Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:55 AM GMT

PDB ID	:	2VA1
Title	:	CRYSTAL STRUCTURE OF UMP KINASE FROM UREAPLASMA PARVUM
Authors	:	Egeblad-Welin, L.; Welin, M.; Wang, L.; Eriksson, S.
Deposited on	:	2007-08-28
Resolution	:	2.50 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

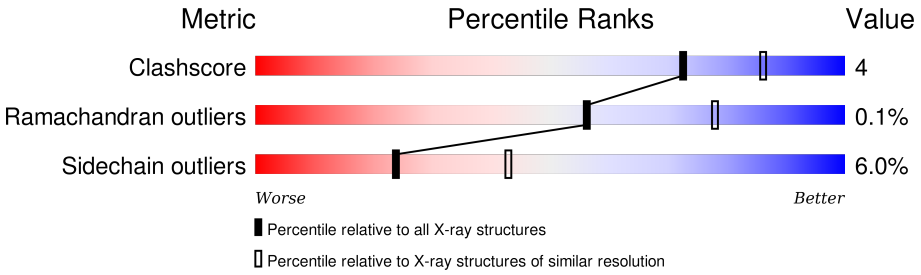
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	75% 11% • 12%
1	B	256	82% 9% • 8%
1	C	256	77% 11% • 11%
1	D	256	80% 7% • 11%
1	E	256	78% 12% • 8%
1	F	256	77% 8% • 12%

2 Entry composition

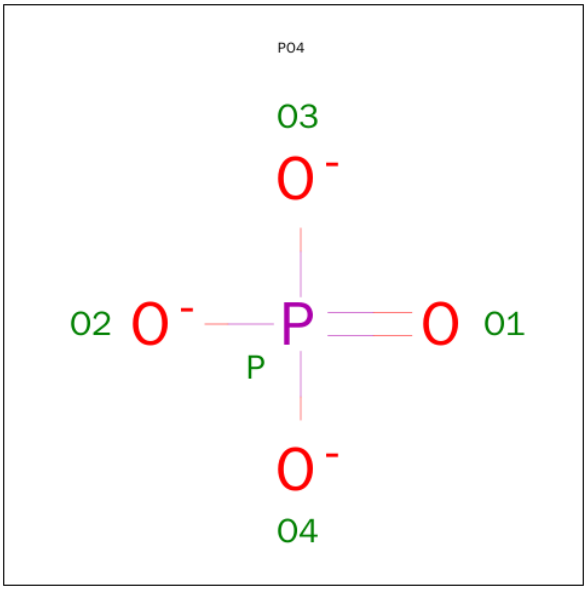
There are 3 unique types of molecules in this entry. The entry contains 10788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1743	1102	295	334	12			
1	B	235	Total	C	N	O	S	0	0	0
			1798	1136	306	342	14			
1	C	227	Total	C	N	O	S	0	0	0
			1746	1104	294	336	12			
1	D	228	Total	C	N	O	S	0	0	0
			1757	1111	298	335	13			
1	E	235	Total	C	N	O	S	0	0	0
			1812	1145	308	346	13			
1	F	226	Total	C	N	O	S	0	0	0
			1744	1103	296	333	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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	E	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	33	Total O 33 33	0	0
3	B	27	Total O 27 27	0	0
3	C	27	Total O 27 27	0	0
3	D	23	Total O 23 23	0	0
3	E	31	Total O 31 31	0	0
3	F	17	Total O 17 17	0	0

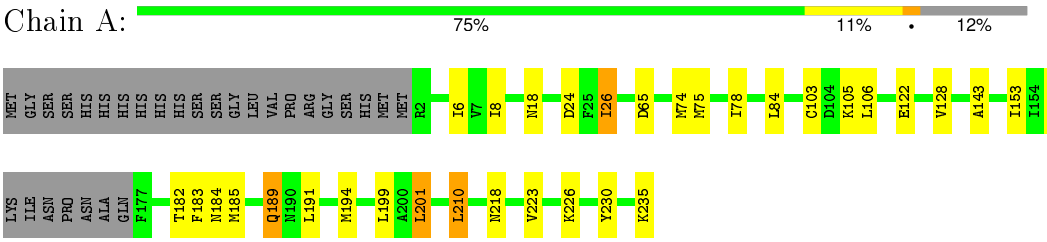
3 Residue-property plots (i)

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.

