Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:46 PM BST

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)

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

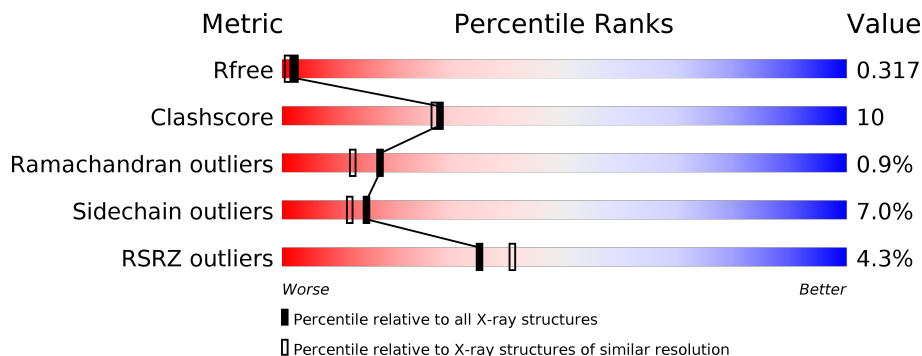|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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	Percentile Ranks	Value
Rfree		0.317
Clashscore		10
Ramachandran outliers		0.9%
Sidechain outliers		7.0%
RSRZ outliers		4.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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	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 crite-

ria:

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

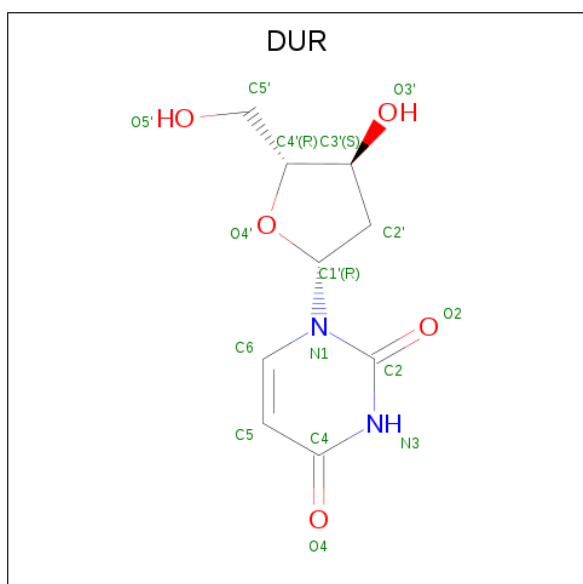*Continued on next page...*

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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: O_4P) (labeled as "Ligand of Interest" by author).

PO4

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

- Molecule 3 is 2'-DEOXYURIDINE (three-letter code: DUR) (formula: $C_9H_{12}N_2O_5$) (labeled as "Ligand of Interest" by author).

DUR

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

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

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.
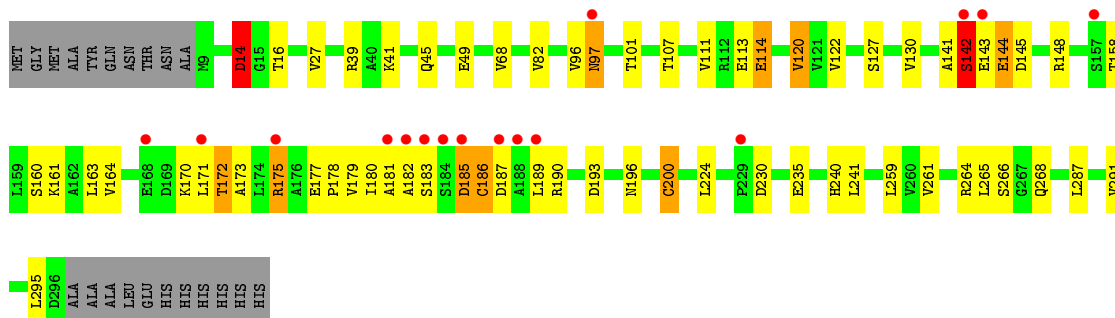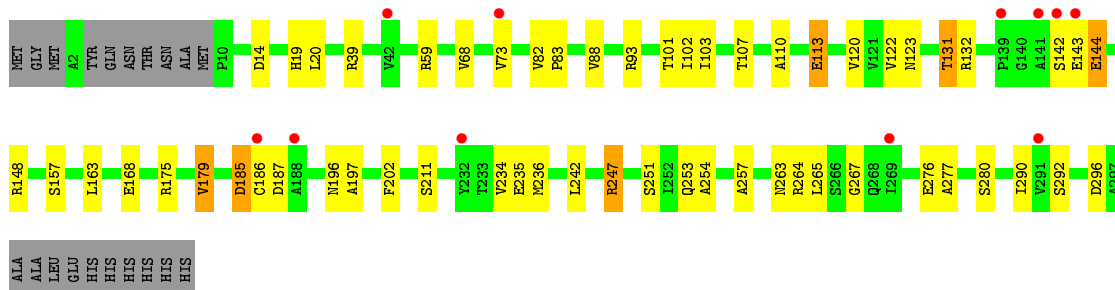
- Molecule 1: Uridine phosphorylase
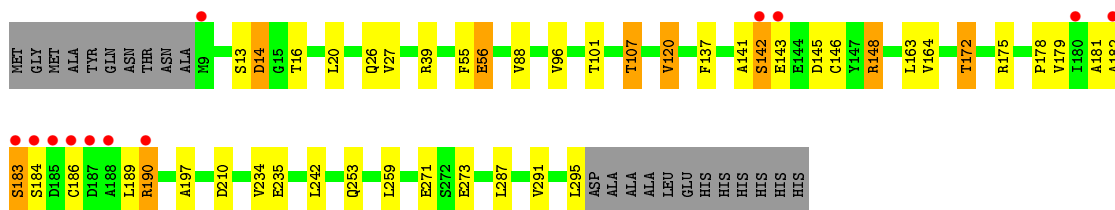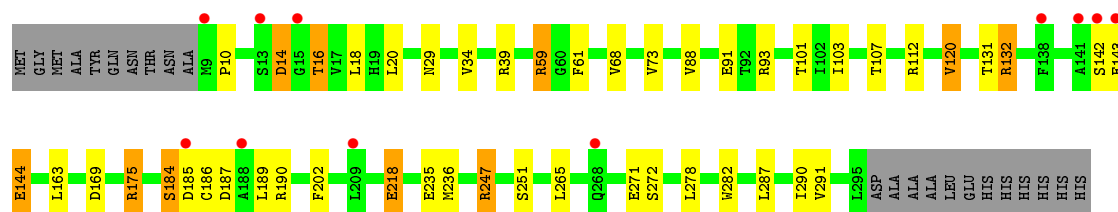

- Molecule 1: Uridine phosphorylase

- Molecule 1: Uridine phosphorylase

• Molecule 1: Uridine phosphorylase

Chain D:

4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [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]	$<|L|> = 0.57$, $<L^2> = 0.42$	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.*

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[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, 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(^{o})	Ideal(^{o})
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 (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	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.

