Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2026 – 08:06 AM EST

PDB ID	:	9Z3O / pdb_00009z3o
Title	:	Complex of phosphorylated p38-alpha and MK2 with a molecular glue
Authors	:	Bell, J.A.
Deposited on	:	2025-11-07
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

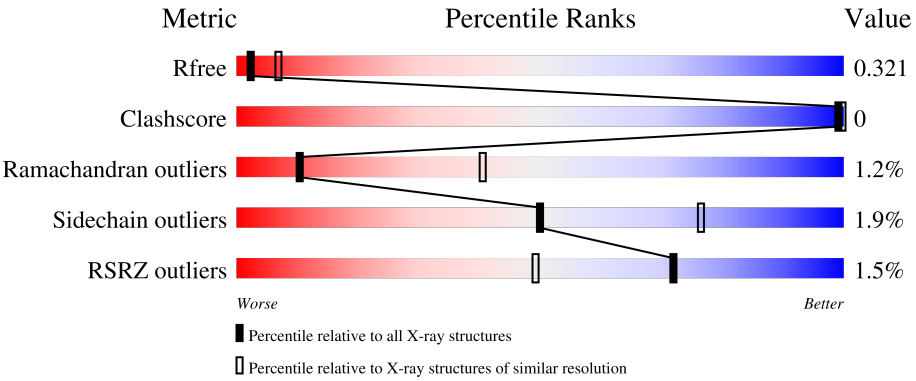
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	89% 7%
1	B	363	2% 87% 9%
2	C	363	91% 5%
2	D	363	89% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22785 atoms, of which 11410 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	351	Total	C	H	N	O	P	S	0	0	0
			5666	1813	2821	483	533	3	13			
1	B	351	Total	C	H	N	O	P	S	0	0	0
			5665	1813	2820	483	533	3	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q16539
A	-1	GLY	-	expression tag	UNP Q16539
A	0	GLY	-	expression tag	UNP Q16539
B	-2	GLY	-	expression tag	UNP Q16539
B	-1	GLY	-	expression tag	UNP Q16539
B	0	GLY	-	expression tag	UNP Q16539

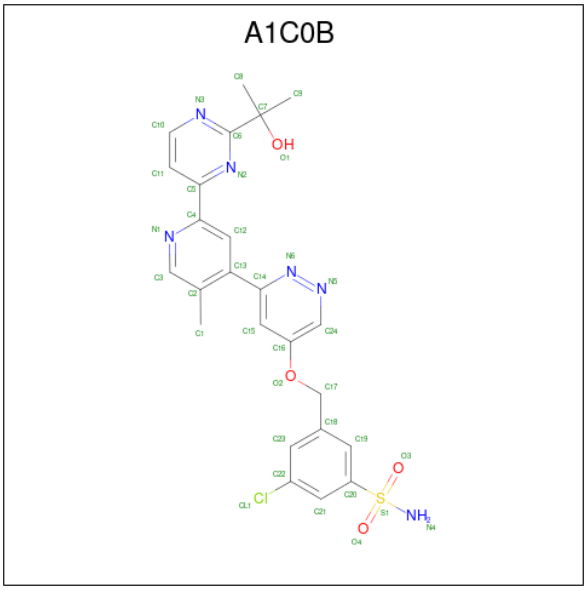
- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	344	Total	C	H	N	O	S	0	0	0
			5629	1774	2839	484	512	20			
2	D	348	Total	C	H	N	O	S	0	0	0
			5677	1789	2864	488	516	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLY	-	expression tag	UNP P49137
C	39	GLY	-	expression tag	UNP P49137
C	40	GLY	-	expression tag	UNP P49137
D	38	GLY	-	expression tag	UNP P49137
D	39	GLY	-	expression tag	UNP P49137
D	40	GLY	-	expression tag	UNP P49137

- Molecule 3 is 3-chloro-5-({[(6P)-6-{2-[2-(2-hydroxypropan-2-yl)pyrimidin-4-yl]-5-methylpyridin-4-yl}pyridazin-4-yl]oxy}methyl)benzene-1-sulfonamide (CCD ID: A1C0B) (formula: $C_{24}H_{23}ClN_6O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	S	0	0
			59	24	1	23	6	4	1		
3	B	1	Total	C	Cl	H	N	O	S	0	0
			59	24	1	23	6	4	1		

