



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:09 pm BST

PDB ID : 4XS2
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2015-01-21
Resolution : 2.73 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

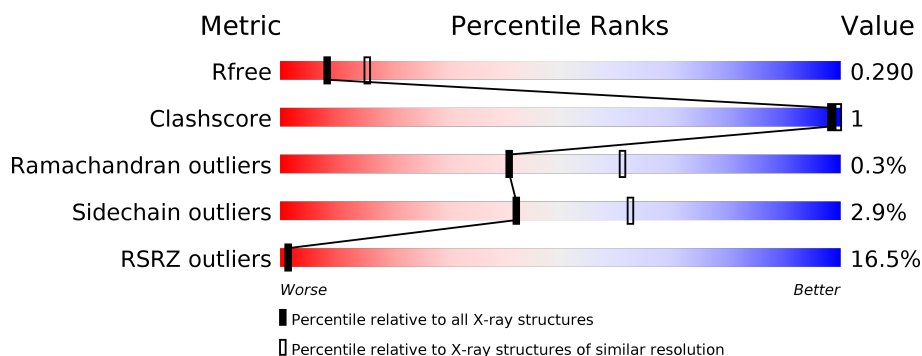
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 $\leq 5\%$. 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	301	<div> <div>17%</div> <div>91%</div> <div>5%</div> </div>
1	B	301	<div> <div>17%</div> <div>90%</div> <div>7%</div> </div>
1	C	301	<div> <div>14%</div> <div>90%</div> <div>6%</div> </div>
1	D	301	<div> <div>13%</div> <div>90%</div> <div>7%</div> </div>

2 Entry composition [i](#)

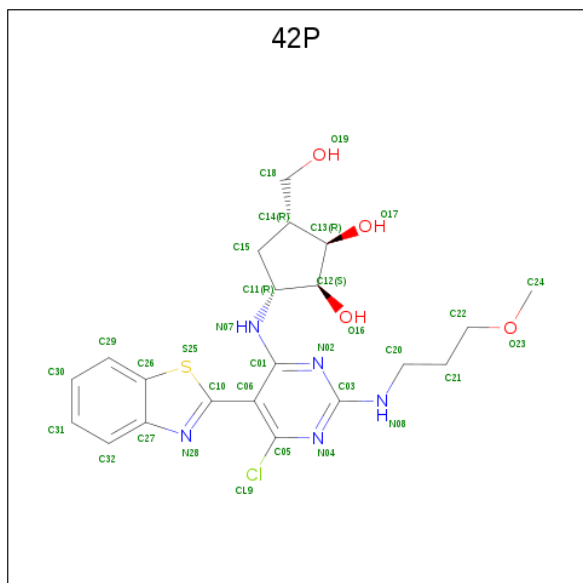
There are 3 unique types of molecules in this entry. The entry contains 9049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	4
			2244	1405	378	444	3	14			
1	B	281	Total	C	N	O	P	S	0	0	3
			2212	1387	373	435	3	14			
1	C	284	Total	C	N	O	P	S	0	0	2
			2223	1397	373	436	3	14			
1	D	280	Total	C	N	O	P	S	0	0	3
			2209	1383	374	435	3	14			

- Molecule 2 is (1R,2S,3R,5R)-3-({5-(1,3-benzothiazol-2-yl)-6-chloro-2-[(3-methoxypropyl)amino]pyrimidin-4-yl}amino)-5-(hydroxymethyl)cyclopentane-1,2-diol (three-letter code: 42P) (formula: C₂₁H₂₆ClN₅O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			32	21	1	5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	S	
			32	21	1	5	4	1	0
2	C	1	Total	C	Cl	N	O	S	
			32	21	1	5	4	1	0
2	D	1	Total	C	Cl	N	O	S	
			32	21	1	5	4	1	0

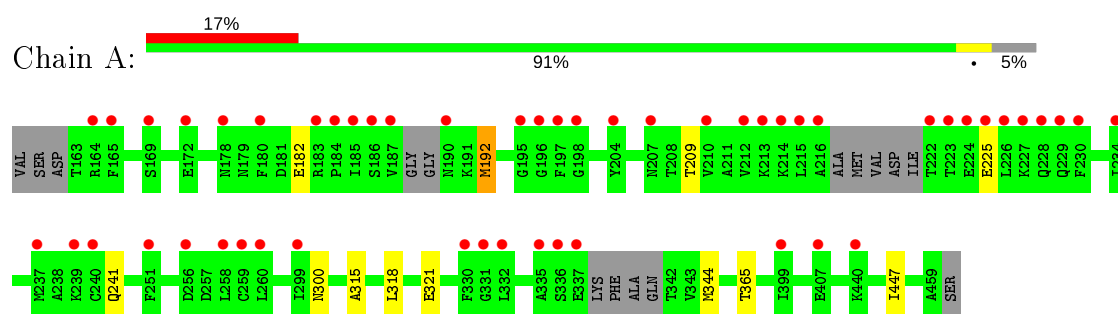
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O		
			6	6	0	0
3	B	7	Total	O		
			7	7	0	0
3	C	9	Total	O		
			9	9	0	0
3	D	11	Total	O		
			11	11	0	0

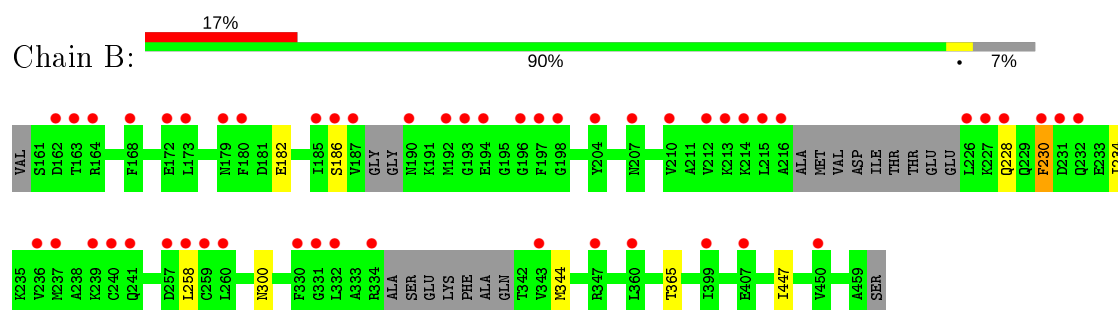
3 Residue-property plots [i](#)

