



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:36 AM UTC

PDB ID : 9ET4 / pdb_00009et4
Title : CDK2-cyclin A in complex with FragLite 9
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 : 2.64 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

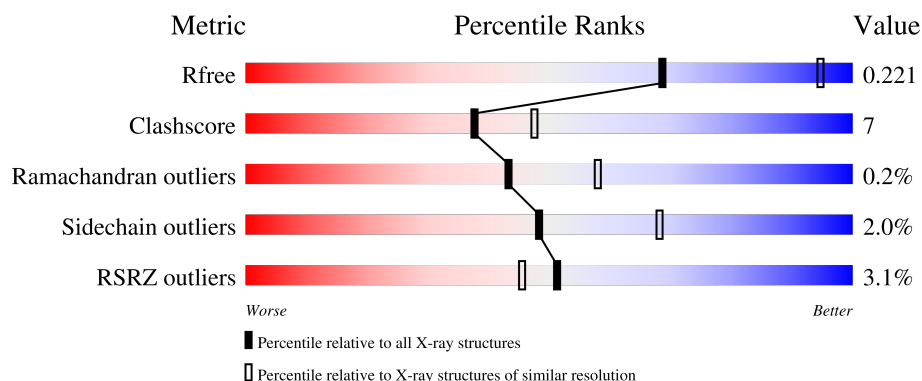
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 $\leq 5\%$. 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	B	268	79% 18% ..
1	D	268	85% 12% .
2	A	302	6% 76% 18% ..
2	C	302	3% 76% 21% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9214 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-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	262	Total	C	N	O	S	0	0	0
			2110	1366	344	390	10			
1	B	261	Total	C	N	O	S	0	0	0
			2103	1361	343	389	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274

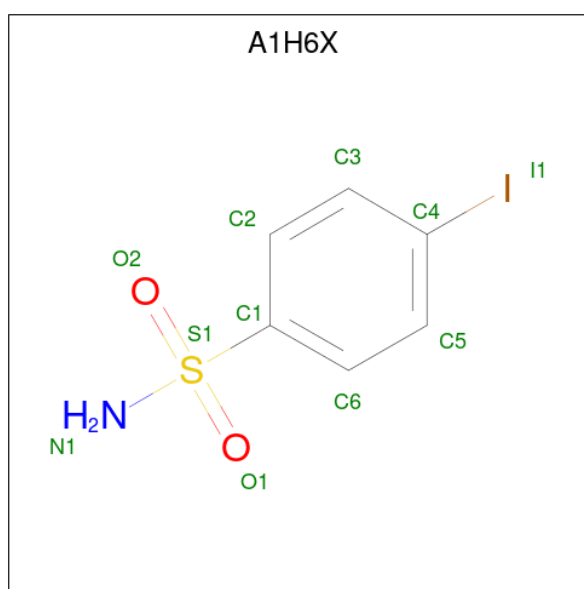
- Molecule 2 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	291	Total	C	N	O	P S	0	2	0
			2354	1527	400	418	1 8			
2	C	296	Total	C	N	O	P S	0	0	0
			2374	1540	401	424	1 8			

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 3 is 4-iodanylbenzenesulfonamide (CCD ID: A1H6X) (formula: $C_6H_6INO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	S	0	1
			22	12	2	2	4	2		
3	A	1	Total	C	I	N	O	S	0	0
			11	6	1	1	2	1		
3	B	1	Total	C	I	N	O	S	0	0
			11	6	1	1	2	1		
3	C	1	Total	C	I	N	O	S	0	0
			11	6	1	1	2	1		
3	C	1	Total	C	I	N	O	S	0	0
			11	6	1	1	2	1		

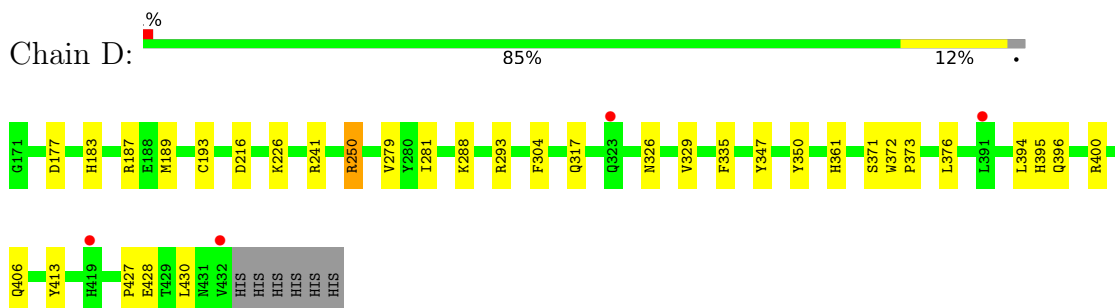
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	39	Total 39	O 39	0	0
4	A	75	Total 75	O 75	0	0
4	B	61	Total 61	O 61	0	0
4	C	32	Total 32	O 32	0	0

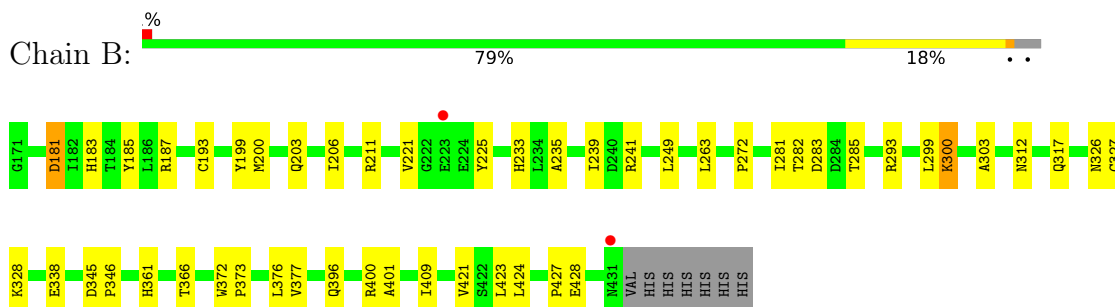
3 Residue-property plots [i](#)

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.