All (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
1:A:107:THR:HG23	2:A:401:PO4:O1	1.76	0.84
1:A:14:ASP:HB3	1:A:16:THR:HG23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:O	1:A:143:GLU:N	2.12	0.83
1:B:185:ASP:O	1:B:187:ASP:N	2.14	0.81
1:A:172:THR:OG1	1:A:175:ARG:NH2	2.14	0.80
1:B:161:LYS:NZ	4:B:503:HOH:O	2.13	0.80
1:B:160:SER:O	1:B:164:VAL:HG23	1.80	0.79
1:D:236:MET:SD	4:D:590:HOH:O	2.40	0.79
1:C:236:MET:HE3	3:C:402:DUR:H2'2	1.66	0.78
1:A:271:GLU:OE1	1:A:273:GLU:N	2.16	0.77
1:C:168:GLU:OE1	4:C:501:HOH:O	2.03	0.77
1:C:276:GLU:OE2	4:C:502:HOH:O	2.08	0.71
1:A:210:ASP:OD2	4:A:501:HOH:O	2.09	0.70
1:C:39:ARG:HH22	1:C:107:THR:HG22	1.57	0.70
1:A:175:ARG:O	1:A:181:ALA:HB2	1.92	0.70
1:C:39:ARG:NH2	1:C:107:THR:HG22	2.07	0.70
1:D:20:LEU:HD21	1:D:88:VAL:HA	1.74	0.69
1:D:131:THR:HG23	4:D:589:HOH:O	1.92	0.69
1:B:189:LEU:HD12	1:B:189:LEU:O	1.93	0.68
1:B:39:ARG:NH2	1:B:107:THR:HG22	2.08	0.68
1:D:202:PHE:HA	1:D:236:MET:HE2	1.76	0.68
1:B:14:ASP:HB3	1:B:16:THR:HG23	1.76	0.67
1:B:171:LEU:O	1:B:175:ARG:HD3	1.95	0.67
1:B:200:CYS:SG	4:B:588:HOH:O	2.46	0.67
1:D:189:LEU:HD13	1:D:278:LEU:HD21	1.78	0.66
1:C:131:THR:HG23	4:C:545:HOH:O	1.96	0.66
1:D:14:ASP:HB3	1:D:16:THR:HG23	1.78	0.65
1:B:120:VAL:HG13	1:B:259:LEU:HD23	1.79	0.65
1:B:190:ARG:NE	4:B:504:HOH:O	2.14	0.65
1:B:107:THR:HG23	2:B:401:PO4:O2	1.96	0.65
1:A:39:ARG:HH22	1:A:107:THR:HG22	1.62	0.65
1:A:287:LEU:O	1:A:291:VAL:HG22	1.98	0.64
1:B:177:GLU:O	1:B:181:ALA:N	2.25	0.64
1:C:280:SER:OG	4:C:503:HOH:O	2.12	0.64
1:D:185:ASP:O	1:D:187:ASP:N	2.32	0.63
1:C:107:THR:HG23	2:C:401:PO4:O1	1.98	0.63
1:D:39:ARG:NH2	1:D:107:THR:HG22	2.14	0.63
1:A:39:ARG:NH2	1:A:107:THR:HG22	2.14	0.62
1:B:82:VAL:HG13	1:B:240:HIS:CG	2.34	0.62
1:C:113:GLU:N	1:C:113:GLU:OE1	2.32	0.62
1:B:185:ASP:N	1:B:185:ASP:OD1	2.31	0.62
1:B:170:LYS:NZ	4:B:509:HOH:O	2.33	0.62
1:C:82:VAL:HG23	4:C:528:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:HG22	1:C:257:ALA:HB2	1.81	0.61
1:C:202:PHE:HD1	1:C:236:MET:CE	2.14	0.61
1:D:107:THR:HG23	2:D:401:PO4:O3	2.01	0.61
1:A:190:ARG:NE	4:A:504:HOH:O	2.29	0.61
1:D:107:THR:OG1	3:D:402:DUR:O4'	2.18	0.60
1:C:107:THR:OG1	3:C:402:DUR:O4'	2.19	0.60
1:A:120:VAL:HG13	1:A:259:LEU:HD23	1.83	0.60
1:D:236:MET:HE3	3:D:402:DUR:H2'2	1.83	0.60
1:B:27:VAL:HG13	1:B:96:VAL:CG2	2.31	0.59
1:A:101:THR:HG23	1:A:295:LEU:HD23	1.84	0.59
1:C:202:PHE:HA	1:C:236:MET:HE2	1.85	0.58
1:B:177:GLU:O	1:B:180:ILE:N	2.37	0.58
1:D:202:PHE:HB2	1:D:236:MET:CE	2.34	0.58
1:D:236:MET:HE3	3:D:402:DUR:O2	2.04	0.58
1:A:183:SER:OG	1:A:184:SER:N	2.36	0.58
1:D:202:PHE:HD1	1:D:236:MET:CE	2.17	0.57
1:A:56:GLU:OE1	1:B:45:GLN:NE2	2.36	0.56
1:B:172:THR:HA	1:B:175:ARG:CZ	2.36	0.56
1:B:175:ARG:HB3	1:B:186:CYS:SG	2.46	0.55
3:A:402:DUR:O5'	1:C:19:HIS:NE2	2.34	0.55
1:C:185:ASP:O	1:C:187:ASP:N	2.40	0.55
1:D:39:ARG:HH22	1:D:107:THR:HG22	1.71	0.55
1:D:202:PHE:CA	1:D:236:MET:HE2	2.36	0.54
1:C:236:MET:CE	3:C:402:DUR:H2'2	2.37	0.54
1:C:211:SER:CB	4:C:510:HOH:O	2.56	0.54
1:B:130:VAL:HG21	1:B:224:LEU:HD11	1.89	0.53
1:B:122:VAL:O	1:B:193:ASP:HA	2.09	0.53
1:D:112:ARG:NH2	4:D:512:HOH:O	2.42	0.53
1:A:179:VAL:O	1:A:183:SER:HB3	2.08	0.53
1:C:236:MET:HE3	3:C:402:DUR:O2	2.09	0.53
1:B:122:VAL:CB	1:B:164:VAL:HG22	2.39	0.53
1:A:27:VAL:HG13	1:A:96:VAL:CG2	2.40	0.52
1:D:101:THR:HG21	4:D:549:HOH:O	2.09	0.52
1:C:211:SER:HB3	4:C:510:HOH:O	2.10	0.50
1:B:178:PRO:HA	1:B:182:ALA:H	1.77	0.50
1:C:264:ARG:HD3	4:C:558:HOH:O	2.11	0.50
1:B:178:PRO:HA	1:B:181:ALA:HB3	1.93	0.50
1:B:122:VAL:HG11	1:B:164:VAL:HG22	1.92	0.50
1:B:287:LEU:O	1:B:291:VAL:HG22	2.12	0.50
1:D:34:VAL:HB	1:D:39:ARG:HD2	1.94	0.50
1:B:172:THR:HA	1:B:175:ARG:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD22	1:D:91:GLU:HB2	1.93	0.49
1:B:172:THR:HG22	1:B:173:ALA:N	2.28	0.49
1:B:185:ASP:HB3	4:B:615:HOH:O	2.11	0.49
1:B:107:THR:OG1	3:B:402:DUR:O4'	2.30	0.49
1:B:101:THR:HG23	1:B:295:LEU:HD23	1.95	0.49
1:C:202:PHE:HB2	1:C:236:MET:CE	2.43	0.49
1:A:26:GLN:HB3	1:A:55:PHE:CZ	2.48	0.49
1:C:175:ARG:HD2	4:C:566:HOH:O	2.12	0.49
1:B:82:VAL:HG13	1:B:240:HIS:CB	2.43	0.48
1:D:175:ARG:NH2	4:D:504:HOH:O	2.26	0.48
1:C:103:ILE:HD12	1:C:290:ILE:HB	1.95	0.48
1:D:169:ASP:O	4:D:501:HOH:O	2.20	0.47
1:B:143:GLU:HG2	1:B:143:GLU:O	2.13	0.47
1:C:20:LEU:HD21	1:C:88:VAL:HA	1.94	0.47
1:B:142:SER:O	1:B:144:GLU:OE2	2.32	0.47
1:C:202:PHE:HD1	1:C:236:MET:HE1	1.78	0.47
1:C:101:THR:HA	1:C:253:GLN:O	2.14	0.47
1:C:202:PHE:CD1	1:C:236:MET:CE	2.97	0.47
1:C:82:VAL:HB	1:C:83:PRO:HD3	1.96	0.47
1:D:189:LEU:CD1	1:D:278:LEU:HD21	2.44	0.46
1:D:202:PHE:CB	1:D:236:MET:HE2	2.44	0.46
1:D:287:LEU:O	1:D:291:VAL:HG22	2.15	0.46
1:B:122:VAL:CG1	1:B:164:VAL:HG22	2.46	0.46
1:C:123:ASN:ND2	1:C:196:ASN:HB2	2.30	0.46
1:C:179:VAL:HG11	1:C:277:ALA:HB2	1.97	0.46
1:D:202:PHE:CD1	1:D:236:MET:CE	2.98	0.46
1:A:253:GLN:HG2	4:A:537:HOH:O	2.16	0.45
1:A:178:PRO:O	1:A:182:ALA:HB3	2.16	0.45
1:B:82:VAL:HG13	1:B:240:HIS:HB2	1.98	0.45
1:C:110:ALA:O	1:C:264:ARG:HG2	2.17	0.45
1:D:103:ILE:HD12	1:D:290:ILE:HB	1.99	0.45
1:D:93:ARG:NH1	1:D:251:SER:HB2	2.32	0.45
1:B:241:LEU:HD12	1:B:241:LEU:O	2.17	0.45
1:B:266:SER:C	1:B:268:GLN:H	2.21	0.45
1:B:41:LYS:O	1:B:45:GLN:HG2	2.16	0.45
1:B:114:GLU:HG2	1:B:114:GLU:O	2.17	0.44
1:B:172:THR:O	1:B:175:ARG:NE	2.50	0.44
1:C:93:ARG:NH1	1:C:251:SER:HB2	2.33	0.44
1:A:178:PRO:O	1:A:182:ALA:N	2.51	0.44
1:B:122:VAL:HG11	1:B:164:VAL:CG2	2.47	0.44
1:D:120:VAL:HG22	1:D:282:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:HB2	1:B:196:ASN:HB3	1.99	0.43
1:A:107:THR:CG2	2:A:401:PO4:O1	2.58	0.43
1:B:122:VAL:HB	1:B:164:VAL:HG22	1.99	0.43
1:C:202:PHE:CD1	1:C:236:MET:HE1	2.54	0.43
1:D:10:PRO:HB2	1:D:18:LEU:HD11	2.00	0.43
1:B:172:THR:HA	1:B:175:ARG:NE	2.33	0.43
1:D:68:VAL:HG23	1:D:73:VAL:HG11	1.99	0.43
1:D:142:SER:O	1:D:144:GLU:HG2	2.18	0.43
1:D:20:LEU:HD12	1:D:61:PHE:CD2	2.54	0.43
1:A:20:LEU:HD21	1:A:88:VAL:HA	2.00	0.43
1:A:181:ALA:O	1:A:183:SER:O	2.37	0.43
1:B:266:SER:C	4:B:534:HOH:O	2.57	0.43
1:B:111:VAL:HG12	1:B:264:ARG:HB2	2.01	0.42
1:C:68:VAL:HG23	1:C:73:VAL:HG11	2.02	0.42
1:C:102:ILE:O	1:C:254:ALA:HA	2.19	0.42
1:B:230:ASP:O	4:B:505:HOH:O	2.20	0.42
1:D:202:PHE:HB2	1:D:236:MET:HE1	1.99	0.42
1:A:137:PHE:CZ	1:A:146:CYS:HB3	2.54	0.42
1:B:171:LEU:O	1:B:175:ARG:CD	2.66	0.42
1:B:97:ASN:C	1:B:97:ASN:OD1	2.58	0.42
1:C:197:ALA:O	1:C:234:VAL:HA	2.19	0.42
1:C:247:ARG:HD3	1:C:247:ARG:HA	1.85	0.42
1:B:68:VAL:HG12	1:B:291:VAL:HG21	2.02	0.42
1:A:210:ASP:CB	4:A:501:HOH:O	2.67	0.42
1:D:68:VAL:HG23	1:D:73:VAL:CG1	2.50	0.42
1:B:39:ARG:NH2	1:B:107:THR:CG2	2.80	0.42
1:B:172:THR:CB	4:B:508:HOH:O	2.67	0.41
1:C:142:SER:C	1:C:144:GLU:H	2.24	0.41
1:D:132:ARG:NH1	4:D:519:HOH:O	2.51	0.41
1:D:14:ASP:CB	1:D:16:THR:HG23	2.48	0.41
1:A:197:ALA:O	1:A:234:VAL:HA	2.20	0.41
1:C:197:ALA:HB3	1:C:234:VAL:HG22	2.02	0.41
1:D:218:GLU:CD	1:D:218:GLU:H	2.22	0.41
1:C:202:PHE:CA	1:C:236:MET:HE2	2.49	0.41
1:A:148:ARG:HH12	1:C:148:ARG:HH11	1.67	0.41
1:C:263:ASN:O	1:C:267:GLY:N	2.54	0.41
1:D:190:ARG:HH11	1:D:190:ARG:HG2	1.86	0.40
1:D:247:ARG:NE	4:D:502:HOH:O	2.25	0.40
1:B:172:THR:HG22	4:B:508:HOH:O	2.20	0.40
1:C:142:SER:O	1:C:144:GLU:N	2.45	0.40
1:D:202:PHE:CD1	1:D:236:MET:HE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:O	1:B:183:SER:OG	2.25	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	285/309 (92%)	270 (95%)	14 (5%)	1 (0%)	34	32
1	B	286/309 (93%)	265 (93%)	18 (6%)	3 (1%)	15	11
1	C	286/309 (93%)	271 (95%)	11 (4%)	4 (1%)	11	6
1	D	285/309 (92%)	273 (96%)	10 (4%)	2 (1%)	22	18
All	All	1142/1236 (92%)	1079 (94%)	53 (5%)	10 (1%)	17	12

