



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2016 – 05:00 PM 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

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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

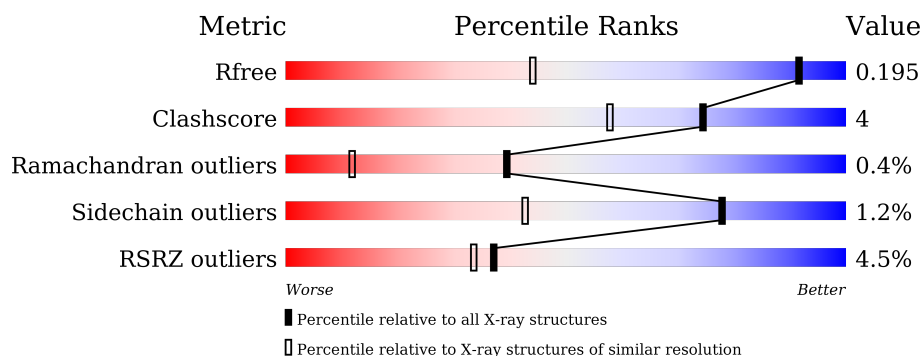
1 Overall quality at a glance ⓘ

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}	91344	1475 (1.34-1.26)
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)
RSRZ outliers	91569	1476 (1.34-1.26)

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>5%</div> <div>92%</div> <div>8%</div> <div>.</div> </div>
1	B	253	<div> <div>12%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	253	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	D	253	<div> <div>6%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	E	253	<div> <div>%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	F	253	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>..</div> </div>

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	NA	E	301	-	-	-	X
3	EDO	B	305	-	-	-	X
3	EDO	C	303	-	-	-	X
3	EDO	E	304	-	-	-	X
3	EDO	F	304	-	-	X	X
3	EDO	F	305	-	-	-	X
5	SO4	D	302	-	-	-	X
5	SO4	E	302	-	-	-	X
6	EOH	B	306	-	-	-	X

2 Entry composition

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
1	A	251	Total	C	N	O	S	0	10	0
			1924	1208	329	372	15			
1	B	251	Total	C	N	O	S	0	11	0
			1940	1221	334	369	16			
1	C	250	Total	C	N	O	S	0	11	0
			1933	1212	336	371	14			
1	D	251	Total	C	N	O	S	0	12	0
			1941	1222	334	370	15			
1	E	251	Total	C	N	O	S	0	14	0
			1951	1227	335	374	15			
1	F	251	Total	C	N	O	S	0	8	0
			1915	1201	333	367	14			

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



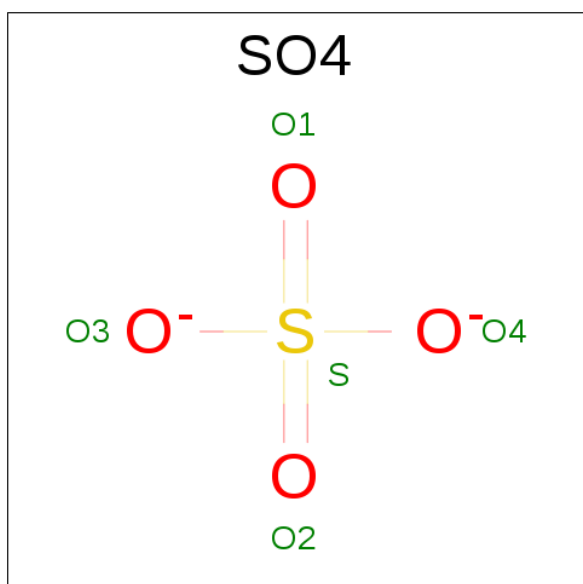
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



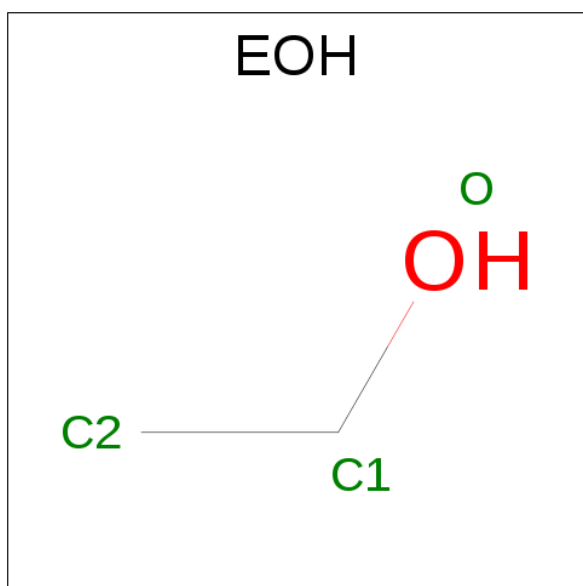
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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: C₂H₆O).



