



# Full wwPDB X-ray Structure Validation Report

Feb 19, 2024 – 03:55 AM EST

PDB ID : 4IP0  
Title : X-Ray Structure of the Complex Uridine Phosphorylase from *Vibrio cholerae* with Phosphate Ion at 1.29 Å Resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2013-01-09  
Resolution : 1.29 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 : 1.8.5 (274361), 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

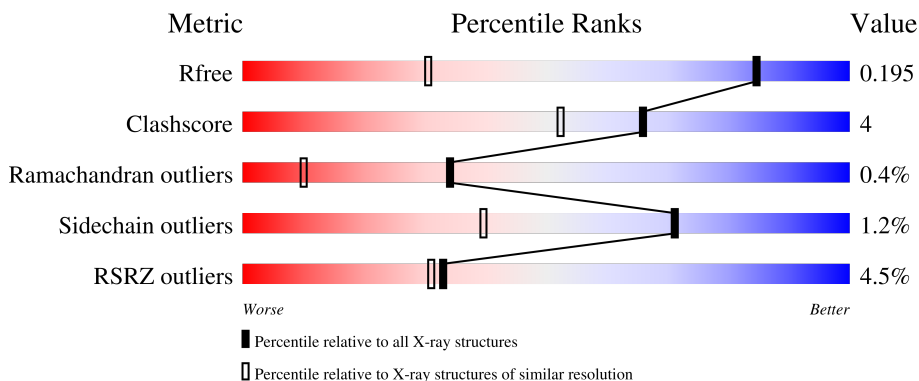
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.29 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.



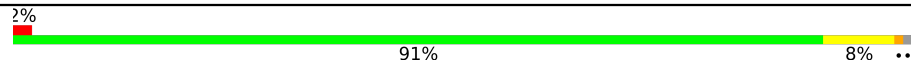
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	 5% 92% 8%
1	B	253	 11% 88% 11%
1	C	253	 2% 90% 8%
1	D	253	 6% 89% 10%
1	E	253	 % 91% 8%

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Mol	Chain	Length	Quality of chain
1	F	253	 A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a 91% quality score. There is a small red segment at the beginning, labeled '2%', and a small yellow segment at the end, labeled '8%'. The text '91%' is centered below the green portion of the bar.

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	EDO	F	304	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13706 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 1924	C 1208	N 329	O 372	S 15	0	10	0
1	B	251	Total 1940	C 1221	N 334	O 369	S 16	0	11	0
1	C	250	Total 1933	C 1212	N 336	O 371	S 14	0	11	0
1	D	251	Total 1941	C 1222	N 334	O 370	S 15	0	12	0
1	E	251	Total 1951	C 1227	N 335	O 374	S 15	0	14	0
1	F	251	Total 1915	C 1201	N 333	O 367	S 14	0	8	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



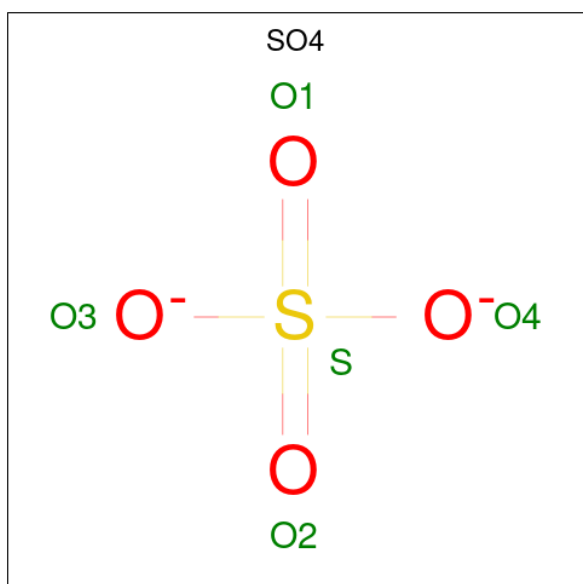
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