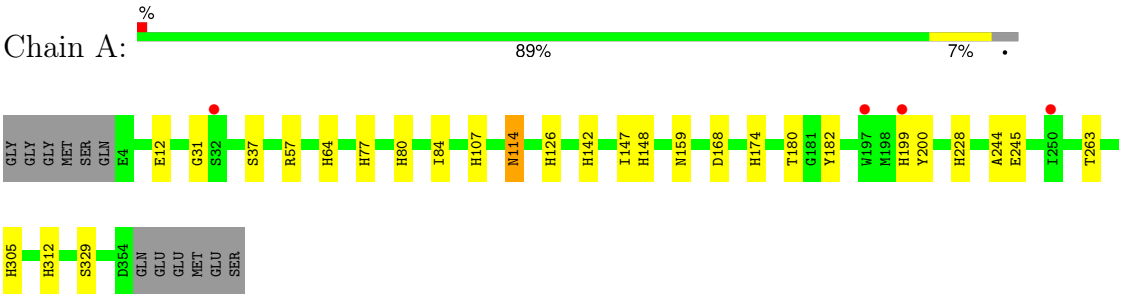
- Molecule 4 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	H	O		0	0
			15	10	5			
4	B	2	Total	H	O		0	0
			6	4	2			
4	C	1	Total	H	O		0	0
			3	2	1			
4	D	2	Total	H	O		0	0
			6	4	2			

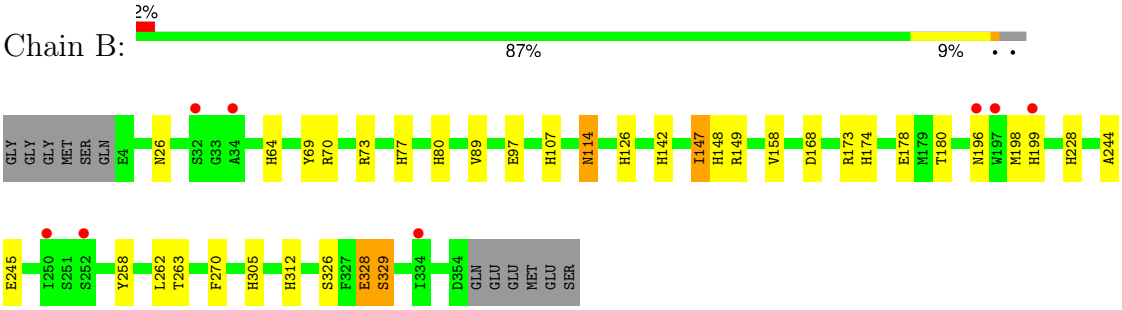
3 Residue-property plots

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.

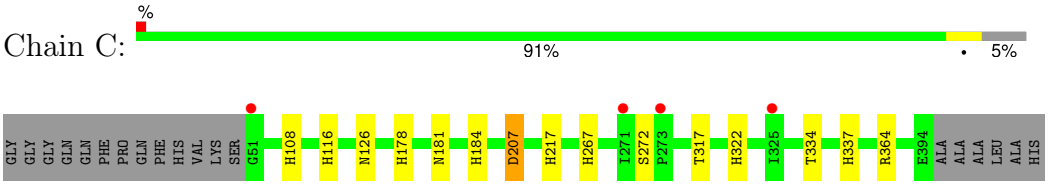
• Molecule 1: Mitogen-activated protein kinase 14



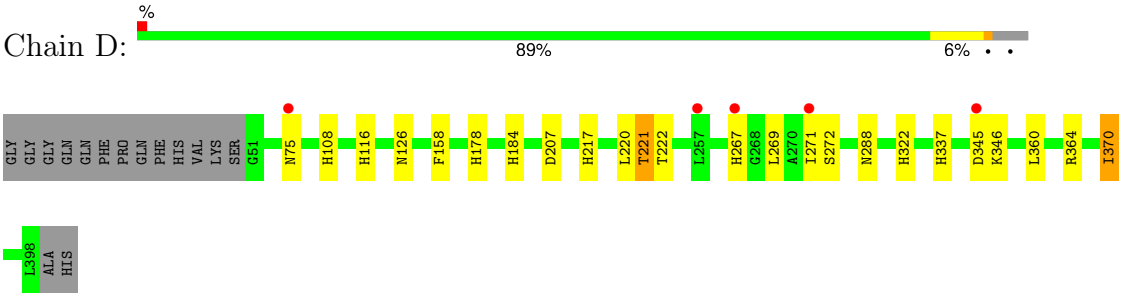
• Molecule 1: Mitogen-activated protein kinase 14