All (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
1	D	14	ASP
1	D	186	CYS
1	B	14	ASP
1	C	186	CYS
1	C	113	GLU

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%)	14	11
1	B	238/253 (94%)	219 (92%)	19 (8%)	12	8
1	C	237/253 (94%)	223 (94%)	14 (6%)	19	17
1	D	237/253 (94%)	221 (93%)	16 (7%)	16	13
All	All	949/1012 (94%)	883 (93%)	66 (7%)	15	12

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	14	ASP
1	A	56	GLU
1	A	107	THR
1	A	120	VAL
1	A	142	SER
1	A	145	ASP
1	A	148	ARG
1	A	163	LEU
1	A	164	VAL
1	A	172	THR
1	A	183	SER
1	A	186	CYS
1	A	189	LEU
1	A	190	ARG
1	A	235	GLU
1	A	242	LEU
1	B	14	ASP
1	B	49	GLU
1	B	97	ASN
1	B	113	GLU
1	B	114	GLU
1	B	120	VAL
1	B	142	SER

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Mol	Chain	Res	Type
1	B	144	GLU
1	B	145	ASP
1	B	148	ARG
1	B	158	THR
1	B	163	LEU
1	B	172	THR
1	B	175	ARG
1	B	179	VAL
1	B	185	ASP
1	B	235	GLU
1	B	261	VAL
1	B	265	LEU
1	C	59	ARG
1	C	120	VAL
1	C	131	THR
1	C	143	GLU
1	C	144	GLU
1	C	157	SER
1	C	163	LEU
1	C	179	VAL
1	C	185	ASP
1	C	235	GLU
1	C	242	LEU
1	C	247	ARG
1	C	265	LEU
1	C	292	SER
1	D	16	THR
1	D	29	ASN
1	D	59	ARG
1	D	120	VAL
1	D	132	ARG
1	D	143	GLU
1	D	144	GLU
1	D	163	LEU
1	D	175	ARG
1	D	184	SER
1	D	218	GLU
1	D	235	GLU
1	D	247	ARG
1	D	265	LEU
1	D	271	GLU
1	D	272	SER

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 monosaccharides 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	#$|Z| > 2$
3	DUR	D	402	-	14,17,17	5.03	10 (71%)	14,24,24	1.49	3 (21%)
3	DUR	B	402	-	14,17,17	5.09	9 (64%)	14,24,24	0.95	1 (7%)
3	DUR	C	402	-	14,17,17	5.42	10 (71%)	14,24,24	1.67	3 (21%)
3	DUR	A	402	-	14,17,17	5.33	8 (57%)	14,24,24	0.83	1 (7%)
2	PO4	B	401	-	4,4,4	1.43	1 (25%)	6,6,6	0.75	0
2	PO4	A	401	-	4,4,4	1.35	0	6,6,6	1.22	1 (16%)
2	PO4	D	401	-	4,4,4	1.25	1 (25%)	6,6,6	0.64	0
2	PO4	C	401	-	4,4,4	1.03	0	6,6,6	1.07	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	DUR	C	402	-	-	0/3/18/18	0/2/2/2
3	DUR	D	402	-	-	0/3/18/18	0/2/2/2
3	DUR	A	402	-	-	2/3/18/18	0/2/2/2
3	DUR	B	402	-	-	3/3/18/18	0/2/2/2

All (39) bond length outliers are listed below:

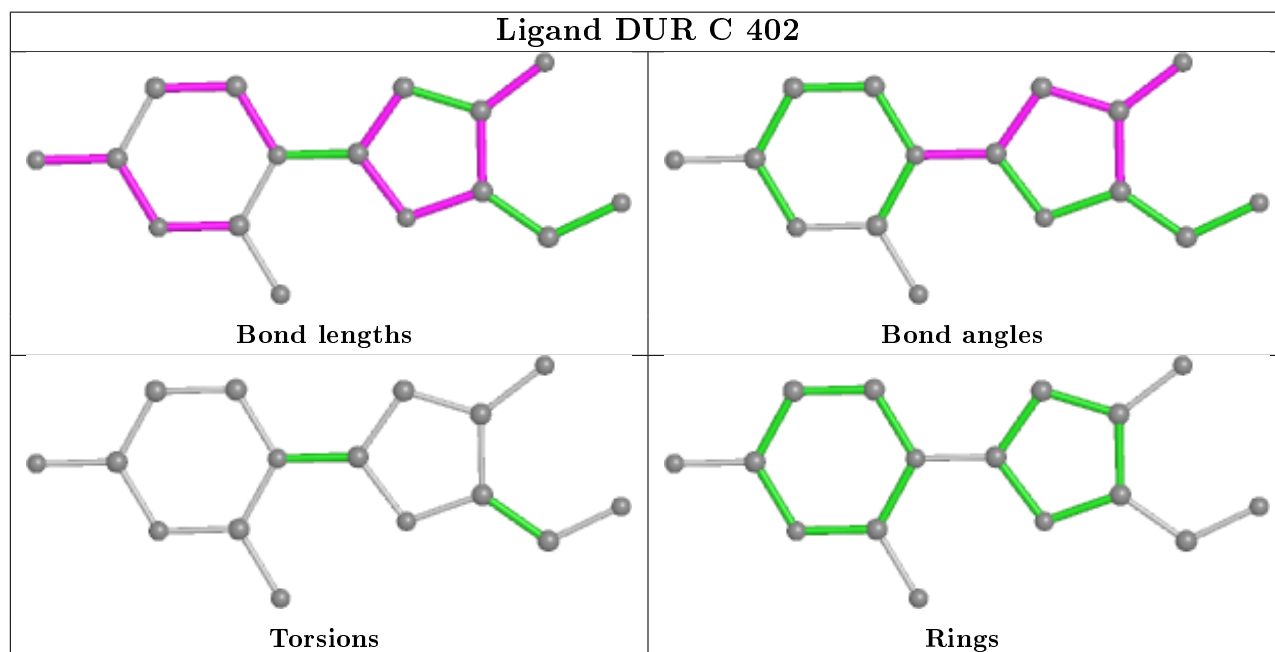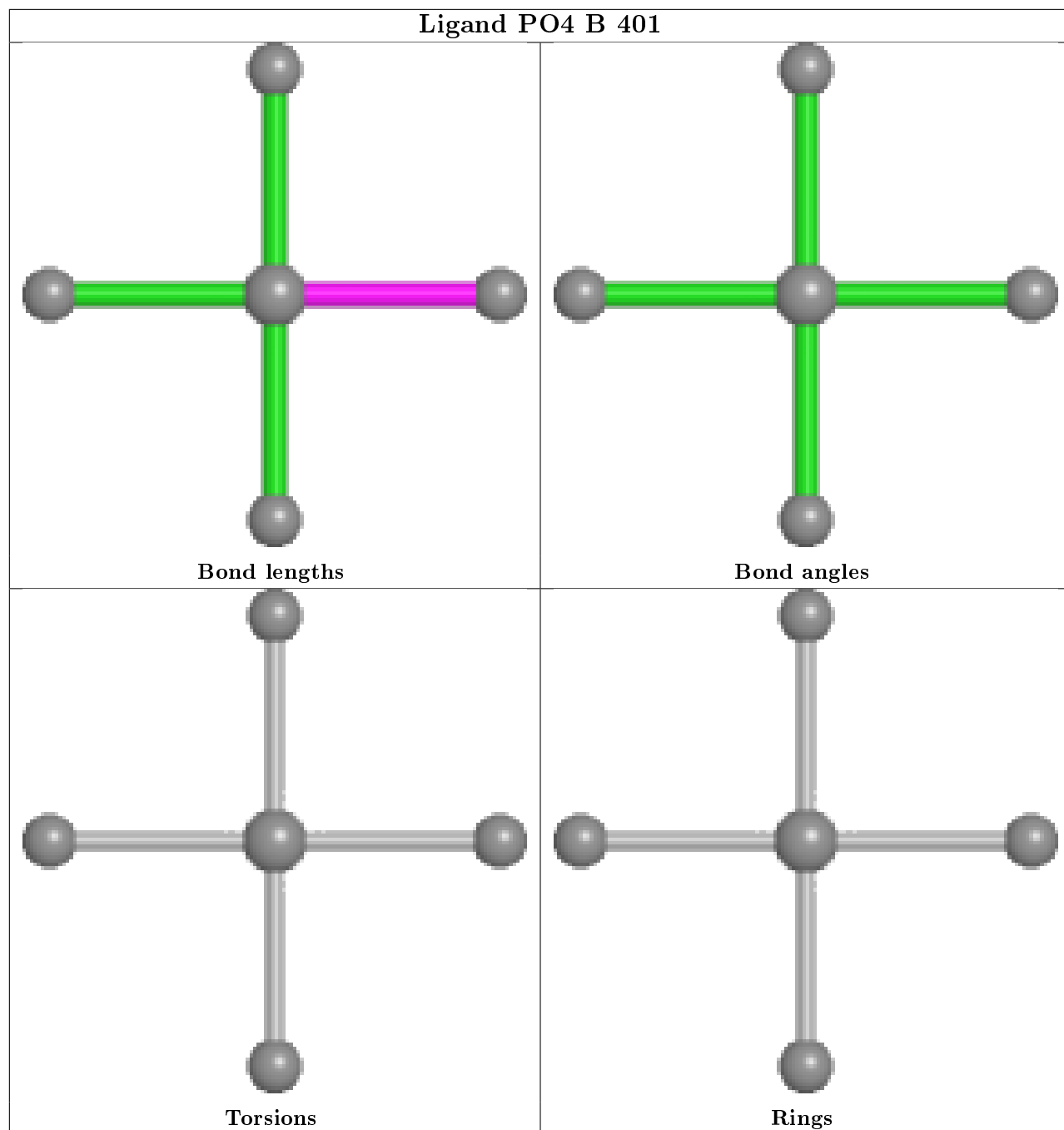| Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	DUR	O4'-C1'	10.57	1.66	1.42
3	A	402	DUR	O4'-C1'	9.45	1.63	1.42
3	D	402	DUR	O4'-C1'	9.24	1.63	1.42
3	A	402	DUR	C4-N3	8.79	1.48	1.33
3	B	402	DUR	O4'-C1'	8.53	1.61	1.42
3	B	402	DUR	C6-N1	7.90	1.45	1.35
3	C	402	DUR	C4-N3	7.88	1.46	1.33
3	C	402	DUR	C6-N1	7.55	1.45	1.35
3	D	402	DUR	C6-N1	7.41	1.45	1.35
3	D	402	DUR	C4-N3	7.35	1.45	1.33
3	C	402	DUR	O4'-C4'	-7.25	1.28	1.45
3	B	402	DUR	C2-N3	7.14	1.52	1.38
3	B	402	DUR	C4-N3	6.92	1.45	1.33
3	A	402	DUR	C2-N3	6.91	1.51	1.38
3	A	402	DUR	O4'-C4'	-6.85	1.29	1.45
3	A	402	DUR	C6-N1	6.83	1.44	1.35
3	B	402	DUR	C2'-C1'	-6.81	1.33	1.52
3	D	402	DUR	O4'-C4'	-6.72	1.30	1.45
3	A	402	DUR	C2'-C1'	-6.41	1.34	1.52
3	D	402	DUR	C2'-C1'	-6.37	1.34	1.52
3	B	402	DUR	O4'-C4'	-6.35	1.30	1.45
3	C	402	DUR	C2'-C1'	-6.31	1.34	1.52
3	C	402	DUR	C2-N3	5.59	1.49	1.38
3	D	402	DUR	C2-N3	5.25	1.48	1.38
3	A	402	DUR	C6-C5	5.16	1.49	1.38
3	C	402	DUR	C6-C5	4.79	1.48	1.38
3	B	402	DUR	C6-C5	4.71	1.48	1.38
3	D	402	DUR	C6-C5	4.64	1.48	1.38
3	C	402	DUR	O3'-C3'	-4.08	1.34	1.43
3	A	402	DUR	O3'-C3'	-3.28	1.36	1.43
3	D	402	DUR	O4-C4	-3.02	1.17	1.24
3	B	402	DUR	O3'-C3'	-2.66	1.37	1.43
3	D	402	DUR	O3'-C3'	-2.47	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	DUR	O4-C4	-2.39	1.18	1.24
3	B	402	DUR	C3'-C4'	2.32	1.59	1.53
3	D	402	DUR	C3'-C4'	2.28	1.59	1.53
2	B	401	PO4	P-O2	-2.28	1.47	1.54
2	D	401	PO4	P-O2	-2.26	1.47	1.54
3	C	402	DUR	C3'-C4'	2.16	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	DUR	O3'-C3'-C2'	-2.78	100.95	110.90
3	C	402	DUR	C2'-C1'-N1	-2.71	108.03	114.27
3	C	402	DUR	O3'-C3'-C4'	2.68	120.35	110.10
3	D	402	DUR	O3'-C3'-C4'	2.58	119.96	110.10
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
2	A	401	PO4	O4-P-O2	2.12	114.79	107.97
3	D	402	DUR	O4'-C4'-C3'	2.12	110.62	105.67
3	D	402	DUR	C2'-C1'-N1	-2.04	109.57	114.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	DUR	O4'-C1'-N1-C6
3	A	402	DUR	C3'-C4'-C5'-O5'
3	A	402	DUR	O4'-C4'-C5'-O5'
3	B	402	DUR	C3'-C4'-C5'-O5'
3	B	402	DUR	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 16 short contacts:

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

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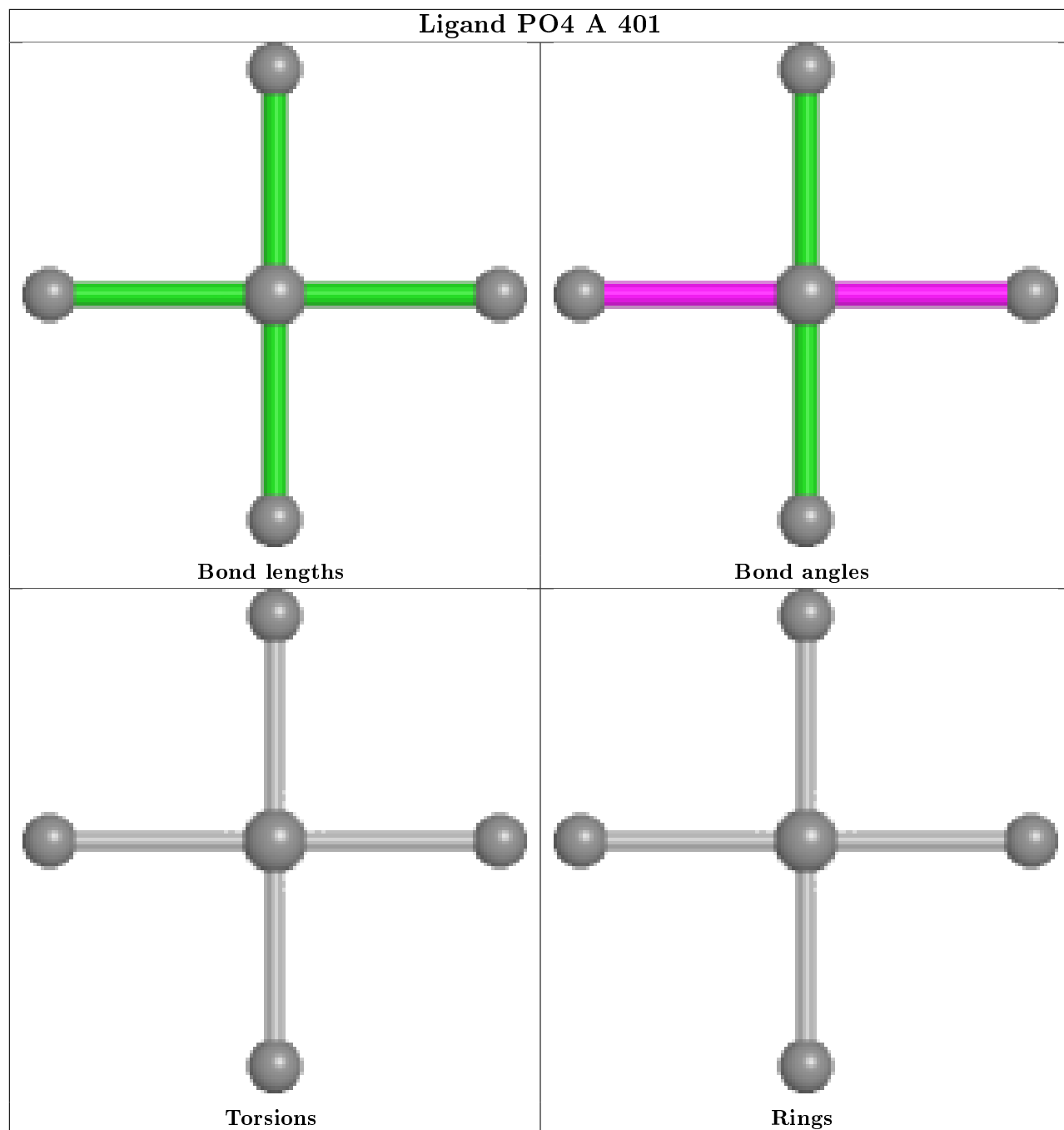| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DUR D 402

Ligand DUR B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand DUR C 402

Bond lengths

Bond angles

Torsions

Rings

Ligand DUR A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand PO4 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PO4 A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PO4 D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PO4 C 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	42	14, 25, 54, 88	0
1	B	288/309 (93%)	0.45	16 (5%)	24	29	13, 25, 61, 95	0
1	C	289/309 (93%)	0.50	11 (3%)	40	46	14, 28, 56, 110	0
1	D	287/309 (92%)	0.31	11 (3%)	40	46	14, 28, 48, 101	0
All	All	1151/1236 (93%)	0.37	50 (4%)	35	41	13, 27, 56, 110	0

All (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
1	A	143	GLU	5.7
1	B	184	SER	5.4
1	C	141	ALA	5.1
1	C	142	SER	4.8
1	B	168	GLU	4.7
1	B	142	SER	4.7
1	C	291	VAL	4.5
1	B	187	ASP	3.7
1	B	175	ARG	3.6
1	D	142	SER	3.6
1	A	185	ASP	3.5
1	C	143	GLU	3.4
1	C	269	ILE	3.3
1	B	157	SER	3.2
1	B	189	LEU	3.2
1	B	183	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	141	ALA	3.0
1	C	186	CYS	2.9
1	B	188	ALA	2.8
1	A	180	ILE	2.8
1	B	97	ASN	2.6
1	C	73	VAL	2.5
1	C	188	ALA	2.5
1	D	138	PHE	2.5
1	D	143	GLU	2.5
1	A	187	ASP	2.5
1	B	185	ASP	2.5
1	A	188	ALA	2.5
1	A	183	SER	2.4
1	D	9	MET	2.4
1	B	171	LEU	2.3
1	C	42	VAL	2.3
1	A	142	SER	2.3
1	B	229	PRO	2.3
1	A	9	MET	2.3
1	A	186	CYS	2.3
1	A	190	ARG	2.3
1	D	185	ASP	2.3
1	D	188	ALA	2.1
1	C	232	TYR	2.1
1	C	139	PRO	2.1
1	D	268	GLN	2.1
1	D	13	SER	2.0
1	D	15	GLY	2.0
1	D	209	LEU	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
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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
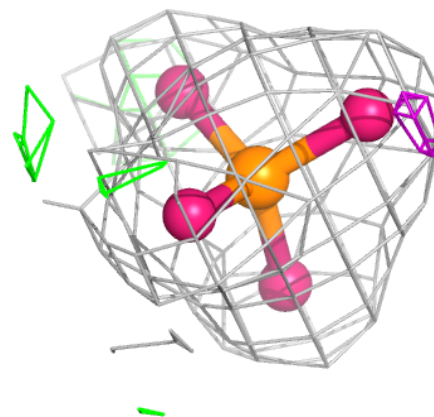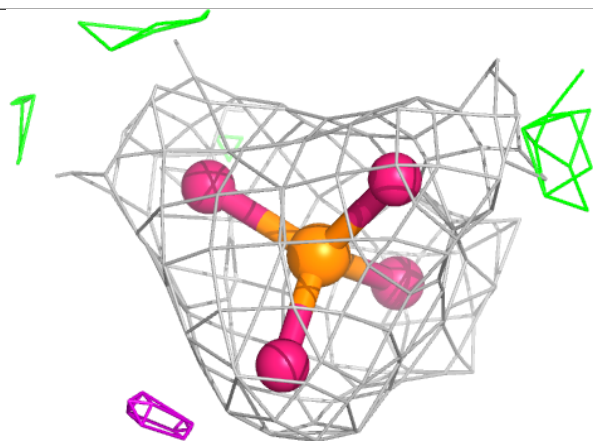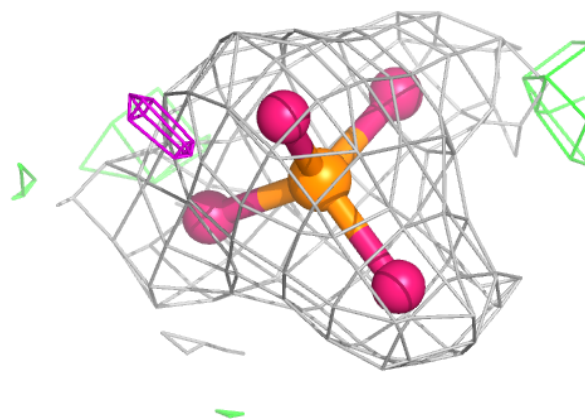

