



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 2VX3 / pdb_00002vx3
Title : Crystal structure of the human dual specificity tyrosine- phosphorylation-regulated kinase 1A
Authors : Roos, A.K.; Soundararajan, M.; Pike, A.C.W.; Federov, O.; King, O.; Burgess-Brown, N.; Philips, C.; Filippakopoulos, P.; Arrowsmith, C.H.; Wikstrom, M.; Edwards, A.; von Delft, F.; Bountra, C.; Knapp, S.
Deposited on : 2008-06-30
Resolution : 2.40 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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

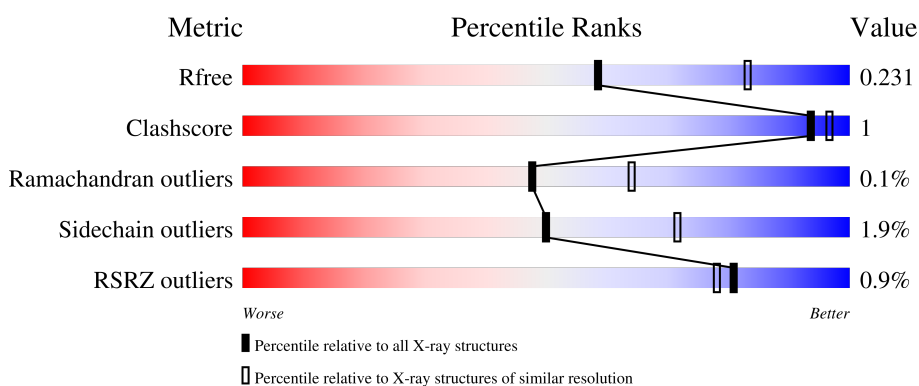
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	A	382	 % 86% 9%
1	B	382	 % 83% 6% 11%
1	C	382	 % 85% 11%
1	D	382	 % 85% 5% 10%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11571 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 DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	347	2828	1815	489	506	1	17	0	2	0
1	B	341	2760	1780	472	490	1	17	0	1	0
1	C	339	2726	1760	462	487	1	16	0	0	0
1	D	343	2772	1789	474	491	1	17	0	2	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	expression tag	UNP Q13627
A	105	HIS	-	expression tag	UNP Q13627
A	106	HIS	-	expression tag	UNP Q13627
A	107	HIS	-	expression tag	UNP Q13627
A	108	HIS	-	expression tag	UNP Q13627
A	109	HIS	-	expression tag	UNP Q13627
A	110	HIS	-	expression tag	UNP Q13627
A	111	SER	-	expression tag	UNP Q13627
A	112	SER	-	expression tag	UNP Q13627
A	113	GLY	-	expression tag	UNP Q13627
A	114	VAL	-	expression tag	UNP Q13627
A	115	ASP	-	expression tag	UNP Q13627
A	116	LEU	-	expression tag	UNP Q13627
A	117	GLY	-	expression tag	UNP Q13627
A	118	THR	-	expression tag	UNP Q13627
A	119	GLU	-	expression tag	UNP Q13627
A	120	ASN	-	expression tag	UNP Q13627
A	121	LEU	-	expression tag	UNP Q13627
A	122	TYR	-	expression tag	UNP Q13627
A	123	PHE	-	expression tag	UNP Q13627

