



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 11:55 AM EST

PDB ID : 4OEH
Title : X-ray Structure of Uridine Phosphorylase from *Vibrio cholerae* Complexed with Uracil at 1.91 Å Resolution
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.
Deposited on : 2014-01-13
Resolution : 1.91 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

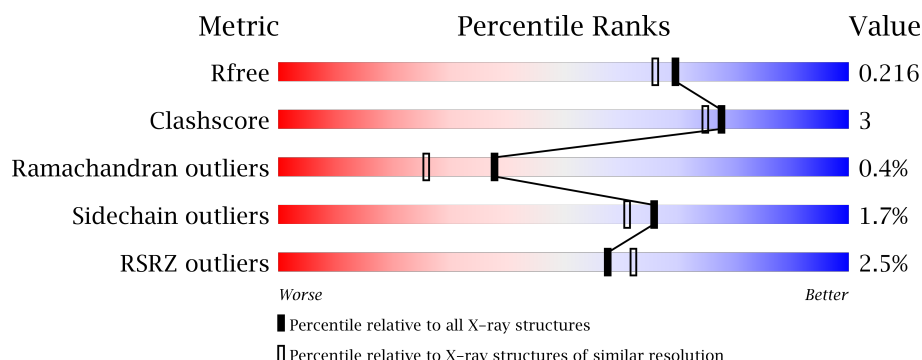
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>0.1%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	B	253	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	C	253	<div> <div>5%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	253	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	E	253	<div> <div>92%</div> <div>6%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

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
3	GOL	B	302	-	-	-	X
3	GOL	D	301	-	-	-	X
3	GOL	E	302	-	-	-	X
3	GOL	F	302	-	-	-	X
3	GOL	F	303	-	-	-	X
4	EDO	C	302	-	-	X	X
4	EDO	C	303	-	-	-	X
6	PEG	B	303	-	-	X	X
7	NA	F	305	-	-	-	X

2 Entry composition [i](#)

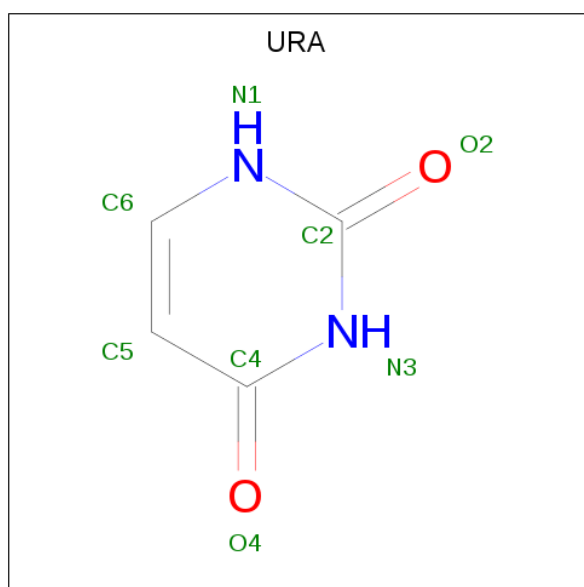
There are 8 unique types of molecules in this entry. The entry contains 12849 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	251	Total	C	N	O	S	0	8	0
			1925	1210	334	368	13			
1	B	252	Total	C	N	O	S	0	6	0
			1922	1203	334	371	14			
1	C	251	Total	C	N	O	S	0	8	0
			1926	1209	336	367	14			
1	D	250	Total	C	N	O	S	0	6	0
			1903	1194	332	364	13			
1	E	251	Total	C	N	O	S	0	5	0
			1896	1190	327	364	15			
1	F	251	Total	C	N	O	S	0	3	0
			1891	1184	328	366	13			

- Molecule 2 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	2	2		
2	B	1	Total	C	N	O	0	0
			8	4	2	2		
2	E	1	Total	C	N	O	0	0
			8	4	2	2		
2	F	1	Total	C	N	O	0	0
			8	4	2	2		