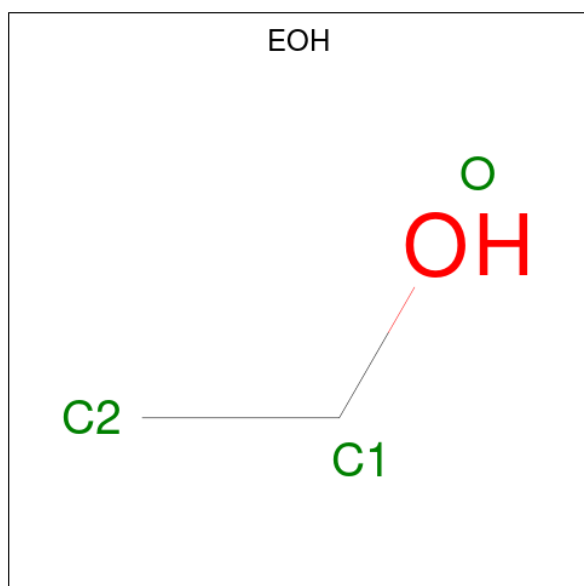
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 3 2 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total K 1 1	0	0

- Molecule 9 is water.

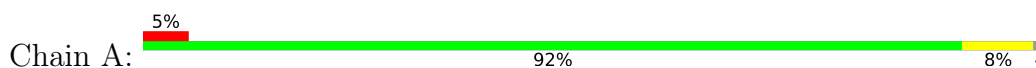
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	357	Total O 361 361	0	4
9	B	300	Total O 302 302	0	2
9	C	367	Total O 371 371	0	4
9	D	303	Total O 308 308	0	5
9	E	336	Total O 336 336	0	0
9	F	335	Total O 338 338	0	3



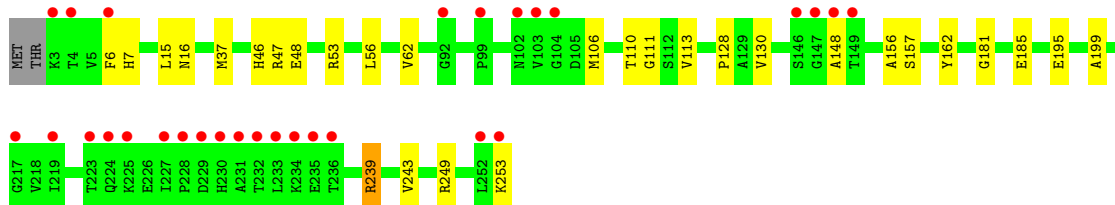
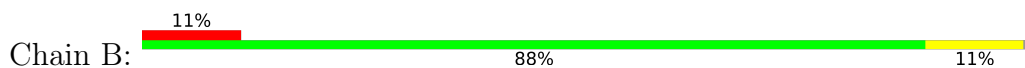
### 3 Residue-property plots [i](#)

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.

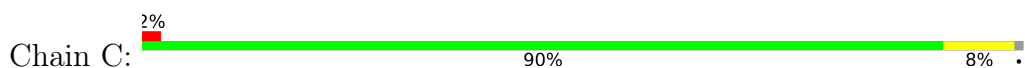
- Molecule 1: Uridine phosphorylase



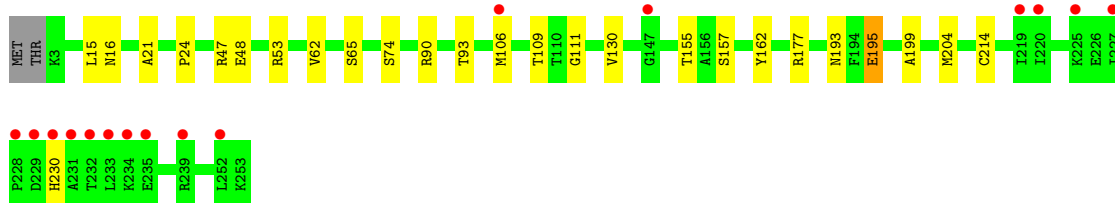
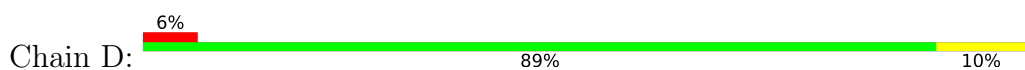
- Molecule 1: Uridine phosphorylase



