



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:08 AM GMT

PDB ID : 3DDO  
Title : X-RAY Structure of the Uridine Phosphorylase from Salmonella Typhimurium  
in Complex with by Phosphate Ion at 1.5A Resolution  
Authors : Lashkov, A.A.; Mikhailov, A.M.; Gabdoulkhakov, A.G.  
Deposited on : 2008-06-06  
Resolution : 1.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

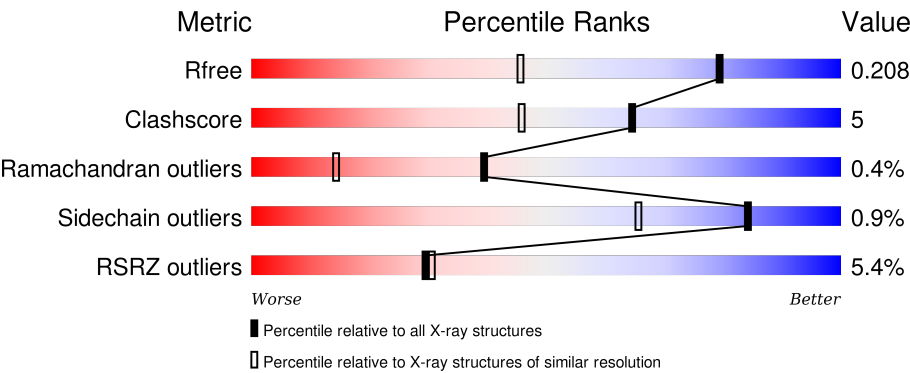
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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 <sub>free</sub>	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 <=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>8%</div><div>85%10%5%</div></div>
1	B	253	<div><div>2%</div><div>90%6%.</div></div>
1	C	253	<div><div>7%</div><div>85%13%.</div></div>
1	D	253	<div><div>6%</div><div>91%8%.</div></div>
1	E	253	<div><div>7%</div><div>87%9%.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	253	 2% 89% 7%

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	PO4	C	5	-	-	-	X

## 2 Entry composition [i](#)

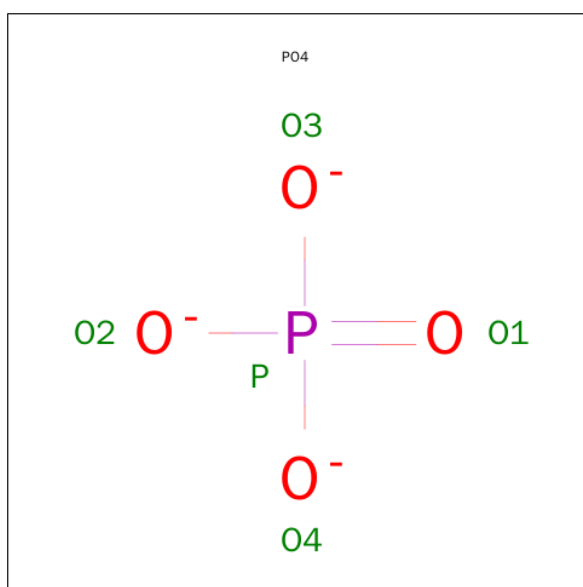
There are 3 unique types of molecules in this entry. The entry contains 12812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	240	Total	C	N	O	S	0	7	0
			1825	1150	320	344	11			
1	B	244	Total	C	N	O	S	0	3	0
			1848	1162	326	349	11			
1	C	249	Total	C	N	O	S	0	6	0
			1912	1195	343	362	12			
1	D	251	Total	C	N	O	S	0	2	0
			1895	1187	334	362	12			
1	E	242	Total	C	N	O	S	0	3	0
			1832	1151	321	349	11			
1	F	243	Total	C	N	O	S	0	2	0
			1831	1150	324	346	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