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

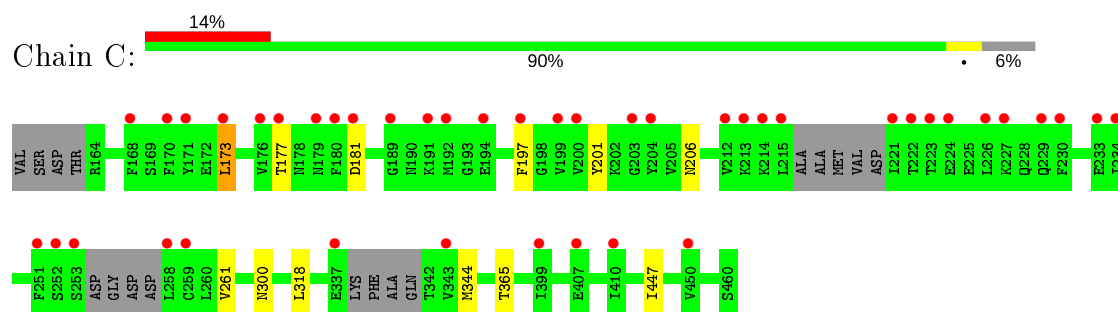
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4

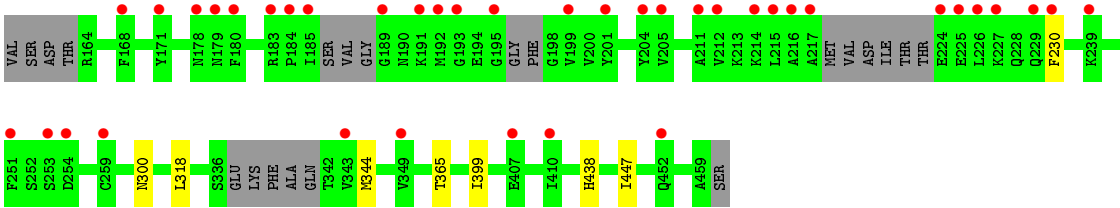


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.97Å 139.99Å 87.62Å 90.00° 125.47° 90.00°	Depositor
Resolution (Å)	31.47 – 2.73 31.47 – 2.73	Depositor EDS
% Data completeness (in resolution range)	95.6 (31.47-2.73) 86.2 (31.47-2.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.264 , 0.285 0.268 , 0.290	Depositor DCC
R_{free} test set	1817 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.257 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9049	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 27.07 % 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 2.3486e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: TPO, 42P, SEP

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	0.45	0/2247	0.56	0/3026
1	B	0.45	0/2215	0.57	0/2982
1	C	0.48	0/2226	0.58	0/2998
1	D	0.46	0/2210	0.57	0/2974
All	All	0.46	0/8898	0.57	0/11980

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	2244	0	2200	3	0
1	B	2212	0	2172	2	0
1	C	2223	0	2190	4	0
1	D	2209	0	2170	1	0
2	A	32	0	26	2	0
2	B	32	0	26	0	0
2	C	32	0	26	0	0
2	D	32	0	26	0	0
3	A	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	0	0
3	C	9	0	0	0	0
3	D	11	0	0	0	0
All	All	9049	0	8836	10	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 1.

All (10) 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:C:173:LEU:HD21	1:C:261:VAL:CG2	2.42	0.50
1:A:315:ALA:O	2:A:501:42P:H12	2.13	0.48
1:C:173:LEU:HD11	1:C:261:VAL:CG2	2.43	0.48
1:C:173:LEU:HD21	1:C:261:VAL:HG22	1.97	0.47
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.97	0.46
1:B:230:PHE:CE1	1:B:234:ILE:HD11	2.51	0.46
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.98	0.45
1:A:192:MET:HB3	2:A:501:42P:H3	1.98	0.45
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.98	0.45
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.97	0.44

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	276/301 (92%)	262 (95%)	14 (5%)	0	100	100
1	B	271/301 (90%)	260 (96%)	10 (4%)	1 (0%)	34	55
1	C	274/301 (91%)	258 (94%)	14 (5%)	2 (1%)	22	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	268/301 (89%)	255 (95%)	13 (5%)	0	100	100
All	All	1089/1204 (90%)	1035 (95%)	51 (5%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	PHE
1	C	206	ASN
1	B	186	SER

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	245/259 (95%)	236 (96%)	9 (4%)	34	54
1	B	242/259 (93%)	236 (98%)	6 (2%)	47	67
1	C	242/259 (93%)	235 (97%)	7 (3%)	42	62
1	D	241/259 (93%)	235 (98%)	6 (2%)	47	67
All	All	970/1036 (94%)	942 (97%)	28 (3%)	42	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	192	MET
1	A	209	THR
1	A	225	GLU
1	A	241	GLN
1	A	318	LEU
1	A	321	GLU
1	A	344	MET
1	A	365	THR
1	B	182	GLU
1	B	228	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	230	PHE
1	B	258	LEU
1	B	344	MET
1	B	365	THR
1	C	173	LEU
1	C	177	THR
1	C	181	ASP
1	C	201	TYR
1	C	318	LEU
1	C	344	MET
1	C	365	THR
1	D	230	PHE
1	D	318	LEU
1	D	344	MET
1	D	365	THR
1	D	399	ILE
1	D	438	HIS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	346	1	8,9,10	0.78	0	8,12,14	1.51	3 (37%)
1	TPO	C	342	1	8,10,11	0.90	0	10,14,16	1.20	2 (20%)
1	TPO	B	342	1	8,10,11	0.80	0	10,14,16	1.30	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	D	346	1	8,9,10	0.87	0	8,12,14	1.24	0
1	TPO	D	342	1	8,10,11	0.78	0	10,14,16	1.32	2 (20%)
1	TPO	C	345	1	8,10,11	1.34	1 (12%)	10,14,16	1.04	0
1	SEP	B	346	1	8,9,10	0.87	0	8,12,14	1.31	1 (12%)
1	TPO	A	345	1	8,10,11	1.15	1 (12%)	10,14,16	1.03	0
1	TPO	D	345	1	8,10,11	1.27	1 (12%)	10,14,16	0.86	0
1	TPO	B	345	1	8,10,11	1.32	1 (12%)	10,14,16	1.02	0
1	SEP	C	346	1	8,9,10	0.81	0	8,12,14	1.14	0
1	TPO	A	342	1	8,10,11	0.97	0	10,14,16	1.22	2 (20%)