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



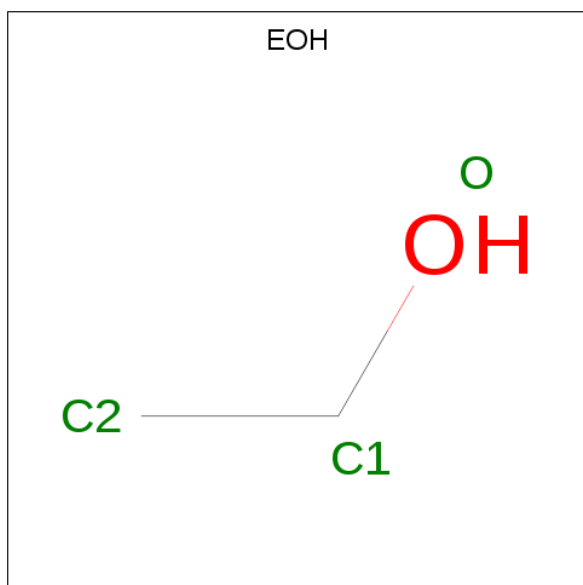
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



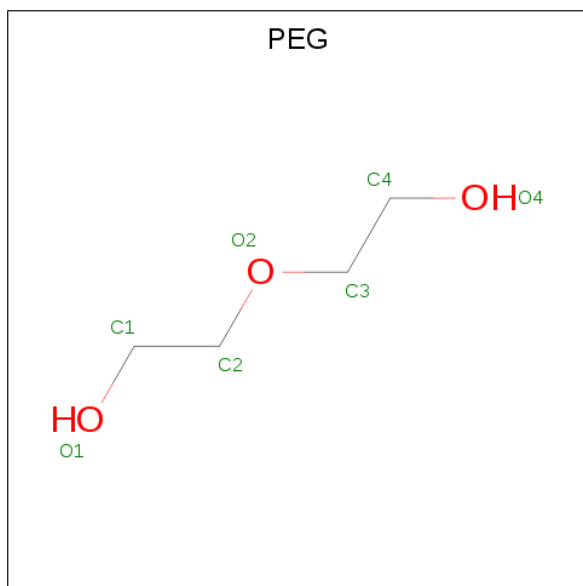
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		
5	D	1	Total	C	O	0	0
			3	2	1		
5	F	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	249	Total 250	O 250	0	1
8	B	196	Total 197	O 197	0	1
8	C	201	Total 201	O 201	0	0
8	D	200	Total 200	O 200	0	0
8	E	219	Total 219	O 219	0	0
8	F	210	Total 210	O 210	0	0

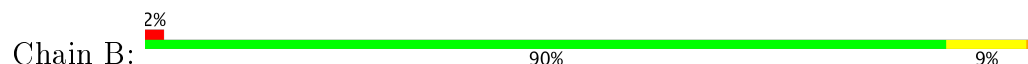
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

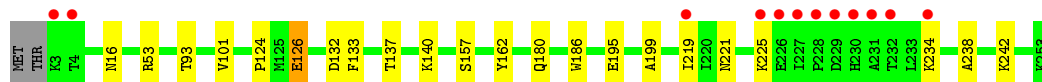
- Molecule 1: Uridine phosphorylase



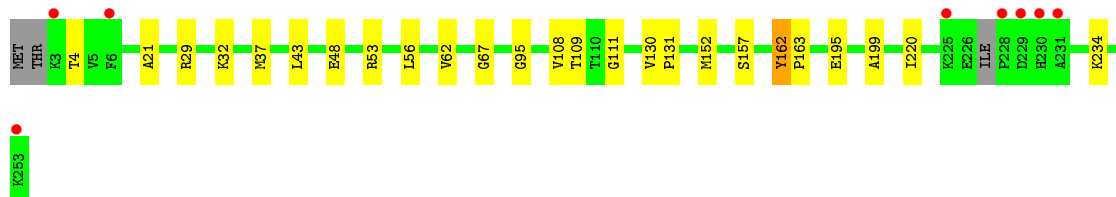
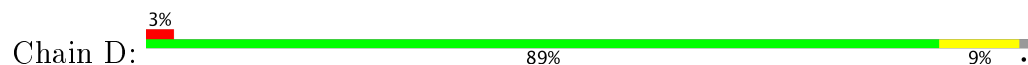
- Molecule 1: Uridine phosphorylase