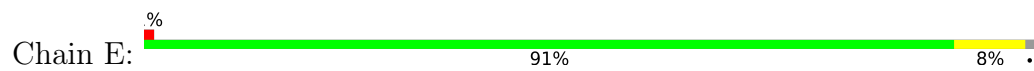
- Molecule 1: Uridine phosphorylase



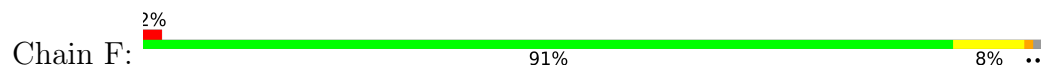
- Molecule 1: Uridine phosphorylase



- 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, $\alpha$ , $\beta$ , $\gamma$	63.67Å 71.06Å 87.91Å 69.63° 72.56° 85.73°	Depositor
Resolution (Å)	18.93 – 1.29 18.93 – 1.29	Depositor EDS
% Data completeness (in resolution range)	94.7 (18.93-1.29) 95.2 (18.93-1.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.29Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.172 , 0.200 0.169 , 0.195	Depositor DCC
$R_{free}$ test set	16562 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.8	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.1	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	0.93	EDS
Total number of atoms	13706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: NA, CL, EOH, EDO, PO4, K, SO4

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	0.42	0/1982	0.59	0/2687
1	B	0.39	0/2001	0.57	0/2709
1	C	0.43	0/1989	0.62	0/2698
1	D	0.44	0/2005	0.57	0/2716
1	E	0.42	0/2021	0.60	0/2738
1	F	0.42	0/1967	0.60	0/2664
All	All	0.42	0/11965	0.59	0/16212