• Molecule 2: MAP kinase-activated protein kinase 2



• Molecule 2: MAP kinase-activated protein kinase 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	133.00Å 133.00Å 344.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.85 – 3.00 47.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.85-3.00) 99.9 (47.85-3.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.01Å)	Xtriage
Refinement program	PRIME-X	Depositor
R, R_{free}	0.292 , 0.327 0.283 , 0.321	Depositor DCC
R_{free} test set	1751 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	81.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22785	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, A1C0B, TPO

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	0.64	1/2869 (0.0%)	1.15	15/3890 (0.4%)
1	B	0.64	1/2869 (0.0%)	1.15	20/3890 (0.5%)
2	C	0.60	0/2848	1.13	11/3843 (0.3%)
2	D	0.59	0/2871	1.15	12/3875 (0.3%)
All	All	0.62	2/11457 (0.0%)	1.14	58/15498 (0.4%)

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	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	HIS	CG-CD2	5.47	1.41	1.35
1	A	174	HIS	CG-CD2	5.29	1.41	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	126	ASN	CA-CB-CG	7.42	120.02	112.60
1	B	114	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	114	ASN	CA-CB-CG	6.45	119.05	112.60
1	B	196	ASN	CA-CB-CG	6.34	118.94	112.60
1	B	244	ALA	N-CA-C	6.27	118.91	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	SER	CB-CA-C	6.25	116.02	109.83
2	D	126	ASN	CA-CB-CG	6.21	118.81	112.60
2	D	158	PHE	CA-CB-CG	6.13	119.93	113.80
2	C	184	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	B	199	HIS	ND1-CE1-NE2	5.96	114.36	108.40
2	D	108	HIS	ND1-CE1-NE2	5.91	114.31	108.40
2	C	108	HIS	ND1-CE1-NE2	5.89	114.29	108.40
2	D	322	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	B	148	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	A	64	HIS	ND1-CE1-NE2	5.87	114.27	108.40
2	C	337	HIS	ND1-CE1-NE2	5.85	114.25	108.40
2	C	322	HIS	ND1-CE1-NE2	5.85	114.25	108.40
2	D	184	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	A	312	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	142	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	107	HIS	ND1-CE1-NE2	5.83	114.23	108.40
2	D	178	HIS	ND1-CE1-NE2	5.83	114.23	108.40
2	C	178	HIS	ND1-CE1-NE2	5.82	114.22	108.40
2	C	267	HIS	ND1-CE1-NE2	5.82	114.22	108.40
1	B	312	HIS	ND1-CE1-NE2	5.81	114.21	108.40
1	A	142	HIS	ND1-CE1-NE2	5.81	114.21	108.40
1	A	148	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	B	305	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	A	199	HIS	ND1-CE1-NE2	5.80	114.20	108.40
2	D	217	HIS	ND1-CE1-NE2	5.80	114.20	108.40
2	C	116	HIS	ND1-CE1-NE2	5.79	114.19	108.40
2	D	337	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	A	77	HIS	ND1-CE1-NE2	5.78	114.18	108.40
2	D	116	HIS	ND1-CE1-NE2	5.77	114.17	108.40
1	A	228	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	107	HIS	ND1-CE1-NE2	5.76	114.16	108.40
2	C	217	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	126	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	B	77	HIS	ND1-CE1-NE2	5.75	114.15	108.40
1	A	80	HIS	ND1-CE1-NE2	5.75	114.14	108.40
1	B	228	HIS	ND1-CE1-NE2	5.74	114.14	108.40
1	B	80	HIS	ND1-CE1-NE2	5.74	114.14	108.40
1	B	126	HIS	ND1-CE1-NE2	5.74	114.14	108.40
2	D	267	HIS	ND1-CE1-NE2	5.71	114.11	108.40
1	B	64	HIS	ND1-CE1-NE2	5.70	114.10	108.40
1	A	305	HIS	ND1-CE1-NE2	5.66	114.06	108.40
2	D	288	ASN	N-CA-C	5.51	121.99	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	337	HIS	CA-C-N	5.43	127.87	120.54
2	C	337	HIS	C-N-CA	5.43	127.87	120.54
1	B	199	HIS	CA-CB-CG	5.34	119.14	113.80
1	B	174	HIS	ND1-CE1-NE2	5.18	113.58	108.40
1	A	159	ASN	CA-CB-CG	5.17	117.78	112.60
1	B	270	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	26	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	244	ALA	N-CA-C	5.16	117.57	111.33
1	A	312	HIS	CA-CB-CG	5.12	118.92	113.80
2	D	370	ILE	CA-CB-CG1	5.11	119.08	110.40
1	B	147	ILE	CB-CA-C	5.01	118.22	110.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLY	Peptide
1	A	329	SER	Peptide
1	B	329	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	2845	2821	2816	0	0
1	B	2845	2820	2816	4	0
2	C	2790	2839	2837	0	0
2	D	2813	2864	2863	1	0
3	A	36	23	0	1	0
3	B	36	23	0	1	0
4	A	5	10	0	0	0
4	B	2	4	0	0	0
4	C	1	2	0	0	0
4	D	2	4	0	0	0
All	All	11375	11410	11332	6	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 0.

