Full wwPDB X-ray Structure Validation Report (i)

Mar 30, 2025 – 04:14 am BST

PDB ID	:	9ESX / pdb_00009esx
Title	:	CDK2-cyclin A in complex with FragLite 17
Authors	:	Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on	:	2024-03-26
Resolution	:	2.37 Å(reported)

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

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

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

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

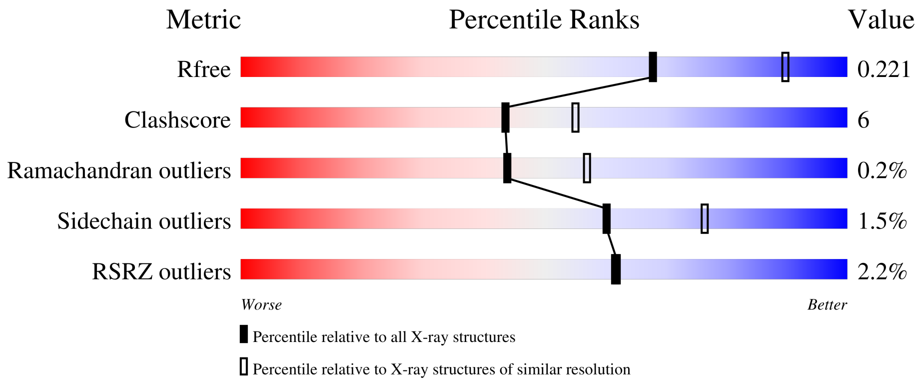
MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.37 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}	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	302	4% / 84% 13% • •
1	C	302	4% / 86% 12% ••
2	B	268	89% 9% •
2	D	268	88% 9% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9294 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total 2355	C 1526	N 398	O 422	P 1	S 8	0	0	0
1	C	298	Total 2400	C 1556	N 407	O 428	P 1	S 8	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total 2116	C 1369	N 345	O 391	S 11	0	1	0
2	D	262	Total 2118	C 1370	N 345	O 393	S 10	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

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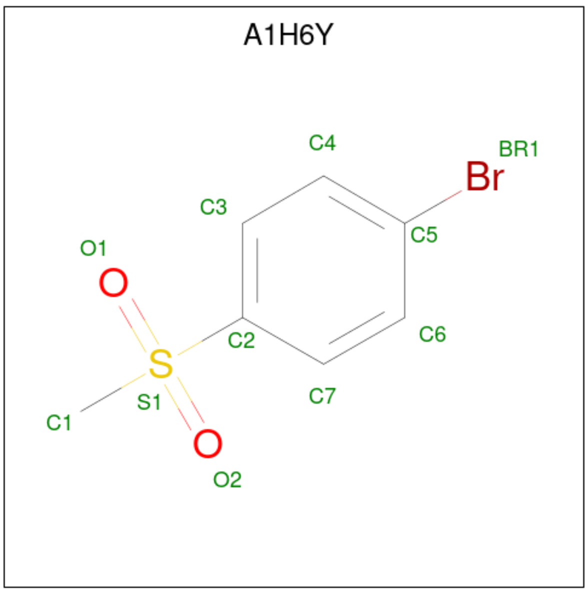
Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is 1-bromanyl-4-methylsulfonyl-benzene (CCD ID: A1H6Y) (formula: $C_7H_7BrO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br C O S 11 1 7 2 1	0	0
3	A	1	Total Br C O S 11 1 7 2 1	0	0
3	B	1	Total Br C O S 11 1 7 2 1	0	0
3	C	1	Total Br C O S 11 1 7 2 1	0	0

- Molecule 4 is water.

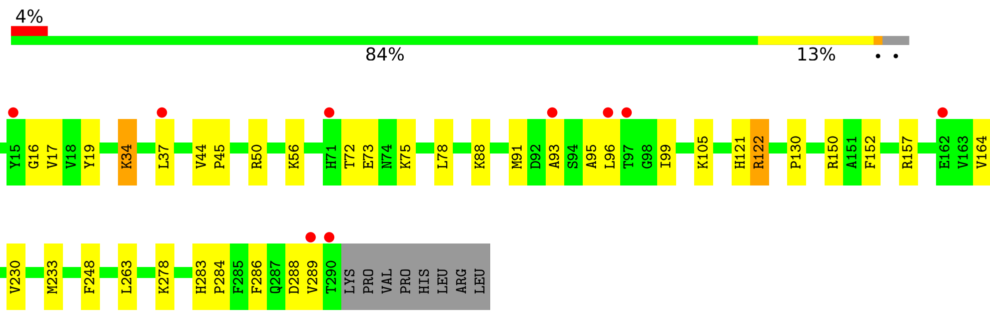
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	86	Total 86	O 86	0	0
4	C	55	Total 55	O 55	0	0
4	D	35	Total 35	O 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