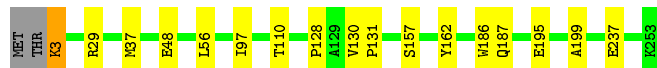
- Molecule 1: Uridine phosphorylase



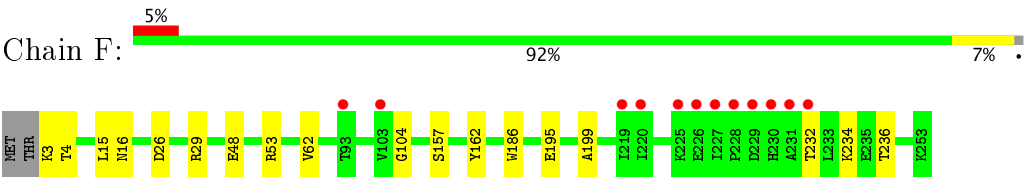
- Molecule 1: Uridine phosphorylase



- 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, α , β , γ	64.25Å 71.76Å 89.32Å 69.14° 72.15° 85.79°	Depositor
Resolution (Å)	44.28 – 1.91 44.28 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.28-1.91) 83.3 (44.28-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.172 , 0.216 0.172 , 0.216	Depositor DCC
R_{free} test set	5184 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12849	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, URA, NA, EOH, EDO, PEG

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	0/1977	0.57	0/2675
1	B	0.43	0/1965	0.57	0/2659
1	C	0.45	1/1976 (0.1%)	0.55	0/2673
1	D	0.45	0/1949	0.55	0/2639
1	E	0.46	1/1942 (0.1%)	0.56	0/2634
1	F	0.45	1/1925 (0.1%)	0.57	0/2612
All	All	0.45	3/11734 (0.0%)	0.56	0/15892

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	186	TRP	CD2-CE2	5.48	1.48	1.41
1	E	186	TRP	CD2-CE2	5.47	1.48	1.41
1	C	186	TRP	CD2-CE2	5.29	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1925	0	1959	9	0
1	B	1922	0	1930	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1926	0	1947	14	0
1	D	1903	0	1916	24	0
1	E	1896	0	1908	18	0
1	F	1891	0	1890	10	0
2	A	8	0	3	0	0
2	B	8	0	3	0	0
2	E	8	0	3	0	0
2	F	8	0	3	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	12	0	16	0	0
4	A	4	0	6	0	0
4	C	8	0	12	5	0
4	E	4	0	6	0	0
5	A	3	0	6	0	0
5	D	3	0	6	0	0
5	F	3	0	6	0	0
6	B	7	0	10	5	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	A	250	0	0	1	0
8	B	197	0	0	3	0
8	C	201	0	0	0	0
8	D	200	0	0	0	0
8	E	219	0	0	0	0
8	F	210	0	0	1	0
All	All	12849	0	11670	79	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 3.

