Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:23 AM EDT

PDB ID	:	2I8A
Title	:	Salmonella typhimurium liganded by phosphate ion at 1.64A resolution
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Deposited on	:	2006-09-01
Resolution	:	1.64 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

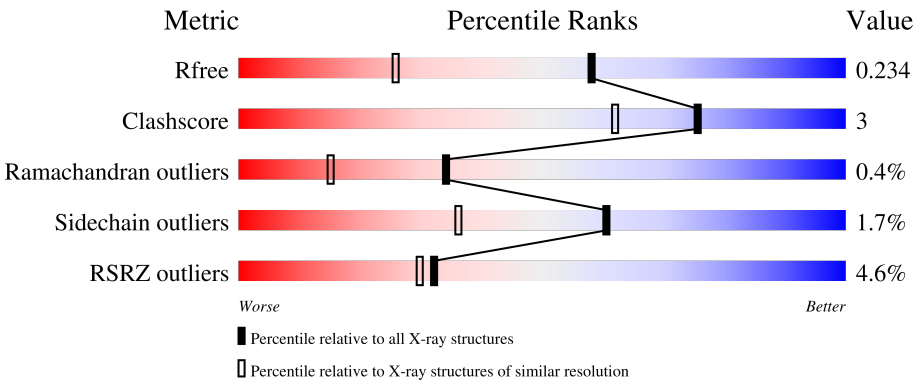
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 >=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 <=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	252	7% 88% 12%
1	B	252	4% 85% 10% 5%
1	C	252	4% 88% 7% 5%
1	D	252	3% 91% 5% •
1	E	252	6% 90% 8% • •

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Mol	Chain	Length	Quality of chain
1	F	252	3% 90% 7%

2 Entry composition (i)

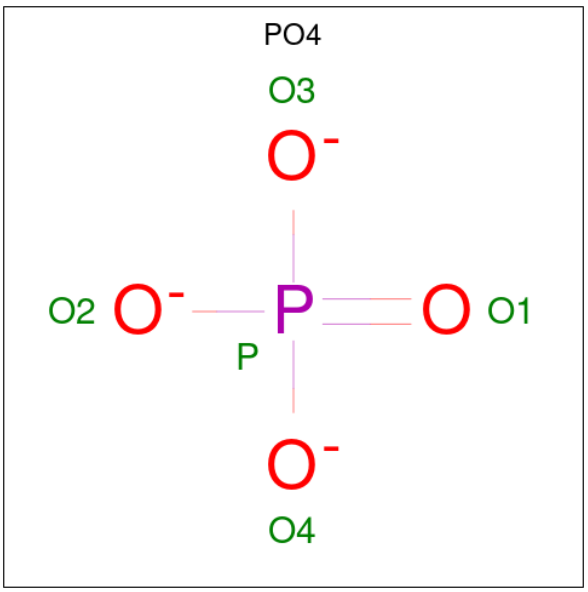
There are 3 unique types of molecules in this entry. The entry contains 12217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1988	1253	342	379	14	0	18	0
1	B	239	1897	1201	334	350	12	0	17	0
1	C	239	1864	1173	328	352	11	0	12	0
1	D	244	1905	1200	332	362	11	0	12	0
1	E	248	1938	1219	342	365	12	0	13	0
1	F	245	1901	1201	330	358	12	0	12	0

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



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

- Molecule 3 is water.

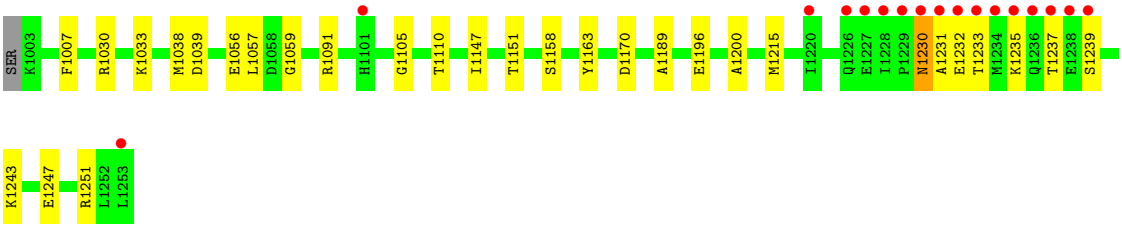
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	134	136	136	0	2
3	B	107	108	108	0	1
3	C	107	107	107	0	0
3	D	112	112	112	0	0
3	E	116	116	116	0	0
3	F	112	115	115	0	3

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.