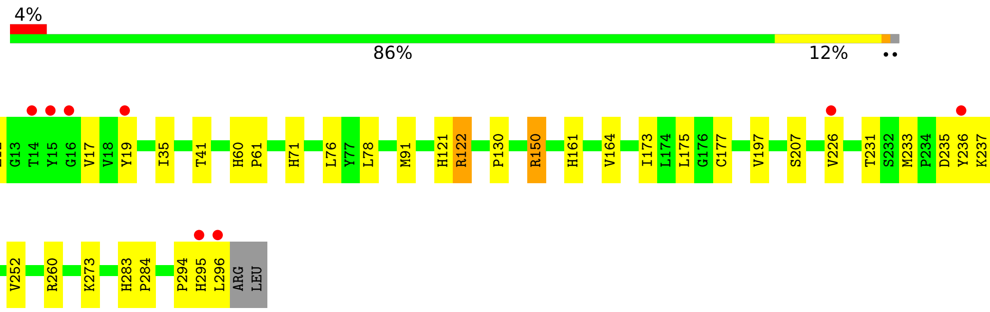
- Molecule 1: Cyclin-dependent kinase 2

Chain A:



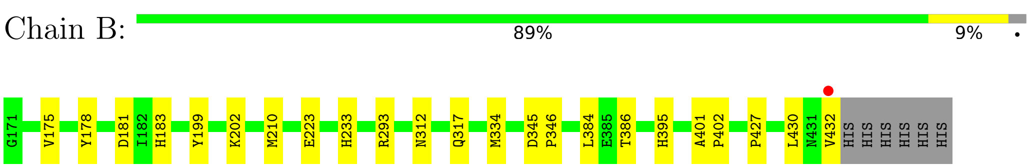
- Molecule 1: Cyclin-dependent kinase 2

Chain C:



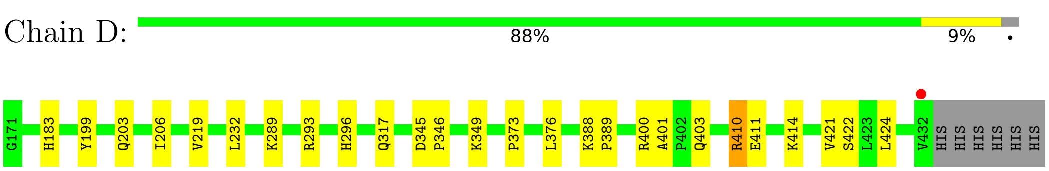
- Molecule 2: Cyclin-A2

Chain B:



- Molecule 2: Cyclin-A2

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.12Å 133.91Å 147.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.90 – 2.37 73.90 – 2.37	Depositor EDS
% Data completeness (in resolution range)	92.4 (73.90-2.37) 92.3 (73.90-2.37)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.222 , 0.229 0.218 , 0.221	Depositor DCC
R_{free} test set	2879 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 30.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9294	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, A1H6Y

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	0.52	0/2403	0.84	0/3259
1	C	0.48	0/2450	0.83	0/3324
2	B	0.49	0/2166	0.82	0/2945
2	D	0.49	0/2168	0.80	0/2948
All	All	0.50	0/9187	0.82	0/12476

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	C	0	2
2	D	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ARG	Sidechain
1	A	50	ARG	Sidechain
1	C	150	ARG	Sidechain
1	C	245	ARG	Sidechain
2	D	400	ARG	Sidechain
2	D	410	ARG	Sidechain

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	2355	0	2389	44	0
1	C	2400	0	2438	31	0
2	B	2116	0	2132	23	0
2	D	2118	0	2131	14	0
3	A	22	0	0	0	0
3	B	11	0	0	1	0
3	C	11	0	0	0	0
4	A	85	0	0	1	0
4	B	86	0	0	3	0
4	C	55	0	0	1	0
4	D	35	0	0	0	0
All	All	9294	0	9090	108	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 6.