All (79) 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:D:53[B]:ARG:NH1	1:D:53[B]:ARG:HB2	1.64	1.09
1:D:53[B]:ARG:HH11	1:D:53[B]:ARG:HB2	1.22	1.01
1:B:242[B]:LYS:HA	1:B:242[B]:LYS:HE2	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:303:PEG:H42	8:B:480:HOH:O	1.60	0.98
1:D:130[B]:VAL:CG2	1:E:130[B]:VAL:CG2	2.51	0.88
1:D:130[B]:VAL:HG22	1:E:130[B]:VAL:HG21	1.60	0.82
1:D:53[B]:ARG:CB	1:D:53[B]:ARG:HH11	1.96	0.79
1:C:132:ASP:HA	4:C:302:EDO:H11	1.67	0.77
1:E:128:PRO:HB2	1:E:130[A]:VAL:HG13	1.74	0.69
1:B:137:THR:HG23	6:B:303:PEG:H32	1.73	0.69
1:D:130[B]:VAL:HG22	1:E:130[B]:VAL:CG2	2.20	0.68
1:D:130[B]:VAL:CG2	1:E:130[B]:VAL:HG21	2.17	0.68
1:C:238:ALA:O	1:C:242:LYS:HG2	1.94	0.67
8:B:565:HOH:O	1:C:140:LYS:HE2	1.94	0.67
6:B:303:PEG:H41	1:C:137:THR:CG2	2.24	0.66
6:B:303:PEG:H41	1:C:137:THR:HG23	1.77	0.66
1:A:3:LYS:HE2	8:A:614:HOH:O	1.96	0.65
1:A:148:ALA:HB2	1:A:239:ARG:HD3	1.80	0.64
1:E:29:ARG:NH1	1:E:237:GLU:HG2	2.13	0.63
1:C:93:THR:HB	1:C:219:ILE:HG12	1.81	0.63
1:F:104:GLY:HA2	1:F:236:THR:CG2	2.29	0.62
1:A:15:LEU:HG	1:A:62:VAL:HG21	1.82	0.61
1:D:37:MET:HG2	1:D:56:LEU:HD13	1.82	0.61
1:F:16:ASN:HB2	1:F:53:ARG:HD2	1.82	0.60
1:D:130[B]:VAL:HG21	1:E:130[B]:VAL:HG22	1.85	0.58
1:B:37:MET:HG2	1:B:56:LEU:HD13	1.84	0.58
1:D:130[B]:VAL:CG2	1:E:130[B]:VAL:HG22	2.32	0.58
1:B:242[B]:LYS:CA	1:B:242[B]:LYS:HE2	2.28	0.58
1:E:3:LYS:HD2	1:E:3:LYS:N	2.20	0.56
1:D:130[A]:VAL:HG21	1:E:110:THR:O	2.06	0.56
1:D:130[B]:VAL:HG21	1:E:130[B]:VAL:CG2	2.34	0.55
1:D:53[B]:ARG:CB	1:D:53[B]:ARG:NH1	2.55	0.55
1:F:104:GLY:HA2	1:F:236:THR:HG21	1.89	0.54
1:A:37:MET:HG2	1:A:56:LEU:HD13	1.90	0.53
1:F:3:LYS:HG2	8:F:480:HOH:O	2.06	0.53
1:C:132:ASP:HA	4:C:302:EDO:C1	2.38	0.52
1:F:232:THR:O	1:F:236:THR:HG23	2.10	0.51
1:B:110:THR:HG21	4:C:302:EDO:H22	1.92	0.51
1:B:29[B]:ARG:NH1	1:B:237:GLU:HB3	2.26	0.51
1:C:133:PHE:HB2	4:C:302:EDO:H22	1.92	0.51
1:F:15:LEU:HG	1:F:62:VAL:HG21	1.93	0.50
1:C:16:ASN:HB2	1:C:53:ARG:HD2	1.94	0.50
1:A:15:LEU:HG	1:A:62:VAL:CG2	2.42	0.49