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
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	C	342	1	-	0/9/11/13	-
1	TPO	B	342	1	-	0/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	TPO	D	342	1	-	0/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	0/5/8/10	-
1	TPO	A	342	1	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	TPO	CB-CA	2.53	1.59	1.53
1	A	345	TPO	CB-CA	2.25	1.58	1.53
1	B	345	TPO	CB-CA	2.19	1.58	1.53
1	D	345	TPO	CB-CA	2.19	1.58	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	TPO	P-OG1-CB	-2.53	115.56	123.21
1	A	342	TPO	P-OG1-CB	-2.50	115.65	123.21
1	C	342	TPO	P-OG1-CB	-2.47	115.76	123.21
1	B	342	TPO	P-OG1-CB	-2.45	115.82	123.21
1	A	346	SEP	O3P-P-OG	2.23	112.67	106.73
1	B	346	SEP	OG-P-O1P	2.18	112.58	106.47
1	A	342	TPO	O3P-P-OG1	2.09	115.38	105.99
1	A	346	SEP	OG-CB-CA	2.09	110.17	108.14
1	B	342	TPO	O2P-P-OG1	2.08	115.32	105.99
1	D	342	TPO	O2P-P-OG1	2.08	115.31	105.99
1	C	342	TPO	O3P-P-OG1	2.06	115.22	105.99
1	A	346	SEP	P-OG-CB	-2.03	112.69	118.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	345	TPO	N-CA-CB-OG1
1	A	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O2P
1	C	345	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	42P	B	501	-	33,35,35	2.08	9 (27%)	36,49,49	2.68	11 (30%)
2	42P	A	501	-	33,35,35	2.14	10 (30%)	36,49,49	3.08	10 (27%)
2	42P	D	501	-	33,35,35	1.87	9 (27%)	36,49,49	2.48	9 (25%)
2	42P	C	501	-	33,35,35	1.74	8 (24%)	36,49,49	2.64	9 (25%)

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	42P	B	501	-	-	6/12/32/32	0/4/4/4
2	42P	A	501	-	-	6/12/32/32	0/4/4/4
2	42P	D	501	-	-	7/12/32/32	0/4/4/4
2	42P	C	501	-	-	1/12/32/32	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	42P	C05-C06	7.46	1.48	1.39
2	B	501	42P	C05-C06	7.45	1.48	1.39
2	D	501	42P	C05-C06	6.62	1.47	1.39
2	C	501	42P	C05-C06	5.38	1.45	1.39
2	B	501	42P	C05-N04	4.35	1.39	1.32
2	D	501	42P	C05-N04	3.69	1.38	1.32
2	A	501	42P	C10-S25	3.43	1.78	1.73
2	B	501	42P	C31-C32	3.39	1.44	1.36
2	A	501	42P	C05-N04	3.38	1.37	1.32
2	C	501	42P	C05-N04	3.30	1.37	1.32
2	C	501	42P	C10-S25	3.22	1.78	1.73
2	B	501	42P	C30-C29	3.14	1.43	1.36
2	A	501	42P	C30-C29	3.14	1.43	1.36
2	A	501	42P	C31-C32	3.05	1.43	1.36
2	D	501	42P	C10-N28	3.05	1.35	1.31
2	A	501	42P	C10-N28	2.94	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	42P	C10-S25	2.82	1.77	1.73
2	C	501	42P	C10-N28	2.81	1.35	1.31
2	C	501	42P	C30-C29	2.77	1.43	1.36
2	C	501	42P	C31-C32	2.74	1.42	1.36
2	B	501	42P	C10-N28	2.70	1.35	1.31
2	A	501	42P	C01-N02	2.62	1.39	1.34
2	C	501	42P	C01-N02	2.58	1.39	1.34
2	B	501	42P	C03-N08	2.52	1.38	1.34
2	D	501	42P	C03-N08	2.51	1.38	1.34
2	B	501	42P	O17-C13	2.49	1.48	1.43
2	A	501	42P	C06-C01	2.48	1.48	1.42
2	D	501	42P	C30-C29	2.47	1.42	1.36
2	C	501	42P	C03-N08	2.35	1.38	1.34
2	D	501	42P	C31-C32	2.28	1.41	1.36
2	B	501	42P	C12-C11	2.21	1.56	1.53
2	A	501	42P	C32-C27	2.19	1.45	1.41
2	D	501	42P	C01-N02	2.11	1.38	1.34
2	A	501	42P	C03-N08	2.04	1.37	1.34
2	D	501	42P	C31-C30	2.04	1.43	1.38
2	B	501	42P	C01-N02	2.02	1.38	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	42P	C06-C05-CL9	14.53	128.92	119.27
2	C	501	42P	C06-C05-CL9	11.67	127.03	119.27
2	B	501	42P	C06-C05-CL9	11.29	126.78	119.27
2	D	501	42P	C06-C05-CL9	10.56	126.29	119.27
2	A	501	42P	C10-N28-C27	5.46	114.60	103.78
2	D	501	42P	C10-N28-C27	5.42	114.52	103.78
2	B	501	42P	C10-N28-C27	5.23	114.14	103.78
2	C	501	42P	C10-N28-C27	5.17	114.04	103.78
2	C	501	42P	C20-N08-C03	4.43	131.40	123.75
2	A	501	42P	CL9-C05-N04	-4.39	108.15	115.56
2	C	501	42P	CL9-C05-N04	-4.16	108.54	115.56
2	A	501	42P	C20-N08-C03	3.78	130.28	123.75
2	B	501	42P	C13-C12-C11	3.73	108.46	102.55
2	B	501	42P	CL9-C05-N04	-3.73	109.28	115.56
2	D	501	42P	CL9-C05-N04	-3.56	109.56	115.56
2	A	501	42P	C14-C15-C11	3.28	107.25	103.32
2	D	501	42P	C14-C15-C11	3.20	107.14	103.32
2	B	501	42P	C15-C11-C12	3.07	108.04	103.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	42P	C27-C26-S25	-2.99	107.89	111.85
2	D	501	42P	C15-C11-C12	2.96	107.87	103.17
2	B	501	42P	C27-C26-S25	-2.87	108.05	111.85
2	C	501	42P	C26-C27-N28	2.75	114.44	108.04
2	B	501	42P	C26-C27-N28	2.72	114.38	108.04
2	A	501	42P	C26-C27-N28	2.68	114.27	108.04
2	B	501	42P	C15-C14-C13	2.60	109.05	102.66
2	D	501	42P	C26-C27-N28	2.60	114.09	108.04
2	C	501	42P	N07-C01-N02	-2.58	113.29	118.84
2	A	501	42P	C06-C05-N04	-2.57	122.87	125.96
2	D	501	42P	C27-C26-S25	-2.53	108.49	111.85
2	A	501	42P	C13-C12-C11	2.52	106.54	102.55
2	C	501	42P	C14-C15-C11	2.44	106.24	103.32
2	B	501	42P	C20-N08-C03	2.40	127.90	123.75
2	B	501	42P	N07-C01-N02	-2.36	113.75	118.84
2	C	501	42P	C27-C26-S25	-2.28	108.82	111.85
2	D	501	42P	C13-C12-C11	2.17	105.98	102.55
2	A	501	42P	N07-C01-N02	-2.16	114.19	118.84
2	D	501	42P	C20-N08-C03	2.13	127.43	123.75
2	B	501	42P	C03-N02-C01	2.10	121.19	116.39
2	C	501	42P	C12-C11-N07	-2.03	108.27	112.32