All (108) 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)
2:B:175:VAL:CG1	2:B:178:TYR:HB2	1.80	1.10
2:B:175:VAL:HG11	2:B:178:TYR:HB2	1.45	0.96
2:B:223:GLU:HG2	4:B:747:HOH:O	1.65	0.95
1:C:294:PRO:HG2	1:C:296:LEU:HD23	1.48	0.95
1:C:294:PRO:HG2	1:C:296:LEU:CD2	1.97	0.95
1:A:9:LYS:HE3	1:A:17:VAL:HG23	1.50	0.92
1:C:294:PRO:CG	1:C:296:LEU:HD21	2.12	0.79
1:C:294:PRO:CG	1:C:296:LEU:CD2	2.63	0.77
1:A:96:LEU:CD1	1:A:96:LEU:H	1.97	0.76
1:A:121:HIS:O	1:A:122:ARG:HG3	1.91	0.71
2:B:210:MET:HG2	3:B:601:A1H6Y:C1	2.21	0.70
1:A:37:LEU:HD11	1:A:44:VAL:HA	1.73	0.69
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.22	0.69
1:A:96:LEU:N	1:A:96:LEU:HD12	2.08	0.68
1:A:93:ALA:O	1:A:96:LEU:HD11	1.93	0.68
2:B:175:VAL:HG12	2:B:178:TYR:HB2	1.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LEU:HB3	2:B:432:VAL:HG23	1.77	0.67
1:C:294:PRO:HB2	1:C:296:LEU:HD21	1.75	0.67
1:A:286:PHE:O	1:A:289:VAL:HG23	1.94	0.66
1:C:294:PRO:HB2	1:C:296:LEU:CD2	2.25	0.66
1:A:177:CYS:SG	1:A:233:MET:HG2	2.36	0.65
1:A:9:LYS:HE3	1:A:17:VAL:CG2	2.27	0.64
1:C:294:PRO:CB	1:C:296:LEU:HD21	2.27	0.64
1:A:96:LEU:CD1	1:A:96:LEU:N	2.61	0.64
1:A:105:LYS:HG2	1:A:289:VAL:HG22	1.79	0.63
1:A:37:LEU:CD1	1:A:44:VAL:HA	2.29	0.62
1:C:161:HIS:HE1	1:C:173:ILE:O	1.83	0.62
1:A:96:LEU:H	1:A:96:LEU:HD12	1.64	0.62
1:C:294:PRO:CB	1:C:296:LEU:CD2	2.79	0.60
1:A:152:PHE:CE2	2:B:175:VAL:HG21	2.37	0.60
2:B:175:VAL:HG12	2:B:175:VAL:O	2.00	0.60
1:A:175:LEU:CD1	1:A:233:MET:HE1	2.32	0.60
1:A:177:CYS:HB2	4:A:722:HOH:O	2.01	0.59
1:A:121:HIS:C	1:A:122:ARG:HG3	2.24	0.58
1:C:12:GLU:HG2	1:C:17:VAL:HG22	1.85	0.58
1:A:93:ALA:C	1:A:96:LEU:HD11	2.25	0.57
2:B:430:LEU:CB	2:B:432:VAL:HG23	2.34	0.56
1:A:152:PHE:HE2	2:B:175:VAL:HG21	1.71	0.56
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.40	0.56
2:B:386:THR:HB	4:B:750:HOH:O	2.07	0.55
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.90	0.54
1:A:177:CYS:SG	1:A:233:MET:CE	2.97	0.53
1:A:78:LEU:N	1:A:78:LEU:HD23	2.23	0.53
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.90	0.52
2:D:411:GLU:HA	2:D:414:LYS:HD2	1.90	0.52
1:C:177:CYS:HB2	4:C:607:HOH:O	2.09	0.52
1:A:248:PHE:HE2	1:A:263:LEU:HD23	1.74	0.52
1:A:91:MET:HA	1:A:95:ALA:HB3	1.90	0.52
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.74	0.52
1:C:17:VAL:HG11	1:C:19:TYR:CZ	2.45	0.51
1:A:177:CYS:SG	1:A:233:MET:SD	3.09	0.51
2:D:289:LYS:HG2	2:D:293:ARG:HD3	1.92	0.50
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.29	0.50
2:B:233:HIS:HD2	4:B:748:HOH:O	1.94	0.49
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.93	0.49
2:B:312:ASN:ND2	2:B:334:MET:SD	2.86	0.49
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:HD12	1:C:78:LEU:HD13	1.93	0.49
2:D:203:GLN:HB3	2:D:206:ILE:HG13	1.94	0.49
2:B:175:VAL:CG1	2:B:178:TYR:CB	2.73	0.48
2:B:175:VAL:HG13	2:B:178:TYR:HD2	1.79	0.48
1:C:175:LEU:HA	1:C:235:ASP:HB2	1.96	0.47
1:C:197:VAL:HG11	1:C:252:VAL:HG12	1.96	0.47
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.96	0.47
1:A:286:PHE:HA	1:A:289:VAL:HG23	1.97	0.47
1:A:286:PHE:CA	1:A:289:VAL:HG23	2.44	0.47
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.79	0.47
1:C:248:PHE:CB	1:C:260:ARG:HD2	2.45	0.46
1:C:121:HIS:O	1:C:122:ARG:HG3	2.15	0.46
1:A:175:LEU:HD12	1:A:233:MET:HE1	1.98	0.46
1:A:16:GLY:HA3	1:A:34:LYS:O	2.17	0.45
2:B:430:LEU:HB3	2:B:432:VAL:CG2	2.45	0.45
1:C:161:HIS:CE1	1:C:173:ILE:O	2.67	0.44
1:A:96:LEU:H	1:A:96:LEU:HD13	1.77	0.44
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.00	0.44
2:B:395:HIS:HE1	2:B:427:PRO:O	2.00	0.44
2:D:219:VAL:HG22	2:D:232:LEU:HD21	1.99	0.44
1:A:17:VAL:HG13	1:A:19:TYR:CE1	2.53	0.43
1:C:76:LEU:HD12	1:C:76:LEU:HA	1.81	0.43
1:C:295:HIS:CD2	1:C:295:HIS:H	2.34	0.43
2:D:346:PRO:O	2:D:349:LYS:HG2	2.18	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.83	0.43
2:D:421:VAL:HA	2:D:424:LEU:HG	2.01	0.43
1:A:56:LYS:HB3	1:A:56:LYS:HE3	1.79	0.43
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.54	0.43
2:D:414:LYS:HG3	2:D:422:SER:OG	2.19	0.43
1:A:157:ARG:HE	1:A:157:ARG:HB2	1.52	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.49	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.84	0.42
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.55	0.42
1:A:95:ALA:HB1	1:A:99:ILE:HG12	2.01	0.42
1:C:237:LYS:HD2	1:C:237:LYS:HA	1.86	0.42
1:A:34:LYS:HB3	1:A:34:LYS:HE3	1.80	0.42
1:C:231:THR:HA	1:C:236:TYR:CD2	2.55	0.41
1:C:121:HIS:C	1:C:122:ARG:HG3	2.39	0.41
1:A:72:THR:HG22	1:A:73:GLU:H	1.86	0.41
1:C:197:VAL:HG11	1:C:252:VAL:HG13	2.01	0.41
2:B:395:HIS:HB2	2:B:430:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HA	1:A:233:MET:SD	2.60	0.41
1:C:91:MET:HE2	1:C:130:PRO:HB3	2.02	0.41
1:C:226:VAL:O	1:C:273:LYS:NZ	2.54	0.41
2:D:203:GLN:HB3	2:D:206:ILE:CG1	2.51	0.41
2:B:401:ALA:N	2:B:402:PRO:CD	2.84	0.40
1:C:71:HIS:HD2	2:D:296:HIS:NE2	2.20	0.40
1:C:9:LYS:HE3	1:C:17:VAL:HG13	2.03	0.40
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.91	0.40
2:B:384:LEU:HD23	2:B:384:LEU:HA	1.93	0.40
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.36	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	291/302 (96%)	281 (97%)	9 (3%)	1 (0%)	37	49
1	C	296/302 (98%)	285 (96%)	10 (3%)	1 (0%)	37	49
2	B	261/268 (97%)	257 (98%)	4 (2%)	0	100	100
2	D	261/268 (97%)	254 (97%)	7 (3%)	0	100	100
All	All	1109/1140 (97%)	1077 (97%)	30 (3%)	2 (0%)	44	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	A	164	VAL