All (6) 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:B:70:ARG:HE	1:B:328:GLU:HB2	1.78	0.46
1:B:258:TYR:CG	2:D:271:ILE:HG21	2.51	0.45
3:B:401:A1C0B:C1	3:B:401:A1C0B:C15	2.97	0.42
1:B:69:TYR:CZ	1:B:73:ARG:HD2	2.55	0.42
1:B:149:ARG:CZ	1:B:173:ARG:HB2	2.50	0.41
3:A:401:A1C0B:C15	3:A:401:A1C0B:C1	2.98	0.41

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	346/363 (95%)	321 (93%)	21 (6%)	4 (1%)	10	40
1	B	346/363 (95%)	325 (94%)	17 (5%)	4 (1%)	10	40
2	C	342/363 (94%)	317 (93%)	22 (6%)	3 (1%)	14	48
2	D	346/363 (95%)	325 (94%)	15 (4%)	6 (2%)	7	32
All	All	1380/1452 (95%)	1288 (93%)	75 (5%)	17 (1%)	10	40

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	GLU
1	A	37	SER
1	B	168	ASP
1	B	198	MET
1	A	168	ASP
2	C	181	ASN

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Mol	Chain	Res	Type
2	D	221	THR
2	D	346	LYS
2	C	272	SER
2	D	207	ASP
2	D	222	THR
2	D	269	LEU
2	D	272	SER
2	C	207	ASP
1	A	57	ARG
1	B	326	SER
1	A	84	ILE

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	308/317 (97%)	303 (98%)	5 (2%)	55	79
1	B	308/317 (97%)	300 (97%)	8 (3%)	40	72
2	C	310/322 (96%)	306 (99%)	4 (1%)	61	81
2	D	311/322 (97%)	304 (98%)	7 (2%)	44	74
All	All	1237/1278 (97%)	1213 (98%)	24 (2%)	50	76

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

Mol	Chain	Res	Type
1	A	12	GLU
1	A	114	ASN
1	A	147	ILE
1	A	200	TYR
1	A	245	GLU
1	B	89	VAL
1	B	97	GLU
1	B	114	ASN
1	B	147	ILE
1	B	158	VAL

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Mol	Chain	Res	Type
1	B	245	GLU
1	B	262	LEU
1	B	328	GLU
2	C	207	ASP
2	C	317	THR
2	C	334	THR
2	C	364	ARG
2	D	75	ASN
2	D	220	LEU
2	D	221	THR
2	D	345	ASP
2	D	360	LEU
2	D	364	ARG
2	D	370	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	201	ASN
1	A	269	ASN
1	B	260	GLN
1	B	272	ASN
2	C	80	GLN
2	C	113	GLN
2	C	217	HIS
2	C	304	ASN
2	D	175	GLN
2	D	217	HIS
2	D	321	ASN
2	D	333	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	TPO	A	180	1	8,10,11	1.25	1 (12%)	10,14,16	0.80	0
1	PTR	A	182	1	15,16,17	1.22	1 (6%)	17,22,24	0.68	0
1	TPO	A	263	1	8,10,11	1.12	1 (12%)	10,14,16	0.97	0
1	PTR	B	182	1	15,16,17	1.14	0	17,22,24	0.60	0
1	TPO	B	180	1	8,10,11	1.16	1 (12%)	10,14,16	1.04	1 (10%)
1	TPO	B	263	1	8,10,11	1.31	1 (12%)	10,14,16	1.04	1 (10%)