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	42P	N04-C03-N08-C20
2	A	501	42P	C12-C11-N07-C01
2	A	501	42P	C13-C14-C18-O19
2	A	501	42P	C15-C14-C18-O19
2	D	501	42P	C13-C14-C18-O19
2	D	501	42P	C15-C14-C18-O19
2	D	501	42P	N08-C20-C21-C22
2	B	501	42P	N02-C03-N08-C20
2	A	501	42P	C20-C21-C22-O23
2	D	501	42P	C20-C21-C22-O23
2	A	501	42P	C21-C22-O23-C24
2	C	501	42P	C21-C22-O23-C24
2	D	501	42P	C12-C11-N07-C01
2	B	501	42P	C15-C14-C18-O19
2	D	501	42P	C21-C22-O23-C24
2	B	501	42P	N08-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501	42P	C15-C11-N07-C01
2	D	501	42P	C15-C11-N07-C01
2	B	501	42P	C13-C14-C18-O19
2	B	501	42P	C20-C21-C22-O23

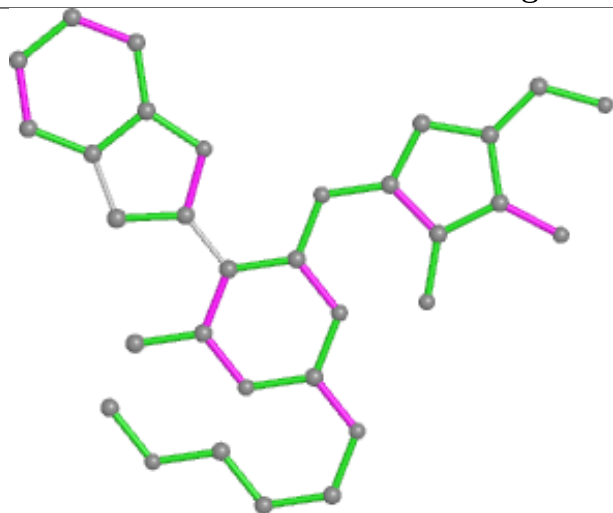
There are no ring outliers.

1 monomer is involved in 2 short contacts:

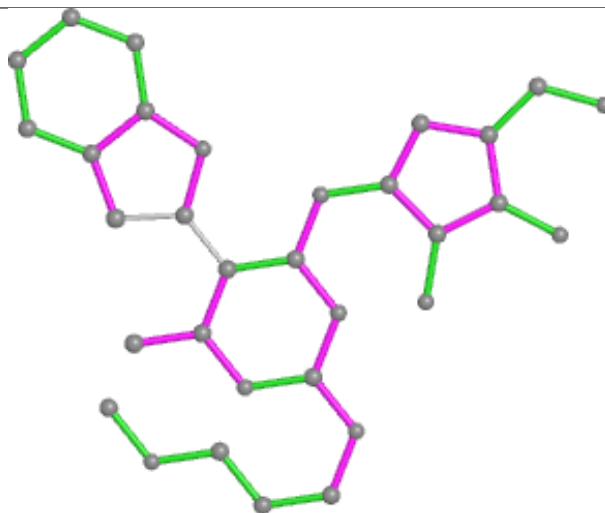
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	42P	2	0

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 than 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.