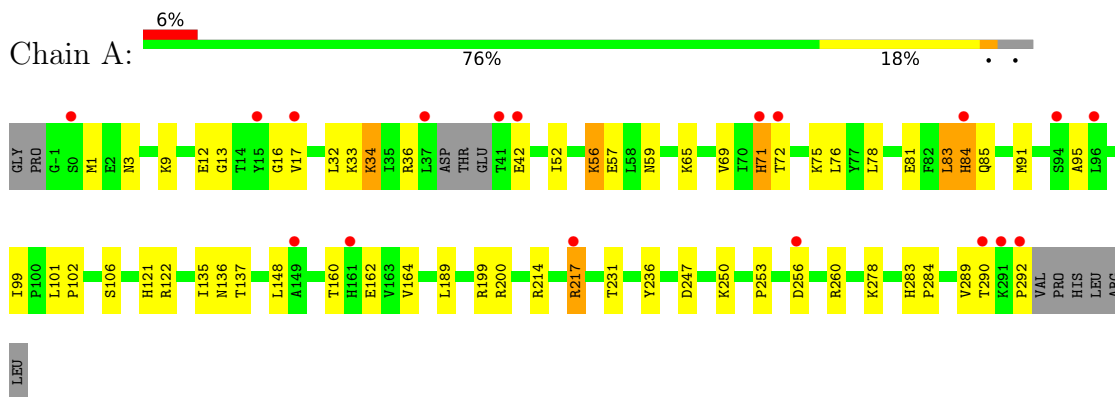
• Molecule 1: Cyclin-A2



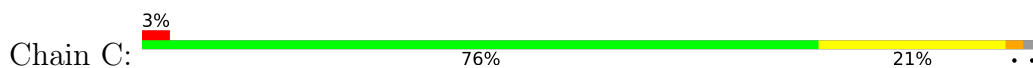
• Molecule 1: Cyclin-A2

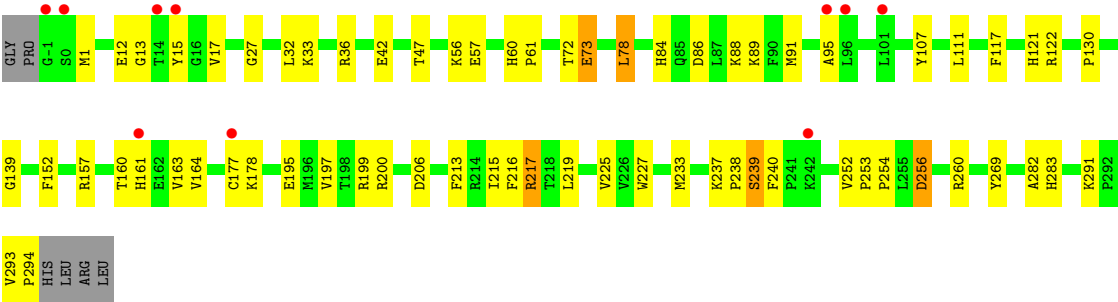


• Molecule 2: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-dependent kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.83Å 133.20Å 147.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.93 – 2.64 98.73 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.8 (98.93-2.64) 95.8 (98.73-2.64)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.220 , 0.222 0.220 , 0.221	Depositor DCC
R_{free} test set	2152 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9214	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, A1H6X

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	B	0.64	0/2153	1.17	10/2927 (0.3%)
1	D	0.60	0/2160	1.17	2/2937 (0.1%)
2	A	0.69	0/2402	1.25	6/3255 (0.2%)
2	C	0.65	0/2423	1.17	3/3287 (0.1%)
All	All	0.65	0/9138	1.19	21/12406 (0.2%)

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	B	0	2
1	D	0	2
2	A	0	3
2	C	0	2
All	All	0	9

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	71	HIS	CB-CA-C	-8.22	97.51	111.31
2	A	247	ASP	CB-CA-C	6.50	119.59	109.84
2	C	42	GLU	CB-CG-CD	6.33	123.36	112.60
2	C	256	ASP	CA-CB-CG	5.83	118.44	112.60
2	A	250	LYS	N-CA-C	-5.76	106.42	113.50
2	C	206	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	203	GLN	CB-CA-C	5.70	115.81	110.17
1	B	327	CYS	CB-CA-C	-5.69	101.70	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	TYR	N-CA-C	-5.63	106.57	113.50
1	B	377	VAL	N-CA-C	-5.62	105.04	110.72
1	B	428	GLU	CB-CG-CD	5.54	122.02	112.60
2	A	253	PRO	N-CA-C	5.48	117.38	110.70
1	B	285	THR	N-CA-C	-5.47	105.47	111.82
2	A	247	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	326	ASN	CA-C-N	5.41	127.84	120.54
1	B	326	ASN	C-N-CA	5.41	127.84	120.54
1	B	272	PRO	N-CA-CB	5.38	106.02	103.22
1	B	181	ASP	CA-CB-CG	5.28	117.88	112.60
2	A	71	HIS	CA-CB-CG	5.27	119.07	113.80
1	D	350	TYR	CB-CA-C	5.01	117.90	109.48
1	D	177	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	200	ARG	Sidechain
2	A	217	ARG	Sidechain
2	A	84[A]	HIS	Mainchain
1	B	187	ARG	Sidechain
1	B	293	ARG	Sidechain
2	C	217	ARG	Sidechain
2	C	36	ARG	Sidechain
1	D	187	ARG	Sidechain
1	D	250	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	B	2103	0	2119	26	0
1	D	2110	0	2128	18	0
2	A	2354	0	2390	44	0
2	C	2374	0	2415	45	0
3	A	33	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	0	0	0
3	C	22	0	0	3	0
4	A	75	0	0	0	0
4	B	61	0	0	1	0
4	C	32	0	0	1	0
4	D	39	0	0	0	0
All	All	9214	0	9052	126	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 7.