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	TPO	A	180	1	-	5/9/11/13	-
1	PTR	A	182	1	-	0/10/11/13	0/1/1/1
1	TPO	A	263	1	-	0/9/11/13	-
1	PTR	B	182	1	-	0/10/11/13	0/1/1/1
1	TPO	B	180	1	-	3/9/11/13	-
1	TPO	B	263	1	-	6/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	TPO	P-OG1	2.76	1.64	1.59
1	A	180	TPO	P-OG1	2.39	1.63	1.59
1	B	180	TPO	P-OG1	2.37	1.63	1.59
1	A	263	TPO	P-OG1	2.35	1.63	1.59
1	A	182	PTR	P-OH	2.16	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263	TPO	CG2-CB-CA	2.50	118.14	113.26
1	B	180	TPO	P-OG1-CB	-2.10	117.63	123.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	180	TPO	N-CA-CB-OG1
1	A	180	TPO	CA-CB-OG1-P
1	A	180	TPO	CG2-CB-OG1-P
1	B	180	TPO	N-CA-CB-OG1
1	B	263	TPO	N-CA-CB-CG2
1	B	263	TPO	N-CA-CB-OG1
1	B	263	TPO	C-CA-CB-CG2
1	B	263	TPO	O-C-CA-CB
1	B	263	TPO	CA-CB-OG1-P
1	B	263	TPO	CB-OG1-P-O1P
1	A	180	TPO	O-C-CA-CB
1	B	180	TPO	C-CA-CB-CG2
1	B	180	TPO	O-C-CA-CB
1	A	180	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	A1C0B	A	401	-	38,39,39	1.37	3 (7%)	55,58,58	0.90	2 (3%)
3	A1C0B	B	401	-	38,39,39	1.40	3 (7%)	55,58,58	0.85	2 (3%)

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	A1C0B	A	401	-	-	6/25/25/25	0/4/4/4
3	A1C0B	B	401	-	-	6/25/25/25	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	A1C0B	S1-N4	5.70	1.71	1.60
3	A	401	A1C0B	S1-N4	5.53	1.71	1.60
3	B	401	A1C0B	O1-C7	-2.31	1.41	1.44
3	A	401	A1C0B	O1-C7	-2.25	1.41	1.44
3	A	401	A1C0B	O3-S1	2.10	1.47	1.43
3	B	401	A1C0B	O3-S1	2.08	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	A1C0B	C20-S1-N4	-2.75	104.57	108.40
3	A	401	A1C0B	C9-C7-C8	2.28	113.32	110.53
3	B	401	A1C0B	C9-C7-C8	2.26	113.29	110.53
3	B	401	A1C0B	C20-S1-N4	-2.24	105.28	108.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1C0B	C19-C20-S1-O3
3	B	401	A1C0B	C15-C16-O2-C17
3	A	401	A1C0B	C21-C20-S1-N4
3	B	401	A1C0B	C21-C20-S1-N4
3	A	401	A1C0B	C21-C20-S1-O3
3	B	401	A1C0B	C19-C20-S1-N4
3	A	401	A1C0B	C15-C16-O2-C17
3	A	401	A1C0B	C19-C20-S1-N4
3	B	401	A1C0B	C19-C20-S1-O3
3	A	401	A1C0B	C24-C16-O2-C17
3	B	401	A1C0B	C24-C16-O2-C17
3	B	401	A1C0B	C21-C20-S1-O3

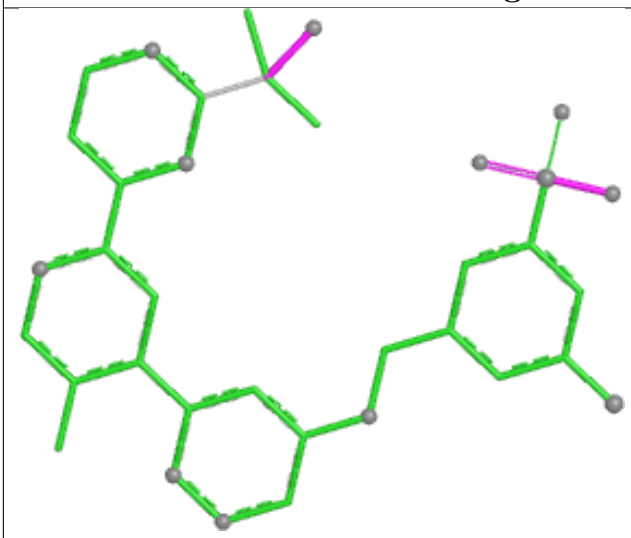
There are no ring outliers.