1:B:214[B]:CYS:SG	8:B:515:HOH:O	2.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53[B]:ARG:CZ	1:D:53[B]:ARG:HB2	2.37	0.49
1:B:137:THR:HG23	6:B:303:PEG:C3	2.40	0.49
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.95	0.49
1:F:104:GLY:HA2	1:F:236:THR:HG22	1.93	0.49
1:D:29:ARG:HH11	1:D:32:LYS:HD3	1.78	0.49
1:E:48:GLU:HB3	1:F:48:GLU:HB3	1.94	0.48
1:E:37:MET:HG2	1:E:56:LEU:HD13	1.96	0.48
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.96	0.47
1:C:124:PRO:HB2	1:C:126[B]:GLU:OE1	2.15	0.47
1:A:177:ARG:NH2	1:C:180:GLN:O	2.48	0.47
1:A:48:GLU:HB3	1:B:48:GLU:HB3	1.97	0.46
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.98	0.46
1:F:26:ASP:HB3	1:F:29:ARG:HG2	1.97	0.46
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.98	0.45
1:B:252:LEU:O	1:B:253:LYS:HB3	2.16	0.45
1:C:132:ASP:CA	4:C:302:EDO:H11	2.44	0.44
1:A:234[B]:LYS:HD3	1:A:234[B]:LYS:HA	1.58	0.44
1:D:108:VAL:HB	1:D:152:MET:SD	2.57	0.44
1:B:29[B]:ARG:HA	1:B:32:LYS:HD2	2.00	0.44
1:D:43:LEU:HD21	1:D:53[A]:ARG:HD3	2.00	0.43
1:B:227:ILE:HA	1:B:228:PRO:HD3	1.90	0.43
1:A:157:SER:HB3	1:A:199:ALA:HB2	2.01	0.42
1:C:101:VAL:O	1:C:221:ASN:ND2	2.52	0.42
1:E:130[B]:VAL:HG13	1:E:131:PRO:HD2	2.02	0.42
1:D:48:GLU:HG3	1:D:67:GLY:HA3	2.00	0.41
1:D:21:ALA:HB2	1:D:62[A]:VAL:HG13	2.01	0.41
1:E:97:ILE:HD12	1:E:187[A]:GLN:HG3	2.01	0.41
1:D:95:GLY:HA2	1:D:220:ILE:O	2.21	0.41
1:E:128:PRO:HB2	1:E:130[A]:VAL:CG1	2.47	0.41
1:D:157:SER:HB3	1:D:199:ALA:HB2	2.01	0.41
1:B:106:MET:HG3	1:B:148:ALA:HB1	2.02	0.41
1:D:111:GLY:HA3	1:E:130[A]:VAL:HG11	2.04	0.40
1:D:162:TYR:HB2	1:D:163:PRO:CD	2.51	0.40
1:B:21:ALA:HA	1:B:62:VAL:O	2.21	0.40
1:D:109:THR:O	1:D:131:PRO:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	257/253 (102%)	254 (99%)	2 (1%)	1 (0%)	38	26
1	B	256/253 (101%)	253 (99%)	2 (1%)	1 (0%)	38	26
1	C	256/253 (101%)	250 (98%)	5 (2%)	1 (0%)	38	26
1	D	252/253 (100%)	248 (98%)	3 (1%)	1 (0%)	38	26
1	E	254/253 (100%)	250 (98%)	3 (1%)	1 (0%)	38	26
1	F	252/253 (100%)	248 (98%)	3 (1%)	1 (0%)	38	26
All	All	1527/1518 (101%)	1503 (98%)	18 (1%)	6 (0%)	38	26

