



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2019 – 08:24 PM EDT

PDB ID : 6K5K
Title : Structural and catalytic analysis of two diverse uridine phosphorylases in the oomycete *Phytophthora capsici*.
Authors : Yang, C.C.; Zhang, X.G.
Deposited on : 2019-05-29
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

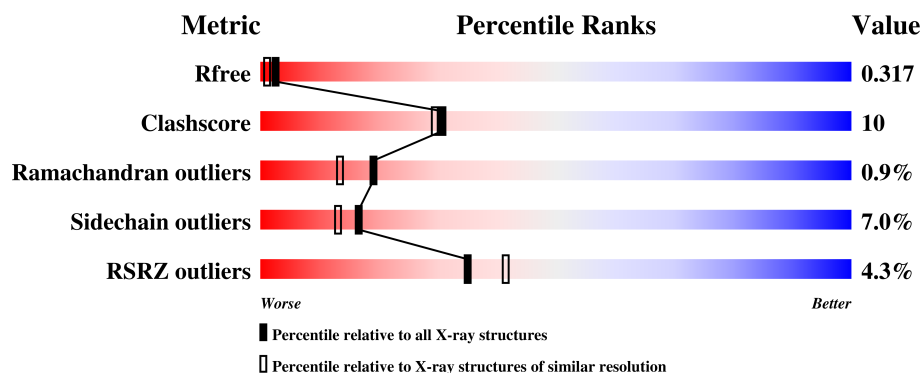
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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	309	 4% 78% 12% • 7%
1	B	309	 5% 72% 17% • • 7%
1	C	309	 4% 75% 17% • 6%
1	D	309	 4% 77% 12% • 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	A	401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17862 atoms, of which 8639 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	287	Total	C	H	N	O	S	0	0	0
			4294	1340	2147	375	420	12			
1	B	288	Total	C	H	N	O	S	0	0	0
			4305	1344	2150	376	423	12			
1	C	289	Total	C	H	N	O	S	0	0	0
			4308	1345	2151	377	424	11			
1	D	287	Total	C	H	N	O	S	0	0	0
			4293	1340	2146	375	420	12			

There are 52 discrepancies between the modelled and reference sequences:

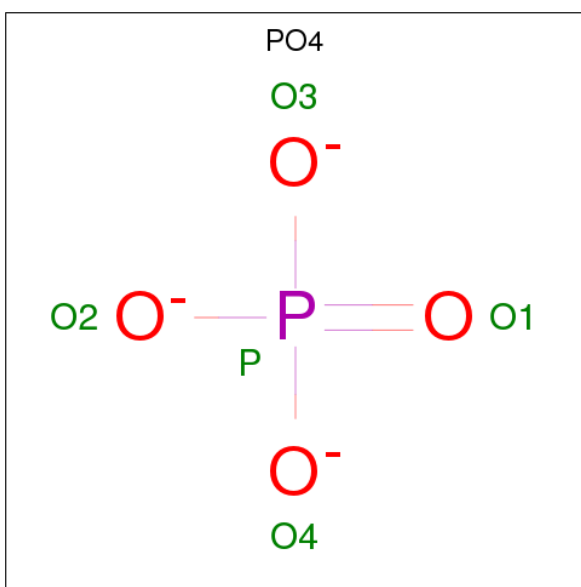
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A0A410UCT3
A	0	GLY	-	expression tag	UNP A0A410UCT3
A	297	ALA	-	expression tag	UNP A0A410UCT3
A	298	ALA	-	expression tag	UNP A0A410UCT3
A	299	ALA	-	expression tag	UNP A0A410UCT3
A	300	LEU	-	expression tag	UNP A0A410UCT3
A	301	GLU	-	expression tag	UNP A0A410UCT3
A	302	HIS	-	expression tag	UNP A0A410UCT3
A	303	HIS	-	expression tag	UNP A0A410UCT3
A	304	HIS	-	expression tag	UNP A0A410UCT3
A	305	HIS	-	expression tag	UNP A0A410UCT3
A	306	HIS	-	expression tag	UNP A0A410UCT3
A	307	HIS	-	expression tag	UNP A0A410UCT3
B	-1	MET	-	expression tag	UNP A0A410UCT3
B	0	GLY	-	expression tag	UNP A0A410UCT3
B	297	ALA	-	expression tag	UNP A0A410UCT3
B	298	ALA	-	expression tag	UNP A0A410UCT3
B	299	ALA	-	expression tag	UNP A0A410UCT3
B	300	LEU	-	expression tag	UNP A0A410UCT3
B	301	GLU	-	expression tag	UNP A0A410UCT3
B	302	HIS	-	expression tag	UNP A0A410UCT3