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 [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	1924	0	1945	12	0
1	B	1940	0	1977	23	0
1	C	1933	0	1944	19	0
1	D	1941	0	1977	20	0
1	E	1951	0	1988	18	0
1	F	1915	0	1933	16	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	8	0	12	4	0
3	E	4	0	6	0	0
3	F	8	0	12	4	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	F	10	0	0	0	0
5	B	10	0	0	0	0
5	D	5	0	0	0	0
5	E	10	0	0	0	0
6	B	3	0	6	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
8	D	1	0	0	0	0
9	A	361	0	0	0	0
9	B	302	0	0	1	0
9	C	371	0	0	0	0
9	D	308	0	0	3	0
9	E	336	0	0	3	0
9	F	338	0	0	2	0
All	All	13706	0	11812	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (94) 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:C:196:MET:HG3	3:C:303:EDO:H12	1.47	0.97
1:D:90[B]:ARG:NH2	1:D:195:GLU:OE2	2.18	0.76
1:E:128:PRO:HB2	1:E:130[B]:VAL:HG13	1.67	0.76
1:B:148:ALA:HB2	1:B:239:ARG:HE	1.51	0.75
1:A:128:PRO:HB2	1:A:130[A]:VAL:HG13	1.68	0.74
1:C:128:PRO:HB2	1:C:130[B]:VAL:HG23	1.69	0.73
1:E:16[A]:ASN:HB2	1:E:53:ARG:HD2	1.71	0.72
1:D:16:ASN:HB2	1:D:53:ARG:HD2	1.73	0.71
1:E:155[B]:THR:HG21	1:E:195[B]:GLU:HG3	1.73	0.70
1:B:15:LEU:HD22	1:B:62[B]:VAL:HG11	1.74	0.70
1:E:29[A]:ARG:NH2	9:E:725:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:HH11	3:C:304:EDO:H22	1.57	0.67
1:D:90[A]:ARG:NE	9:D:697:HOH:O	2.32	0.61
1:C:4[A]:THR:N	1:C:10:VAL:O	2.33	0.61
1:D:15:LEU:HD22	1:D:62[B]:VAL:HG11	1.81	0.61
1:B:128:PRO:HB2	1:B:130[B]:VAL:HG23	1.81	0.61
1:A:16[A]:ASN:HB2	1:A:53:ARG:HD2	1.84	0.59
1:F:196:MET:HG3	3:F:304:EDO:H12	1.84	0.59
1:B:111:GLY:HA3	1:C:130[B]:VAL:HG21	1.84	0.59
1:E:15:LEU:HG	1:E:62:VAL:HG21	1.86	0.57
1:B:130[B]:VAL:HG22	1:C:130[B]:VAL:HG22	1.85	0.56
1:E:155[B]:THR:CG2	1:E:195[B]:GLU:HG3	2.34	0.56
1:E:128:PRO:HB2	1:E:130[B]:VAL:CG1	2.35	0.56
1:F:178[A]:ARG:NH1	9:F:613:HOH:O	2.39	0.56
1:F:16[B]:ASN:HB2	1:F:53:ARG:HD2	1.89	0.55
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.89	0.55
1:E:90[A]:ARG:NH1	9:E:590:HOH:O	2.39	0.54
1:B:16:ASN:HB2	1:B:53:ARG:HD2	1.89	0.54
1:B:106[B]:MET:HE1	1:B:243:VAL:HG21	1.90	0.54
1:B:185:GLU:OE1	1:D:177:ARG:HB2	2.08	0.54
1:C:4[A]:THR:HG22	1:C:11:THR:HG22	1.90	0.53
1:B:110:THR:O	1:C:130[A]:VAL:HG21	2.09	0.53
1:D:111:GLY:HA3	1:E:130[B]:VAL:HG11	1.90	0.52
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.91	0.52
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.92	0.52
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.91	0.52
1:B:157:SER:HB3	1:B:199:ALA:HB2	1.91	0.52
1:E:90[B]:ARG:NH1	9:E:590:HOH:O	2.43	0.51
1:D:93:THR:O	9:D:685:HOH:O	2.19	0.51
1:F:128:PRO:HB2	1:F:130:VAL:HG13	1.93	0.51
1:B:130[A]:VAL:HG21	1:C:110:THR:O	2.11	0.51
1:E:15:LEU:HG	1:E:62:VAL:CG2	2.42	0.49
1:D:90[A]:ARG:NH1	9:D:490:HOH:O	2.45	0.49
1:D:130[B]:VAL:CG1	1:E:130[B]:VAL:HG12	2.42	0.49
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.93	0.49
1:C:48:GLU:HB3	1:D:48:GLU:HB3	1.95	0.49
1:A:130[A]:VAL:HG12	1:F:130:VAL:CG1	2.43	0.49
1:B:148:ALA:HB2	1:B:239:ARG:NE	2.24	0.49
1:B:249:ARG:O	1:B:253:LYS:HG3	2.13	0.48
1:F:165:GLN:HE22	3:F:304:EDO:H21	1.79	0.48