All (126) 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:C:15:TYR:CE2	2:C:47:THR:HG21	1.89	1.06
2:C:15:TYR:CD2	2:C:47:THR:HG21	2.13	0.82
2:C:15:TYR:CE2	2:C:47:THR:CG2	2.62	0.82
2:A:121:HIS:O	2:A:122:ARG:HG3	1.87	0.73
2:C:12:GLU:HG2	2:C:13:GLY:H	1.55	0.71
2:A:81:GLU:O	3:A:601[A]:A1H6X:I1	2.82	0.67
2:C:121:HIS:O	2:C:122:ARG:HG3	1.94	0.67
2:A:56:LYS:HE3	1:B:303:ALA:O	1.95	0.66
1:B:225:TYR:HE2	1:B:281:ILE:HG21	1.62	0.64
1:D:326:ASN:HD22	1:D:329:VAL:HG23	1.63	0.64
2:A:12:GLU:HG2	2:A:13:GLY:H	1.63	0.64
2:C:121:HIS:C	2:C:122:ARG:HG3	2.23	0.63
2:C:12:GLU:HG2	2:C:13:GLY:N	2.13	0.63
2:C:177:CYS:SG	2:C:233:MET:SD	2.95	0.62
2:A:283:HIS:ND1	2:A:284:PRO:HD2	2.16	0.61
1:D:396:GLN:HE21	1:D:400:ARG:NE	1.99	0.60
2:A:12:GLU:HG2	2:A:13:GLY:N	2.16	0.60
1:B:249:LEU:HG	2:C:27:GLY:HA3	1.82	0.60
2:A:121:HIS:C	2:A:122:ARG:HG3	2.25	0.59
2:A:16:GLY:HA3	2:A:34:LYS:O	2.03	0.59
2:C:15:TYR:CD2	2:C:47:THR:CG2	2.84	0.58
2:A:33:LYS:HD3	2:A:78:LEU:HD12	1.84	0.58
2:C:88:LYS:HB2	2:C:130:PRO:HB2	1.85	0.58
2:A:91:MET:HA	2:A:95:ALA:HB3	1.87	0.57
2:C:197:VAL:CG1	2:C:254:PRO:HG2	2.34	0.57
1:B:396:GLN:HB3	1:B:400:ARG:NH2	2.20	0.57
2:C:56:LYS:HD2	3:C:502:A1H6X:C5	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:HE1	2:A:32:LEU:HD13	1.88	0.55
2:A:9:LYS:HE2	2:A:17:VAL:HG13	1.86	0.55
2:A:106:SER:HB2	2:A:292:PRO:HD2	1.88	0.55
2:A:290:THR:OG1	2:A:292:PRO:HD3	2.06	0.55
1:D:183:HIS:HB2	1:D:317:GLN:HE22	1.73	0.54
2:A:33:LYS:CD	2:A:78:LEU:HD12	2.38	0.54
1:D:395:HIS:HB2	1:D:430:LEU:HD11	1.89	0.53
2:A:214:ARG:HG3	2:A:217:ARG:HH11	1.74	0.53
1:D:373:PRO:HD2	1:D:376:LEU:HD12	1.91	0.53
1:B:233:HIS:HD2	4:B:837:HOH:O	1.91	0.52
1:D:216:ASP:HB2	1:D:406:GLN:HG2	1.90	0.52
1:D:396:GLN:HE21	1:D:400:ARG:CZ	2.22	0.52
2:A:278:LYS:NZ	1:B:181:ASP:OD2	2.38	0.52
1:B:200:MET:HE3	1:B:211:ARG:HB2	1.92	0.52
2:A:231:THR:HA	2:A:236:TYR:CD2	2.45	0.52
2:A:101:LEU:HB3	2:A:102:PRO:HD3	1.92	0.51
1:D:189:MET:HE2	2:C:57:GLU:OE2	2.11	0.51
1:B:366:THR:HG23	1:B:427:PRO:HD3	1.93	0.50
2:C:84:HIS:HB2	4:C:628:HOH:O	2.11	0.50
1:B:396:GLN:HB3	1:B:400:ARG:CZ	2.40	0.50
2:C:1:MET:HE1	2:C:32:LEU:HD13	1.92	0.50
2:A:84[A]:HIS:CE1	2:A:137:THR:HG23	2.48	0.49
2:A:56:LYS:HE2	3:A:603:A1H6X:C5	2.43	0.49
1:D:395:HIS:HE1	1:D:427:PRO:O	1.96	0.49
2:C:215:ILE:HG23	2:C:219:LEU:HD12	1.94	0.49
2:C:256:ASP:O	2:C:260:ARG:HG3	2.13	0.49
2:A:52:ILE:HG12	2:A:78:LEU:HD21	1.95	0.48
1:B:328:LYS:HD2	1:B:424:LEU:HD11	1.95	0.48
2:C:33:LYS:HE3	3:C:501:A1H6X:O1	2.12	0.48
2:C:95:ALA:O	2:C:199:ARG:NH1	2.47	0.48
2:A:91:MET:HG2	2:A:99:ILE:HD11	1.95	0.47
2:C:195:GLU:O	2:C:199:ARG:N	2.46	0.47
2:A:36:ARG:CZ	2:A:75:LYS:HE2	2.44	0.47
2:A:69:VAL:HG22	2:A:78:LEU:HD23	1.97	0.47
2:C:291:LYS:HG2	2:C:291:LYS:O	2.15	0.47
2:C:86:ASP:CG	2:C:89:LYS:HG2	2.39	0.47
2:C:117:PHE:O	2:C:121:HIS:ND1	2.47	0.47
2:C:86:ASP:OD2	2:C:89:LYS:HG2	2.14	0.47
1:B:221:VAL:HG21	1:B:281:ILE:HD12	1.97	0.47
2:A:72:THR:OG1	2:A:75:LYS:HB2	2.14	0.46
2:A:42:GLU:H	2:A:42:GLU:HG3	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:CD2	1:D:361:HIS:C	2.94	0.46
2:A:83:LEU:HD23	2:A:136:ASN:HB3	1.98	0.46
1:D:304:PHE:HD2	3:C:502:A1H6X:N1	2.13	0.46
2:C:12:GLU:HG3	2:C:17:VAL:HG22	1.97	0.46
1:B:263:LEU:HD22	1:B:299:LEU:HD21	1.97	0.46
2:C:253:PRO:N	2:C:254:PRO:HD2	2.30	0.46
1:D:347:TYR:OH	1:D:394:LEU:HA	2.16	0.45
1:D:279:VAL:HG21	1:D:288:LYS:HA	1.99	0.45
2:C:78:LEU:HD23	2:C:78:LEU:N	2.32	0.45
2:A:85:GLN:HE21	2:A:135:ILE:HD11	1.82	0.44
2:A:12:GLU:CG	2:A:13:GLY:H	2.30	0.44
2:A:256[A]:ASP:O	2:A:260:ARG:HG3	2.17	0.44
1:B:338:GLU:HB3	1:B:409:ILE:HD13	2.00	0.44
2:C:88:LYS:HA	2:C:91:MET:HE2	2.00	0.44
2:A:59:ASN:OD1	2:A:65:LYS:HE3	2.18	0.43
2:C:216:PHE:HE2	2:C:240:PHE:CD2	2.36	0.43
2:A:52:ILE:HG12	2:A:78:LEU:CD2	2.48	0.43
2:C:227:TRP:CE3	2:C:269:TYR:HB3	2.53	0.43
2:C:60:HIS:CG	2:C:61:PRO:HD2	2.53	0.43
1:B:200:MET:SD	1:B:206:ILE:HG13	2.59	0.43
1:D:193:CYS:O	1:D:241:ARG:HD2	2.18	0.42
2:A:283:HIS:CE1	2:A:284:PRO:HD2	2.53	0.42
2:C:12:GLU:CG	2:C:13:GLY:N	2.82	0.42
1:D:335:PHE:HB2	1:D:413:TYR:CD2	2.55	0.42
1:B:372:TRP:HA	1:B:373:PRO:HD3	1.79	0.42
2:C:107:TYR:O	2:C:111:LEU:HG	2.19	0.42
2:A:71:HIS:HA	2:A:76:LEU:HD12	2.02	0.42
1:B:400:ARG:O	1:B:401:ALA:C	2.62	0.42
1:B:421:VAL:C	1:B:423:LEU:H	2.28	0.42
2:C:239:SER:O	2:C:240:PHE:C	2.61	0.42
1:B:183:HIS:HB2	1:B:317:GLN:HE22	1.82	0.42
1:B:235:ALA:O	1:B:239:ILE:HG13	2.19	0.42
1:B:361:HIS:CD2	1:B:361:HIS:C	2.96	0.42
2:C:12:GLU:HA	2:C:17:VAL:HA	2.02	0.42
2:A:289:VAL:HG22	2:A:290:THR:N	2.35	0.41
2:C:195:GLU:HG3	2:C:200:ARG:O	2.20	0.41
2:C:12:GLU:CG	2:C:13:GLY:H	2.28	0.41
2:C:122:ARG:HA	2:C:152:PHE:CE2	2.55	0.41
2:C:237:LYS:HA	2:C:238:PRO:HD3	1.90	0.41
2:C:72:THR:HG22	2:C:73:GLU:H	1.85	0.41
2:A:12:GLU:CG	2:A:13:GLY:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:HIS:CD2	1:B:300:LYS:HD2	2.56	0.41
2:A:189:LEU:HD23	2:A:189:LEU:HA	1.87	0.41
2:C:139:GLY:HA2	2:C:294:PRO:HD3	2.01	0.41
2:A:36:ARG:NH2	2:A:75:LYS:HE2	2.36	0.41
1:B:372:TRP:CZ2	1:B:376:LEU:HB3	2.56	0.41
1:D:293:ARG:HH11	2:A:3:ASN:HA	1.85	0.41
2:A:52:ILE:HD11	2:A:78:LEU:HD21	2.02	0.40
2:C:161:HIS:O	2:C:163:VAL:N	2.52	0.40
2:C:282:ALA:O	2:C:283:HIS:C	2.65	0.40
1:D:396:GLN:NE2	1:D:400:ARG:CZ	2.84	0.40
2:A:57:GLU:HB2	1:B:185:TYR:OH	2.22	0.40
2:C:213:PHE:HB3	2:C:217:ARG:HH21	1.87	0.40
1:D:371:SER:O	1:D:372:TRP:C	2.65	0.40
1:B:193:CYS:O	1:B:241:ARG:HD2	2.22	0.40
2:A:33:LYS:NZ	3:A:601[B]:A1H6X:O1	2.50	0.40
1:B:282:THR:O	1:B:283:ASP:C	2.65	0.40
1:B:345:ASP:HA	1:B:346:PRO:HA	1.83	0.40