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

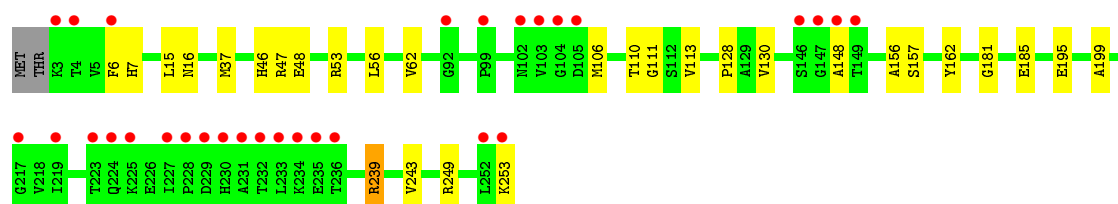
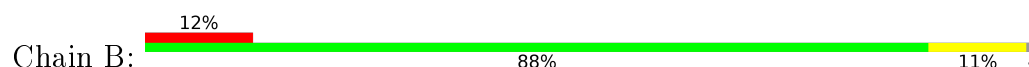
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

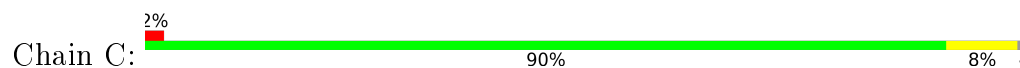
- Molecule 1: Uridine phosphorylase



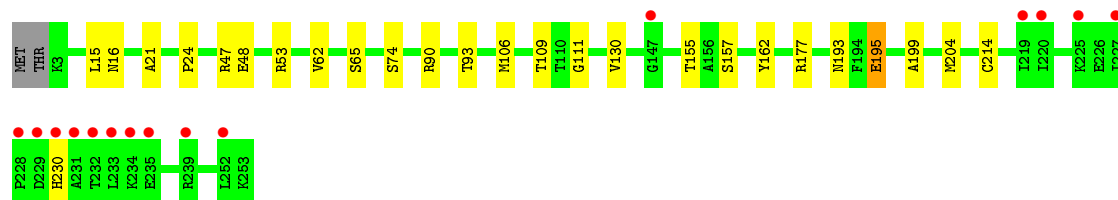
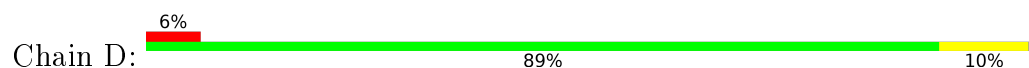
- Molecule 1: Uridine phosphorylase



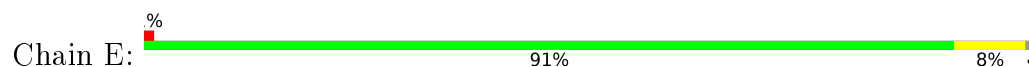
- Molecule 1: Uridine phosphorylase

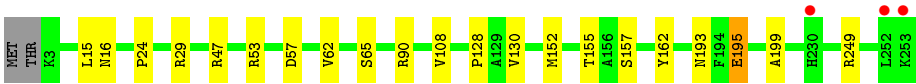


- Molecule 1: Uridine phosphorylase

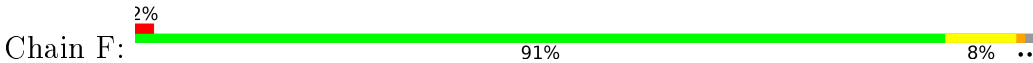


- Molecule 1: Uridine phosphorylase





● 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	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) 84.8 (18.93-1.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.172 , 0.200 0.167 , 0.195	Depositor DCC
R_{free} test set	16508 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	7.8	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13706	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 4.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, K, EOH, EDO, SO4, PO4