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	256/264 (97%)	251 (98%)	5 (2%)	50	68
1	C	262/264 (99%)	257 (98%)	5 (2%)	52	70
2	B	235/240 (98%)	232 (99%)	3 (1%)	65	80
2	D	235/240 (98%)	233 (99%)	2 (1%)	75	87
All	All	988/1008 (98%)	973 (98%)	15 (2%)	60	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	75	LYS
1	A	122	ARG
1	A	150	ARG
1	A	200	ARG
2	B	199	TYR
2	B	202	LYS
2	B	293	ARG
1	C	41	THR
1	C	122	ARG
1	C	150	ARG
1	C	207	SER
1	C	233	MET
2	D	199	TYR
2	D	403	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN

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Mol	Chain	Res	Type
2	B	296	HIS
2	B	312	ASN
2	B	317	GLN
2	B	378	GLN
2	B	395	HIS
2	B	431	ASN
1	C	71	HIS
1	C	161	HIS
1	C	246	GLN
1	C	287	GLN
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	370	GLN
2	D	395	HIS
2	D	403	GLN
2	D	425	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

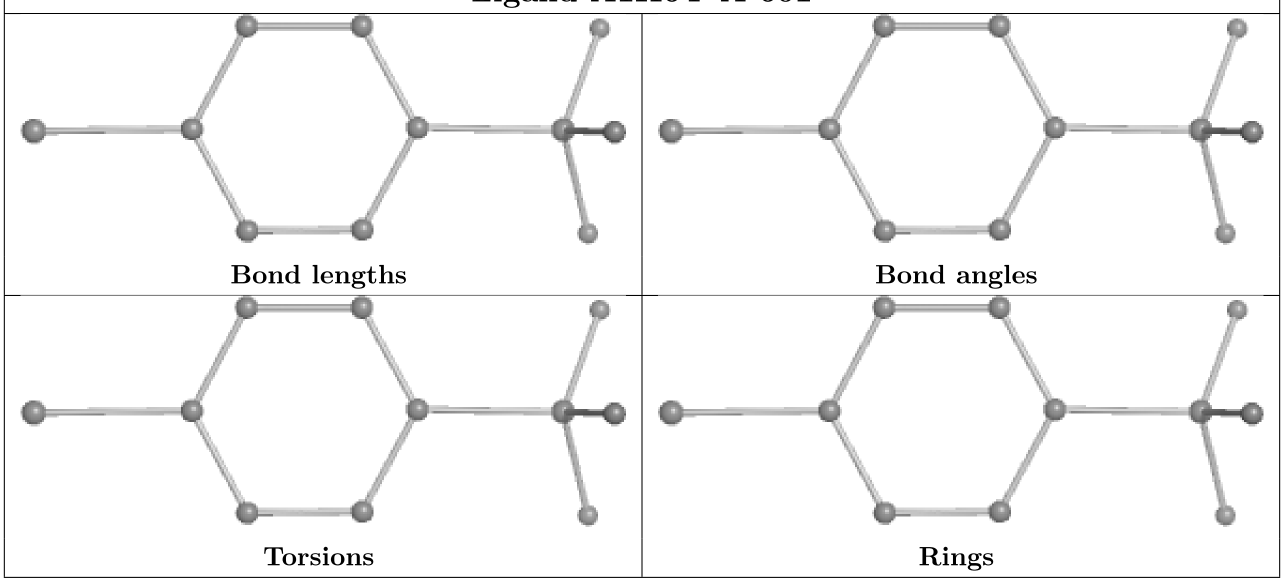
There are no torsion outliers.