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	B	259/268 (97%)	256 (99%)	3 (1%)	0	100	100
1	D	260/268 (97%)	256 (98%)	4 (2%)	0	100	100
2	A	288/302 (95%)	278 (96%)	9 (3%)	1 (0%)	36	50
2	C	293/302 (97%)	282 (96%)	10 (3%)	1 (0%)	36	50
All	All	1100/1140 (96%)	1072 (98%)	26 (2%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

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

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	B	233/240 (97%)	231 (99%)	2 (1%)	70	82
1	D	234/240 (98%)	230 (98%)	4 (2%)	53	72
2	A	256/264 (97%)	250 (98%)	6 (2%)	44	65
2	C	259/264 (98%)	251 (97%)	8 (3%)	35	55
All	All	982/1008 (97%)	962 (98%)	20 (2%)	48	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	226	LYS
1	D	250	ARG
1	D	281	ILE
1	D	428	GLU
2	A	34	LYS
2	A	56	LYS
2	A	83	LEU
2	A	148	LEU
2	A	162	GLU
2	A	199	ARG
1	B	300	LYS
1	B	312	ASN
2	C	73	GLU
2	C	78	LEU
2	C	157	ARG
2	C	178	LYS
2	C	225	VAL
2	C	239	SER
2	C	252	VAL
2	C	293	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	228	GLN
1	D	233	HIS
1	D	254	GLN
1	D	317	GLN
1	D	326	ASN
1	D	370	GLN
1	D	395	HIS
1	D	396	GLN
2	A	62	ASN
2	A	71	HIS
2	A	74	ASN
2	A	85	GLN
1	B	179	HIS
1	B	183	HIS
1	B	228	GLN
1	B	233	HIS
1	B	254	GLN
1	B	312	ASN
1	B	317	GLN
1	B	370	GLN
1	B	378	GLN
1	B	395	HIS
1	B	425	ASN
2	C	74	ASN
2	C	246	GLN
2	C	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
2	TPO	C	160	2	8,10,11	0.67	0	10,14,16	1.07	1 (10%)
2	TPO	A	160	2	8,10,11	0.71	0	10,14,16	1.03	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
2	TPO	C	160	2	-	1/9/11/13	-
2	TPO	A	160	2	-	1/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	160	TPO	O-C-CA	-2.52	118.30	124.77
2	A	160	TPO	O-C-CA	-2.51	118.31	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	160	TPO	O-C-CA-CB
2	C	160	TPO	O-C-CA-CB

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](#)

6 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	A1H6X	C	501	-	11,11,11	0.63	0	16,16,16	1.35	3 (18%)
3	A1H6X	A	601[A]	-	11,11,11	0.48	0	16,16,16	0.88	0
3	A1H6X	A	603	-	11,11,11	0.41	0	16,16,16	0.84	0
3	A1H6X	B	701	-	11,11,11	0.49	0	16,16,16	1.20	1 (6%)
3	A1H6X	C	502	-	11,11,11	0.37	0	16,16,16	0.80	0
3	A1H6X	A	601[B]	-	11,11,11	0.57	0	16,16,16	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H6X	C	501	-	-	4/6/6/6	0/1/1/1
3	A1H6X	A	601[A]	-	-	4/6/6/6	0/1/1/1
3	A1H6X	A	603	-	-	4/6/6/6	0/1/1/1
3	A1H6X	B	701	-	-	0/6/6/6	0/1/1/1
3	A1H6X	C	502	-	-	5/6/6/6	0/1/1/1
3	A1H6X	A	601[B]	-	-	5/6/6/6	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	A1H6X	O2-S1-N1	2.18	110.50	107.35
3	C	501	A1H6X	C3-C4-C5	2.16	123.50	120.64
3	B	701	A1H6X	C2-C1-C6	2.11	123.22	120.47
3	C	501	A1H6X	C2-C1-C6	2.03	123.12	120.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601[B]	A1H6X	C6-C1-S1-N1
3	A	603	A1H6X	C6-C1-S1-O1
3	A	603	A1H6X	C2-C1-S1-O1
3	A	603	A1H6X	C6-C1-S1-N1
3	C	502	A1H6X	C6-C1-S1-N1
3	A	601[B]	A1H6X	C2-C1-S1-N1
3	A	603	A1H6X	C2-C1-S1-N1
3	C	501	A1H6X	C2-C1-S1-N1
3	C	502	A1H6X	C2-C1-S1-N1
3	A	601[A]	A1H6X	C2-C1-S1-O2
3	C	501	A1H6X	C6-C1-S1-N1
3	A	601[A]	A1H6X	C6-C1-S1-O2
3	A	601[A]	A1H6X	C6-C1-S1-N1
3	A	601[A]	A1H6X	C2-C1-S1-N1
3	C	501	A1H6X	C6-C1-S1-O1
3	C	501	A1H6X	C2-C1-S1-O1
3	A	601[B]	A1H6X	C2-C1-S1-O1
3	C	502	A1H6X	C2-C1-S1-O2
3	C	502	A1H6X	C6-C1-S1-O2
3	A	601[B]	A1H6X	C6-C1-S1-O1
3	C	502	A1H6X	C6-C1-S1-O1
3	A	601[B]	A1H6X	C6-C1-S1-O2

