26	8,10,16,16	20
3	GOL	A	303[C]	6/6	0.85	0.18	10,12,15,16	14
3	GOL	A	303[A]	6/6	0.85	0.18	9,14,27,27	14
7	TRS	F	306	8/8	0.88	0.24	8,10,21,21	20
3	GOL	D	301[B]	6/6	0.92	0.11	14,20,23,23	14
3	GOL	D	301[A]	6/6	0.92	0.11	11,15,17,18	14
3	GOL	F	301[A]	6/6	0.92	0.10	17,19,23,24	14
3	GOL	F	301[B]	6/6	0.92	0.10	10,14,17,18	14
4	MG	A	304	1/1	0.93	0.35	16,16,16,16	1
2	CYT	A	301	8/8	0.95	0.14	9,10,11,11	13
2	CYT	F	304	8/8	0.96	0.07	5,6,8,9	0
2	CYT	D	302	8/8	0.97	0.09	7,8,10,10	13
8	EDO	E	305	4/4	0.97	0.12	7,13,15,15	10
8	EDO	F	305	4/4	0.97	0.12	8,14,16,16	10
3	GOL	B	301[B]	6/6	0.98	0.09	18,21,24,24	14
4	MG	A	305	1/1	0.98	0.18	24,24,24,24	1
4	MG	B	303	1/1	0.98	0.10	22,22,22,22	1
4	MG	E	303	1/1	0.98	0.09	9,9,9,9	1
3	GOL	B	301[A]	6/6	0.98	0.09	11,12,14,15	14
5	NA	E	306	1/1	0.99	0.12	7,7,7,7	1
2	CYT	E	304	8/8	0.99	0.04	5,6,8,8	0
2	CYT	C	302	8/8	0.99	0.04	4,5,7,7	0
2	CYT	B	304	8/8	0.99	0.04	5,5,7,7	0
4	MG	F	302	1/1	0.99	0.06	13,13,13,13	1
4	MG	F	303	1/1	0.99	0.07	9,9,9,9	1
5	NA	A	306	1/1	0.99	0.10	8,8,8,8	1
6	CL	B	302	1/1	1.00	0.03	10,10,10,10	1
6	CL	C	301	1/1	1.00	0.03	10,10,10,10	1
5	NA	C	304	1/1	1.00	0.09	8,8,8,8	1
4	MG	E	301	1/1	1.00	0.04	12,12,12,12	1

6.5 Other polymers (i)

There are no such residues in this entry.