



# wwPDB X-ray Structure Validation Summary Report

Mar 10, 2026 – 03:29 AM UTC

PDB ID : 5C80 / pdb\_00005c80  
Title : X-ray structure uridine phosphorylase from *Vibrio cholerae* in complex with uridine at 2.24 Å resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2015-06-25  
Resolution : 2.24 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](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

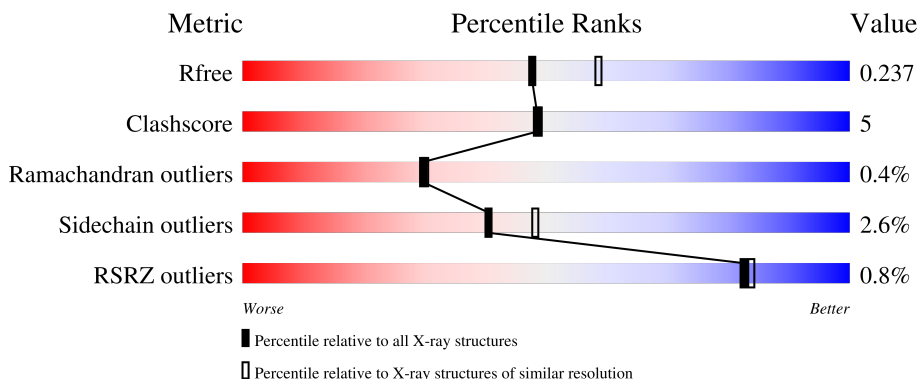
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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))
$R_{free}$	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	 82% 16% ..
1	B	253	 88% 11%
1	C	253	 83% 15% .
1	D	253	 88% 10% ..
1	E	253	 85% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	253	 85% 14% ..

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
3	TRS	C	302[A]	-	X	-	-
3	TRS	F	303[A]	-	X	-	-
3	TRS	F	303[B]	-	X	-	-

## 2 Entry composition [i](#)

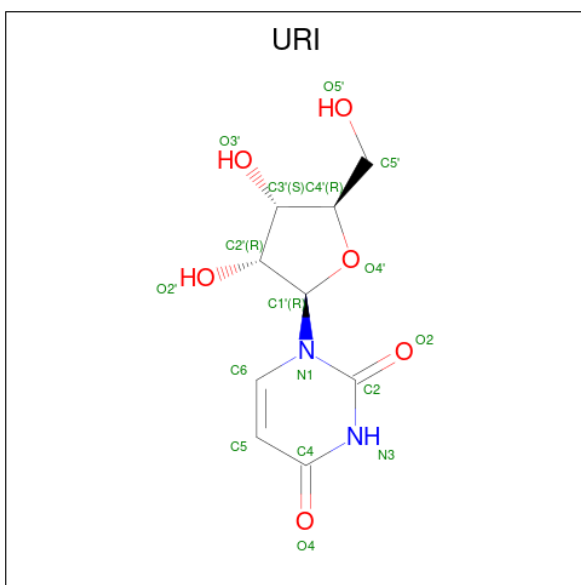
There are 8 unique types of molecules in this entry. The entry contains 12408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

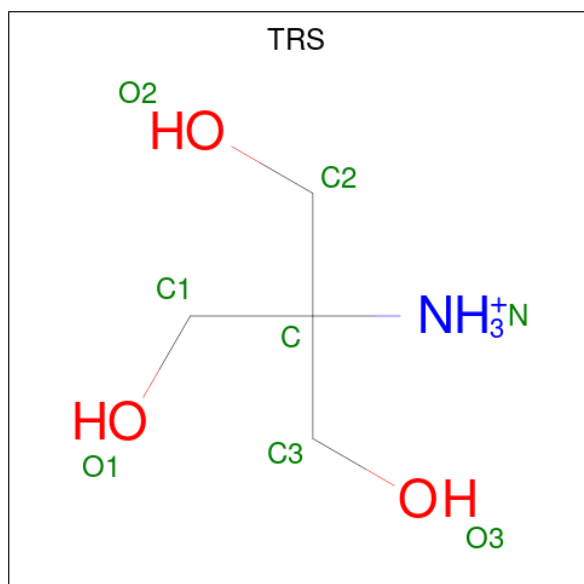
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 1893	C 1186	N 330	O 364	S 13	0	2	0
1	B	252	Total 1886	C 1181	N 328	O 364	S 13	0	0	0
1	C	251	Total 1882	C 1179	N 327	O 362	S 14	0	1	0
1	D	249	Total 1880	C 1180	N 327	O 359	S 14	0	3	0
1	E	251	Total 1879	C 1177	N 327	O 362	S 13	0	0	0
1	F	251	Total 1897	C 1188	N 333	O 363	S 13	0	2	0