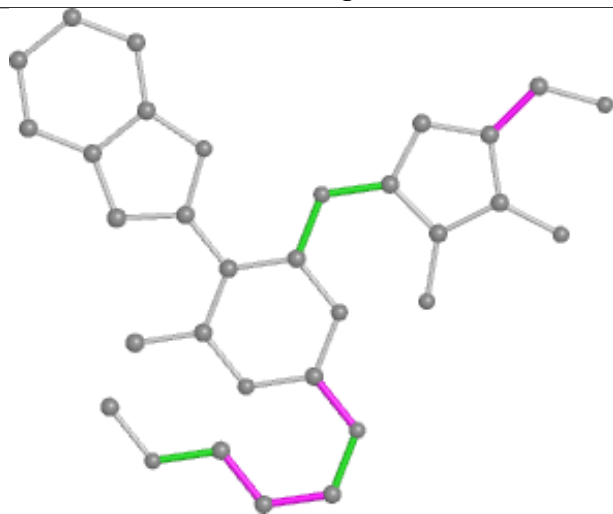
Ligand 42P B 501



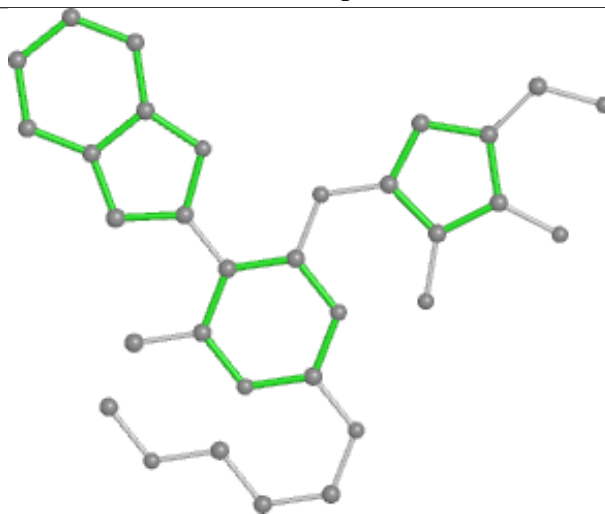
Bond lengths



Bond angles

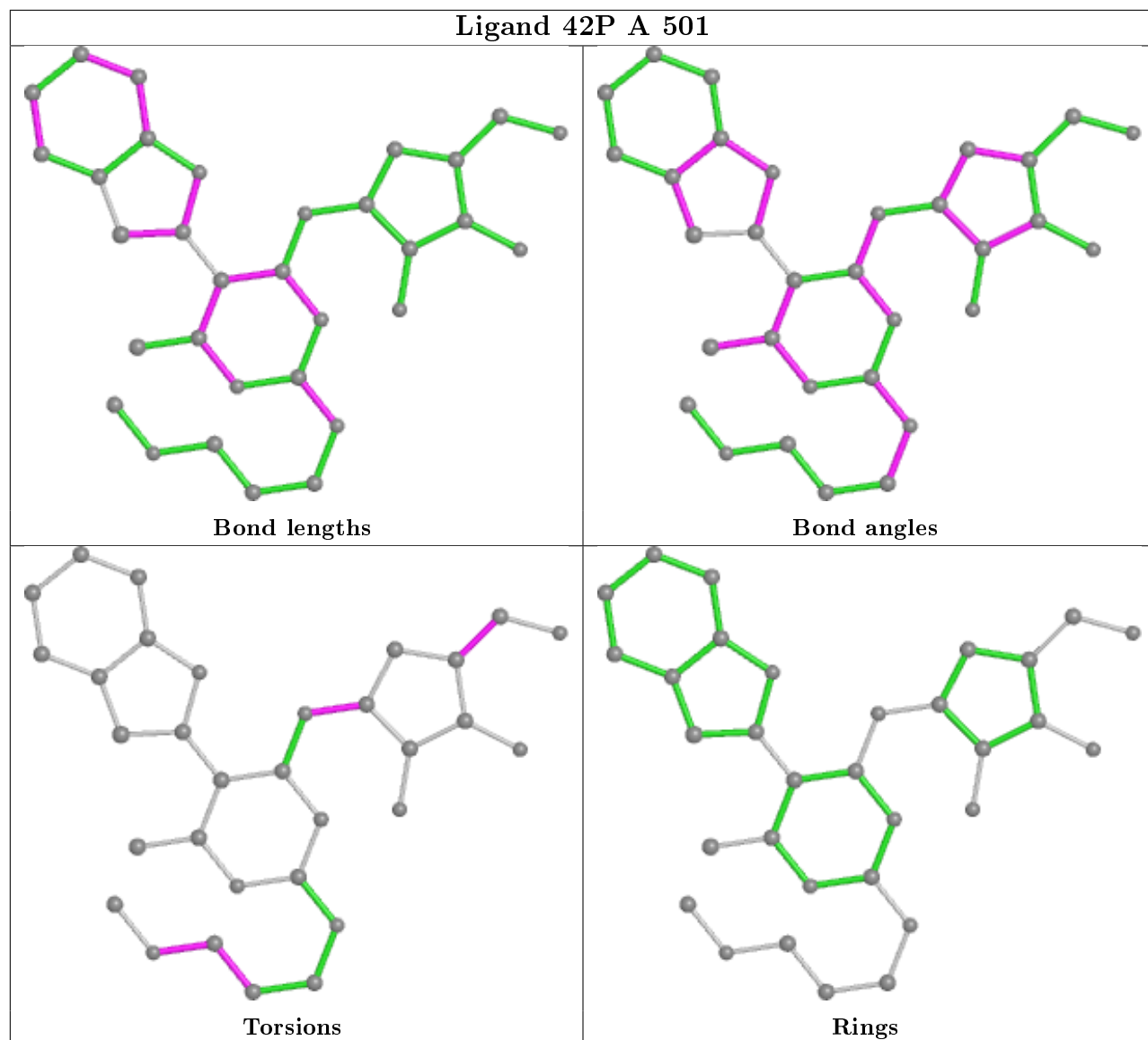


Torsions

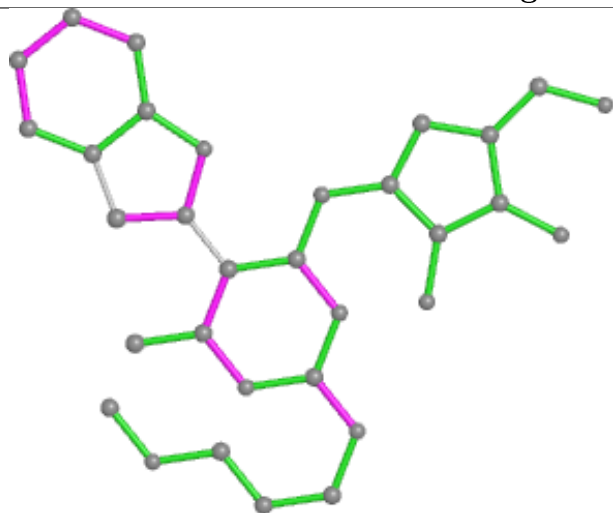


Rings

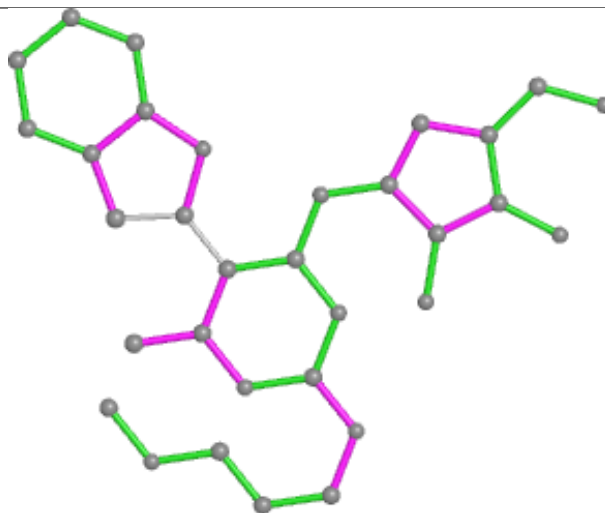
Ligand 42P A 501



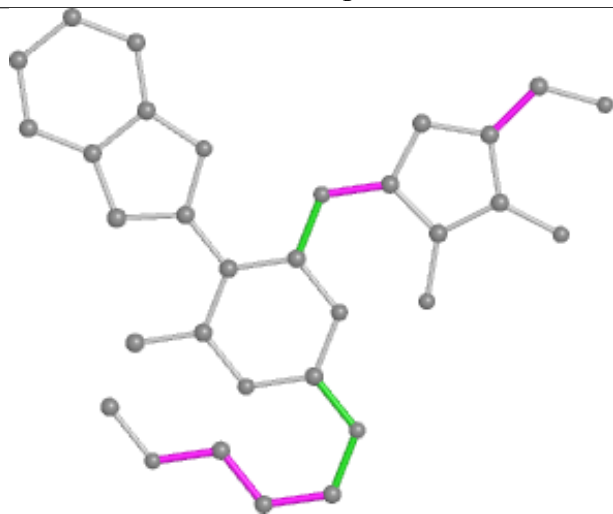
Ligand 42P D 501



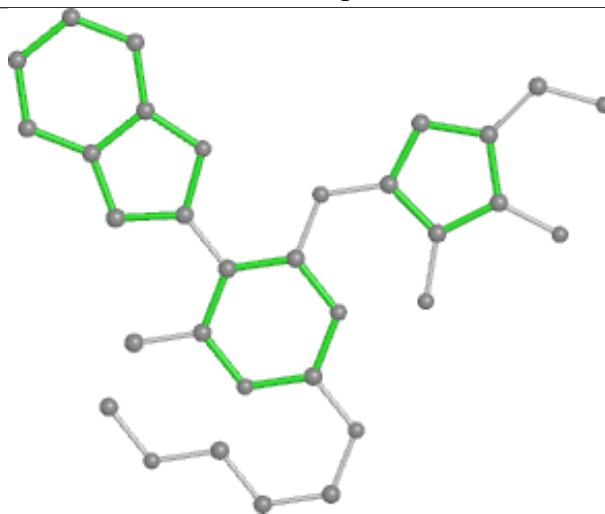
Bond lengths



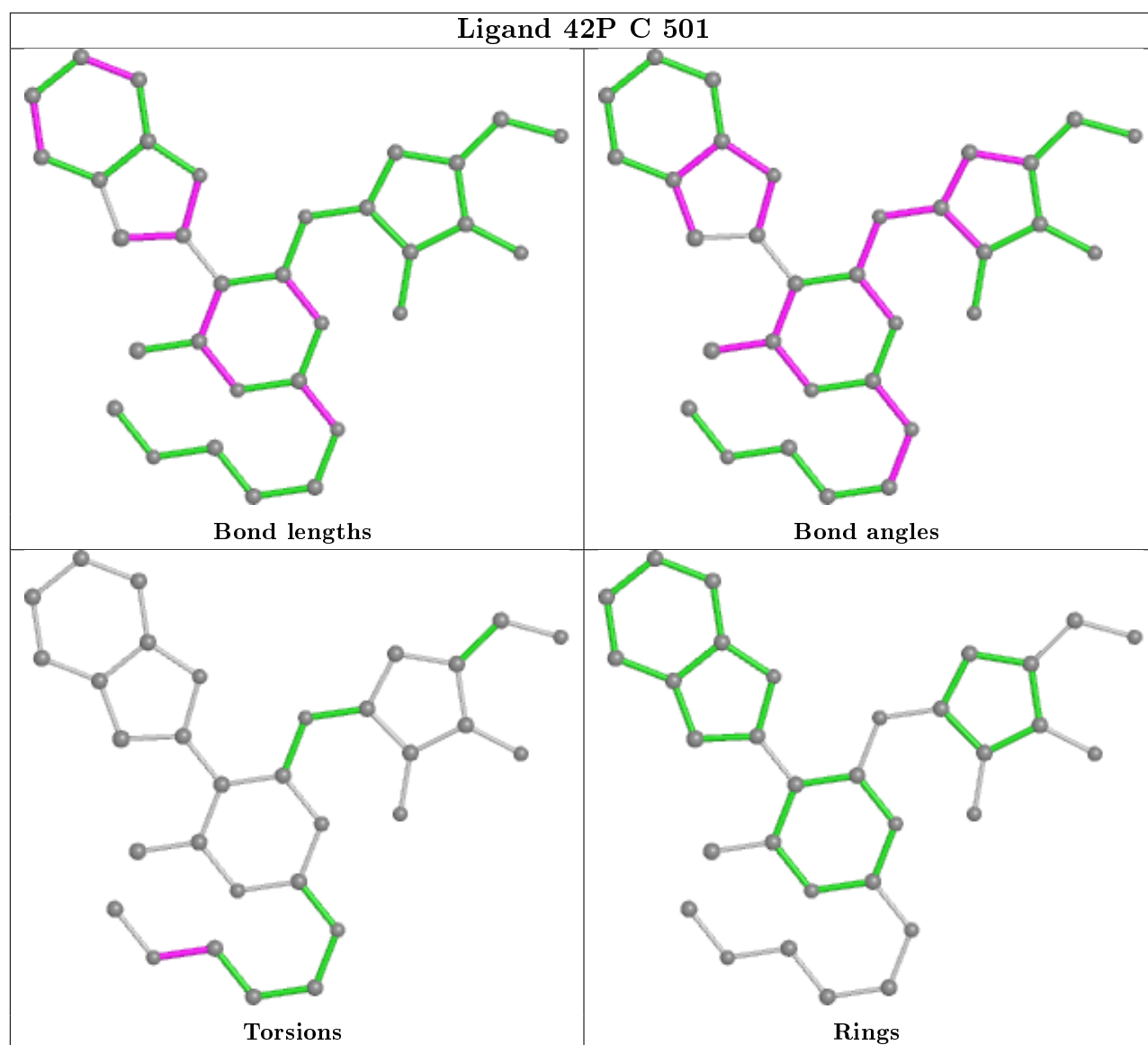
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	283/301 (94%)	1.25	52 (18%) 1 1	31, 69, 135, 154	0
1	B	278/301 (92%)	1.10	51 (18%) 1 1	28, 61, 137, 166	0
1	C	281/301 (93%)	0.90	43 (15%) 2 2	27, 59, 115, 138	0
1	D	277/301 (92%)	0.85	39 (14%) 2 2	26, 58, 124, 142	0
All	All	1119/1204 (92%)	1.03	185 (16%) 1 1	26, 62, 129, 166	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	12.8
1	A	226	LEU	12.1
1	A	195	GLY	11.4
1	B	226	LEU	10.4
1	A	240	CYS	10.2
1	B	227	LYS	9.7
1	D	217	ALA	8.3
1	B	230	PHE	8.1
1	A	223	THR	8.1
1	D	230	PHE	7.9
1	B	240	CYS	7.9
1	B	237	MET	7.8
1	A	230	PHE	7.8
1	A	237	MET	6.8
1	A	215	LEU	6.6
1	B	197	PHE	6.6
1	A	197	PHE	6.2
1	A	204	TYR	6.1
1	C	223	THR	6.1
1	C	258	LEU	6.1
1	B	207	ASN	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	ASN	6.0
1	C	230	PHE	5.8
1	D	216	ALA	5.8
1	A	185	ILE	5.8
1	C	197	PHE	5.7
1	B	204	TYR	5.5
1	A	251	PHE	5.4