Note EDS was not executed.

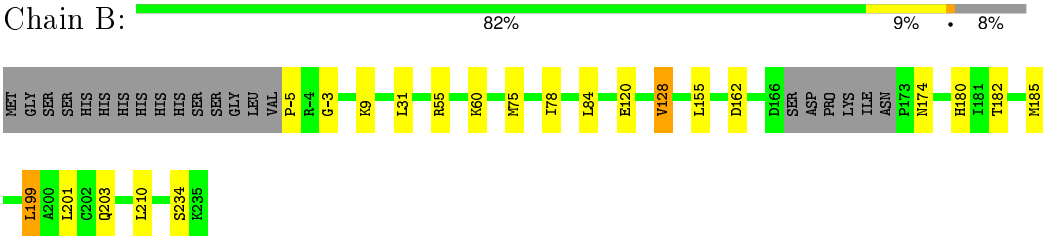
- Molecule 1: URIDYLATE KINASE

Chain A:



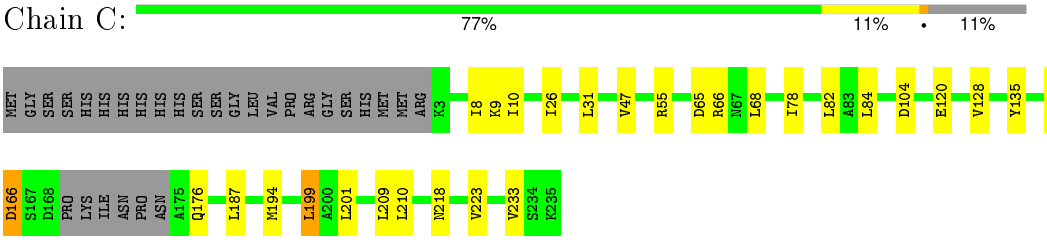
- Molecule 1: URIDYLATE KINASE

Chain B:



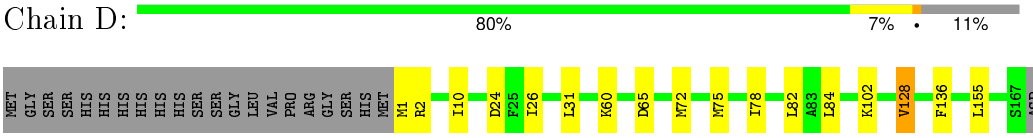
- Molecule 1: URIDYLATE KINASE

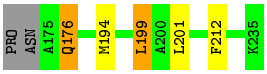
Chain C:



- Molecule 1: URIDYLATE KINASE

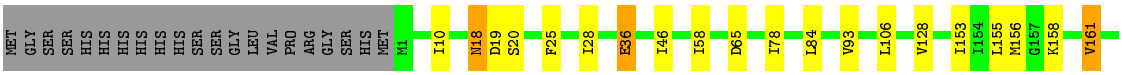
Chain D:





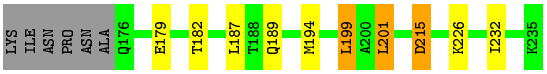
• Molecule 1: URIDYLATE KINASE

Chain E:



• Molecule 1: URIDYLATE KINASE

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.75Å 96.55Å 96.27Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (20.00-2.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10788	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.37	0/1760	0.52	0/2370
1	B	0.36	0/1816	0.56	1/2445 (0.0%)
1	C	0.36	0/1763	0.54	0/2375
1	D	0.37	0/1774	0.52	0/2388
1	E	0.36	0/1832	0.54	0/2470
1	F	0.37	0/1761	0.54	0/2371
All	All	0.37	0/10706	0.54	1/14419 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	-5	PRO	N-CA-CB	5.96	110.45	103.30