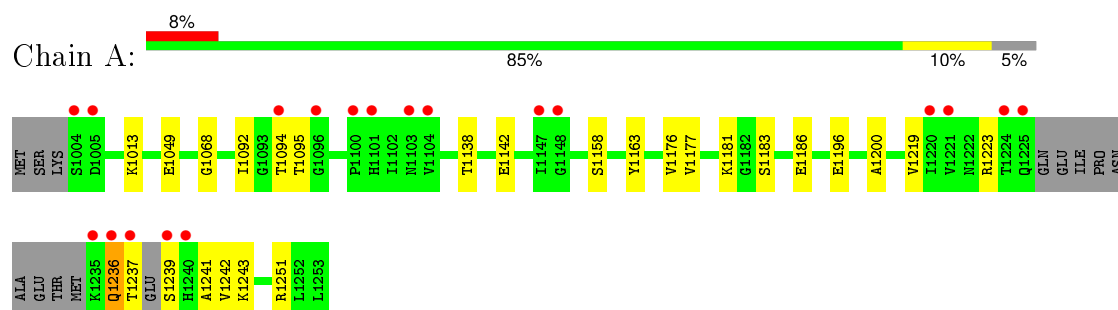
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	263	Total O 263 263	0	0
3	B	251	Total O 251 251	0	0
3	C	277	Total O 277 277	0	0
3	D	305	Total O 305 305	0	0
3	E	250	Total O 250 250	0	0
3	F	298	Total O 298 298	0	0

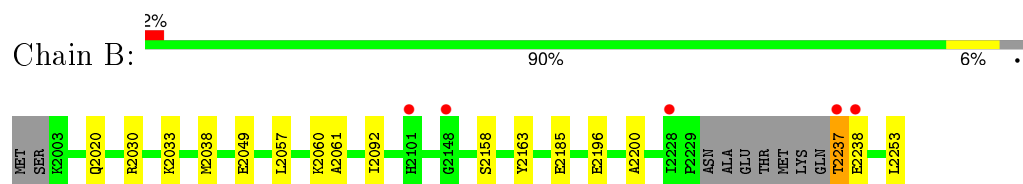
### 3 Residue-property plots [i](#)