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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	209/203 (103%)	207 (99%)	2 (1%)	80	79
1	B	207/203 (102%)	201 (97%)	6 (3%)	48	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	208/203 (102%)	202 (97%)	6 (3%)	48	37
1	D	205/203 (101%)	202 (98%)	3 (2%)	70	66
1	E	205/203 (101%)	203 (99%)	2 (1%)	80	79
1	F	203/203 (100%)	200 (98%)	3 (2%)	70	66
All	All	1237/1218 (102%)	1215 (98%)	22 (2%)	66	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	237	GLU
1	B	3	LYS
1	B	16	ASN
1	B	106	MET
1	B	195	GLU
1	B	233	LEU
1	B	253	LYS
1	C	126[A]	GLU
1	C	126[B]	GLU
1	C	195	GLU
1	C	225[A]	LYS
1	C	225[B]	LYS
1	C	234	LYS
1	D	4	THR
1	D	195	GLU
1	D	234	LYS
1	E	3	LYS
1	E	195	GLU
1	F	4	THR
1	F	195	GLU
1	F	234	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	144	GLN
1	A	230	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	URA	A	301	-	6,8,8	1.07	0	5,10,10	8.64	4 (80%)
3	GOL	A	302	-	5,5,5	0.27	0	5,5,5	0.28	0
4	EDO	A	303	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EOH	A	304	-	2,2,2	0.42	0	1,1,1	0.35	0
2	URA	B	301	-	6,8,8	0.92	0	5,10,10	8.81	4 (80%)
3	GOL	B	302	-	5,5,5	0.36	0	5,5,5	0.07	0
6	PEG	B	303	-	6,6,6	0.38	0	5,5,5	0.54	0
3	GOL	C	301	-	5,5,5	0.21	0	5,5,5	0.34	0
4	EDO	C	302	-	3,3,3	0.30	0	2,2,2	0.70	0
4	EDO	C	303	-	3,3,3	0.51	0	2,2,2	0.33	0
3	GOL	D	301	-	5,5,5	0.33	0	5,5,5	0.28	0
5	EOH	D	302	-	2,2,2	0.41	0	1,1,1	0.35	0
2	URA	E	301	-	6,8,8	1.16	0	5,10,10	8.93	4 (80%)
3	GOL	E	302	-	5,5,5	0.38	0	5,5,5	0.14	0
4	EDO	E	303	-	3,3,3	0.51	0	2,2,2	0.24	0
2	URA	F	301	-	6,8,8	1.00	0	5,10,10	8.92	4 (80%)
3	GOL	F	302	-	5,5,5	0.30	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	303	-	5,5,5	0.30	0	5,5,5	0.35	0
5	EOH	F	304	-	2,2,2	0.41	0	1,1,1	0.34	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	URA	A	301	-	-	0/0/0/0	0/1/1/1
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0
4	EDO	A	303	-	-	0/1/1/1	0/0/0/0
5	EOH	A	304	-	-	0/0/0/0	0/0/0/0
2	URA	B	301	-	-	0/0/0/0	0/1/1/1
3	GOL	B	302	-	-	0/4/4/4	0/0/0/0
6	PEG	B	303	-	-	0/4/4/4	0/0/0/0
3	GOL	C	301	-	-	0/4/4/4	0/0/0/0
4	EDO	C	302	-	-	0/1/1/1	0/0/0/0
4	EDO	C	303	-	-	0/1/1/1	0/0/0/0
3	GOL	D	301	-	-	0/4/4/4	0/0/0/0
5	EOH	D	302	-	-	0/0/0/0	0/0/0/0
2	URA	E	301	-	-	0/0/0/0	0/1/1/1
3	GOL	E	302	-	-	0/4/4/4	0/0/0/0
4	EDO	E	303	-	-	0/1/1/1	0/0/0/0
2	URA	F	301	-	-	0/0/0/0	0/1/1/1
3	GOL	F	302	-	-	0/4/4/4	0/0/0/0
3	GOL	F	303	-	-	0/4/4/4	0/0/0/0
5	EOH	F	304	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	URA	N1-C2-N3	-11.31	120.27	128.40
2	F	301	URA	N1-C2-N3	-10.81	120.63	128.40
2	B	301	URA	N1-C2-N3	-10.74	120.68	128.40
2	A	301	URA	N1-C2-N3	-10.32	120.97	128.40
2	B	301	URA	C5-C6-N1	-4.39	118.86	123.92
2	A	301	URA	C5-C6-N1	-4.33	118.93	123.92
2	F	301	URA	C5-C6-N1	-4.28	118.99	123.92