2 monomers are involved in 2 short contacts:

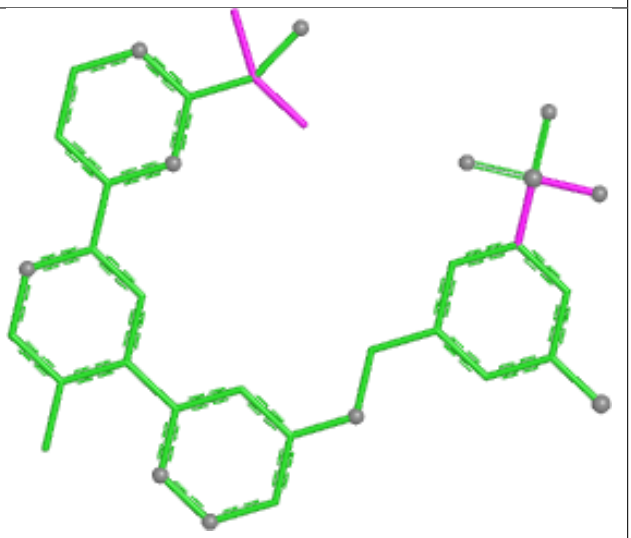
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	A1C0B	1	0
3	B	401	A1C0B	1	0

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.