1:B:46:HIS:HE1	9:B:436:HOH:O	1.97	0.47
1:A:128:PRO:HB2	1:A:130[A]:VAL:CG1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ARG:HB3	1:D:48:GLU:OE1	2.15	0.46
1:C:128:PRO:HB2	1:C:130[B]:VAL:CG2	2.43	0.46
1:D:21:ALA:HB2	1:D:62[B]:VAL:HG23	1.99	0.45
1:C:41[A]:VAL:HG11	1:C:53:ARG:NH2	2.32	0.45
1:E:155[A]:THR:HG22	1:E:193:ASN:OD1	2.17	0.45
1:B:130[B]:VAL:HG21	1:C:111:GLY:HA3	1.99	0.45
1:C:57:ASP:OD2	1:C:249[B]:ARG:HG3	2.17	0.44
1:C:27:PRO:HD2	1:D:47:ARG:HA	1.99	0.44
1:F:21:ALA:HB2	1:F:62:VAL:HG13	1.98	0.44
1:A:74:SER:HA	1:A:204[B]:MET:HE1	1.99	0.44
1:D:155[B]:THR:HG22	1:D:193:ASN:OD1	2.18	0.44
1:B:181:GLY:O	1:B:185:GLU:HG3	2.18	0.43
1:B:6:PHE:HD2	1:B:7:HIS:CE1	2.36	0.43
1:F:74:SER:HA	1:F:204[B]:MET:HE1	2.00	0.43
1:A:155[A]:THR:HG22	1:A:193:ASN:OD1	2.18	0.43
1:D:24:PRO:O	1:D:65:SER:HA	2.17	0.43
1:D:109:THR:OG1	1:D:155[B]:THR:HG21	2.19	0.43
1:A:130[A]:VAL:HG11	1:F:111:GLY:HA3	1.99	0.43
1:A:130[A]:VAL:HG12	1:F:130:VAL:HG12	2.00	0.43
1:B:106[B]:MET:SD	1:B:243:VAL:HG21	2.59	0.43
1:E:108:VAL:HB	1:E:152:MET:SD	2.59	0.43
1:C:165:GLN:HE22	3:C:303:EDO:C2	2.32	0.42
1:B:128:PRO:HB2	1:B:130[B]:VAL:CG2	2.49	0.42
1:E:47:ARG:HA	1:F:27:PRO:HD2	2.01	0.42
1:B:37:MET:HG2	1:B:56:LEU:HD13	2.02	0.42
1:E:24:PRO:O	1:E:65:SER:HA	2.18	0.42
1:A:108:VAL:HB	1:A:152:MET:SD	2.60	0.41
1:A:109:THR:OG1	1:A:155[A]:THR:HG21	2.20	0.41
1:F:113:VAL:HB	1:F:156:ALA:HA	2.03	0.41
1:A:24:PRO:O	1:A:65:SER:HA	2.21	0.41
1:B:113:VAL:HB	1:B:156:ALA:HA	2.02	0.41
1:B:47[B]:ARG:HB3	1:B:48:GLU:OE2	2.20	0.41
1:C:113:VAL:HB	1:C:156:ALA:HA	2.02	0.41
1:D:74:SER:HA	1:D:204[B]:MET:HE1	2.03	0.41
1:D:90[B]:ARG:HG2	1:D:214[B]:CYS:SG	2.60	0.41
1:D:109:THR:HG23	1:D:155[B]:THR:HG23	2.03	0.41
1:B:106[B]:MET:CE	1:B:243:VAL:HG21	2.50	0.40
1:F:195:GLU:HA	3:F:304:EDO:C2	2.51	0.40
1:E:57:ASP:OD2	1:E:249:ARG:HG3	2.22	0.40
1:F:234:LYS:HG2	9:F:466:HOH:O	2.21	0.40
1:C:165:GLN:HE22	3:C:303:EDO:H21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:HE22	3:F:304:EDO:C2	2.34	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	259/253 (102%)	254 (98%)	4 (2%)	1 (0%)	34	10
1	B	260/253 (103%)	257 (99%)	2 (1%)	1 (0%)	34	10
1	C	258/253 (102%)	256 (99%)	1 (0%)	1 (0%)	34	10
1	D	261/253 (103%)	257 (98%)	3 (1%)	1 (0%)	34	10
1	E	263/253 (104%)	260 (99%)	2 (1%)	1 (0%)	34	10
1	F	256/253 (101%)	254 (99%)	1 (0%)	1 (0%)	34	10
All	All	1557/1518 (103%)	1538 (99%)	13 (1%)	6 (0%)	34	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	TYR
1	E	162	TYR
1	F	162	TYR
1	A	162	TYR
1	B	162	TYR
1	C	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	211/203 (104%)	208 (99%)	3 (1%)	67	34
1	B	212/203 (104%)	210 (99%)	2 (1%)	78	53
1	C	210/203 (103%)	207 (99%)	3 (1%)	67	34
1	D	212/203 (104%)	209 (99%)	3 (1%)	67	34
1	E	215/203 (106%)	213 (99%)	2 (1%)	78	53
1	F	207/203 (102%)	203 (98%)	4 (2%)	57	20
All	All	1267/1218 (104%)	1250 (99%)	17 (1%)	71	35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	195	GLU
1	A	225	LYS
1	B	195	GLU
1	B	239	ARG
1	C	4[A]	THR
1	C	4[B]	THR
1	C	195	GLU
1	D	106	MET
1	D	195	GLU
1	D	230	HIS
1	E	195[A]	GLU
1	E	195[B]	GLU
1	F	178[A]	ARG
1	F	178[B]	ARG