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

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:157:SER:HB3	1:F:199:ALA:HB2	1.89	0.55
1:F:16[B]:ASN:HB2	1:F:53:ARG:HD2	1.89	0.55
1:E:90[A]:ARG:NH1	9:E:590:HOH:O	2.39	0.54
1:B:185:GLU:OE1	1:D:177:ARG:HB2	2.08	0.54
1:B:106[B]:MET:HE1	1:B:243:VAL:HG21	1.90	0.54
1:B:16:ASN:HB2	1:B:53:ARG:HD2	1.89	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:B:148:ALA:HB2	1:B:239:ARG:NE	2.24	0.49
1:A:130[A]:VAL:HG12	1:F:130:VAL:CG1	2.43	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:109:THR:OG1	1:D:155[B]:THR:HG21	2.19	0.43
1:D:24:PRO:O	1:D:65:SER:HA	2.17	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:90[B]:ARG:HG2	1:D:214[B]:CYS:SG	2.60	0.41
1:D:74:SER:HA	1:D:204[B]:MET:HE1	2.03	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%)	39	12
1	B	260/253 (103%)	257 (99%)	2 (1%)	1 (0%)	39	12
1	C	258/253 (102%)	256 (99%)	1 (0%)	1 (0%)	39	12
1	D	261/253 (103%)	257 (98%)	3 (1%)	1 (0%)	39	12
1	E	263/253 (104%)	260 (99%)	2 (1%)	1 (0%)	39	12
1	F	256/253 (101%)	254 (99%)	1 (0%)	1 (0%)	39	12
All	All	1557/1518 (103%)	1538 (99%)	13 (1%)	6 (0%)	39	12

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%)	74	36
1	B	212/203 (104%)	210 (99%)	2 (1%)	84	55
1	C	210/203 (103%)	207 (99%)	3 (1%)	74	36
1	D	212/203 (104%)	209 (99%)	3 (1%)	74	36
1	E	215/203 (106%)	213 (99%)	2 (1%)	84	55
1	F	207/203 (102%)	203 (98%)	4 (2%)	65	23
All	All	1267/1218 (104%)	1250 (99%)	17 (1%)	78	38