- Molecule 2 is URIDINE (CCD ID: 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	N	O	0	0
			17	9	2	6		
2	B	1	Total	C	N	O	0	0
			17	9	2	6		
2	C	1	Total	C	N	O	0	0
			17	9	2	6		
2	D	1	Total	C	N	O	0	0
			17	9	2	6		
2	E	1	Total	C	N	O	0	0
			17	9	2	6		
2	F	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



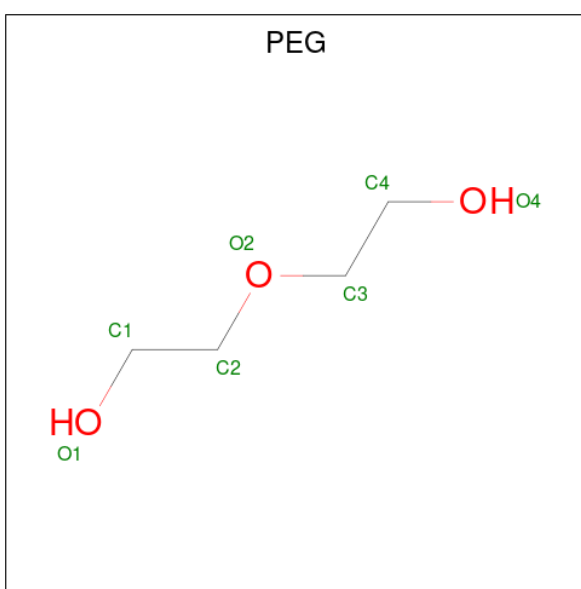
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			16	8	2	6		
3	B	1	Total	C	N	O	0	1
			16	8	2	6		
3	C	1	Total	C	N	O	0	1
			16	8	2	6		
3	D	1	Total	C	N	O	0	1
			16	8	2	6		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	1
			16	8	2	6		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		
3	F	1	Total	C	N	O	0	1
			16	8	2	6		
3	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

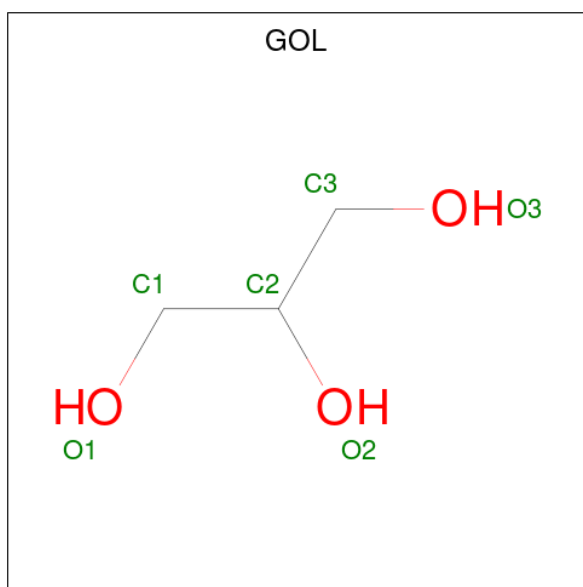
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0