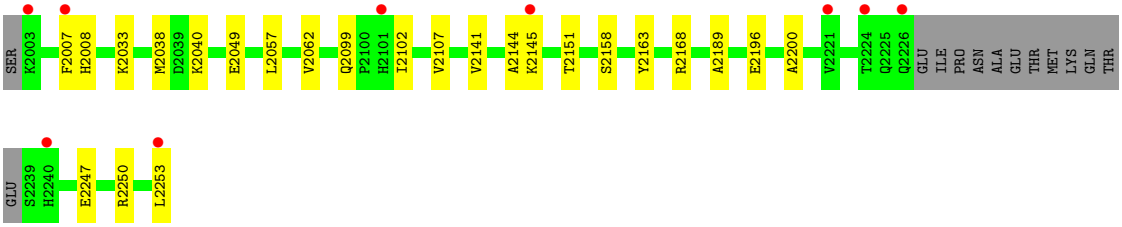
• Molecule 1: Uridine phosphorylase

Chain A:



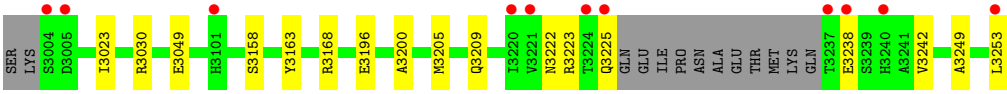
• Molecule 1: Uridine phosphorylase

Chain B:



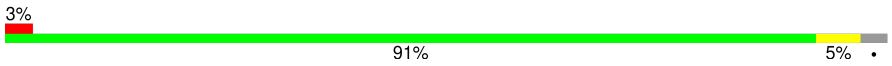
• Molecule 1: Uridine phosphorylase

Chain C:



• Molecule 1: Uridine phosphorylase

Chain D:



- Molecule 1: Uridine phosphorylase

Chain E:

- Molecule 1: Uridine phosphorylase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.60Å 125.03Å 134.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 1.64 26.95 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.4 (27.00-1.64) 95.4 (26.95-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.197 , 0.237 0.196 , 0.234	Depositor DCC
R_{free} test set	8837 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12217	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.47	0/2073	0.61	0/2804
1	B	0.42	0/1979	0.54	0/2671
1	C	0.45	0/1929	0.59	0/2609
1	D	0.45	0/1972	0.60	0/2668
1	E	0.46	0/2004	0.61	0/2708
1	F	0.47	0/1967	0.59	0/2660
All	All	0.45	0/11924	0.59	0/16120