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

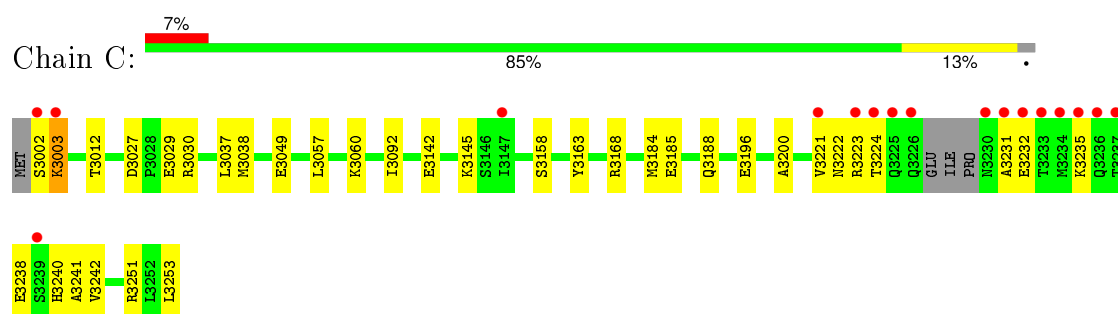
- Molecule 1: Uridine phosphorylase



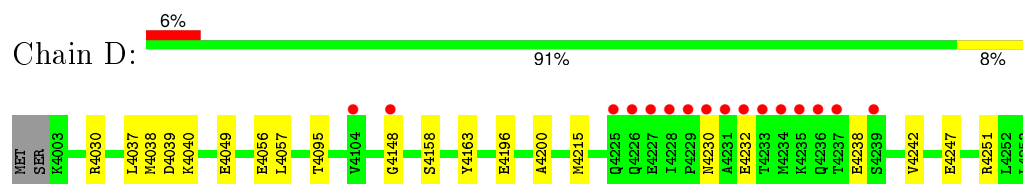
- Molecule 1: Uridine phosphorylase



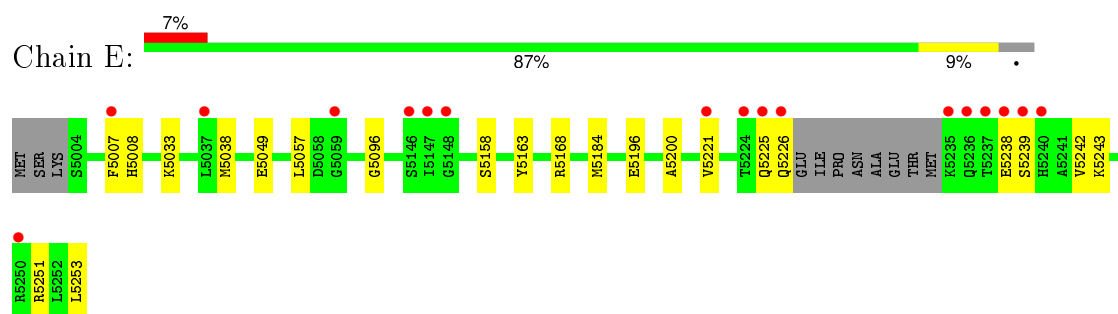
- Molecule 1: Uridine phosphorylase



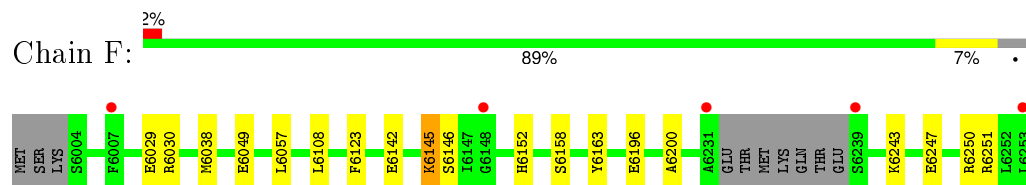
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.60Å 124.92Å 134.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.50 42.17 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.91-1.50) 98.2 (42.17-1.50)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.166 , 0.212 0.163 , 0.208	Depositor DCC
$R_{free}$ test set	11847 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 236950 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.34	0/1874	0.54	0/2539
1	B	0.35	0/1886	0.54	0/2554
1	C	0.35	0/1952	0.55	0/2638
1	D	0.36	0/1932	0.54	0/2618
1	E	0.34	0/1870	0.51	0/2532
1	F	0.36	0/1866	0.53	0/2530
All	All	0.35	0/11380	0.53	0/15411

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	1825	0	1857	22	0
1	B	1848	0	1880	15	0
1	C	1912	0	1943	36	0
1	D	1895	0	1912	14	0
1	E	1832	0	1849	14	0
1	F	1831	0	1854	17	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
3	A	263	0	0	4	0
3	B	251	0	0	2	0
3	C	277	0	0	9	0
3	D	305	0	0	5	0
3	E	250	0	0	4	0
3	F	298	0	0	5	0
All	All	12812	0	11295	114	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.