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	1743	0	1798	24	0
1	B	1798	0	1845	12	0
1	C	1746	0	1798	14	0
1	D	1757	0	1819	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1812	0	1874	18	0
1	F	1744	0	1802	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	33	0	0	0	0
3	B	27	0	0	0	0
3	C	27	0	0	1	0
3	D	23	0	0	0	0
3	E	31	0	0	2	0
3	F	17	0	0	0	0
All	All	10788	0	10936	90	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 (90) 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:55:ARG:HG3	1:F:55:ARG:HH11	1.29	0.94
1:F:55:ARG:HH11	1:F:55:ARG:CG	2.03	0.72
1:B:194:MET:HE2	1:B:199:LEU:HD12	1.73	0.71
1:C:223:VAL:HG12	3:C:2026:HOH:O	1.94	0.68
1:D:194:MET:HB2	1:D:199:LEU:HD13	1.77	0.66
1:A:8:ILE:HG12	1:A:155:LEU:HD12	1.78	0.66
1:D:176:GLN:HE21	1:D:176:GLN:N	1.94	0.66
1:B:155:LEU:HD22	1:B:210:LEU:HD23	1.77	0.65
1:A:24:ASP:OD1	1:A:26:ILE:HG23	1.98	0.63
1:A:210:LEU:HD11	1:A:223:VAL:HG22	1.79	0.63
1:D:194:MET:HE2	1:D:199:LEU:HD12	1.81	0.62
1:E:155:LEU:HD22	1:E:210:LEU:HD23	1.83	0.61
1:E:19:ASP:HB3	1:F:19:ASP:HB3	1.83	0.61
1:A:78:ILE:HG12	1:A:128:VAL:HG13	1.81	0.61
1:B:78:ILE:HG12	1:B:128:VAL:HG13	1.83	0.60
1:D:176:GLN:H	1:D:176:GLN:HE21	1.46	0.60
1:C:82:LEU:HD12	1:D:75:MET:HE1	1.87	0.57
1:C:78:ILE:HG12	1:C:128:VAL:HG13	1.86	0.56
1:C:78:ILE:HG12	1:C:128:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG22	1:B:75:MET:HE1	1.86	0.56
1:A:182:THR:HG22	1:A:185:MET:H	1.71	0.56
1:C:166:ASP:OD1	1:C:176:GLN:HB2	2.05	0.56
1:A:75:MET:HE1	1:B:75:MET:HG2	1.88	0.55
1:A:103:CYS:SG	1:A:106:LEU:HD12	2.47	0.55
1:D:136:PHE:CZ	1:F:136:PHE:CZ	2.96	0.53
1:A:183:PHE:HD1	1:A:235:LYS:HB3	1.73	0.53
1:D:24:ASP:OD1	1:D:26:ILE:HG13	2.08	0.53
1:C:194:MET:HB2	1:C:199:LEU:HD13	1.90	0.53
1:D:10:ILE:HD13	1:D:31:LEU:HD21	1.92	0.52
1:D:72:MET:HA	1:D:75:MET:HE3	1.92	0.52
1:A:6:ILE:HG22	1:A:153:ILE:HG23	1.91	0.52
1:F:194:MET:HB2	1:F:199:LEU:HD13	1.92	0.52
1:B:78:ILE:HG12	1:B:128:VAL:CG1	2.40	0.51
1:A:78:ILE:HG22	1:B:75:MET:CE	2.39	0.51
1:E:106:LEU:HD11	1:F:101:ILE:HD13	1.92	0.51
1:F:55:ARG:NH1	1:F:55:ARG:CG	2.70	0.51
1:D:78:ILE:HG12	1:D:128:VAL:HG13	1.93	0.51
1:F:55:ARG:HG3	1:F:55:ARG:NH1	2.10	0.51
1:C:82:LEU:HD12	1:D:75:MET:CE	2.40	0.50
1:F:93:VAL:O	1:F:95:THR:HG22	2.11	0.50
1:D:136:PHE:CZ	1:F:136:PHE:HZ	2.29	0.50
1:E:106:LEU:HD22	1:F:75:MET:SD	2.51	0.50
1:E:36:GLU:HG2	1:E:93:VAL:CG2	2.42	0.50
1:E:180:HIS:HE1	1:E:234:SER:OG	1.95	0.49