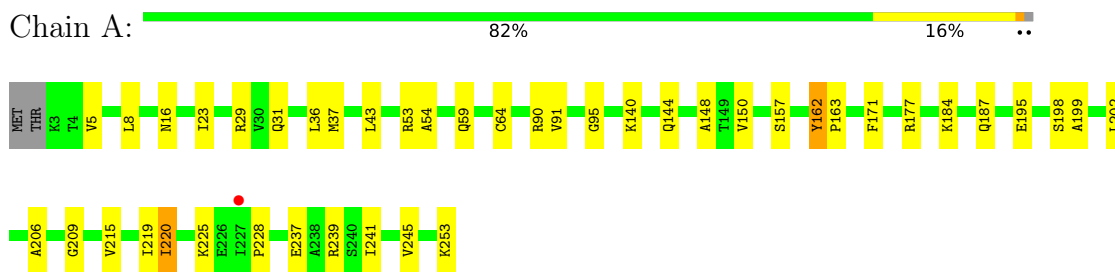
- Molecule 8 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	A	136	Total 136	O 136	0	0
8	B	141	Total 141	O 141	0	0
8	C	129	Total 129	O 129	0	0
8	D	134	Total 134	O 134	0	0
8	E	134	Total 134	O 134	0	0
8	F	148	Total 148	O 148	0	0

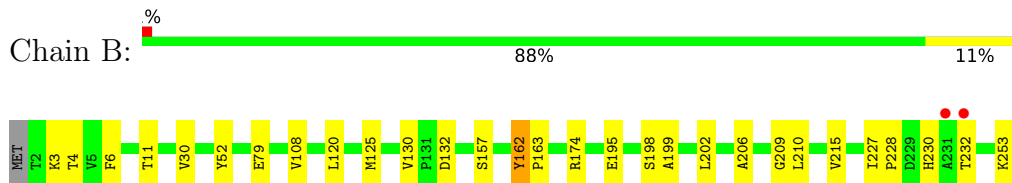
### 3 Residue-property plots [i](#)

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.