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

Some 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 carbohydrates 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	$\# Z > 2$
3	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.39	0
4	PO4	B	301	-	4,4,4	0.65	0	6,6,6	0.23	0
4	PO4	B	302	-	4,4,4	0.67	0	6,6,6	0.23	0
5	SO4	B	303	-	4,4,4	0.19	0	6,6,6	0.10	0
5	SO4	B	304	-	4,4,4	0.19	0	6,6,6	0.31	0
3	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EOH	B	306	-	2,2,2	0.45	0	1,1,1	0.15	0
4	PO4	C	301	-	4,4,4	0.74	0	6,6,6	0.26	0
3	EDO	C	303	-	3,3,3	0.38	0	2,2,2	0.12	0
3	EDO	C	304	-	3,3,3	0.44	0	2,2,2	0.41	0
5	SO4	D	302	-	4,4,4	0.18	0	6,6,6	0.07	0
5	SO4	E	302	-	4,4,4	0.22	0	6,6,6	0.06	0
5	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.12	0
3	EDO	E	304	-	3,3,3	0.45	0	2,2,2	0.37	0
4	PO4	F	301	-	4,4,4	0.68	0	6,6,6	0.29	0
4	PO4	F	302	-	4,4,4	0.57	0	6,6,6	0.24	0
3	EDO	F	304	-	3,3,3	0.45	0	2,2,2	0.25	0
3	EDO	F	305	-	3,3,3	0.43	0	2,2,2	0.44	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	A	302	-	-	0/1/1/1	0/0/0/0
4	PO4	B	301	-	-	0/0/0/0	0/0/0/0
4	PO4	B	302	-	-	0/0/0/0	0/0/0/0
5	SO4	B	303	-	-	0/0/0/0	0/0/0/0
5	SO4	B	304	-	-	0/0/0/0	0/0/0/0
3	EDO	B	305	-	-	0/1/1/1	0/0/0/0
6	EOH	B	306	-	-	0/0/0/0	0/0/0/0
4	PO4	C	301	-	-	0/0/0/0	0/0/0/0
3	EDO	C	303	-	-	0/1/1/1	0/0/0/0
3	EDO	C	304	-	-	0/1/1/1	0/0/0/0
5	SO4	D	302	-	-	0/0/0/0	0/0/0/0
5	SO4	E	302	-	-	0/0/0/0	0/0/0/0
5	SO4	E	303	-	-	0/0/0/0	0/0/0/0
3	EDO	E	304	-	-	0/1/1/1	0/0/0/0
4	PO4	F	301	-	-	0/0/0/0	0/0/0/0
4	PO4	F	302	-	-	0/0/0/0	0/0/0/0
3	EDO	F	304	-	-	0/1/1/1	0/0/0/0
3	EDO	F	305	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	C	304	EDO	1	0
3	F	304	EDO	4	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%)	0.10	12 (4%) 34 30	3, 8, 20, 37	1 (0%)
1	B	251/253 (99%)	0.43	30 (11%) 6 5	3, 10, 25, 34	0
1	C	250/253 (98%)	-0.14	4 (1%) 74 72	3, 6, 15, 27	0
1	D	251/253 (99%)	0.16	15 (5%) 25 22	3, 8, 23, 37	0
1	E	251/253 (99%)	-0.09	3 (1%) 81 80	3, 7, 16, 33	0
1	F	251/253 (99%)	-0.14	4 (1%) 74 72	3, 6, 16, 27	0
All	All	1505/1518 (99%)	0.05	68 (4%) 37 33	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	E	253	LYS	7.0
1	D	230	HIS	6.8
1	A	227	ILE	6.6
1	B	231	ALA	6.4
1	D	227	ILE	6.2
1	B	147	GLY	6.1
1	B	149	THR	5.8
1	B	227	ILE	5.7
1	C	4[A]	THR	5.7
1	B	230	HIS	5.4
1	A	225	LYS	5.2
1	B	6	PHE	5.1
1	A	226	GLU	5.0
1	B	232	THR	4.7
1	D	229	ASP	4.6
1	D	231	ALA	4.5
1	F	253	LYS	4.4
1	B	103	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	229	ASP	4.3
1	B	234	LYS	4.0
1	A	3	LYS	3.9
1	C	6	PHE	3.7
1	B	102	ASN	3.4
1	B	3	LYS	3.4
1	C	253	LYS	3.4
1	B	253	LYS	3.3
1	B	236	THR	3.2
1	B	225	LYS	3.1
1	E	252	LEU	3.1
1	D	232	THR	3.0
1	D	225	LYS	3.0
1	B	233	LEU	3.0
1	B	4	THR	2.9
1	A	4	THR	2.9
1	D	228	PRO	2.9
1	D	233	LEU	2.9
1	B	219	ILE	2.9
1	B	92	GLY	2.8
1	B	104	GLY	2.8
1	D	235	GLU	2.8
1	A	231	ALA	2.8
1	B	224	GLN	2.7
1	B	223	THR	2.7
1	B	148	ALA	2.6
1	B	146	SER	2.5
1	A	230	HIS	2.5
1	F	4	THR	2.5
1	F	6	PHE	2.5
1	B	99	PRO	2.4
1	B	235	GLU	2.4
1	C	230[A]	HIS	2.4
1	B	217	GLY	2.3
1	D	234	LYS	2.3
1	D	219	ILE	2.3
1	A	252	LEU	2.3
1	A	234	LYS	2.2
1	D	252	LEU	2.2
1	F	230	HIS	2.2
1	B	252	LEU	2.2
1	A	235	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	230	HIS	2.1
1	D	220	ILE	2.1
1	B	228	PRO	2.1
1	A	228	PRO	2.0
1	B	105	ASP	2.0
1	D	147	GLY	2.0
1	D	239	ARG	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
3	EDO	F	304	4/4	0.71	0.22	20.82	15,15,15,20	0
6	EOH	B	306	3/3	0.90	0.20	17.76	22,22,23,24	0
3	EDO	B	305	4/4	0.67	0.29	14.13	39,39,39,40	4
3	EDO	C	303	4/4	0.83	0.18	11.17	9,9,11,12	4
3	EDO	E	304	4/4	0.79	0.35	8.87	30,31,32,33	0
5	SO4	D	302	5/5	0.94	0.12	7.80	12,12,14,16	5
3	EDO	F	305	4/4	0.85	0.27	7.59	20,24,27,29	0
5	SO4	E	302	5/5	0.78	0.23	4.78	50,50,50,51	0
2	NA	E	301	1/1	1.00	0.09	2.02	4,4,4,4	0
2	NA	A	301	1/1	1.00	0.09	1.81	5,5,5,5	0
4	PO4	B	302	5/5	0.98	0.13	1.12	10,11,11,11	0
8	K	D	301	1/1	0.98	0.09	-0.10	6,6,6,6	1
4	PO4	F	301	5/5	1.00	0.04	-1.58	4,4,4,4	0
4	PO4	C	301	5/5	0.99	0.04	-2.02	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CL	F	303	1/1	1.00	0.03	-3.81	12,12,12,12	0
7	CL	C	302	1/1	1.00	0.02	-5.39	10,10,10,10	0
3	EDO	A	302	4/4	0.85	0.24	-	35,36,36,36	4
4	PO4	F	302	5/5	0.94	0.21	-	15,15,17,18	0
5	SO4	B	304	5/5	0.93	0.15	-	14,16,17,17	0
3	EDO	C	304	4/4	0.42	0.26	-	38,38,39,40	0
5	SO4	B	303	5/5	0.92	0.31	-	36,37,38,38	0
4	PO4	B	301	5/5	0.82	0.39	-	58,58,58,58	0
5	SO4	E	303	5/5	0.85	0.24	-	32,33,33,33	5

6.5 Other polymers [i](#)

There are no such residues in this entry.