1	F	195	GLU
1	F	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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	$\# Z  > 2$
5	SO4	D	302	-	4,4,4	0.15	0	6,6,6	0.10	0
3	EDO	B	305	-	3,3,3	0.45	0	2,2,2	0.30	0
5	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.41	0
4	PO4	B	302	-	4,4,4	0.91	0	6,6,6	0.44	0
4	PO4	C	301	-	4,4,4	0.90	0	6,6,6	0.78	0
4	PO4	F	301	-	4,4,4	1.18	0	6,6,6	1.05	0
5	SO4	E	303	-	4,4,4	0.15	0	6,6,6	0.09	0
4	PO4	B	301	-	4,4,4	0.89	0	6,6,6	0.44	0
3	EDO	A	302	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	E	304	-	3,3,3	0.47	0	2,2,2	0.31	0
6	EOH	B	306	-	2,2,2	0.45	0	1,1,1	0.13	0
3	EDO	C	303	-	3,3,3	0.38	0	2,2,2	0.09	0
5	SO4	E	302	-	4,4,4	0.15	0	6,6,6	0.05	0
3	EDO	F	304	-	3,3,3	0.46	0	2,2,2	0.20	0
4	PO4	F	302	-	4,4,4	0.87	0	6,6,6	0.49	0
3	EDO	F	305	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	C	304	-	3,3,3	0.46	0	2,2,2	0.34	0
5	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.10	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
3	EDO	B	305	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	E	304	-	-	1/1/1/1	-
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	F	304	-	-	0/1/1/1	-
3	EDO	F	305	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	304	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
3	F	305	EDO	O1-C1-C2-O2
3	B	305	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	EDO	3	0
3	F	304	EDO	4	0
3	C	304	EDO	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%)	0.10	12 (4%) 30 28	3, 8, 20, 37	1 (0%)
1	B	251/253 (99%)	0.44	29 (11%) 4 3	3, 10, 25, 34	0
1	C	250/253 (98%)	-0.13	4 (1%) 72 73	3, 6, 15, 27	0
1	D	251/253 (99%)	0.17	16 (6%) 19 16	3, 8, 23, 37	0
1	E	251/253 (99%)	-0.08	3 (1%) 79 80	3, 7, 16, 33	0
1	F	251/253 (99%)	-0.14	4 (1%) 72 73	3, 6, 16, 27	0
All	All	1505/1518 (99%)	0.06	68 (4%) 33 31	3, 7, 19, 37	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	LYS	7.2
1	D	230	HIS	7.1
1	E	253	LYS	7.0
1	A	227	ILE	6.9
1	B	231	ALA	6.4
1	B	147	GLY	6.2
1	D	227	ILE	6.2
1	B	227	ILE	5.9
1	C	4[A]	THR	5.8
1	B	149	THR	5.7
1	B	230	HIS	5.5
1	A	225	LYS	5.4
1	B	6	PHE	5.3
1	A	226	GLU	5.0
1	B	232	THR	5.0
1	F	253	LYS	4.5
1	D	231	ALA	4.4
1	D	229	ASP	4.4
1	B	229	ASP	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	103	VAL	4.2
1	B	234	LYS	4.1
1	A	3	LYS	3.9
1	C	6	PHE	3.7
1	B	102	ASN	3.6
1	E	252	LEU	3.5
1	C	253	LYS	3.3
1	B	3	LYS	3.3
1	B	253	LYS	3.2
1	B	233	LEU	3.2
1	B	236	THR	3.2
1	D	232	THR	3.1
1	D	225	LYS	3.1
1	B	4	THR	3.1
1	B	225	LYS	3.0
1	D	228	PRO	3.0
1	D	233	LEU	2.9
1	A	4	THR	2.9
1	D	235	GLU	2.9
1	B	148	ALA	2.9
1	B	92	GLY	2.8
1	B	223	THR	2.7
1	B	224	GLN	2.7
1	B	146	SER	2.7
1	B	104	GLY	2.7
1	A	231	ALA	2.7
1	B	219	ILE	2.6
1	B	99	PRO	2.6
1	A	230	HIS	2.6
1	C	230[A]	HIS	2.5
1	F	6	PHE	2.4
1	B	235	GLU	2.4
1	F	4	THR	2.4
1	D	219	ILE	2.4
1	D	234	LYS	2.4
1	D	252	LEU	2.3
1	F	230	HIS	2.3
1	A	252	LEU	2.3
1	B	217	GLY	2.3
1	E	230	HIS	2.2
1	D	239	ARG	2.2
1	B	228	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	234	LYS	2.2
1	D	106	MET	2.1
1	B	252	LEU	2.1
1	D	147	GLY	2.1
1	A	228	PRO	2.1
1	A	235	GLU	2.1
1	D	220	ILE	2.1