Electron density around DUR D 402:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
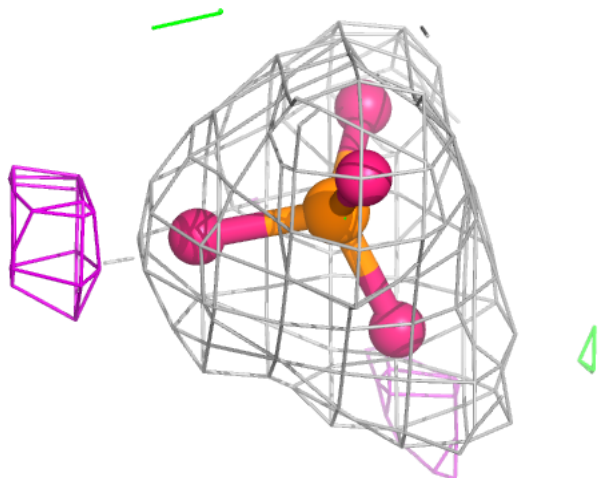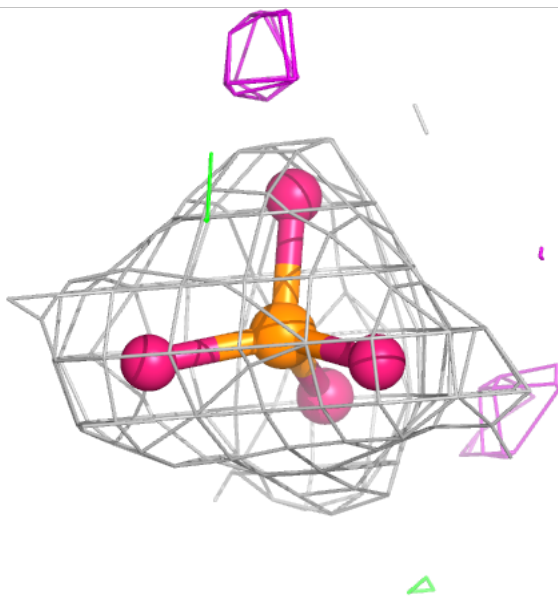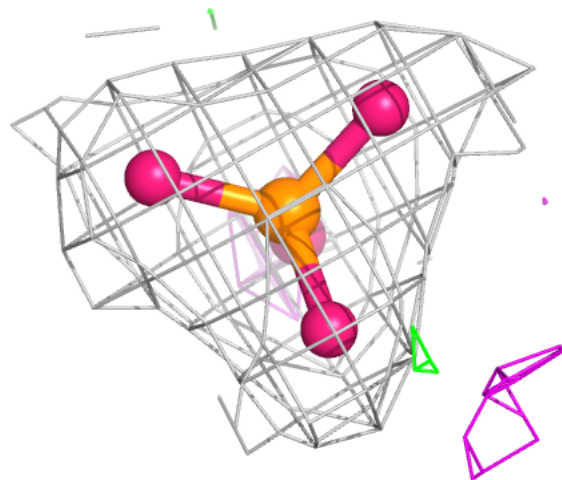and green (positive)