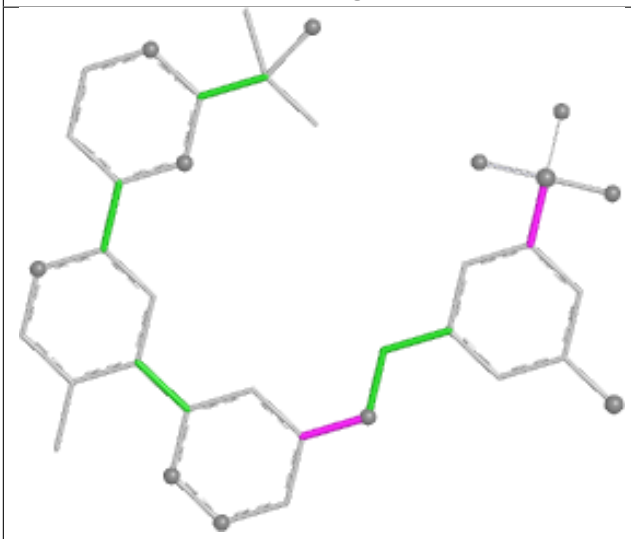
Ligand A1C0B A 401



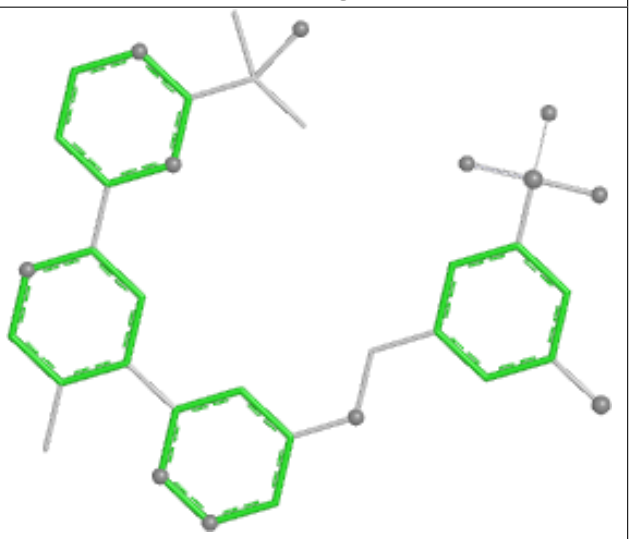
Bond lengths



Bond angles

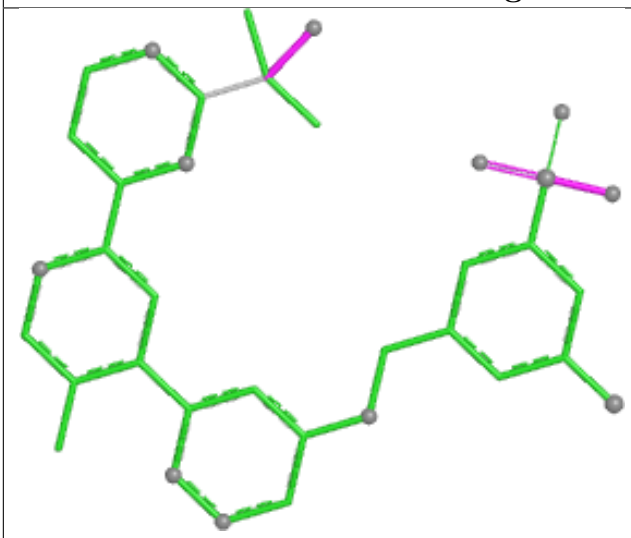


Torsions

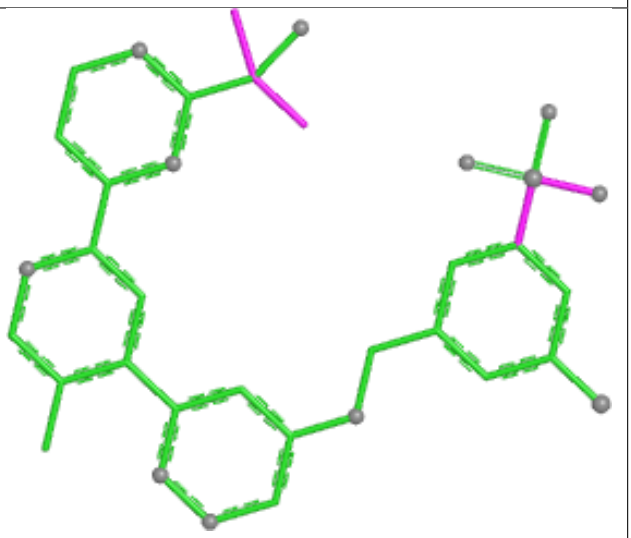


Rings

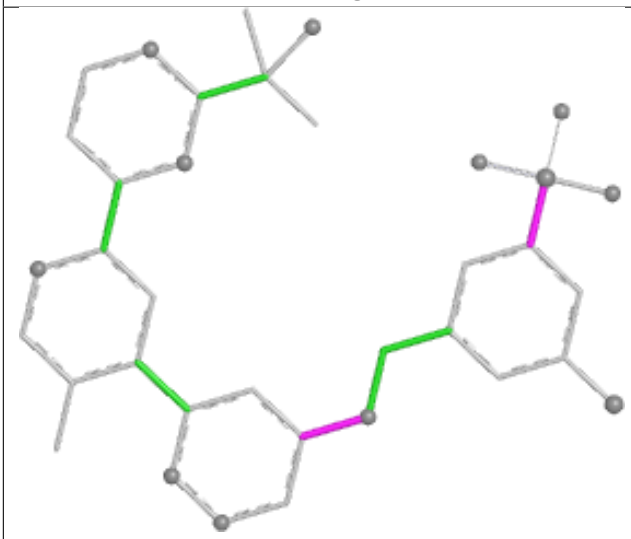
Ligand A1C0B B 401



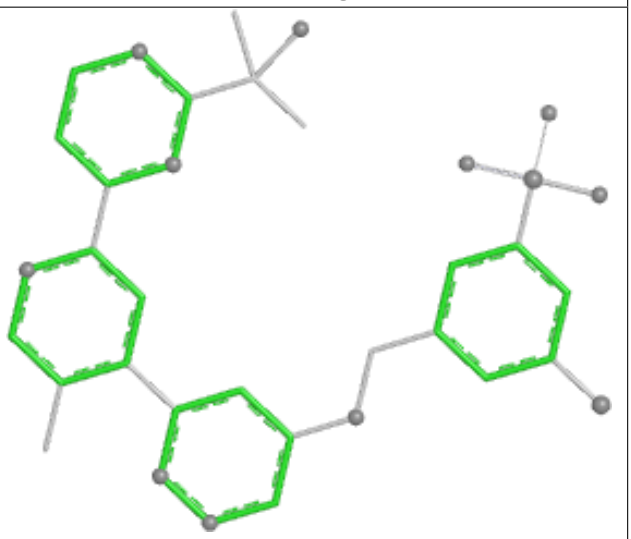
Bond lengths



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, 95^{th} 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	348/363 (95%)	0.01	4 (1%)	78	57	45, 70, 105, 119	0
1	B	348/363 (95%)	-0.07	8 (2%)	61	38	44, 70, 104, 123	0
2	C	344/363 (94%)	0.18	4 (1%)	76	55	56, 91, 116, 133	0
2	D	348/363 (95%)	0.29	5 (1%)	73	51	56, 92, 116, 133	1 (0%)
All	All	1388/1452 (95%)	0.10	21 (1%)	72	49	44, 81, 113, 133	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	ILE	3.0
2	D	257	LEU	2.9
2	C	273	PRO	2.7
2	C	51	GLY	2.7
1	A	250	ILE	2.6
1	B	32	SER	2.6
1	B	34	ALA	2.5
2	D	345	ASP	2.5
1	A	199	HIS	2.5
2	C	325	ILE	2.5
1	B	197	TRP	2.5
2	C	271	ILE	2.4
1	B	250	ILE	2.3
2	D	75	ASN	2.3
1	A	197	TRP	2.3
1	A	32	SER	2.2