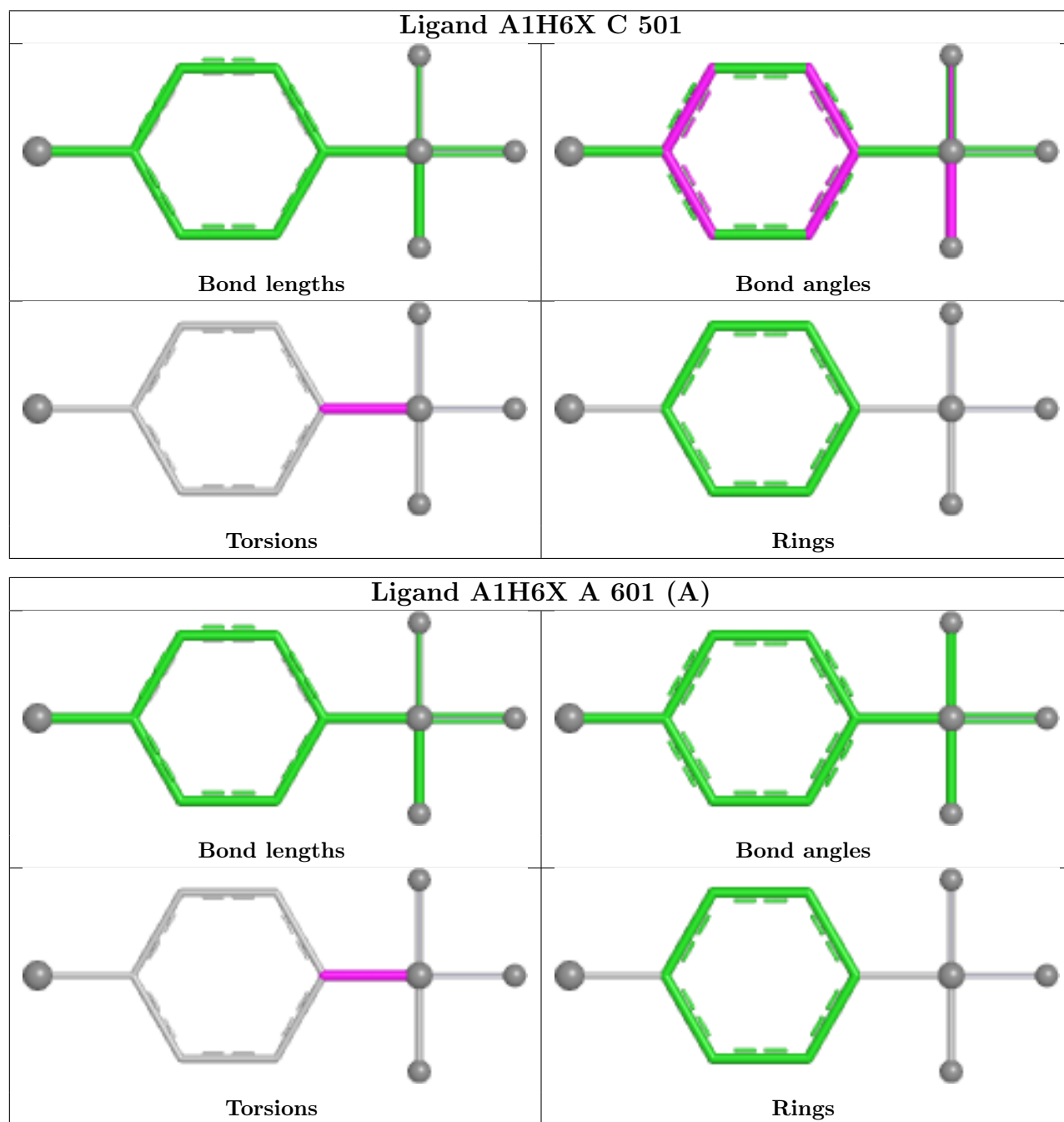
There are no ring outliers.

5 monomers are involved in 6 short contacts:

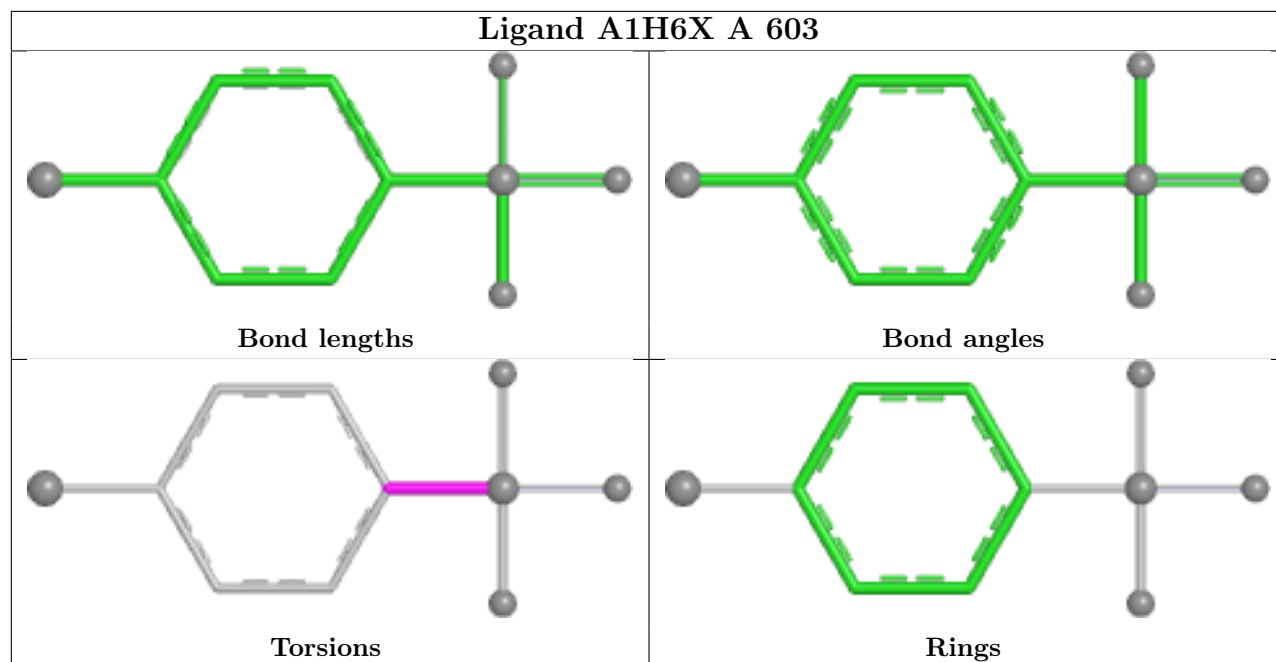
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	A1H6X	1	0
3	A	601[A]	A1H6X	1	0
3	A	603	A1H6X	1	0
3	C	502	A1H6X	2	0
3	A	601[B]	A1H6X	1	0

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 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.