Electron density around DUR B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
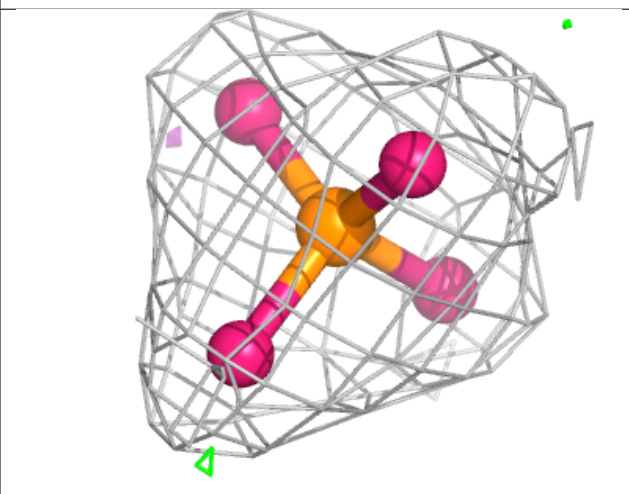mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
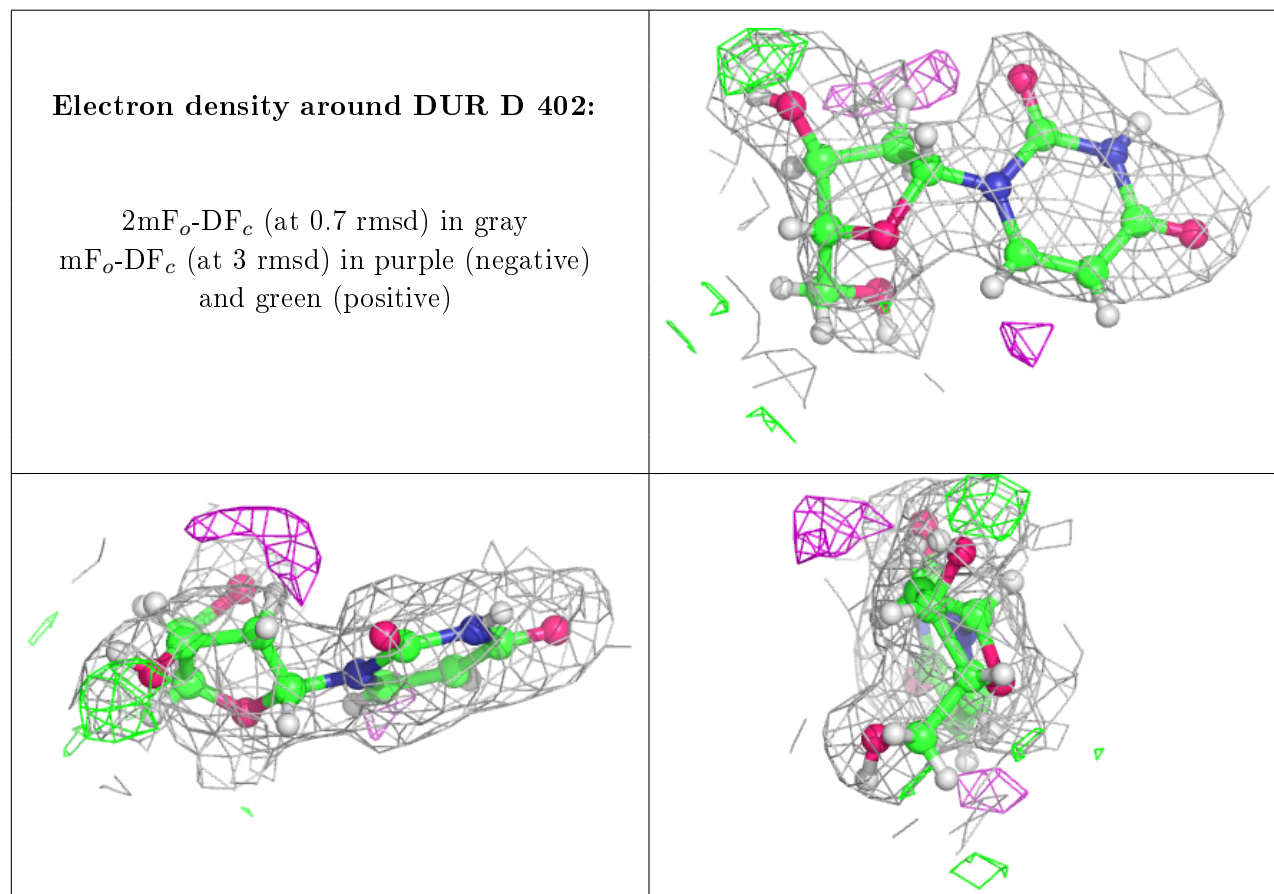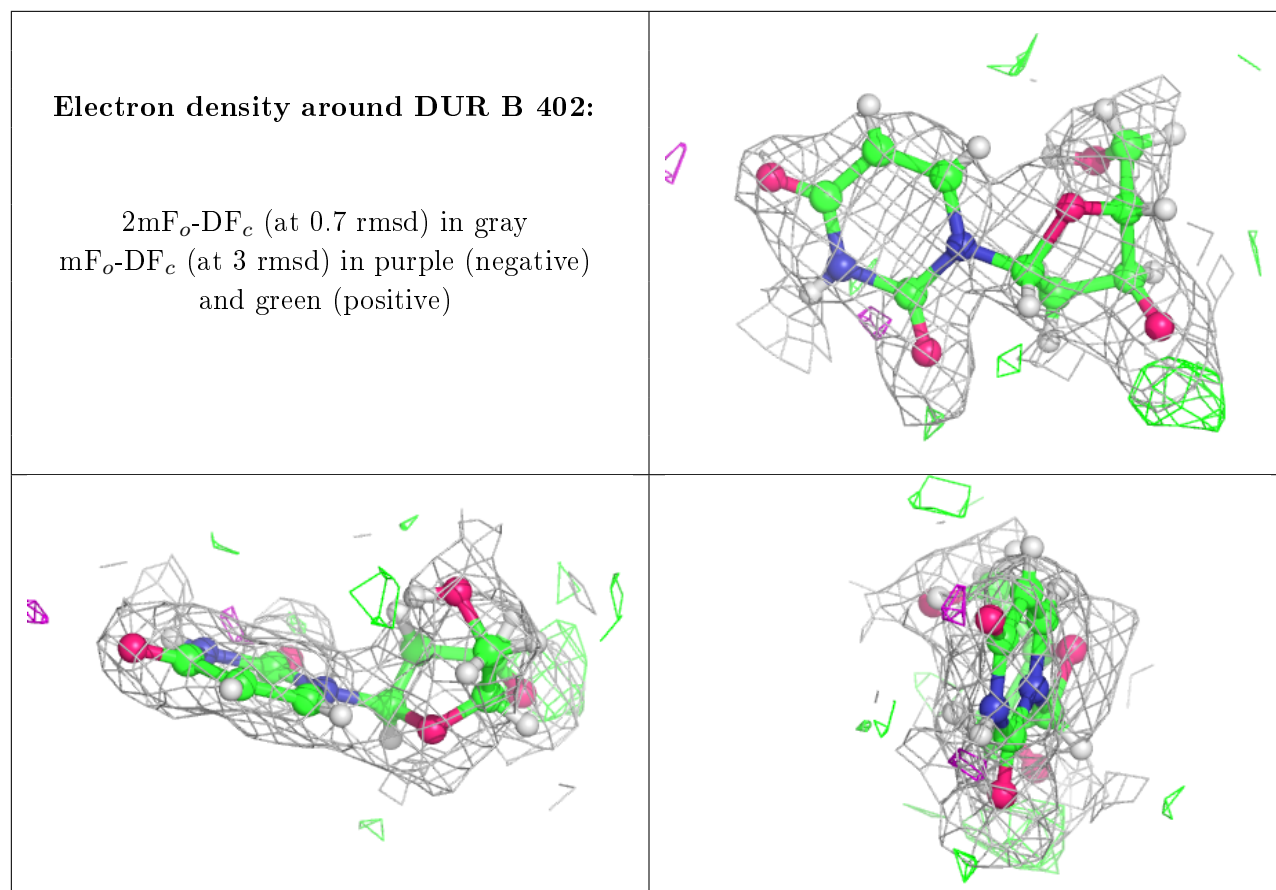
Electron density around DUR C 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around DUR A 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
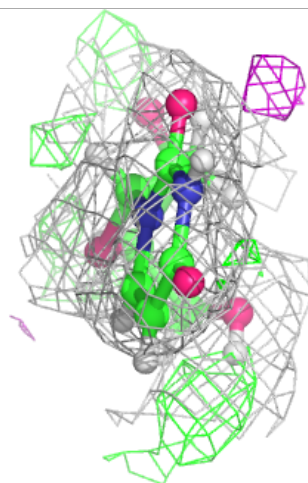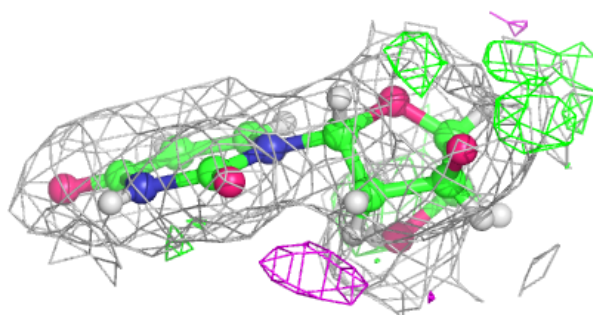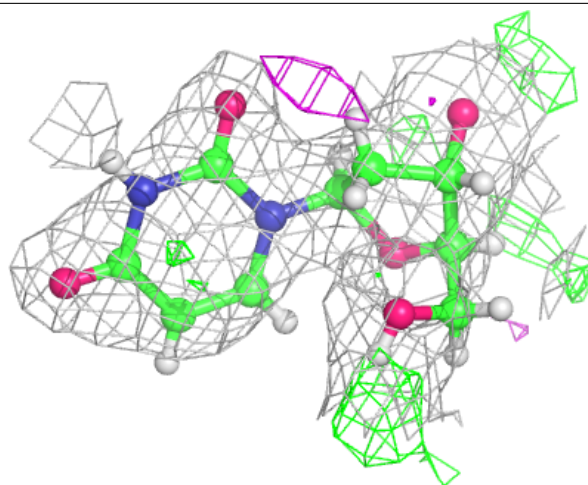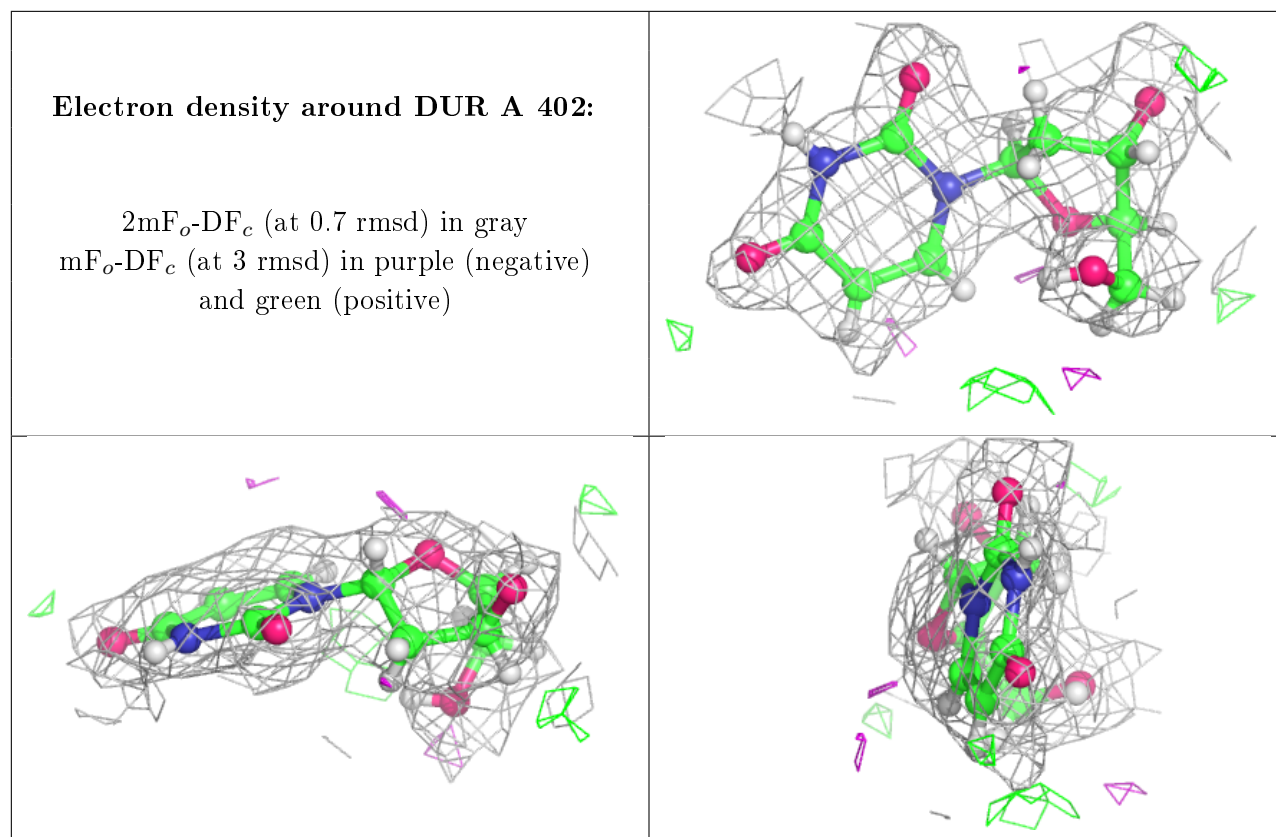