All (114) 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:F:6247:GLU:HG3	1:F:6251:ARG:HH12	1.30	0.96
1:B:2060[A]:LYS:HD2	1:B:2253:LEU:HD22	1.53	0.89
1:F:6247:GLU:HG3	1:F:6251:ARG:NH1	1.87	0.89
1:D:4039:ASP:HB3	3:D:1119:HOH:O	1.71	0.88
1:C:3003:LYS:H	1:C:3003:LYS:HD3	1.41	0.84
1:C:3222:ASN:OD1	1:C:3224:THR:HG22	1.84	0.78
1:C:3251:ARG:HD3	3:C:784:HOH:O	1.84	0.76
1:C:3003:LYS:HE2	1:C:3003:LYS:O	1.84	0.76
1:C:3142:GLU:O	1:C:3145[B]:LYS:HE2	1.86	0.76
1:A:1251:ARG:HD3	3:A:1349:HOH:O	1.87	0.74
1:C:3003:LYS:HG2	1:C:3012:THR:HG21	1.70	0.74
1:F:6247:GLU:CG	1:F:6251:ARG:HH12	1.99	0.73
1:B:2020:GLN:H	1:B:2060[A]:LYS:NZ	1.85	0.73
1:D:4247:GLU:HG3	1:D:4251:ARG:HH12	1.56	0.68
1:B:2060[A]:LYS:HD3	1:B:2061:ALA:O	1.94	0.67
1:D:4040:LYS:HE3	3:D:1119:HOH:O	1.93	0.67
1:D:4030:ARG:HD3	1:D:4238:GLU:OE2	1.95	0.67
1:E:5251:ARG:HD3	3:E:1123:HOH:O	1.95	0.66
1:E:5168:ARG:HD2	3:E:331:HOH:O	1.97	0.62
1:C:3145[A]:LYS:HG2	3:C:382:HOH:O	1.97	0.62
1:C:3092:ILE:HD11	1:C:3241:ALA:HB1	1.81	0.62
1:C:3027:ASP:HB3	1:C:3030:ARG:HG3	1.82	0.61
1:C:3223[A]:ARG:HD3	3:C:1309:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3030:ARG:HD2	1:C:3238:GLU:OE1	1.99	0.61
1:F:6029:GLU:HB2	3:F:1223:HOH:O	2.01	0.61
1:B:2020:GLN:H	1:B:2060[A]:LYS:HZ1	1.49	0.60
1:A:1236:GLN:O	1:A:1239:SER:HB3	2.02	0.59
1:A:1223:ARG:HG2	3:A:1418:HOH:O	2.04	0.57
1:C:3003:LYS:HG2	1:C:3012:THR:CG2	2.33	0.57
1:F:6243:LYS:HD2	3:F:457:HOH:O	2.04	0.56
1:D:4148:GLY:HA2	3:D:955:HOH:O	2.05	0.56
1:C:3168:ARG:HD2	3:C:440:HOH:O	2.05	0.56
1:B:2158:SER:HB3	1:B:2200:ALA:HB2	1.88	0.56
1:F:6145:LYS:HD2	1:F:6146:SER:N	2.22	0.55
1:C:3145[B]:LYS:HE3	3:C:1317:HOH:O	2.06	0.55
1:A:1177[A]:VAL:HG11	1:F:6123:PHE:C	2.27	0.55
1:C:3038:MET:HG2	1:C:3057:LEU:HD21	1.89	0.54
1:A:1239:SER:O	1:A:1243:LYS:HG3	2.08	0.54
1:F:6038:MET:HG2	1:F:6057:LEU:HD13	1.89	0.54
1:E:5038:MET:HG2	1:E:5057:LEU:HD13	1.89	0.54
1:C:3158:SER:HB3	1:C:3200:ALA:HB2	1.90	0.54
1:C:3029:GLU:HB2	3:C:1043:HOH:O	2.07	0.54
1:B:2030:ARG:HH12	1:B:2092:ILE:HG13	1.73	0.53
1:B:2237:THR:HG22	1:B:2238:GLU:H	1.73	0.53
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.92	0.52
1:C:3168:ARG:HH22	1:C:3223[B]:ARG:HH22	1.57	0.52
1:D:4247:GLU:HG3	1:D:4251:ARG:NH1	2.23	0.52
1:F:6030:ARG:HD3	3:F:407:HOH:O	2.10	0.51
1:E:5238:GLU:O	1:E:5242:VAL:HG23	2.11	0.51
1:F:6158:SER:HB3	1:F:6200:ALA:HB2	1.92	0.51
1:C:3232:GLU:HA	1:C:3235:LYS:HE2	1.92	0.51
1:D:4037:LEU:HD22	1:D:4242:VAL:HG12	1.91	0.51
1:C:3003:LYS:CD	1:C:3003:LYS:H	2.17	0.51
1:F:6057:LEU:HG	1:F:6250:ARG:HG2	1.92	0.51
1:B:2057:LEU:HB3	1:B:2253:LEU:HD11	1.93	0.50
1:D:4158:SER:HB3	1:D:4200:ALA:HB2	1.93	0.50
1:B:2030:ARG:HG3	1:B:2033:LYS:HZ2	1.77	0.50
1:C:3003:LYS:N	1:C:3003:LYS:HD3	2.21	0.49
1:B:2020:GLN:H	1:B:2060[A]:LYS:HZ3	1.60	0.49
1:C:3002:SER:HB2	1:C:3003:LYS:NZ	2.27	0.49
1:F:6108:LEU:HD22	1:F:6152:HIS:HB2	1.94	0.49
1:A:1236:GLN:HG3	1:A:1237:THR:HG23	1.95	0.49