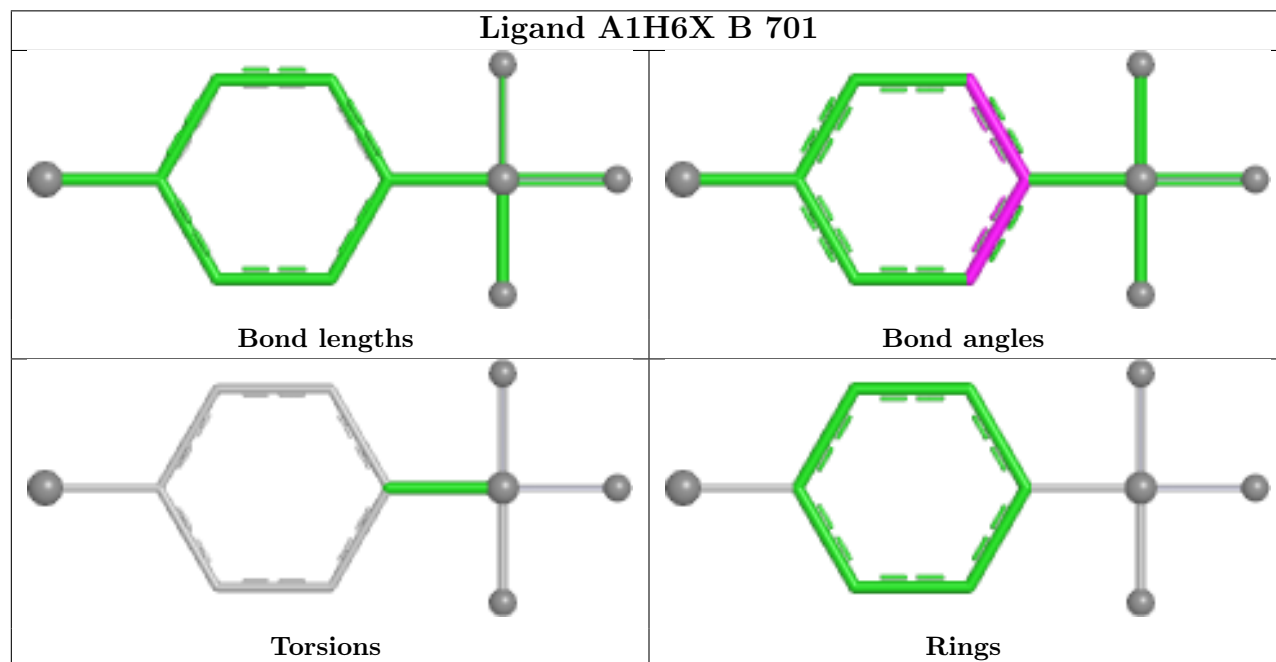
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