1	D	193	GLY	5.4
1	B	173	LEU	5.4
1	B	163	THR	5.3
1	C	214	LYS	5.3
1	C	215	LEU	5.2
1	C	180	PHE	5.2
1	A	336	SER	5.1
1	D	184	PRO	5.1
1	A	164	ARG	5.1
1	A	198	GLY	5.1
1	A	186	SER	5.0
1	B	215	LEU	5.0
1	A	239	LYS	5.0
1	B	185	ILE	5.0
1	B	330	PHE	5.0
1	A	337	GLU	4.9
1	D	168	PHE	4.9
1	A	229	GLN	4.9
1	D	224	GLU	4.7
1	C	221	ILE	4.7
1	A	225	GLU	4.7
1	C	213	LYS	4.7
1	A	187	VAL	4.6
1	C	194	GLU	4.6
1	B	260	LEU	4.4
1	B	216	ALA	4.4
1	B	164	ARG	4.4
1	A	228	GLN	4.4
1	C	259	CYS	4.3
1	D	227	LYS	4.3
1	B	214	LYS	4.3
1	B	334	ARG	4.3
1	D	189	GLY	4.2
1	A	165	PHE	4.2
1	A	180	PHE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203	GLY	4.1
1	B	198	GLY	4.1
1	B	187	VAL	3.9
1	C	181	ASP	3.9
1	A	190	ASN	3.9
1	C	179	ASN	3.9
1	D	192	MET	3.8
1	A	184	PRO	3.8
1	A	196	GLY	3.8
1	C	212	VAL	3.7
1	D	185	ILE	3.7
1	C	173	LEU	3.7
1	C	226	LEU	3.7
1	D	178	ASN	3.6
1	D	407	GLU	3.6
1	C	251	PHE	3.6
1	A	224	GLU	3.6
1	A	227	LYS	3.5
1	B	179	ASN	3.5
1	B	259	CYS	3.5
1	D	191	LYS	3.5
1	C	229	GLN	3.5
1	D	343	VAL	3.4
1	A	222	THR	3.4
1	A	259	CYS	3.4
1	D	215	LEU	3.4
1	B	347	ARG	3.4
1	B	186	SER	3.3
1	C	176	VAL	3.3
1	B	407	GLU	3.3
1	B	399	ILE	3.3
1	B	228	GLN	3.2
1	C	191	LYS	3.2
1	B	193	GLY	3.2
1	D	171	TYR	3.2
1	C	227	LYS	3.1
1	A	183	ARG	3.1
1	D	211	ALA	3.1
1	A	260	LEU	3.0
1	B	190	ASN	3.0
1	A	212	VAL	3.0
1	B	343	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	2.9