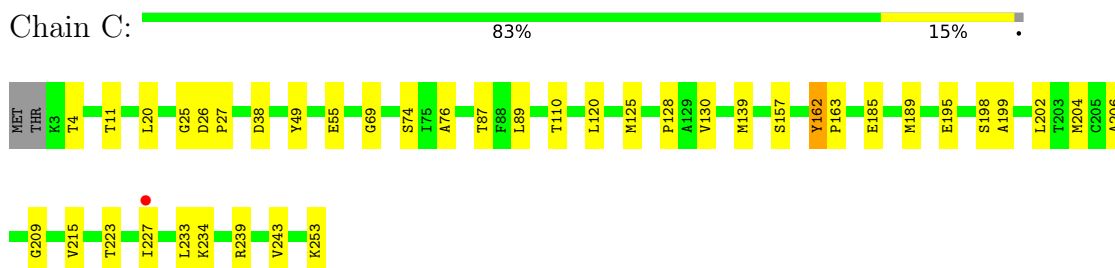
- Molecule 1: Uridine phosphorylase



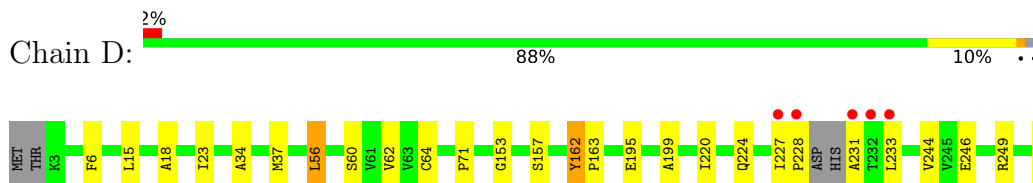
- Molecule 1: Uridine phosphorylase



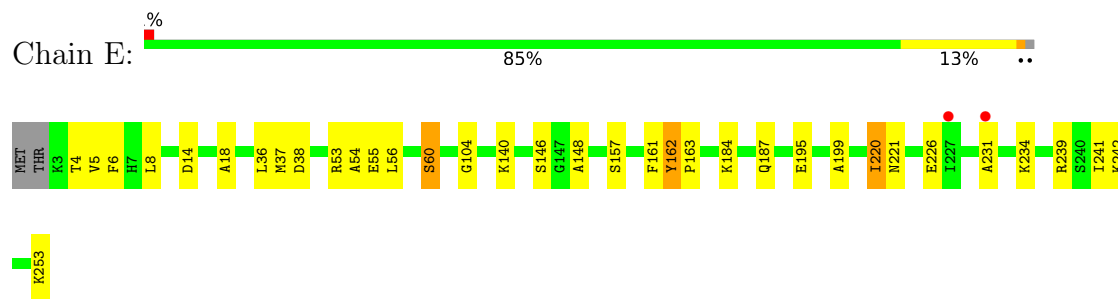
- Molecule 1: Uridine phosphorylase



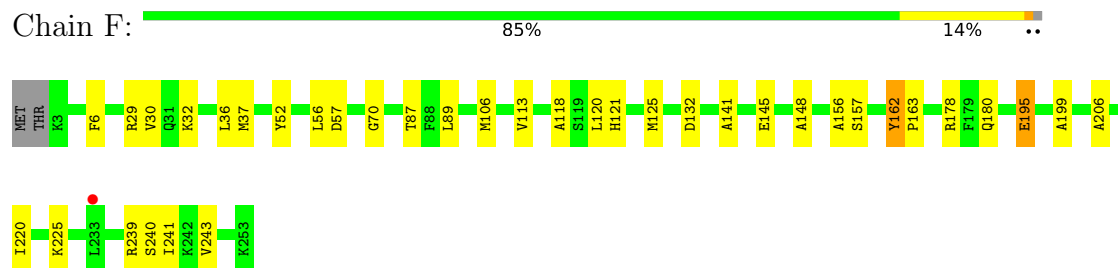
- Molecule 1: Uridine phosphorylase



- 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, $\alpha$ , $\beta$ , $\gamma$	61.26Å 73.11Å 83.14Å 71.81° 77.19° 85.69°	Depositor
Resolution (Å)	45.47 – 2.24 45.47 – 2.24	Depositor EDS
% Data completeness (in resolution range)	90.9 (45.47-2.24) 90.9 (45.47-2.24)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.168 , 0.237 0.169 , 0.237	Depositor DCC
$R_{free}$ test set	2849 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: URI, CL, TRS, PEG, NA, GOL

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	0.64	0/1930	0.95	0/2615
1	B	0.68	0/1917	0.93	2/2599 (0.1%)
1	C	0.67	0/1916	0.97	1/2597 (0.0%)
1	D	0.65	0/1916	0.91	2/2594 (0.1%)
1	E	0.62	0/1910	0.92	2/2589 (0.1%)
1	F	0.68	1/1932 (0.1%)	0.95	1/2618 (0.0%)
All	All	0.66	1/11521 (0.0%)	0.94	8/15612 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	70	GLY	N-CA	5.22	1.49	1.44

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	PHE	N-CA-C	6.78	118.32	111.07
1	E	161	PHE	N-CA-C	-6.33	105.69	113.41
1	D	153	GLY	N-CA-C	6.23	118.55	110.45
1	B	230	HIS	N-CA-C	6.23	118.15	111.36
1	B	6	PHE	N-CA-C	5.77	117.24	111.07

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	1893	0	1902	30	0
1	B	1886	0	1890	14	0
1	C	1882	0	1888	22	0
1	D	1880	0	1895	15	0
1	E	1879	0	1883	16	0
1	F	1897	0	1902	22	0
2	A	17	0	12	1	0
2	B	17	0	12	1	0
2	C	17	0	12	1	0
2	D	17	0	12	1	0
2	E	17	0	12	1	0
2	F	17	0	12	1	0
3	A	16	0	24	2	0
3	B	16	0	24	4	0
3	C	16	0	24	1	0
3	D	24	0	36	2	0
3	E	16	0	24	0	0
3	F	32	0	48	2	0
4	A	7	0	10	1	0
4	B	7	0	10	2	0
4	C	7	0	10	2	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	B	6	0	8	0	0
6	D	6	0	8	0	0
6	F	6	0	8	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
8	A	136	0	0	2	0
8	B	141	0	0	2	0
8	C	129	0	0	4	0
8	D	134	0	0	1	0
8	E	134	0	0	5	0
8	F	148	0	0	3	0
All	All	12408	0	11666	127	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 5.