There are no ring outliers.

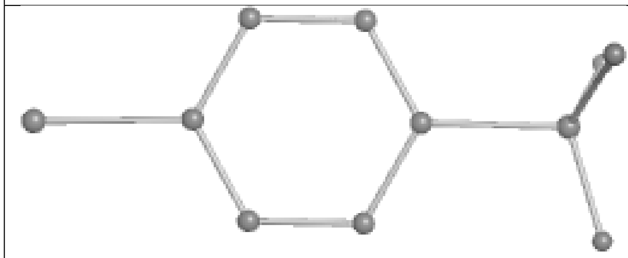
No monomer is involved in short contacts.

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.

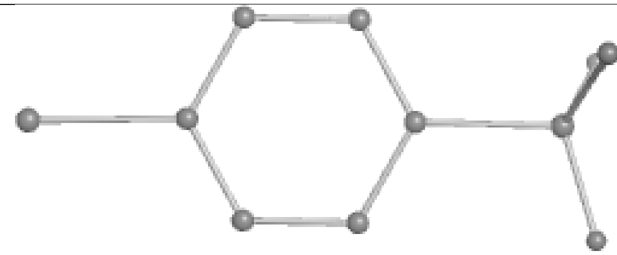
Ligand A1H6Y A 601



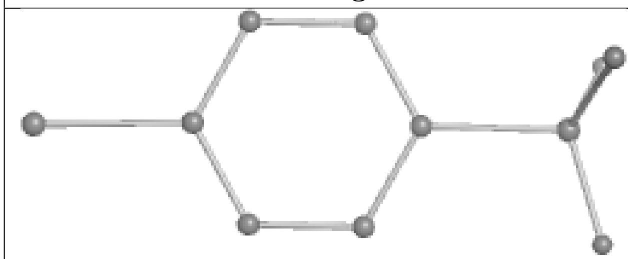
Ligand A1H6Y A 602



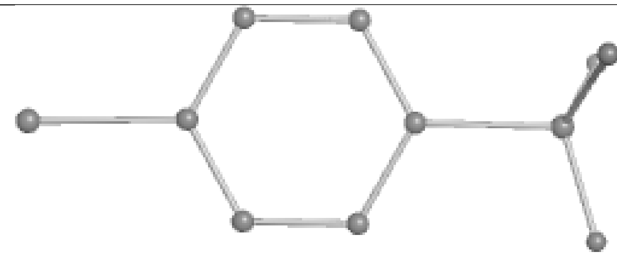
Bond lengths



Bond angles

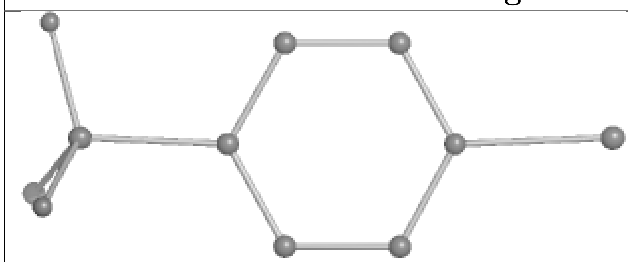


Torsions

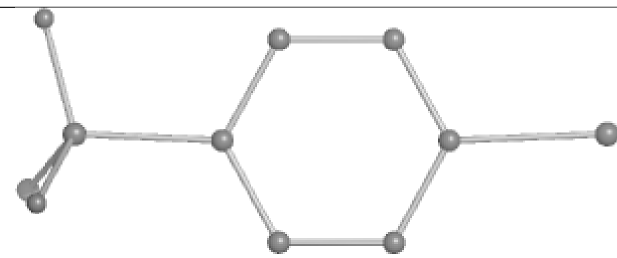


Rings

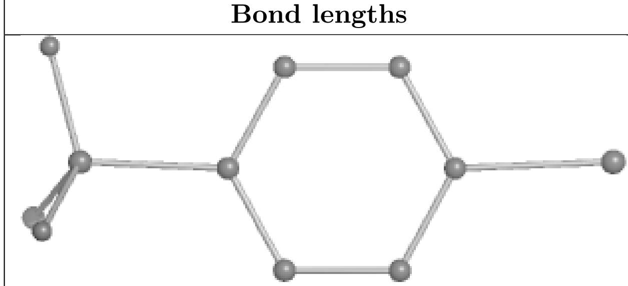
Ligand A1H6Y B 601



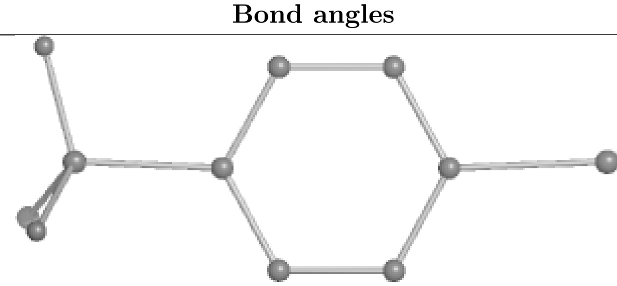
Bond lengths



Bond angles

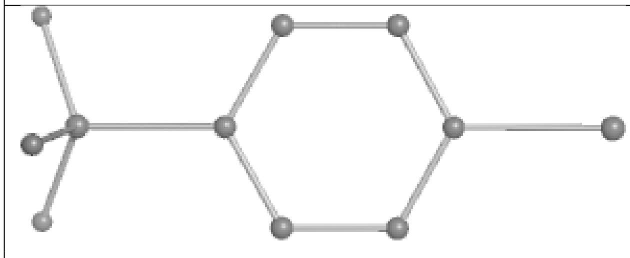


Torsions

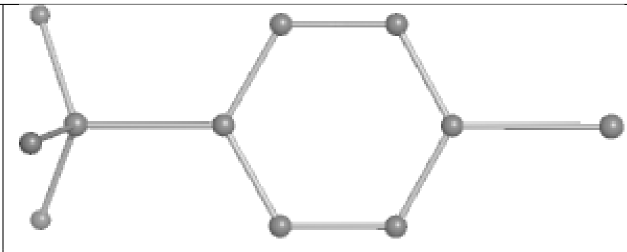


Rings

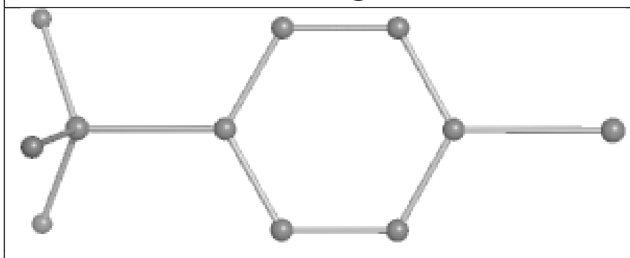
Ligand A1H6Y C 501



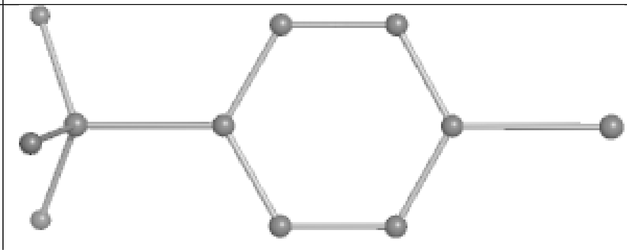
Bond lengths



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 (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, 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	293/302 (97%)	-0.11	11 (3%)	44	45	16, 28, 67, 97	0