1	B	231	ASP	2.9
1	B	213	LYS	2.9
1	C	177	THR	2.9
1	B	212	VAL	2.8
1	D	259	CYS	2.8
1	D	254	ASP	2.8
1	D	239	LYS	2.8
1	D	183	ARG	2.8
1	B	168	PHE	2.8
1	C	222	THR	2.8
1	D	226	LEU	2.8
1	A	178	ASN	2.8
1	C	233	GLU	2.7
1	D	349	VAL	2.7
1	C	337	GLU	2.7
1	A	399	ILE	2.7
1	D	253	SER	2.7
1	A	234	ILE	2.7
1	C	171	TYR	2.7
1	B	450	VAL	2.6
1	D	229	GLN	2.6
1	C	200	VAL	2.6
1	C	253	SER	2.6
1	C	399	ILE	2.6
1	C	199	VAL	2.6
1	B	239	LYS	2.6
1	C	204	TYR	2.6
1	A	330	PHE	2.6
1	A	213	LYS	2.5
1	C	410	ILE	2.5
1	D	212	VAL	2.5
1	D	204	TYR	2.5
1	A	407	GLU	2.5
1	A	331	GLY	2.5
1	B	331	GLY	2.5
1	D	180	PHE	2.5
1	A	256	ASP	2.5
1	D	179	ASN	2.5
1	C	168	PHE	2.5
1	C	170	PHE	2.5
1	D	201	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	332	LEU	2.4
1	C	252	SER	2.4
1	A	210	VAL	2.4
1	A	299	ILE	2.4
1	C	192	MET	2.4
1	A	258	LEU	2.4
1	B	210	VAL	2.4
1	D	251	PHE	2.4
1	B	162	ASP	2.3
1	C	343	VAL	2.3
1	C	224	GLU	2.3
1	A	214	LYS	2.3
1	A	440	LYS	2.3
1	B	172	GLU	2.3
1	B	180	PHE	2.3
1	B	241	GLN	2.2
1	C	407	GLU	2.2
1	D	452	GLN	2.2
1	B	360	LEU	2.2
1	C	189	GLY	2.2
1	A	172	GLU	2.2
1	B	196	GLY	2.2
1	C	450	VAL	2.2
1	B	232	GLN	2.1
1	D	225	GLU	2.1
1	B	257	ASP	2.1
1	B	194	GLU	2.1
1	D	214	LYS	2.1
1	D	199	VAL	2.1
1	B	192	MET	2.1
1	B	236	VAL	2.1
1	C	234	ILE	2.1
1	D	195	GLY	2.1
1	D	205	VAL	2.0
1	A	332	LEU	2.0
1	D	410	ILE	2.0
1	A	335	ALA	2.0
1	A	169	SER	2.0