1:B:2038:MET:HG2	1:B:2057:LEU:HD13	1.94	0.49
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:GLN:HG2	1:A:1237:THR:N	2.29	0.48
1:E:5243:LYS:N	1:E:5243:LYS:HD3	2.28	0.48
1:C:3049:GLU:HB3	1:E:5049[A]:GLU:CG	2.44	0.47
1:A:1177[A]:VAL:HG13	3:F:106:HOH:O	2.14	0.47
1:E:5057:LEU:HB3	1:E:5253:LEU:HD11	1.96	0.47
1:D:4247:GLU:CG	1:D:4251:ARG:HH12	2.27	0.46
3:B:2488:HOH:O	1:C:3185:GLU:HG2	2.14	0.46
1:A:1092[B]:ILE:HD12	1:A:1242:VAL:HA	1.98	0.46
1:C:3168:ARG:HH22	1:C:3223[B]:ARG:NH2	2.13	0.46
1:A:1138:THR:O	1:A:1142:GLU:HG3	2.16	0.46
1:E:5225:GLN:O	1:E:5226:GLN:C	2.54	0.45
1:D:4230:ASN:C	1:D:4232:GLU:H	2.20	0.45
1:C:3231:ALA:O	1:C:3235:LYS:HG2	2.16	0.45
1:C:3092:ILE:HD11	1:C:3241:ALA:CB	2.47	0.44
1:D:4095:THR:HA	3:D:1209:HOH:O	2.16	0.44
1:D:4038:MET:HG2	1:D:4057:LEU:HD13	2.00	0.44
1:A:1236:GLN:CG	1:A:1237:THR:HG23	2.48	0.44
1:A:1092[B]:ILE:CD1	1:A:1242:VAL:HG22	2.46	0.44
1:E:5184:MET:HE2	3:E:1134:HOH:O	2.17	0.44
1:E:5239:SER:O	1:E:5243:LYS:HG2	2.17	0.44
1:A:1013:LYS:HE3	1:A:1013:LYS:HB2	1.84	0.44
1:A:1095:THR:O	1:A:1219:VAL:HA	2.17	0.44
1:A:1176:VAL:O	1:A:1181:LYS:HE3	2.18	0.43
1:C:3188[B]:GLN:HG2	3:C:570:HOH:O	2.17	0.43
1:F:6142:GLU:HA	1:F:6145:LYS:HE3	1.99	0.43
1:A:1049:GLU:HB3	1:F:6049:GLU:HB3	2.00	0.43
1:C:3240:HIS:HD2	3:C:1330:HOH:O	2.01	0.43
1:B:2185:GLU:HG3	3:B:2270:HOH:O	2.18	0.42
3:A:1328:HOH:O	1:F:6029:GLU:HG3	2.18	0.42
1:B:2033:LYS:HE2	1:B:2238:GLU:OE2	2.20	0.42
1:F:6142:GLU:HA	1:F:6145:LYS:HG3	2.01	0.42
1:D:4056:GLU:HG2	3:D:1559:HOH:O	2.19	0.42
1:C:3060:LYS:HB2	1:C:3253:LEU:HD13	2.01	0.42
1:C:3037:LEU:HD12	1:C:3242:VAL:HG12	2.01	0.42
1:F:6251:ARG:HD3	3:F:1151:HOH:O	2.20	0.41
1:C:3221:VAL:HG22	1:C:3222:ASN:N	2.34	0.41
1:A:1092[B]:ILE:HD11	1:A:1242:VAL:HG22	2.02	0.41
1:C:3240:HIS:CD2	3:C:1330:HOH:O	2.73	0.41
1:C:3184:MET:HE1	1:C:3223[A]:ARG:HG3	2.02	0.41
1:E:5033:LYS:HD2	3:E:1132:HOH:O	2.20	0.41
1:C:3184:MET:O	1:C:3188[A]:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2049:GLU:HB3	1:D:4049:GLU:HB3	2.01	0.41
1:C:3223[B]:ARG:HA	1:C:3223[B]:ARG:HD3	1.77	0.40
1:A:1092[A]:ILE:HD11	1:A:1241:ALA:HB1	2.03	0.40
1:A:1049:GLU:HG3	1:A:1068:GLY:HA3	2.02	0.40
1:E:5007[B]:PHE:CD2	1:E:5008:HIS:CE1	3.09	0.40
1:E:5096:GLY:HA2	1:E:5221:VAL:O	2.21	0.40
1:A:1094:THR:HG22	3:A:1453:HOH:O	2.21	0.40
1:A:1183[A]:SER:HA	1:A:1186:GLU:OE1	2.21	0.40
1:B:2057:LEU:HD12	1:B:2057:LEU:HA	1.88	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	241/253 (95%)	238 (99%)	2 (1%)	1 (0%)	39	14
1	B	243/253 (96%)	239 (98%)	3 (1%)	1 (0%)	39	14
1	C	251/253 (99%)	247 (98%)	3 (1%)	1 (0%)	39	14
1	D	251/253 (99%)	246 (98%)	4 (2%)	1 (0%)	39	14
1	E	241/253 (95%)	238 (99%)	2 (1%)	1 (0%)	39	14
1	F	241/253 (95%)	239 (99%)	1 (0%)	1 (0%)	39	14
All	All	1468/1518 (97%)	1447 (99%)	15 (1%)	6 (0%)	39	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4163	TYR
1	A	1163	TYR
1	B	2163	TYR