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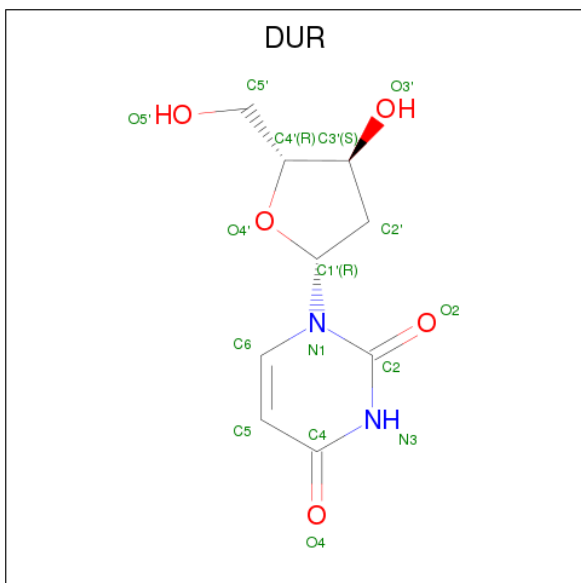
Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP A0A410UCT3
B	304	HIS	-	expression tag	UNP A0A410UCT3
B	305	HIS	-	expression tag	UNP A0A410UCT3
B	306	HIS	-	expression tag	UNP A0A410UCT3
B	307	HIS	-	expression tag	UNP A0A410UCT3
C	-1	MET	-	expression tag	UNP A0A410UCT3
C	0	GLY	-	expression tag	UNP A0A410UCT3
C	297	ALA	-	expression tag	UNP A0A410UCT3
C	298	ALA	-	expression tag	UNP A0A410UCT3
C	299	ALA	-	expression tag	UNP A0A410UCT3
C	300	LEU	-	expression tag	UNP A0A410UCT3
C	301	GLU	-	expression tag	UNP A0A410UCT3
C	302	HIS	-	expression tag	UNP A0A410UCT3
C	303	HIS	-	expression tag	UNP A0A410UCT3
C	304	HIS	-	expression tag	UNP A0A410UCT3
C	305	HIS	-	expression tag	UNP A0A410UCT3
C	306	HIS	-	expression tag	UNP A0A410UCT3
C	307	HIS	-	expression tag	UNP A0A410UCT3
D	-1	MET	-	expression tag	UNP A0A410UCT3
D	0	GLY	-	expression tag	UNP A0A410UCT3
D	297	ALA	-	expression tag	UNP A0A410UCT3
D	298	ALA	-	expression tag	UNP A0A410UCT3
D	299	ALA	-	expression tag	UNP A0A410UCT3
D	300	LEU	-	expression tag	UNP A0A410UCT3
D	301	GLU	-	expression tag	UNP A0A410UCT3
D	302	HIS	-	expression tag	UNP A0A410UCT3
D	303	HIS	-	expression tag	UNP A0A410UCT3
D	304	HIS	-	expression tag	UNP A0A410UCT3
D	305	HIS	-	expression tag	UNP A0A410UCT3
D	306	HIS	-	expression tag	UNP A0A410UCT3
D	307	HIS	-	expression tag	UNP A0A410UCT3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is 2'-DEOXYURIDINE (three-letter code: DUR) (formula: $C_9H_{12}N_2O_5$).