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

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
1	SEP	C	346	10/11	0.68	0.23	91,94,99,100	0
1	TPO	D	342	11/12	0.70	0.22	94,96,101,101	0
1	TPO	C	342	11/12	0.70	0.23	99,100,105,105	0
1	TPO	A	342	11/12	0.76	0.23	109,111,113,113	0
1	TPO	A	345	11/12	0.77	0.16	100,101,102,103	0
1	SEP	A	346	10/11	0.77	0.16	100,102,106,107	0
1	SEP	B	346	10/11	0.77	0.18	98,100,104,104	0
1	TPO	B	345	11/12	0.79	0.20	96,99,100,100	0
1	TPO	B	342	11/12	0.81	0.21	98,100,102,102	0
1	SEP	D	346	10/11	0.81	0.17	87,91,97,97	0
1	TPO	C	345	11/12	0.88	0.19	89,90,93,94	0
1	TPO	D	345	11/12	0.89	0.16	87,88,91,91	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

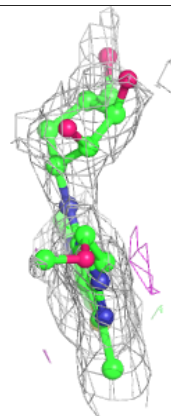
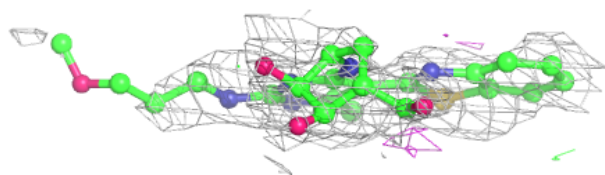
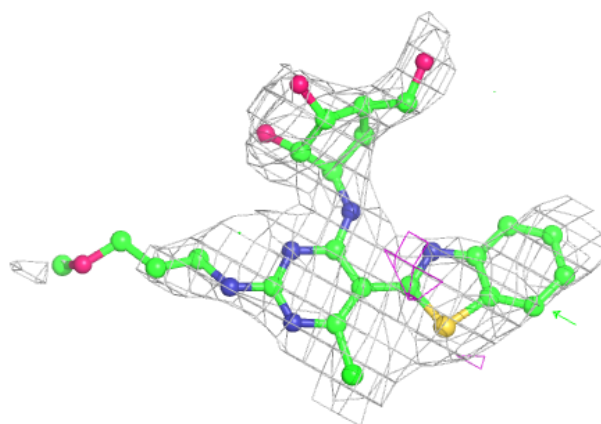
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	42P	A	501	32/32	0.76	0.31	94,98,101,102	0
2	42P	C	501	32/32	0.81	0.30	99,108,112,114	0
2	42P	D	501	32/32	0.82	0.29	85,88,90,91	0
2	42P	B	501	32/32	0.84	0.23	69,73,82,85	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.

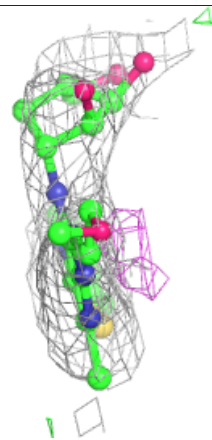
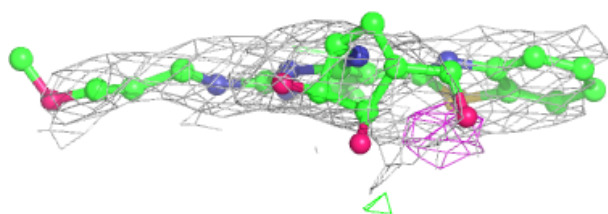
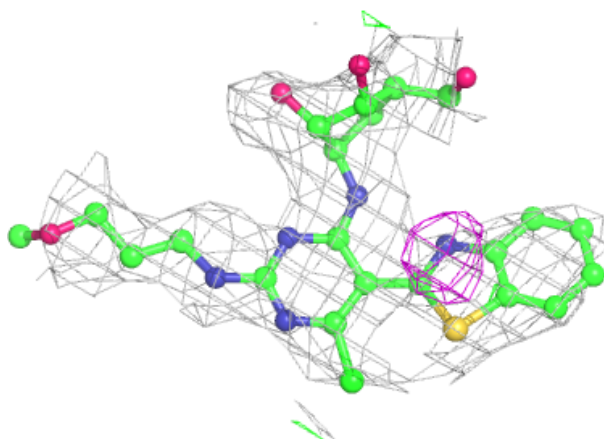
Electron density around 42P A 501:

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



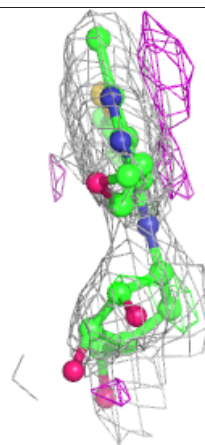
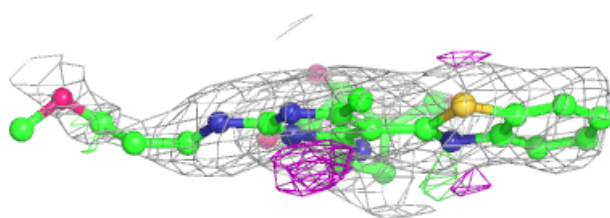
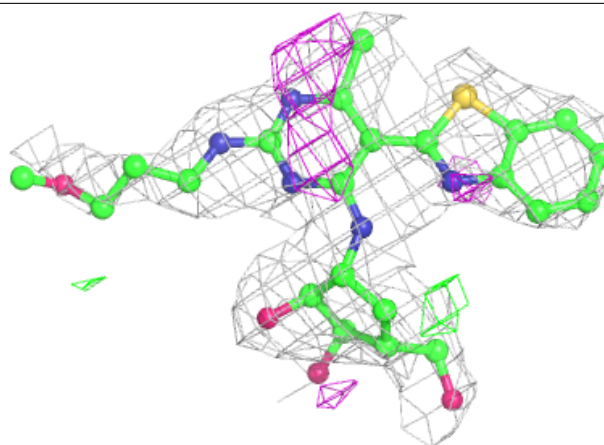
Electron density around 42P C 501:

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



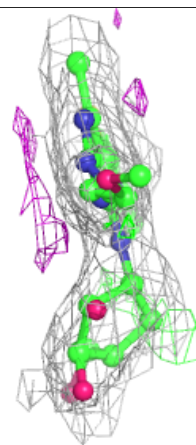
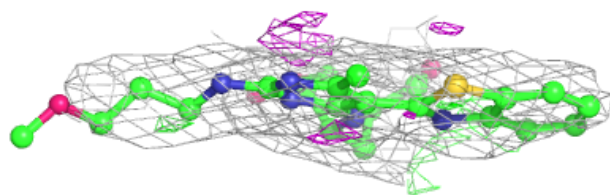
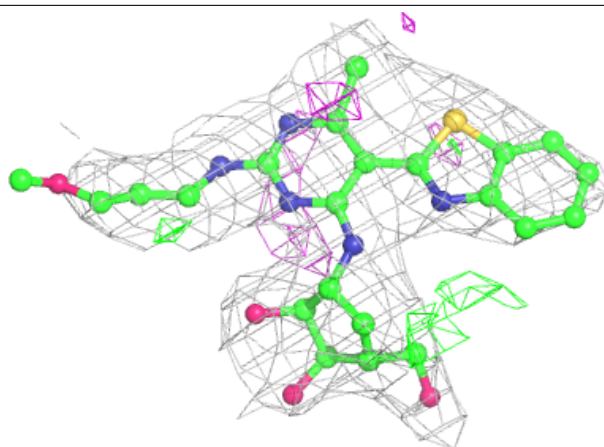
Electron density around 42P D 501:

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



Electron density around 42P B 501:

$2mF_o-DF_c$ (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.