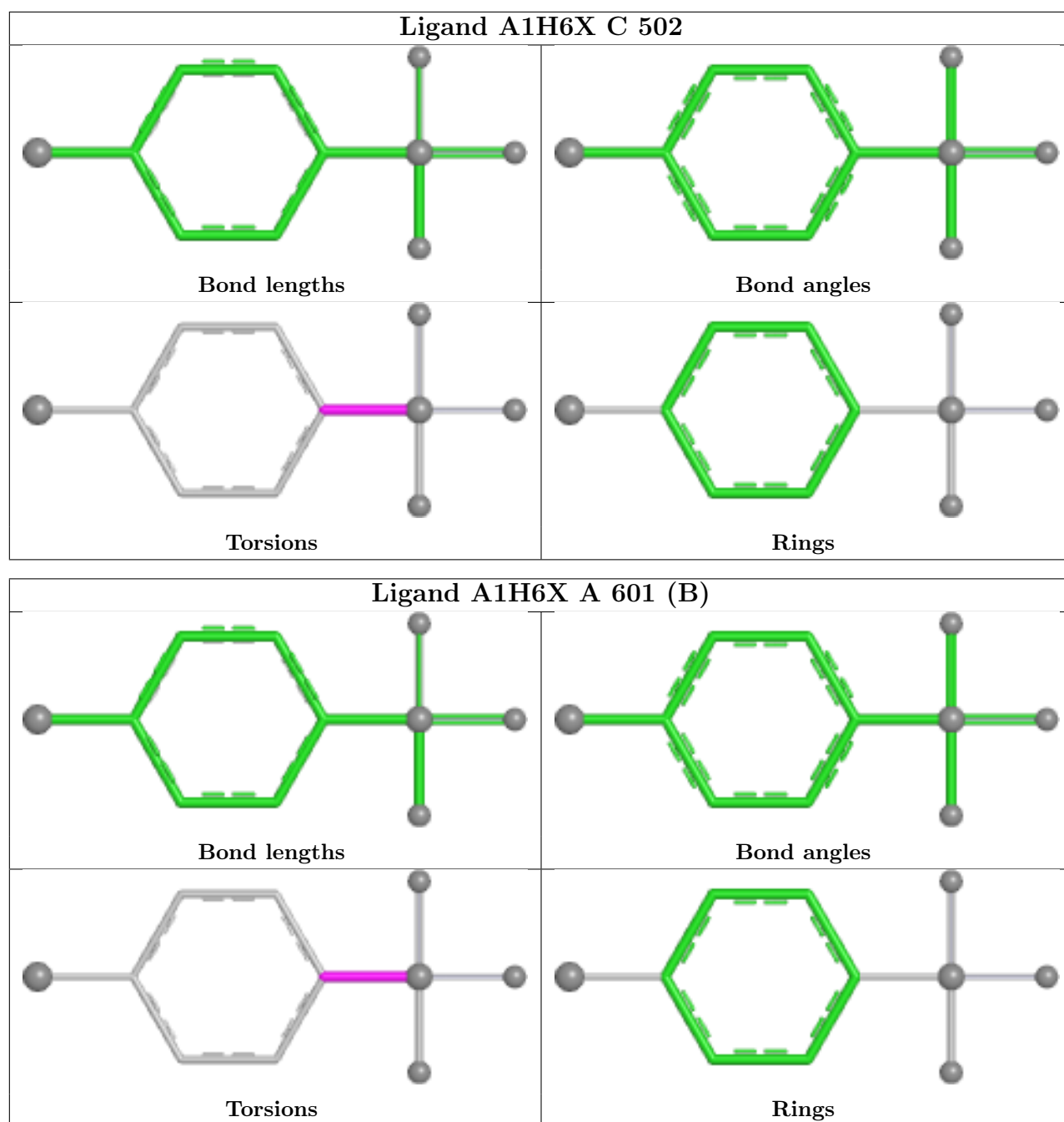


Ligand A1H6X A 603



Ligand A1H6X B 701





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	B	261/268 (97%)	-0.21	2 (0%) 82 80	40, 56, 82, 117	0
1	D	262/268 (97%)	0.08	4 (1%) 72 69	43, 65, 99, 147	0
2	A	290/302 (96%)	-0.05	18 (6%) 26 22	26, 52, 101, 132	2 (0%)
2	C	295/302 (97%)	0.12	10 (3%) 48 42	44, 63, 105, 155	0
All	All	1108/1140 (97%)	-0.01	34 (3%) 51 45	26, 58, 100, 155	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	VAL	6.6
2	C	15	TYR	4.8
2	C	-1	GLY	4.3
2	A	292	PRO	4.0
1	B	431	ASN	3.9
2	A	72	THR	3.8
2	C	0	SER	3.8
1	D	391	LEU	3.8
2	A	17	VAL	3.7
1	B	223	GLU	3.5
1	D	323	GLN	3.4
2	A	84[A]	HIS	3.1
2	A	41	THR	3.1
2	A	161	HIS	3.0
2	A	15	TYR	2.8
2	A	291	LYS	2.8
2	A	42	GLU	2.6
2	A	71	HIS	2.6
2	A	290	THR	2.6
2	A	0	SER	2.5
2	A	149	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	37	LEU	2.4
2	A	94	SER	2.3
2	A	96	LEU	2.3
2	A	256[A]	ASP	2.3
2	C	242	LYS	2.2
2	C	14	THR	2.2
2	C	161	HIS	2.2
2	C	101	LEU	2.1
2	C	95	ALA	2.1
2	A	217	ARG	2.1
2	C	96	LEU	2.0
2	C	177	CYS	2.0
1	D	419	HIS	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, 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	TPO	C	160	11/12	0.95	0.08	48,55,61,63	0
2	TPO	A	160	11/12	0.96	0.07	43,49,54,55	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

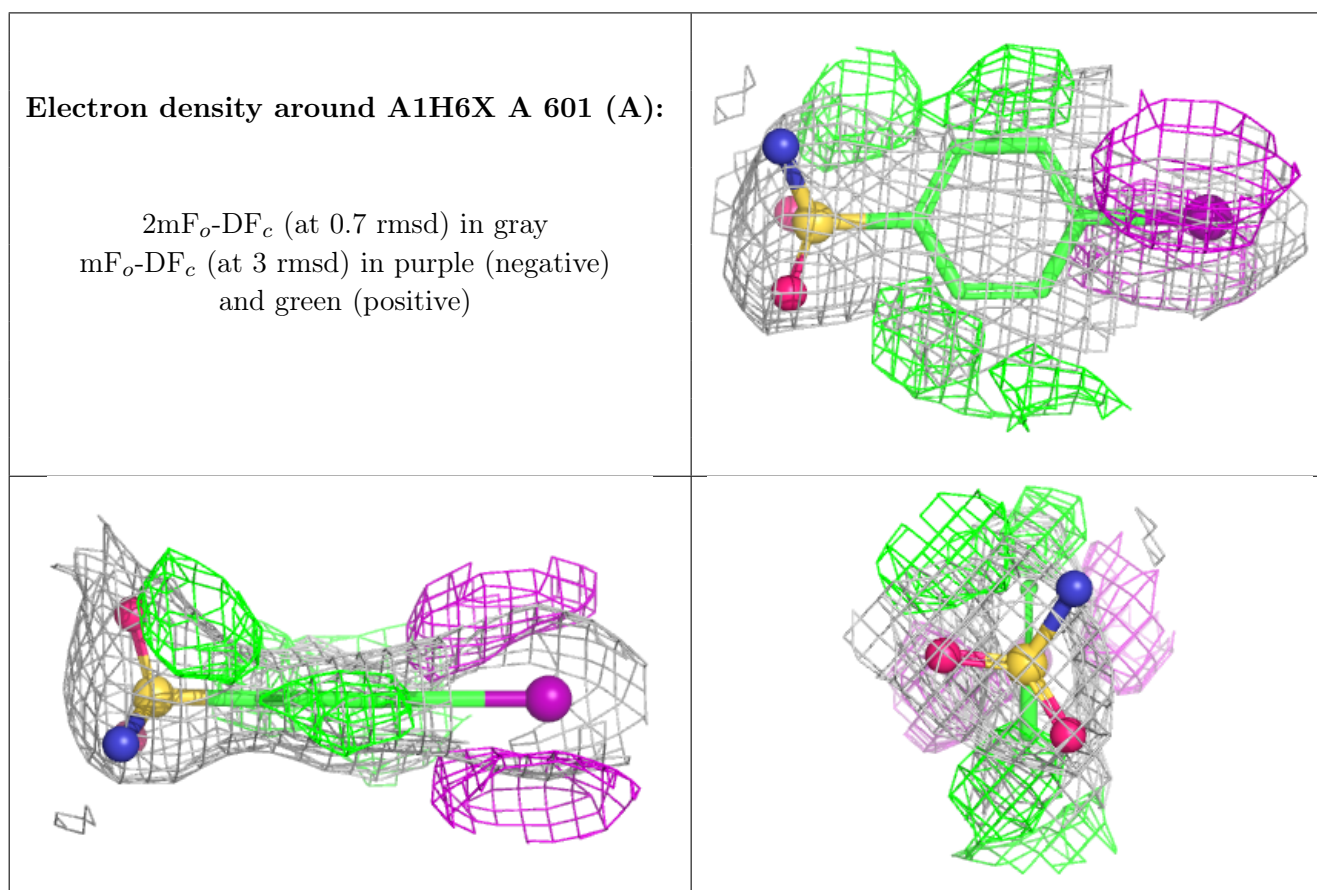
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1H6X	A	601[A]	11/11	0.78	0.27	74,83,108,141	11
3	A1H6X	A	601[B]	11/11	0.78	0.27	73,80,129,170	11
3	A1H6X	C	501	11/11	0.85	0.22	86,113,139,152	0

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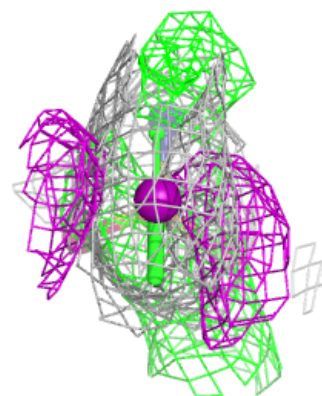
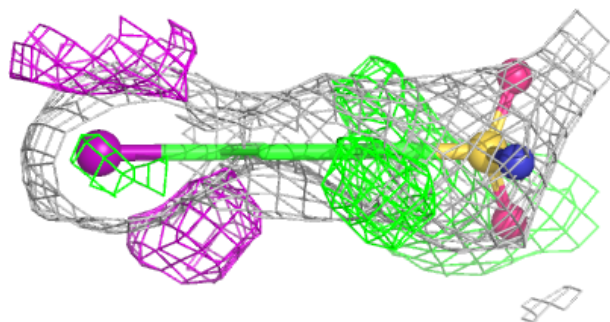
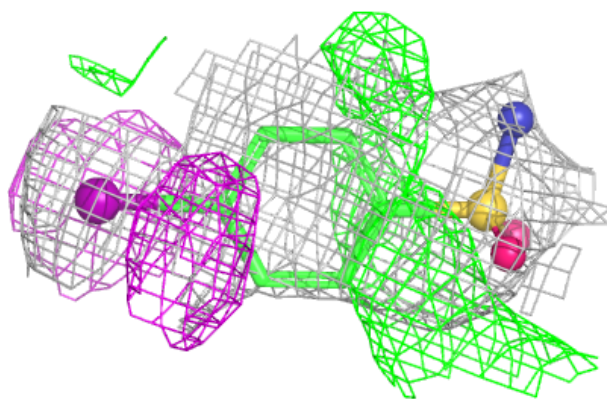
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1H6X	A	603	11/11	0.90	0.14	94,109,123,148	0
3	A1H6X	C	502	11/11	0.92	0.14	114,126,148,150	0
3	A1H6X	B	701	11/11	0.93	0.14	88,118,143,150	0

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.