The worst 5 of 127 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:206:ALA:HA	3:A:302[A]:TRS:H31	1.55	0.87
1:F:206:ALA:HA	3:F:303[A]:TRS:H11	1.56	0.86
1:A:148:ALA:HB2	1:A:239:ARG:HD3	1.60	0.82
3:B:302[A]:TRS:O3	8:B:401:HOH:O	1.97	0.81
1:A:29:ARG:HE	1:A:237:GLU:HG3	1.46	0.80

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	251/253 (99%)	245 (98%)	5 (2%)	1 (0%)	30	30
1	B	250/253 (99%)	240 (96%)	9 (4%)	1 (0%)	30	30
1	C	250/253 (99%)	244 (98%)	5 (2%)	1 (0%)	30	30
1	D	248/253 (98%)	238 (96%)	9 (4%)	1 (0%)	30	30
1	E	249/253 (98%)	246 (99%)	2 (1%)	1 (0%)	30	30
1	F	251/253 (99%)	246 (98%)	4 (2%)	1 (0%)	30	30
All	All	1499/1518 (99%)	1459 (97%)	34 (2%)	6 (0%)	30	30

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	TYR
1	D	162	TYR
1	E	162	TYR
1	A	162	TYR
1	B	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	203/203 (100%)	197 (97%)	6 (3%)	36	43
1	B	202/203 (100%)	197 (98%)	5 (2%)	42	50
1	C	202/203 (100%)	197 (98%)	5 (2%)	42	50
1	D	202/203 (100%)	197 (98%)	5 (2%)	42	50
1	E	201/203 (99%)	194 (96%)	7 (4%)	32	37
1	F	203/203 (100%)	200 (98%)	3 (2%)	57	66
All	All	1213/1218 (100%)	1182 (97%)	31 (3%)	40	48

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	234	LYS
1	E	253	LYS
1	D	195	GLU
1	F	57	ASP
1	E	220	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	100	HIS
1	E	180	GLN
1	F	187	GLN
1	B	31	GLN
1	C	59	GLN