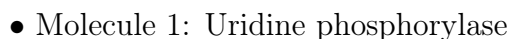
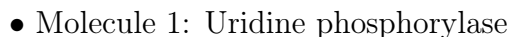
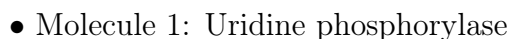


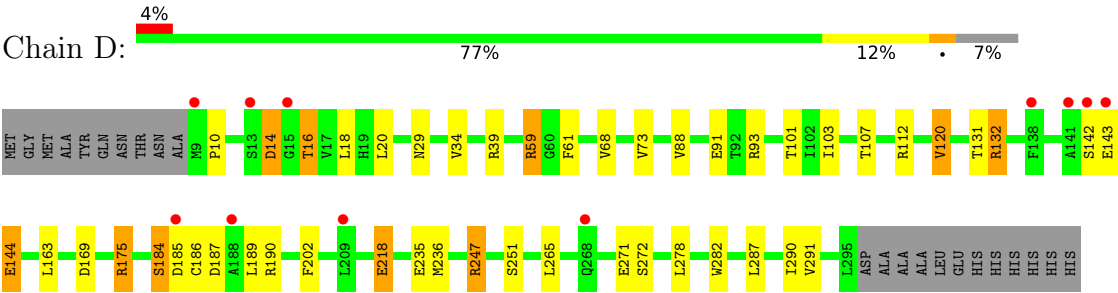
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	9	11	2	5		
3	B	1	Total	C	H	N	O	0	0
			27	9	11	2	5		
3	C	1	Total	C	H	N	O	0	0
			27	9	11	2	5		
3	D	1	Total	C	H	N	O	0	0
			28	9	12	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	140	Total	O	0	0
			140	140		
4	C	136	Total	O	0	0
			136	136		
4	D	128	Total	O	0	0
			128	128		

- Molecule 1: Uridine phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.79Å 97.38Å 188.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 2.10 48.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.69-2.10) 99.4 (48.69-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.246 , 0.317 0.246 , 0.317	Depositor DCC
R_{free} test set	3655 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17862	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5795e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DUR

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	0.59	0/2181	0.73	0/2961
1	B	0.68	1/2189 (0.0%)	0.77	0/2972
1	C	0.61	0/2190	0.74	1/2972 (0.0%)
1	D	0.60	0/2181	0.73	1/2961 (0.0%)
All	All	0.62	1/8741 (0.0%)	0.74	2/11866 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	CYS	CB-SG	6.22	1.92	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	59	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	184	SER	Peptide

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	2147	2147	2144	28	0
1	B	2155	2150	2148	58	0
1	C	2157	2151	2149	45	0
1	D	2147	2146	2144	41	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	16	11	11	2	0
3	B	16	11	12	1	0
3	C	16	11	11	5	0
3	D	16	12	12	3	0
4	A	129	0	0	4	0
4	B	140	0	0	9	0
4	C	136	0	0	10	0
4	D	128	0	0	8	0
All	All	9223	8639	8631	172	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 10.

The worst 5 of 172 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)
3:C:402:DUR:C1'	3:C:402:DUR:O4'	1.66	1.22
3:A:402:DUR:O4'	3:A:402:DUR:C1'	1.63	1.18
1:C:236:MET:SD	4:C:592:HOH:O	2.10	1.10
1:B:141:ALA:O	1:B:143:GLU:N	2.04	0.90
1:B:39:ARG:HH22	1:B:107:THR:HG22	1.42	0.84

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	285/309 (92%)	270 (95%)	14 (5%)	1 (0%)	36	34
1	B	286/309 (93%)	265 (93%)	18 (6%)	3 (1%)	17	12
1	C	286/309 (93%)	271 (95%)	11 (4%)	4 (1%)	12	7
1	D	285/309 (92%)	273 (96%)	10 (4%)	2 (1%)	24	19
All	All	1142/1236 (92%)	1079 (94%)	53 (5%)	10 (1%)	19	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	B	142	SER
1	B	186	CYS
1	C	14	ASP
1	C	296	ASP