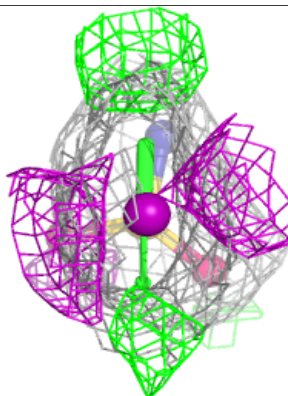
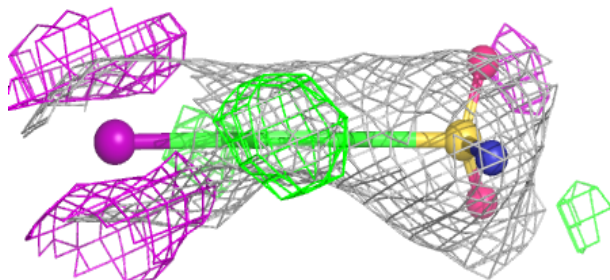
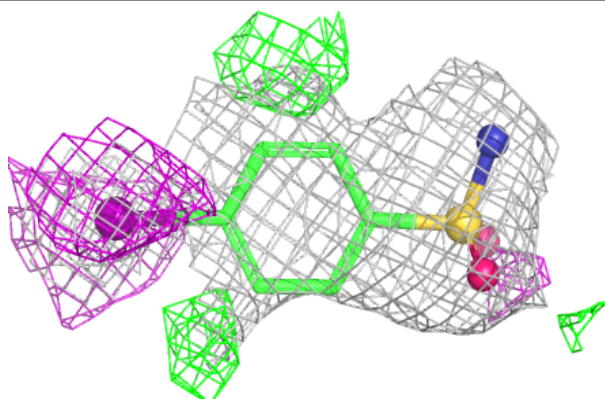


Electron density around A1H6X A 601 (B):

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

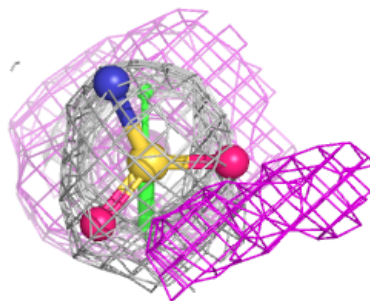
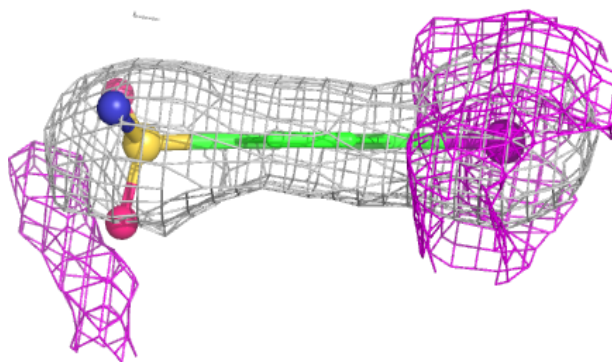
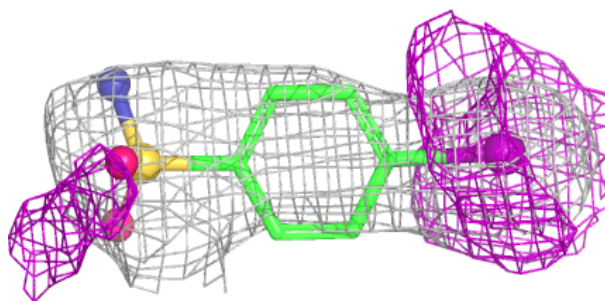
**Electron density around A1H6X C 501:**

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

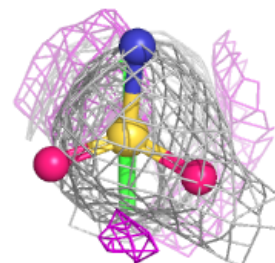
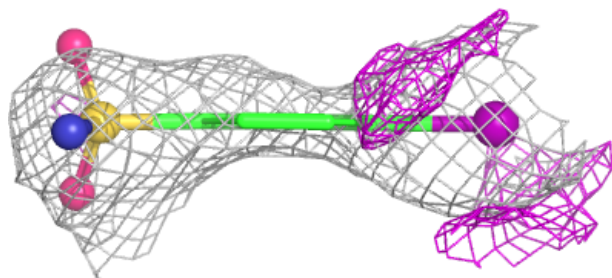
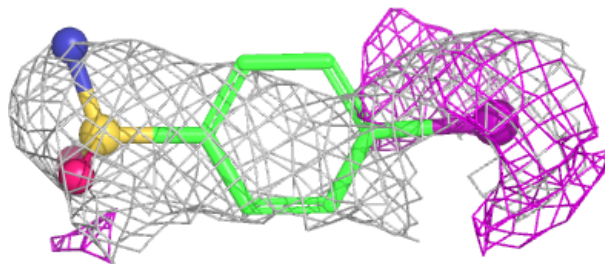


Electron density around A1H6X A 603:

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

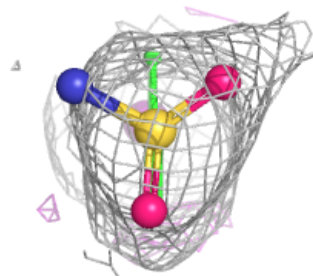
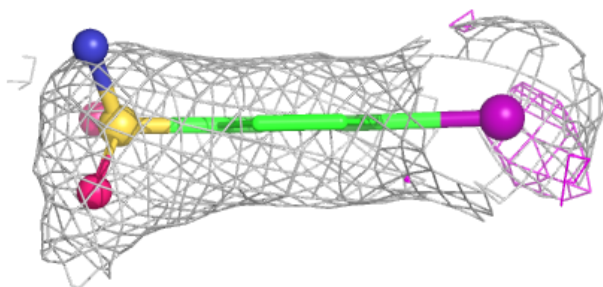
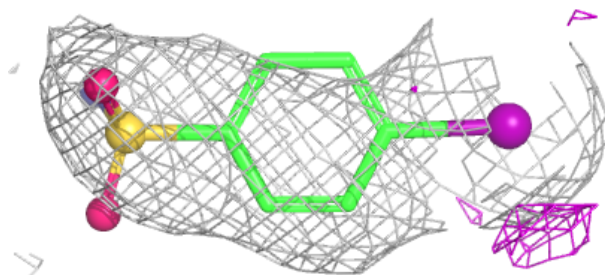
**Electron density around A1H6X C 502:**

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



Electron density around A1H6X B 701:

$2mF_o - DF_c$ (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.