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	1988	0	2045	23	0
1	B	1897	0	1964	14	0
1	C	1864	0	1905	9	0
1	D	1905	0	1936	7	0
1	E	1938	0	1982	16	0
1	F	1901	0	1952	8	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	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	136	0	0	3	0
3	B	108	0	0	2	0
3	C	107	0	0	2	0
3	D	112	0	0	3	0
3	E	116	0	0	1	0
3	F	115	0	0	0	0
All	All	12217	0	11784	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (73) 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:A:1039[B]:ASP:HB3	1:A:1056[B]:GLU:CG	1.72	1.18
1:A:1039[B]:ASP:CB	1:A:1056[B]:GLU:HG3	1.81	1.09
1:D:4185[B]:GLU:HG3	3:D:57:HOH:O	1.69	0.90
1:B:2144:ALA:HB1	1:B:2151:THR:HG21	1.59	0.84
1:E:5149:ALA:HB2	1:E:5240[B]:HIS:HE1	1.45	0.82
1:A:1039[B]:ASP:HB3	1:A:1056[B]:GLU:HG3	0.86	0.79
1:A:1039[B]:ASP:OD1	1:A:1056[B]:GLU:HG2	1.84	0.77
1:E:5030[B]:ARG:HH12	1:E:5092[B]:ILE:HG13	1.50	0.76
1:E:5149:ALA:HB2	1:E:5240[B]:HIS:CE1	2.23	0.73
1:E:5149:ALA:CB	1:E:5240[B]:HIS:HE1	2.05	0.70
1:A:1056[B]:GLU:OE1	1:A:1059:GLY:HA2	1.94	0.68
1:A:1030:ARG:CZ	3:A:513:HOH:O	2.42	0.67
1:A:1039[B]:ASP:CB	1:A:1056[B]:GLU:CG	2.58	0.66
1:D:4229:PRO:HA	1:D:4230:ASN:C	2.15	0.66
1:A:1230:ASN:HD22	1:A:1230:ASN:H	1.44	0.66
1:A:1231:ALA:O	1:A:1235:LYS:HG2	2.01	0.61
1:F:6182:GLY:O	1:F:6185[B]:GLU:HG3	2.01	0.60
1:B:2141:VAL:O	1:B:2145[B]:LYS:HG2	2.02	0.59
1:E:5178:ARG:HA	1:E:5181:LYS:HE2	1.86	0.58
1:A:1110:THR:OG1	1:A:1215[B]:MET:HE3	2.06	0.55
1:B:2144:ALA:CB	1:B:2151:THR:HG21	2.35	0.55
1:A:1007:PHE:HB2	1:D:4228:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039[B]:ASP:OD1	1:A:1056[B]:GLU:CG	2.53	0.53
1:C:3168[B]:ARG:NH2	1:F:6007[B]:PHE:CE1	2.77	0.53
1:F:6158:SER:HB3	1:F:6200:ALA:HB2	1.91	0.53
1:E:5246:VAL:O	1:E:5250[B]:ARG:HG3	2.09	0.52
1:A:1056[B]:GLU:OE1	1:A:1059:GLY:CA	2.58	0.51
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.91	0.51
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.91	0.51
1:B:2158:SER:HB3	1:B:2200:ALA:HB2	1.93	0.51
1:D:4175:ARG:NH2	3:D:523:HOH:O	2.42	0.51
1:C:3222:ASN:HB3	1:C:3225:GLN:HG2	1.94	0.50
1:C:3238:GLU:O	1:C:3242:VAL:HG23	2.13	0.49
1:E:5030[B]:ARG:HH12	1:E:5092[B]:ILE:CG1	2.24	0.49
1:A:1233:THR:O	1:A:1237[A]:THR:HG23	2.14	0.48