1:E:158:LYS:HB3	1:E:161:VAL:HG23	1.94	0.49
1:D:78:ILE:HG12	1:D:128:VAL:CG1	2.44	0.48
1:E:10:ILE:HD12	1:E:46:ILE:HG23	1.95	0.48
1:A:6:ILE:HG22	1:A:153:ILE:CG2	2.44	0.48
1:E:65:ASP:HB3	3:E:2003:HOH:O	2.12	0.48
1:E:194:MET:HB2	1:E:199:LEU:HD13	1.96	0.47
1:A:105:LYS:HE2	3:E:2006:HOH:O	2.13	0.47
1:D:136:PHE:CE2	1:F:136:PHE:HZ	2.32	0.47
1:C:10:ILE:HD12	1:C:31:LEU:HD11	1.96	0.47
1:A:183:PHE:HD1	1:A:235:LYS:CB	2.28	0.46
1:E:184:ASN:HA	1:E:187:LEU:HD23	1.97	0.46
1:B:182:THR:HA	1:B:234:SER:O	2.16	0.45
1:E:166:ASP:HB2	1:E:189:GLN:HE22	1.82	0.45
1:F:102:LYS:NZ	1:F:104:ASP:OD1	2.43	0.45
1:D:155:LEU:HB3	1:D:212:PHE:HE2	1.82	0.45
1:E:182:THR:HG22	1:E:235:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:PHE:HZ	1:F:136:PHE:CZ	2.35	0.44
1:E:153:ILE:HD11	1:E:210:LEU:HB2	1.99	0.44
1:C:66:ARG:HG2	1:C:135:TYR:CE2	2.53	0.44
1:C:209:LEU:HB2	1:C:233:VAL:HB	1.98	0.44
1:F:65:ASP:OD2	1:F:65:ASP:C	2.55	0.44
1:A:226:LYS:HD2	1:A:230:TYR:OH	2.18	0.44
1:F:9:LYS:C	1:F:9:LYS:HD2	2.38	0.44
1:F:159:ASN:HA	1:F:215:ASP:OD1	2.17	0.43
1:B:60:LYS:HA	1:B:60:LYS:HE2	1.99	0.43
1:A:78:ILE:HG12	1:A:128:VAL:CG1	2.47	0.43
1:A:75:MET:CE	1:B:75:MET:HG2	2.47	0.43
1:A:184:ASN:HD21	1:A:235:LYS:HE2	1.84	0.43
1:A:189:GLN:HB3	1:A:191:LEU:HG	1.99	0.42
1:E:18:ASN:HD22	1:E:20:SER:H	1.67	0.42
1:A:210:LEU:CD1	1:A:223:VAL:HG22	2.47	0.42
1:B:194:MET:HB2	1:B:199:LEU:HD13	2.01	0.42
1:C:68:LEU:HD11	1:D:82:LEU:HB3	2.02	0.42
1:E:78:ILE:HG12	1:E:128:VAL:CG1	2.50	0.42
1:C:8:ILE:HG12	1:C:155:LEU:HD12	2.01	0.42
1:F:143:ALA:HB1	1:F:201:LEU:HB3	2.02	0.41
1:E:25:PHE:HA	1:E:28:ILE:HG22	2.02	0.41
1:A:194:MET:HE2	1:A:199:LEU:HD23	2.03	0.41
1:B:180:HIS:HE1	1:B:234:SER:OG	2.04	0.41
1:E:209:LEU:HB2	1:E:233:VAL:HB	2.02	0.41
1:C:47:VAL:HG21	1:C:142:ALA:HA	2.02	0.41
1:C:104:ASP:OD1	1:F:102:LYS:HE3	2.22	0.40
1:A:143:ALA:HB1	1:A:201:LEU:HB3	2.03	0.40
1:A:74:MET:O	1:A:78:ILE:HG13	2.22	0.40
1:F:118:ALA:HA	1:F:123:GLN:HE21	1.87	0.40
1:A:153:ILE:HD11	1:A:210:LEU:HD23	2.02	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	222/256 (87%)	213 (96%)	9 (4%)	0	100 100
1	B	231/256 (90%)	223 (96%)	7 (3%)	1 (0%)	39 61
1	C	223/256 (87%)	218 (98%)	5 (2%)	0	100 100
1	D	224/256 (88%)	218 (97%)	6 (3%)	0	100 100
1	E	233/256 (91%)	225 (97%)	8 (3%)	0	100 100
1	F	222/256 (87%)	218 (98%)	4 (2%)	0	100 100
All	All	1355/1536 (88%)	1315 (97%)	39 (3%)	1 (0%)	56 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-3	GLY