### 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](#)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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
4	PEG	C	303	-	6,6,6	0.46	0	5,5,5	0.45	0
6	GOL	D	304	-	5,5,5	0.52	0	5,5,5	0.47	0
3	TRS	D	303	-	7,7,7	0.40	0	9,9,9	1.23	1 (11%)
3	TRS	A	302[B]	-	7,7,7	0.33	0	9,9,9	0.49	0
6	GOL	F	305	-	5,5,5	0.46	0	5,5,5	0.45	0
2	URI	F	301	-	18,18,18	1.15	1 (5%)	26,26,26	2.17	11 (42%)
3	TRS	F	304	-	7,7,7	0.44	0	9,9,9	1.19	1 (11%)
3	TRS	B	302[A]	-	7,7,7	0.50	0	9,9,9	0.85	0
3	TRS	E	302[A]	-	7,7,7	0.41	0	9,9,9	0.68	0
2	URI	E	301	-	18,18,18	1.20	3 (16%)	26,26,26	2.27	9 (34%)
2	URI	C	301	-	18,18,18	1.26	2 (11%)	26,26,26	2.31	10 (38%)
3	TRS	F	303[B]	-	7,7,7	0.43	0	9,9,9	5.32	6 (66%)
3	TRS	A	302[A]	-	7,7,7	0.47	0	9,9,9	1.18	1 (11%)
2	URI	A	301	-	18,18,18	1.32	2 (11%)	26,26,26	2.24	12 (46%)
2	URI	B	301	-	18,18,18	1.20	1 (5%)	26,26,26	2.14	10 (38%)
3	TRS	C	302[B]	-	7,7,7	0.38	0	9,9,9	0.44	0
3	TRS	F	302	-	7,7,7	0.43	0	9,9,9	0.89	0
3	TRS	F	303[A]	-	7,7,7	0.31	0	9,9,9	5.47	6 (66%)
3	TRS	D	302[B]	-	7,7,7	0.48	0	9,9,9	0.99	0
4	PEG	A	303	-	6,6,6	0.41	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	303	-	5,5,5	0.23	0	5,5,5	0.43	0
4	PEG	B	304	-	6,6,6	0.36	0	5,5,5	0.50	0
3	TRS	C	302[A]	-	7,7,7	0.46	0	9,9,9	5.54	6 (66%)
3	TRS	D	302[A]	-	7,7,7	0.33	0	9,9,9	0.48	0
2	URI	D	301	-	18,18,18	1.07	1 (5%)	26,26,26	2.24	9 (34%)
3	TRS	B	302[B]	-	7,7,7	0.44	0	9,9,9	0.77	0
3	TRS	E	302[B]	-	7,7,7	0.37	0	9,9,9	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	C	303	-	-	2/4/4/4	-
6	GOL	D	304	-	-	2/4/4/4	-
3	TRS	D	303	-	-	3/9/9/9	-
3	TRS	A	302[B]	-	-	3/9/9/9	-
6	GOL	F	305	-	-	2/4/4/4	-
2	URI	F	301	-	-	4/6/22/22	0/2/2/2
3	TRS	F	304	-	-	3/9/9/9	-
3	TRS	B	302[A]	-	-	6/9/9/9	-
3	TRS	E	302[A]	-	-	8/9/9/9	-
2	URI	E	301	-	-	4/6/22/22	0/2/2/2
2	URI	C	301	-	-	3/6/22/22	0/2/2/2
3	TRS	F	303[B]	-	-	6/9/9/9	-
3	TRS	A	302[A]	-	-	5/9/9/9	-
2	URI	A	301	-	-	2/6/22/22	0/2/2/2
2	URI	B	301	-	-	4/6/22/22	0/2/2/2
3	TRS	C	302[B]	-	-	8/9/9/9	-
3	TRS	F	302	-	-	5/9/9/9	-
3	TRS	F	303[A]	-	-	6/9/9/9	-
3	TRS	D	302[B]	-	-	3/9/9/9	-
4	PEG	A	303	-	-	3/4/4/4	-
6	GOL	B	303	-	-	0/4/4/4	-
4	PEG	B	304	-	-	3/4/4/4	-
3	TRS	C	302[A]	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	D	302[A]	-	-	3/9/9/9	-
2	URI	D	301	-	-	4/6/22/22	0/2/2/2
3	TRS	B	302[B]	-	-	8/9/9/9	-
3	TRS	E	302[B]	-	-	0/9/9/9	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	URI	C4-N3	-2.69	1.34	1.38
2	C	301	URI	C2-N1	2.63	1.42	1.38
2	A	301	URI	C2-N1	2.60	1.42	1.38
2	D	301	URI	C2-N1	2.50	1.42	1.38
2	C	301	URI	C4-N3	-2.48	1.34	1.38

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302[A]	TRS	C3-C-N	-9.87	83.00	108.17
3	F	303[B]	TRS	C1-C-N	-9.30	84.46	108.17
3	F	303[A]	TRS	C2-C-N	-9.15	84.83	108.17
3	F	303[A]	TRS	C1-C-N	-8.71	85.96	108.17
3	F	303[A]	TRS	C3-C-N	-8.66	86.09	108.17

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	URI	C2'-C1'-N1-C2
2	D	301	URI	C2'-C1'-N1-C2
3	A	302[A]	TRS	C2-C-C1-O1
3	A	302[A]	TRS	C3-C-C1-O1
3	A	302[B]	TRS	C2-C-C1-O1