1	C	297/302 (98%)	0.00	11 (3%)	45	46	17, 31, 63, 136	1 (0%)
2	B	262/268 (97%)	-0.31	1 (0%)	89	88	17, 30, 53, 88	1 (0%)
2	D	262/268 (97%)	0.06	1 (0%)	89	88	19, 32, 50, 78	1 (0%)
All	All	1114/1140 (97%)	-0.09	24 (2%)	62	62	16, 30, 58, 136	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	THR	6.2
2	D	432	VAL	5.7
1	C	15	TYR	5.2
1	C	295	HIS	3.7
1	A	-2	PRO	3.7
1	C	296	LEU	3.6
1	C	-1	GLY	3.4
1	A	15	TYR	3.4
1	A	71	HIS	3.1
1	C	14	THR	3.0
1	C	19	TYR	2.9
1	A	37	LEU	2.8
1	A	162	GLU	2.8
2	B	432	VAL	2.8
1	A	0	SER	2.6
1	A	96	LEU	2.5
1	A	93	ALA	2.4
1	A	97	THR	2.4
1	C	16	GLY	2.2
1	C	226	VAL	2.2
1	C	236	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	12	GLU	2.1
1	A	289	VAL	2.0
1	C	242	LYS	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	C	160	11/12	0.97	0.05	20,25,28,29	0
1	TPO	A	160	11/12	0.98	0.05	19,26,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