1:F:6060:LYS:HB2	1:F:6253:LEU:HD13	1.96	0.47
3:C:461:HOH:O	1:E:5175:ARG:HD2	2.15	0.46
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.96	0.46
1:F:6108:LEU:HD22	1:F:6152:HIS:HB2	1.98	0.46
1:A:1232:GLU:O	1:A:1235:LYS:N	2.46	0.45
1:B:2038:MET:SD	1:B:2062:VAL:HG21	2.55	0.45
1:A:1247:GLU:HG3	1:A:1251[A]:ARG:HH12	1.81	0.45
1:D:4158:SER:HB3	1:D:4200:ALA:HB2	1.97	0.45
1:C:3223:ARG:HG2	3:C:627:HOH:O	2.16	0.45
1:F:6038:MET:HG2	1:F:6057[A]:LEU:HD13	1.98	0.45
1:B:2057:LEU:HB3	1:B:2253:LEU:HD11	1.98	0.45
1:B:2099:GLN:HB2	1:B:2102:ILE:HD12	1.99	0.44
1:C:3049:GLU:HB3	1:F:6049:GLU:HB3	1.99	0.44
1:B:2007[A]:PHE:HD2	1:B:2008:HIS:CE1	2.35	0.44
1:B:2107:VAL:O	1:B:2151:THR:HA	2.17	0.44
1:E:5003:LYS:HZ3	1:E:5003:LYS:N	2.16	0.44
1:A:1189:ALA:HB3	3:A:657:HOH:O	2.16	0.44
1:B:2049[A]:GLU:CG	1:E:5049:GLU:HB3	2.48	0.43
1:B:2247[B]:GLU:OE1	1:B:2250:ARG:HD3	2.18	0.43
1:A:1151[B]:THR:HG21	3:A:391:HOH:O	2.18	0.43
1:C:3158:SER:HB3	1:C:3200:ALA:HB2	2.01	0.42
1:B:2189:ALA:HB3	3:B:439:HOH:O	2.20	0.42
1:C:3023[B]:ILE:HD11	1:C:3249:ALA:HB2	2.01	0.42
1:E:5038:MET:HG2	1:E:5057:LEU:HD21	2.01	0.42
1:A:1105:GLY:HA2	1:A:1237[A]:THR:HG22	2.01	0.42
1:A:1239:SER:O	1:A:1243:LYS:HG3	2.19	0.42
1:E:5220:ILE:HG21	1:E:5234:MET:HG3	2.02	0.41
1:B:2168:ARG:HD2	3:B:216:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3205:MET:O	1:C:3209[B]:GLN:HG2	2.20	0.41
1:E:5038:MET:SD	1:E:5062[B]:VAL:HG21	2.60	0.41
1:D:4194:ASN:ND2	3:D:647:HOH:O	2.52	0.41
1:F:6230:ASN:O	1:F:6231:ALA:HB2	2.21	0.41
1:C:3249:ALA:O	1:C:3253:LEU:HG	2.21	0.41
1:E:5030[B]:ARG:NH1	1:E:5092[B]:ILE:HG13	2.26	0.41
1:E:5013:LYS:HE2	3:E:692:HOH:O	2.21	0.40
1:A:1091:ARG:HB3	1:A:1215[B]:MET:HG3	2.02	0.40
1:D:4238:GLU:HG3	1:D:4239:SER:H	1.87	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	267/252 (106%)	261 (98%)	5 (2%)	1 (0%)	34	15
1	B	252/252 (100%)	248 (98%)	3 (1%)	1 (0%)	34	15
1	C	247/252 (98%)	241 (98%)	5 (2%)	1 (0%)	34	15
1	D	252/252 (100%)	248 (98%)	3 (1%)	1 (0%)	34	15
1	E	257/252 (102%)	254 (99%)	2 (1%)	1 (0%)	34	15
1	F	253/252 (100%)	250 (99%)	2 (1%)	1 (0%)	34	15
All	All	1528/1512 (101%)	1502 (98%)	20 (1%)	6 (0%)	34	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1163	TYR
1	C	3163	TYR
1	F	6163	TYR