2	E	301	URA	C5-C6-N1	-3.76	119.58	123.92
2	A	301	URA	C4-N3-C2	7.46	120.54	114.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	URA	C4-N3-C2	7.70	120.74	114.13
2	F	301	URA	C4-N3-C2	7.73	120.77	114.13
2	E	301	URA	C4-N3-C2	8.11	121.09	114.13
2	E	301	URA	C6-N1-C2	13.76	121.06	114.41
2	A	301	URA	C6-N1-C2	13.80	121.08	114.41
2	B	301	URA	C6-N1-C2	13.84	121.10	114.41
2	F	301	URA	C6-N1-C2	14.18	121.26	114.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	PEG	5	0
4	C	302	EDO	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	251/253 (99%)	-0.26	2 (0%) 86 88	12, 19, 31, 49	0
1	B	252/253 (99%)	-0.14	4 (1%) 72 76	12, 20, 38, 68	0
1	C	251/253 (99%)	-0.10	12 (4%) 31 35	13, 21, 39, 64	0
1	D	250/253 (98%)	-0.04	8 (3%) 48 52	14, 22, 40, 74	0
1	E	251/253 (99%)	-0.23	0 100 100	13, 18, 30, 39	0
1	F	251/253 (99%)	-0.11	12 (4%) 31 35	13, 19, 38, 63	0
All	All	1506/1518 (99%)	-0.15	38 (2%) 58 62	12, 20, 36, 74	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	5.6
1	C	227	ILE	5.5
1	D	229	ASP	4.9
1	F	227	ILE	4.5
1	C	230	HIS	4.4
1	F	230	HIS	3.8
1	D	253	LYS	3.8
1	F	229	ASP	3.7
1	C	232	THR	3.7
1	D	228	PRO	3.7
1	C	229	ASP	3.5
1	D	231	ALA	3.5
1	D	230	HIS	3.4
1	C	226	GLU	3.3
1	B	253	LYS	3.1
1	C	225[A]	LYS	3.0
1	C	219	ILE	3.0
1	F	228	PRO	3.0
1	A	253	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	226	GLU	2.8
1	A	230	HIS	2.8
1	C	3[A]	LYS	2.8
1	C	228	PRO	2.8
1	F	231	ALA	2.8
1	B	232	THR	2.8
1	C	231	ALA	2.8
1	D	225	LYS	2.7
1	F	232	THR	2.7
1	F	220	ILE	2.6
1	C	4	THR	2.5
1	B	234	LYS	2.4
1	F	225	LYS	2.4
1	F	93	THR	2.3
1	F	219	ILE	2.3
1	C	234	LYS	2.2
1	D	3	LYS	2.2
1	F	103	VAL	2.2
1	D	6	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
6	PEG	B	303	7/7	0.87	0.28	49.00	24,26,29,30	0
4	EDO	C	303	4/4	0.75	0.19	8.73	42,43,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	F	303	6/6	0.83	0.22	5.25	33,35,36,39	0
3	GOL	B	302	6/6	0.82	0.16	3.63	28,29,30,30	0
4	EDO	C	302	4/4	0.91	0.14	3.09	17,18,19,20	0
7	NA	F	305	1/1	0.97	0.15	2.90	21,21,21,21	1
3	GOL	E	302	6/6	0.86	0.15	2.69	26,27,28,28	0
3	GOL	F	302	6/6	0.62	0.20	2.14	35,38,39,39	0
3	GOL	D	301	6/6	0.90	0.12	2.03	36,37,37,38	0
7	NA	B	304	1/1	0.95	0.15	1.93	35,35,35,35	0
3	GOL	A	302	6/6	0.90	0.12	1.48	28,30,31,32	0
7	NA	D	303	1/1	0.91	0.12	1.22	31,31,31,31	1
2	URA	F	301	8/8	0.91	0.18	0.92	23,27,28,28	0
2	URA	A	301	8/8	0.94	0.09	-0.05	17,18,18,19	0
3	GOL	C	301	6/6	0.92	0.08	-0.44	31,32,34,34	0
5	EOH	F	304	3/3	0.93	0.09	-0.74	38,38,38,38	0
2	URA	B	301	8/8	0.96	0.07	-1.20	15,15,15,15	0
2	URA	E	301	8/8	0.98	0.06	-1.59	11,12,12,12	0
4	EDO	A	303	4/4	0.74	0.21	-	49,49,49,50	0
4	EDO	E	303	4/4	0.88	0.14	-	40,41,41,41	0
5	EOH	A	304	3/3	0.92	0.12	-	41,41,43,43	0
5	EOH	D	302	3/3	0.84	0.17	-	47,47,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.