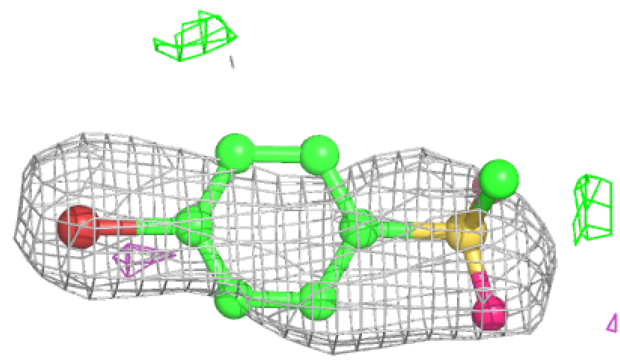
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

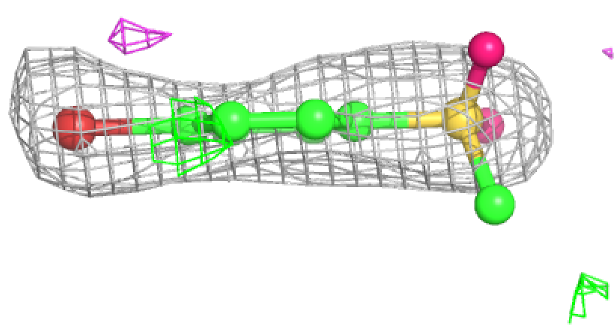
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	A1H6Y	A	602	11/11	0.79	0.19	90,122,170,181	0
3	A1H6Y	B	601	11/11	0.88	0.18	91,117,145,146	0
3	A1H6Y	A	601	11/11	0.96	0.09	34,38,47,48	0
3	A1H6Y	C	501	11/11	0.98	0.06	30,36,41,42	0

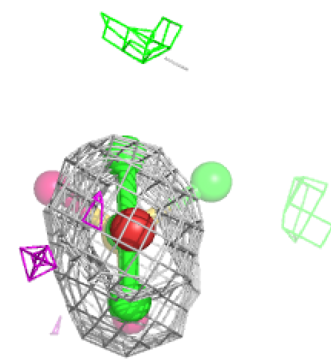
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H6Y A 602:

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

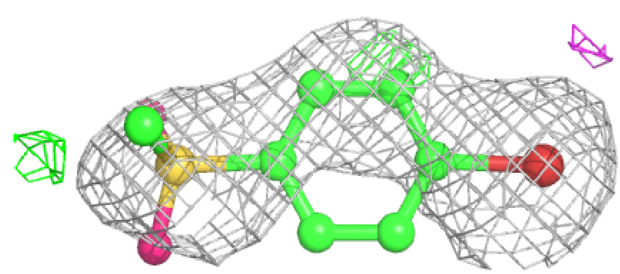


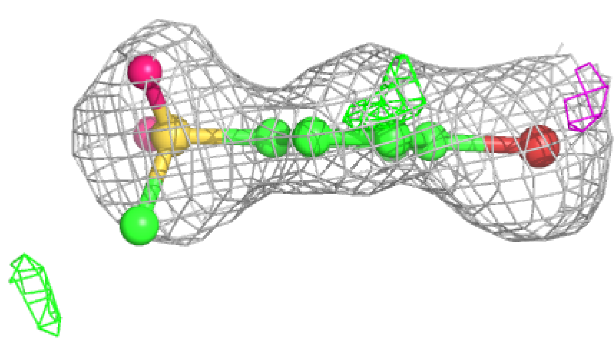


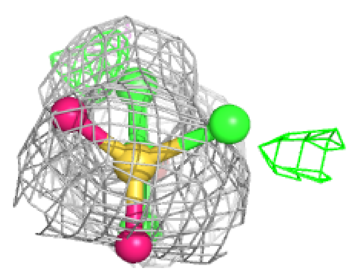


Electron density around A1H6Y B 601:

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

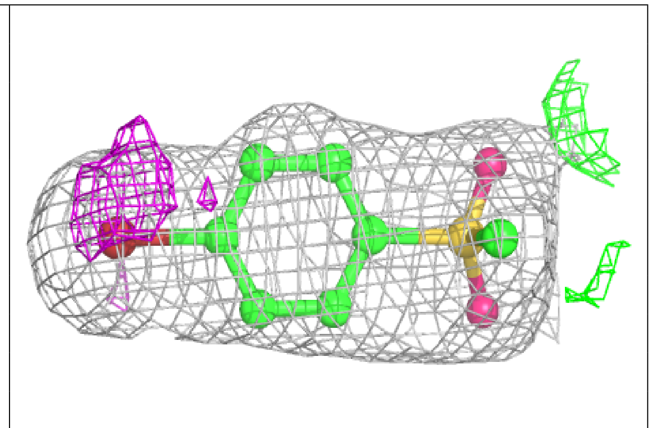


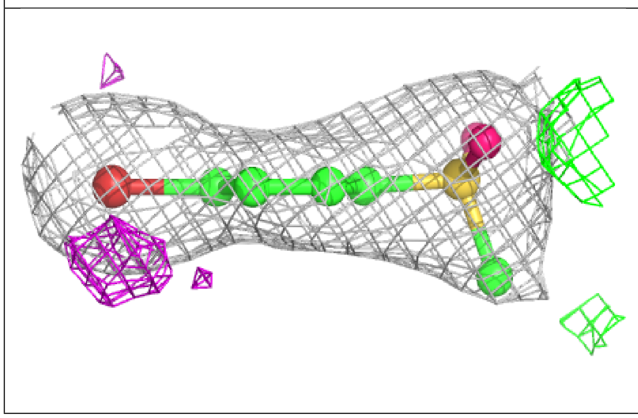


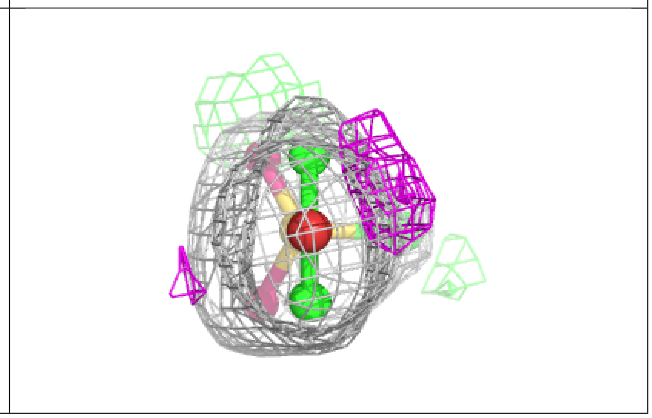


Electron density around A1H6Y A 601:

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

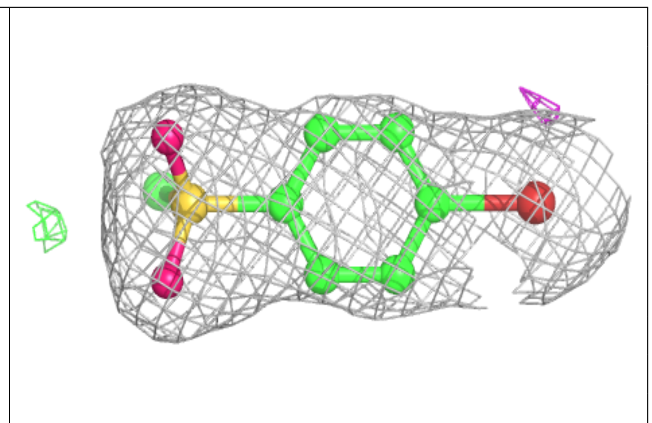


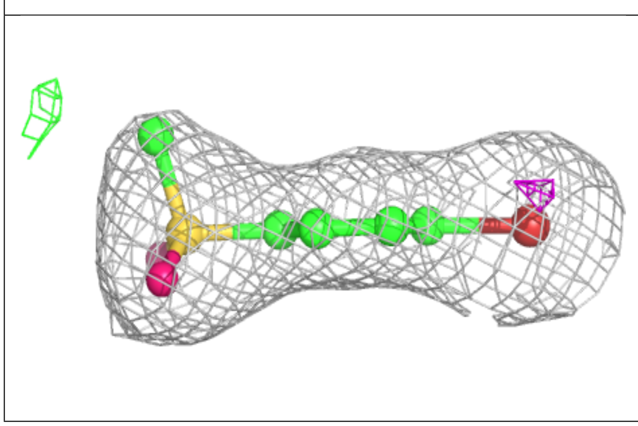


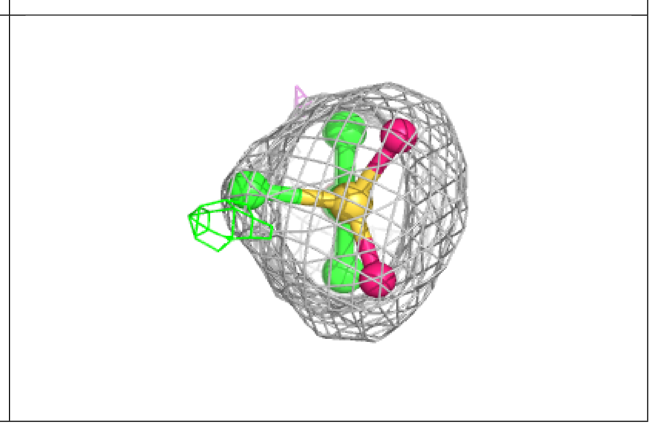


Electron density around A1H6Y C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.