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Mol	Chain	Res	Type
1	B	2163	TYR
1	D	4163	TYR
1	E	5163	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	218/201 (108%)	211 (97%)	7 (3%)	39	12
1	B	206/201 (102%)	203 (98%)	3 (2%)	65	42
1	C	201/201 (100%)	198 (98%)	3 (2%)	65	42
1	D	206/201 (102%)	202 (98%)	4 (2%)	57	32
1	E	209/201 (104%)	205 (98%)	4 (2%)	57	32
1	F	206/201 (102%)	203 (98%)	3 (2%)	65	42
All	All	1246/1206 (103%)	1222 (98%)	24 (2%)	60	32

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033[A]	LYS
1	A	1033[B]	LYS
1	A	1147	ILE
1	A	1170[A]	ASP
1	A	1170[B]	ASP
1	A	1196	GLU
1	A	1230	ASN
1	B	2033	LYS
1	B	2040	LYS
1	B	2196	GLU
1	C	3030[A]	ARG
1	C	3030[B]	ARG
1	C	3196	GLU
1	D	4013	LYS
1	D	4196	GLU

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Mol	Chain	Res	Type
1	D	4239	SER
1	D	4253	LEU
1	E	5003	LYS
1	E	5092[A]	ILE
1	E	5092[B]	ILE
1	E	5196	GLU
1	F	6002	SER
1	F	6196	GLU
1	F	6240	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1225	GLN
1	A	1230	ASN
1	D	4188	GLN
1	D	4240	HIS
1	E	5225	GLN
1	F	6101	HIS
1	F	6225	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 monosaccharides 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	B	7002	-	4,4,4	0.93	0	6,6,6	0.49	0
2	PO4	D	7004	-	4,4,4	0.86	0	6,6,6	0.71	0
2	PO4	E	7005	-	4,4,4	0.96	0	6,6,6	0.41	0
2	PO4	C	7003	-	4,4,4	0.95	0	6,6,6	0.53	0
2	PO4	F	7006	-	4,4,4	1.01	0	6,6,6	0.64	0
2	PO4	A	7001	-	4,4,4	0.91	0	6,6,6	0.54	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 (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, 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	251/252 (99%)	0.03	17 (6%)	17	15	5, 11, 35, 56	12 (4%)
1	B	239/252 (94%)	0.11	9 (3%)	40	38	7, 16, 31, 38	1 (0%)
1	C	239/252 (94%)	0.07	11 (4%)	32	30	7, 14, 32, 40	0
1	D	244/252 (96%)	-0.05	7 (2%)	51	50	5, 13, 25, 33	0
1	E	248/252 (98%)	0.07	15 (6%)	21	19	5, 11, 29, 37	3 (1%)
1	F	245/252 (97%)	-0.08	8 (3%)	46	44	5, 12, 26, 31	1 (0%)
All	All	1466/1512 (96%)	0.02	67 (4%)	32	30	5, 13, 29, 56	17 (1%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1228[A]	ILE	10.0
1	E	5231	ALA	7.6
1	E	5230	ASN	7.1
1	E	5233	THR	6.5
1	F	6002	SER	6.3
1	B	2226	GLN	6.1
1	E	5234	MET	5.6
1	F	6231	ALA	5.3
1	E	5232	GLU	5.3
1	E	5236	GLN	5.1
1	E	5235	LYS	5.0
1	D	4253	LEU	5.0
1	F	6003	LYS	4.9
1	C	3004	SER	4.8
1	B	2101[A]	HIS	4.8
1	A	1237[A]	THR	4.5
1	A	1234	MET	4.3
1	B	2003	LYS	4.2
1	A	1230	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	3237	THR	4.2
1	E	5253	LEU	4.1
1	C	3005	ASP	4.0
1	C	3101[A]	HIS	3.9
1	A	1233	THR	3.9
1	F	6253	LEU	3.8
1	C	3238	GLU	3.8
1	D	4238	GLU	3.8
1	A	1253	LEU	3.8
1	C	3253	LEU	3.8
1	B	2253	LEU	3.8
1	B	2240[A]	HIS	3.7
1	C	3225	GLN	3.7
1	D	4101[A]	HIS	3.5
1	D	4228	ILE	3.5
1	E	5224	THR	3.4
1	A	1231	ALA	3.4
1	A	1235	LYS	3.3
1	D	4230	ASN	3.3
1	A	1232	GLU	3.2
1	A	1101[A]	HIS	3.2
1	E	5226	GLN	3.1
1	A	1236	GLN	3.1
1	B	2224	THR	3.1
1	C	3221	VAL	3.0
1	F	6007[A]	PHE	2.9
1	A	1226	GLN	2.9
1	C	3224	THR	2.9
1	A	1227	GLU	2.7
1	A	1220	ILE	2.7
1	F	6239	SER	2.7
1	B	2007[A]	PHE	2.6
1	C	3240	HIS	2.6
1	E	5225	GLN	2.5
1	F	6145[A]	LYS	2.4
1	D	4059	GLY	2.3
1	A	1229	PRO	2.3
1	E	5003	LYS	2.3
1	E	5147	ILE	2.3
1	A	1238	GLU	2.2
1	D	4148	GLY	2.2
1	E	5239	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1239	SER	2.1
1	C	3220	ILE	2.1
1	E	5238	GLU	2.0
1	B	2221	VAL	2.0
1	B	2145[A]	LYS	2.0
1	F	6146	SER	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 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, 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	B-factors(Å^2)	Q<0.9
2	PO4	B	7002	5/5	0.86	0.19	29,29,30,30	5
2	PO4	E	7005	5/5	0.90	0.17	34,34,35,35	5
2	PO4	C	7003	5/5	0.98	0.06	27,28,28,29	0
2	PO4	D	7004	5/5	0.99	0.06	16,17,17,18	0
2	PO4	A	7001	5/5	0.99	0.04	18,19,19,19	0
2	PO4	F	7006	5/5	0.99	0.07	14,16,16,17	0

6.5 Other polymers (i)

There are no such residues in this entry.