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Mol	Chain	Res	Type
1	C	3163	TYR
1	E	5163	TYR
1	F	6163	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	196/202 (97%)	194 (99%)	2 (1%)	82	62
1	B	197/202 (98%)	195 (99%)	2 (1%)	82	62
1	C	204/202 (101%)	202 (99%)	2 (1%)	82	62
1	D	202/202 (100%)	200 (99%)	2 (1%)	82	62
1	E	195/202 (96%)	194 (100%)	1 (0%)	92	81
1	F	194/202 (96%)	192 (99%)	2 (1%)	82	62
All	All	1188/1212 (98%)	1177 (99%)	11 (1%)	84	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1196	GLU
1	A	1236	GLN
1	B	2196	GLU
1	B	2237	THR
1	C	3003	LYS
1	C	3196	GLU
1	D	4196	GLU
1	D	4215	MET
1	E	5196	GLU
1	F	6145	LYS
1	F	6196	GLU

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

Mol	Chain	Res	Type
1	B	2209	GLN
1	C	3230	ASN
1	C	3236	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	PO4	A	4	-	4,4,4	0.45	0	6,6,6	0.26	0
2	PO4	B	2	-	4,4,4	0.44	0	6,6,6	0.27	0
2	PO4	C	5	-	4,4,4	0.42	0	6,6,6	0.27	0
2	PO4	D	3	-	4,4,4	0.56	0	6,6,6	0.29	0
2	PO4	F	1	-	4,4,4	0.55	0	6,6,6	0.26	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	PO4	A	4	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2	-	-	0/0/0/0	0/0/0/0
2	PO4	C	5	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1	-	-	0/0/0/0	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.

No monomer is involved in short contacts.