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	194/220 (88%)	185 (95%)	9 (5%)	33 57
1	B	197/220 (90%)	184 (93%)	13 (7%)	21 38
1	C	194/220 (88%)	182 (94%)	12 (6%)	23 41
1	D	195/220 (89%)	185 (95%)	10 (5%)	29 52
1	E	202/220 (92%)	191 (95%)	11 (5%)	27 49
1	F	194/220 (88%)	178 (92%)	16 (8%)	14 27
All	All	1176/1320 (89%)	1105 (94%)	71 (6%)	24 43

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	26	ILE
1	A	65	ASP
1	A	84	LEU
1	A	122	GLU
1	A	189	GLN
1	A	201	LEU
1	A	210	LEU
1	A	218	ASN
1	B	9	LYS
1	B	31	LEU
1	B	55	ARG
1	B	84	LEU
1	B	120	GLU
1	B	128	VAL
1	B	162	ASP
1	B	174	ASN
1	B	185	MET
1	B	190	ASN
1	B	199	LEU
1	B	201	LEU
1	B	203	GLN
1	C	9	LYS
1	C	26	ILE
1	C	55	ARG
1	C	65	ASP
1	C	84	LEU
1	C	120	GLU
1	C	166	ASP
1	C	187	LEU
1	C	199	LEU
1	C	201	LEU
1	C	210	LEU
1	C	218	ASN
1	D	1	MET
1	D	2	ARG
1	D	60	LYS
1	D	65	ASP
1	D	84	LEU
1	D	102	LYS
1	D	128	VAL
1	D	176	GLN
1	D	199	LEU

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Mol	Chain	Res	Type
1	D	201	LEU
1	E	18	ASN
1	E	36	GLU
1	E	58	ILE
1	E	84	LEU
1	E	156	MET
1	E	161	VAL
1	E	172	ASN
1	E	187	LEU
1	E	199	LEU
1	E	201	LEU
1	E	214	ILE
1	F	9	LYS
1	F	55	ARG
1	F	75	MET
1	F	84	LEU
1	F	94	ASN
1	F	95	THR
1	F	156	MET
1	F	179	GLU
1	F	182	THR
1	F	187	LEU
1	F	189	GLN
1	F	199	LEU
1	F	201	LEU
1	F	215	ASP
1	F	226	LYS
1	F	232	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	29	ASN
1	A	71	ASN
1	A	108	HIS
1	A	123	GLN
1	A	184	ASN
1	A	189	GLN
1	B	71	ASN
1	B	89	ASN
1	B	108	HIS

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	159	ASN
1	B	174	ASN
1	B	180	HIS
1	B	184	ASN
1	B	190	ASN
1	C	71	ASN
1	C	123	GLN
1	D	71	ASN
1	D	123	GLN
1	D	159	ASN
1	D	176	GLN
1	D	184	ASN
1	D	203	GLN
1	E	18	ASN
1	E	29	ASN
1	E	71	ASN
1	E	123	GLN
1	E	176	GLN
1	E	180	HIS
1	E	189	GLN
1	F	71	ASN
1	F	86	ASN
1	F	94	ASN
1	F	113	ASN
1	F	123	GLN
1	F	176	GLN

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 (i)

6 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	1236	-	4,4,4	0.51	0	6,6,6	0.27	0
2	PO4	B	1236	-	4,4,4	0.51	0	6,6,6	0.28	0
2	PO4	C	1236	-	4,4,4	0.51	0	6,6,6	0.28	0
2	PO4	D	1236	-	4,4,4	0.46	0	6,6,6	0.28	0
2	PO4	E	1236	-	4,4,4	0.46	0	6,6,6	0.27	0
2	PO4	F	1236	-	4,4,4	0.50	0	6,6,6	0.27	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	1236	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1236	-	-	0/0/0/0	0/0/0/0
2	PO4	C	1236	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1236	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1236	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1236	-	-	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.