Electron density around PO4 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
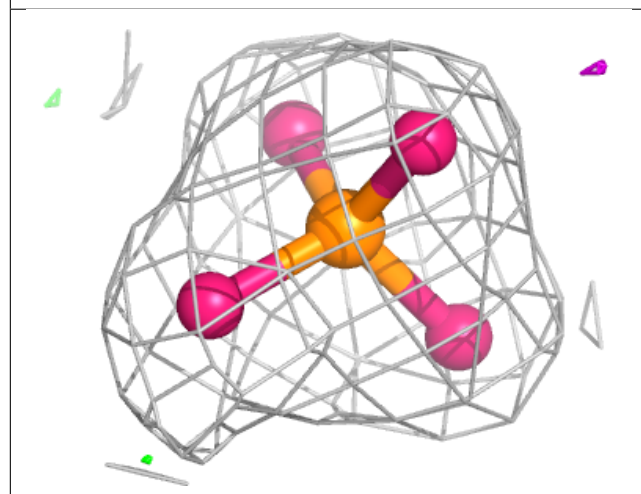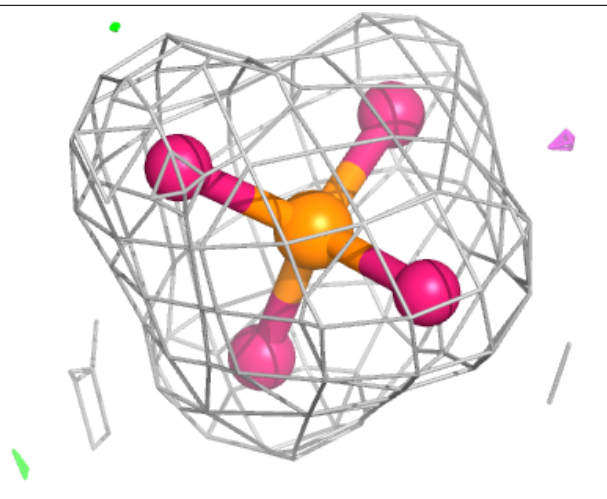mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PO4 A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
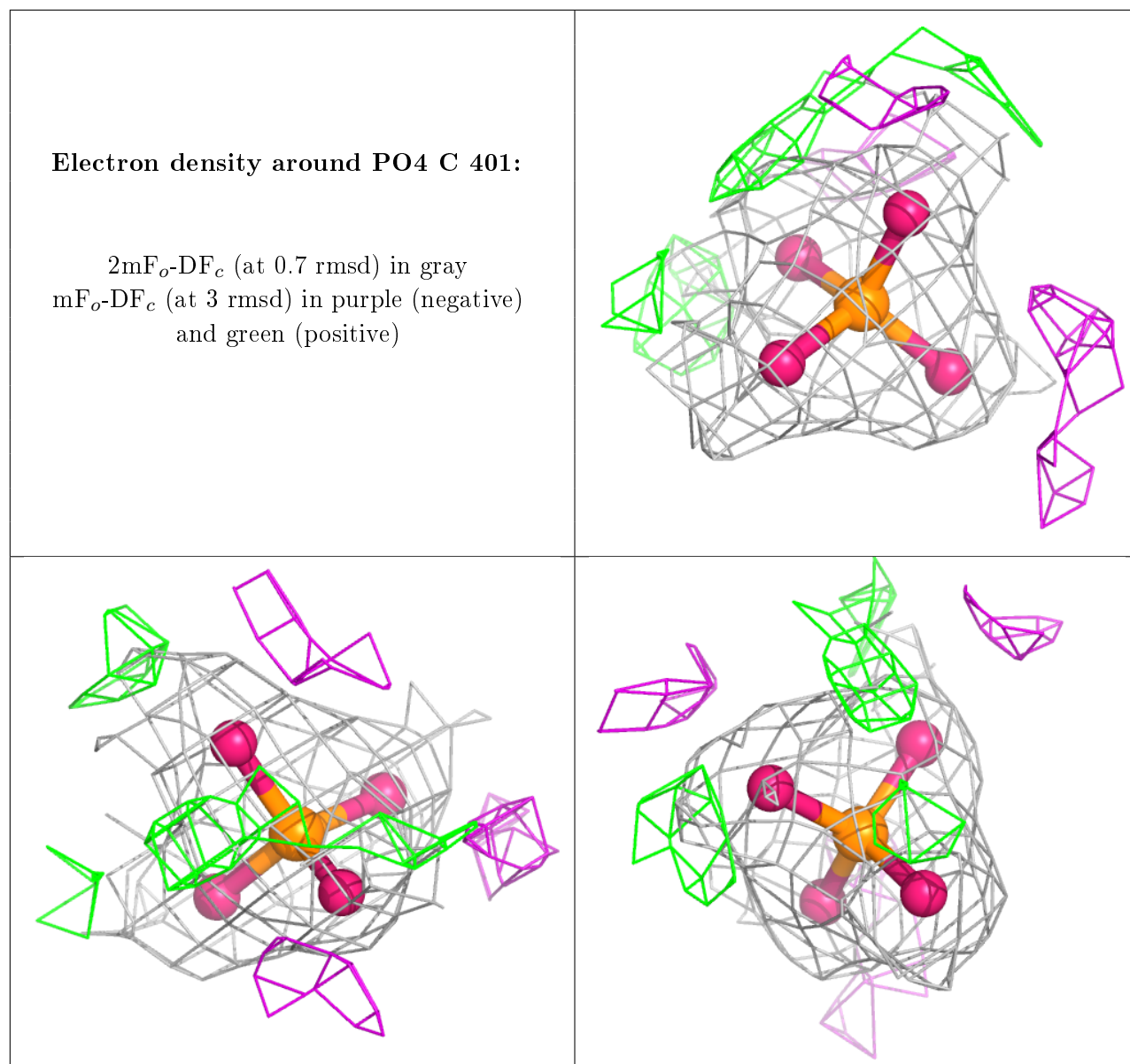and green (positive)

Electron density around PO4 B 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PO4 C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.