## 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, 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	240/253 (94%)	0.34	19 (7%) 15 15	10, 17, 45, 69	0
1	B	244/253 (96%)	0.09	5 (2%) 68 72	8, 15, 35, 70	0
1	C	249/253 (98%)	0.26	17 (6%) 20 20	8, 14, 44, 65	0
1	D	251/253 (99%)	0.14	16 (6%) 23 23	8, 13, 44, 75	0
1	E	242/253 (95%)	0.31	17 (7%) 19 20	10, 19, 43, 71	0
1	F	243/253 (96%)	0.00	5 (2%) 67 70	8, 14, 34, 51	0
All	All	1469/1518 (96%)	0.19	79 (5%) 29 30	8, 15, 41, 75	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5226	GLN	12.4
1	A	1237	THR	9.3
1	B	2237	THR	8.6
1	A	1236	GLN	8.6
1	C	3233	THR	8.6
1	C	3231	ALA	7.9
1	C	3230	ASN	7.4
1	D	4228	ILE	6.5
1	A	1235	LYS	6.5
1	D	4231	ALA	6.4
1	D	4233	THR	6.4
1	E	5237	THR	6.3
1	C	3232	GLU	6.1
1	E	5236	GLN	5.9
1	C	3236	GLN	5.6
1	A	1224	THR	5.3
1	C	3235	LYS	5.2
1	C	3002	SER	4.8
1	C	3234	MET	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	4230	ASN	4.8
1	C	3224	THR	4.4
1	A	1104	VAL	4.2
1	D	4235	LYS	4.2
1	A	1221	VAL	4.1
1	D	4232	GLU	4.1
1	A	1220	ILE	3.8
1	F	6231	ALA	3.8
1	E	5007[A]	PHE	3.8
1	E	5224	THR	3.7
1	E	5221	VAL	3.7
1	E	5235	LYS	3.7
1	D	4229	PRO	3.6
1	D	4226	GLN	3.5
1	A	1225	GLN	3.4
1	C	3221	VAL	3.3
1	D	4239	SER	3.2
1	D	4237	THR	3.0
1	A	1147	ILE	3.0
1	A	1148	GLY	3.0
1	C	3226	GLN	2.9
1	A	1004	SER	2.9
1	A	1239	SER	2.8
1	D	4236	GLN	2.8
1	A	1096	GLY	2.7
1	A	1101[A]	HIS	2.7
1	E	5147	ILE	2.7
1	F	6007	PHE	2.7
1	C	3237	THR	2.6
1	F	6253	LEU	2.6
1	A	1240	HIS	2.6
1	B	2101	HIS	2.6
1	E	5240	HIS	2.6
1	E	5146	SER	2.5
1	B	2238	GLU	2.5
1	A	1103	ASN	2.5
1	D	4227	GLU	2.4
1	D	4234	MET	2.4
1	A	1005	ASP	2.4
1	B	2148	GLY	2.3
1	C	3223[A]	ARG	2.3
1	D	4104	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	5238	GLU	2.3
1	A	1094	THR	2.2
1	D	4148	GLY	2.2
1	A	1100	PRO	2.2
1	D	4225	GLN	2.2
1	C	3239	SER	2.2
1	C	3225	GLN	2.2
1	C	3003	LYS	2.1
1	E	5239	SER	2.1
1	E	5059	GLY	2.1
1	B	2228	ILE	2.1
1	E	5225	GLN	2.1
1	E	5148	GLY	2.0
1	F	6148	GLY	2.0
1	E	5037	LEU	2.0
1	F	6239	SER	2.0
1	E	5250	ARG	2.0
1	C	3147	ILE	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	C	5	5/5	0.92	0.18	2.42	54,55,57,58	0
2	PO4	A	4	5/5	0.98	0.09	-0.22	29,29,31,32	0
2	PO4	D	3	5/5	0.99	0.07	-0.79	18,18,20,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	2	5/5	0.99	0.05	-0.86	16,16,17,19	0
2	PO4	F	1	5/5	0.99	0.06	-1.13	15,15,15,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.