There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	PEG	2	0
3	A	302[B]	TRS	1	0
2	F	301	URI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302[A]	TRS	3	0
2	E	301	URI	1	0
2	C	301	URI	1	0
3	F	303[B]	TRS	1	0
3	A	302[A]	TRS	1	0
2	A	301	URI	1	0
2	B	301	URI	1	0
3	F	303[A]	TRS	1	0
3	D	302[B]	TRS	1	0
4	A	303	PEG	1	0
4	B	304	PEG	2	0
3	C	302[A]	TRS	1	0
3	D	302[A]	TRS	1	0
2	D	301	URI	1	0
3	B	302[B]	TRS	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%)	-0.21	1 (0%) 88 90	13, 27, 55, 78	2 (0%)
1	B	252/253 (99%)	-0.30	2 (0%) 82 84	15, 25, 54, 90	0
1	C	251/253 (99%)	-0.25	1 (0%) 88 90	15, 26, 51, 77	1 (0%)
1	D	249/253 (98%)	-0.18	5 (2%) 65 66	12, 27, 52, 95	3 (1%)
1	E	251/253 (99%)	-0.07	2 (0%) 82 84	18, 30, 58, 97	0
1	F	251/253 (99%)	-0.33	1 (0%) 88 90	9, 25, 45, 86	2 (0%)
All	All	1505/1518 (99%)	-0.23	12 (0%) 82 84	9, 27, 55, 97	8 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	LEU	3.7
1	E	227	ILE	3.5
1	D	227	ILE	3.3
1	F	233	LEU	3.2
1	D	228	PRO	3.2

### 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 oligosaccharides 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	TRS	E	302[A]	8/8	0.79	0.12	13,14,15,16	8
3	TRS	E	302[B]	8/8	0.79	0.12	23,25,26,26	8
6	GOL	F	305	6/6	0.79	0.13	44,47,50,53	0
6	GOL	B	303	6/6	0.82	0.12	55,55,56,56	0
3	TRS	F	304	8/8	0.85	0.09	30,31,32,32	0
6	GOL	D	304	6/6	0.88	0.11	25,27,27,28	0
4	PEG	B	304	7/7	0.88	0.11	42,46,47,49	0
3	TRS	C	302[A]	8/8	0.89	0.11	10,11,12,12	8
3	TRS	C	302[B]	8/8	0.89	0.11	15,16,16,17	8
3	TRS	B	302[A]	8/8	0.89	0.10	7,7,7,7	8
3	TRS	B	302[B]	8/8	0.89	0.10	9,10,10,10	8
3	TRS	F	302	8/8	0.89	0.08	29,31,31,31	0
3	TRS	A	302[A]	8/8	0.90	0.10	7,7,7,7	8
3	TRS	A	302[B]	8/8	0.90	0.10	15,15,15,16	8
3	TRS	D	302[B]	8/8	0.91	0.11	14,15,15,16	8
3	TRS	D	302[A]	8/8	0.91	0.11	21,22,22,23	8
4	PEG	C	303	7/7	0.91	0.10	36,38,40,41	0
3	TRS	F	303[A]	8/8	0.92	0.10	8,9,9,9	8
3	TRS	F	303[B]	8/8	0.92	0.10	15,16,16,16	8
3	TRS	D	303	8/8	0.93	0.08	22,24,25,28	0
2	URI	D	301	17/17	0.93	0.07	25,26,28,32	0
4	PEG	A	303	7/7	0.94	0.08	44,45,47,50	0
2	URI	A	301	17/17	0.94	0.07	21,23,27,30	0
2	URI	C	301	17/17	0.94	0.07	19,23,25,26	0
5	CL	A	304	1/1	0.95	0.08	41,41,41,41	0
2	URI	B	301	17/17	0.95	0.06	27,29,37,37	0
2	URI	E	301	17/17	0.95	0.07	24,26,30,34	0
2	URI	F	301	17/17	0.95	0.07	24,27,33,41	0
5	CL	C	304	1/1	0.96	0.09	56,56,56,56	0
5	CL	B	305	1/1	0.96	0.06	45,45,45,45	0
7	NA	F	307	1/1	0.96	0.06	36,36,36,36	0
5	CL	D	305	1/1	0.97	0.05	55,55,55,55	0
5	CL	F	306	1/1	0.97	0.08	44,44,44,44	0
7	NA	B	306	1/1	0.98	0.05	26,26,26,26	0
5	CL	A	305	1/1	0.98	0.07	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.