## 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
3	EDO	C	304	4/4	0.41	0.26	38,38,39,40	0
3	EDO	B	305	4/4	0.62	0.31	39,39,39,40	4
3	EDO	F	304	4/4	0.76	0.22	15,15,15,20	0
5	SO4	E	302	5/5	0.76	0.24	50,50,50,51	0
3	EDO	E	304	4/4	0.79	0.35	30,31,32,33	0
4	PO4	B	301	5/5	0.80	0.37	58,58,58,58	0
3	EDO	A	302	4/4	0.82	0.27	35,36,36,36	4
3	EDO	C	303	4/4	0.83	0.19	9,9,11,12	4
5	SO4	E	303	5/5	0.84	0.24	32,33,33,33	5
3	EDO	F	305	4/4	0.86	0.28	20,24,27,29	0
6	EOH	B	306	3/3	0.90	0.20	22,22,23,24	0
5	SO4	B	303	5/5	0.92	0.31	36,37,38,38	0
5	SO4	B	304	5/5	0.94	0.15	14,16,17,17	0
4	PO4	F	302	5/5	0.94	0.20	15,15,17,18	0
5	SO4	D	302	5/5	0.95	0.12	12,12,14,16	5
8	K	D	301	1/1	0.97	0.10	6,6,6,6	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	B	302	5/5	0.98	0.13	10,11,11,11	0
4	PO4	C	301	5/5	0.99	0.05	4,4,4,4	0
4	PO4	F	301	5/5	1.00	0.04	4,4,4,4	0
2	NA	A	301	1/1	1.00	0.10	5,5,5,5	0
7	CL	C	302	1/1	1.00	0.03	10,10,10,10	0
7	CL	F	303	1/1	1.00	0.04	12,12,12,12	0
2	NA	E	301	1/1	1.00	0.09	4,4,4,4	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.