1	B	252	SER	2.2
2	D	267	HIS	2.2
1	B	199	HIS	2.2
1	B	196	ASN	2.1
2	D	271	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	TPO	B	263	11/12	0.59	0.19	89,106,140,140	0
1	TPO	B	180	11/12	0.60	0.17	81,95,115,116	0
1	TPO	A	180	11/12	0.75	0.12	108,118,138,139	0
1	PTR	B	182	16/17	0.75	0.15	62,89,139,142	0
1	PTR	A	182	16/17	0.75	0.16	87,108,141,142	0
1	TPO	A	263	11/12	0.77	0.13	97,105,131,131	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

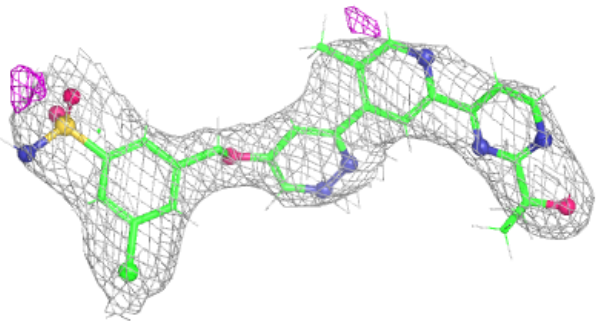
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A1C0B	B	401	36/36	0.91	0.13	64,71,86,87	0
3	A1C0B	A	401	36/36	0.93	0.11	39,54,73,74	0

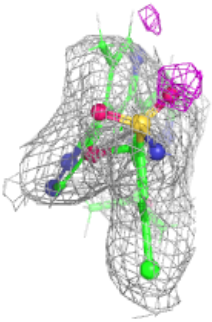
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1C0B B 401:

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

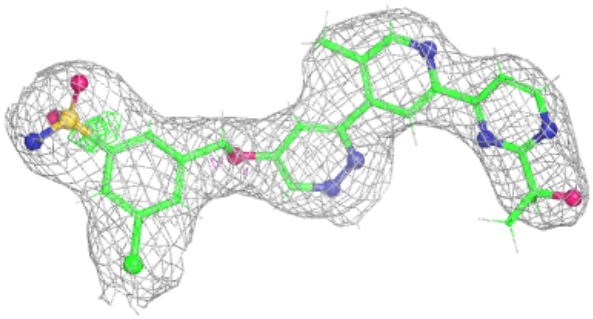


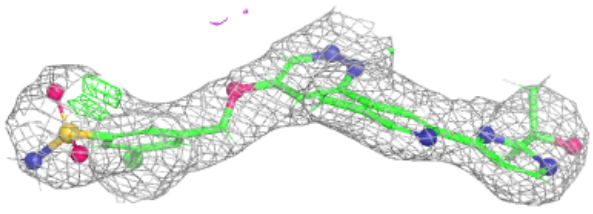


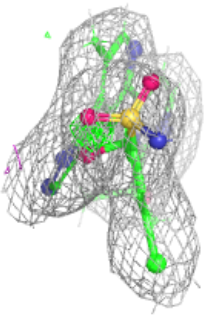


Electron density around A1C0B A 401:

$2mF_o$-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 (i)

There are no such residues in this entry.