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	237/253 (94%)	220 (93%)	17 (7%)	16	12
1	B	238/253 (94%)	219 (92%)	19 (8%)	13	9
1	C	237/253 (94%)	223 (94%)	14 (6%)	21	18
1	D	237/253 (94%)	221 (93%)	16 (7%)	17	14
All	All	949/1012 (94%)	883 (93%)	66 (7%)	16	13

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	172	THR
1	C	59	ARG
1	D	218	GLU
1	B	175	ARG
1	B	235	GLU

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

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](#)

8 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	401	-	4,4,4	1.34	0	6,6,6	1.21	1 (16%)
3	DUR	A	402	-	11,17,17	4.91	6 (54%)	14,24,24	1.00	2 (14%)
2	PO4	B	401	-	4,4,4	1.41	1 (25%)	6,6,6	0.75	0
3	DUR	B	402	-	11,17,17	4.84	7 (63%)	14,24,24	0.95	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	401	-	4,4,4	1.02	0	6,6,6	1.07	0
3	DUR	C	402	-	11,17,17	5.30	8 (72%)	14,24,24	1.86	4 (28%)
2	PO4	D	401	-	4,4,4	1.24	1 (25%)	6,6,6	0.64	0
3	DUR	D	402	-	11,17,17	4.91	8 (72%)	14,24,24	1.55	3 (21%)

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	401	-	-	0/0/0/0	0/0/0/0
3	DUR	A	402	-	-	0/2/18/18	0/2/2/2
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	DUR	B	402	-	-	0/2/18/18	0/2/2/2
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
3	DUR	C	402	-	-	0/2/18/18	0/2/2/2
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
3	DUR	D	402	-	-	0/2/18/18	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	DUR	O4'-C4'	-7.24	1.28	1.45
3	B	402	DUR	C2'-C1'	-6.99	1.33	1.52
3	A	402	DUR	O4'-C4'	-6.84	1.29	1.45
3	D	402	DUR	O4'-C4'	-6.71	1.30	1.45
3	A	402	DUR	C2'-C1'	-6.57	1.34	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	DUR	O3'-C3'-C2'	-2.75	100.95	110.86
3	C	402	DUR	C2'-C1'-N1	-2.71	108.03	114.27
3	A	402	DUR	C2'-C1'-N1	-2.29	108.98	114.27
3	B	402	DUR	C2'-C1'-N1	-2.17	109.26	114.27
3	D	402	DUR	C2'-C1'-N1	-2.04	109.57	114.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PO4	2	0
3	A	402	DUR	2	0
2	B	401	PO4	1	0
3	B	402	DUR	1	0
2	C	401	PO4	1	0
3	C	402	DUR	5	0
2	D	401	PO4	1	0
3	D	402	DUR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/309 (92%)	0.21	12 (4%) 36 43	14, 25, 54, 88	0
1	B	288/309 (93%)	0.45	16 (5%) 24 30	13, 25, 61, 95	0
1	C	289/309 (93%)	0.50	11 (3%) 40 47	14, 28, 56, 110	0
1	D	287/309 (92%)	0.31	11 (3%) 40 47	14, 28, 48, 101	0
All	All	1151/1236 (93%)	0.37	50 (4%) 35 41	13, 27, 56, 110	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLU	9.9
1	B	182	ALA	9.3
1	A	182	ALA	6.9
1	A	184	SER	6.9
1	B	181	ALA	6.0

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. 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(\AA^2)	Q<0.9
3	DUR	D	402	16/16	0.89	0.16	21,30,38,46	0
3	DUR	B	402	16/16	0.89	0.14	15,23,29,30	0
3	DUR	C	402	16/16	0.90	0.14	17,26,37,45	0
3	DUR	A	402	16/16	0.90	0.14	19,26,35,37	0
2	PO4	D	401	5/5	0.98	0.11	18,19,22,25	0
2	PO4	A	401	5/5	0.99	0.15	16,18,20,21	0
2	PO4	B	401	5/5	0.99	0.13	15,17,21,23	0
2	PO4	C	401	5/5	0.99	0.13	17,19,21,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.