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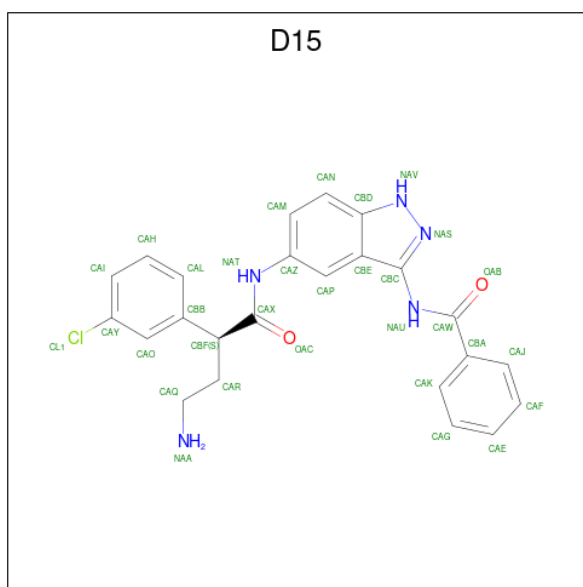
Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLN	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	104	MET	-	expression tag	UNP Q13627
B	105	HIS	-	expression tag	UNP Q13627
B	106	HIS	-	expression tag	UNP Q13627
B	107	HIS	-	expression tag	UNP Q13627
B	108	HIS	-	expression tag	UNP Q13627
B	109	HIS	-	expression tag	UNP Q13627
B	110	HIS	-	expression tag	UNP Q13627
B	111	SER	-	expression tag	UNP Q13627
B	112	SER	-	expression tag	UNP Q13627
B	113	GLY	-	expression tag	UNP Q13627
B	114	VAL	-	expression tag	UNP Q13627
B	115	ASP	-	expression tag	UNP Q13627
B	116	LEU	-	expression tag	UNP Q13627
B	117	GLY	-	expression tag	UNP Q13627
B	118	THR	-	expression tag	UNP Q13627
B	119	GLU	-	expression tag	UNP Q13627
B	120	ASN	-	expression tag	UNP Q13627
B	121	LEU	-	expression tag	UNP Q13627
B	122	TYR	-	expression tag	UNP Q13627
B	123	PHE	-	expression tag	UNP Q13627
B	124	GLN	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	104	MET	-	expression tag	UNP Q13627
C	105	HIS	-	expression tag	UNP Q13627
C	106	HIS	-	expression tag	UNP Q13627
C	107	HIS	-	expression tag	UNP Q13627
C	108	HIS	-	expression tag	UNP Q13627
C	109	HIS	-	expression tag	UNP Q13627
C	110	HIS	-	expression tag	UNP Q13627
C	111	SER	-	expression tag	UNP Q13627
C	112	SER	-	expression tag	UNP Q13627
C	113	GLY	-	expression tag	UNP Q13627
C	114	VAL	-	expression tag	UNP Q13627
C	115	ASP	-	expression tag	UNP Q13627
C	116	LEU	-	expression tag	UNP Q13627
C	117	GLY	-	expression tag	UNP Q13627
C	118	THR	-	expression tag	UNP Q13627
C	119	GLU	-	expression tag	UNP Q13627

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Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASN	-	expression tag	UNP Q13627
C	121	LEU	-	expression tag	UNP Q13627
C	122	TYR	-	expression tag	UNP Q13627
C	123	PHE	-	expression tag	UNP Q13627
C	124	GLN	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	104	MET	-	expression tag	UNP Q13627
D	105	HIS	-	expression tag	UNP Q13627
D	106	HIS	-	expression tag	UNP Q13627
D	107	HIS	-	expression tag	UNP Q13627
D	108	HIS	-	expression tag	UNP Q13627
D	109	HIS	-	expression tag	UNP Q13627
D	110	HIS	-	expression tag	UNP Q13627
D	111	SER	-	expression tag	UNP Q13627
D	112	SER	-	expression tag	UNP Q13627
D	113	GLY	-	expression tag	UNP Q13627
D	114	VAL	-	expression tag	UNP Q13627
D	115	ASP	-	expression tag	UNP Q13627
D	116	LEU	-	expression tag	UNP Q13627
D	117	GLY	-	expression tag	UNP Q13627
D	118	THR	-	expression tag	UNP Q13627
D	119	GLU	-	expression tag	UNP Q13627
D	120	ASN	-	expression tag	UNP Q13627
D	121	LEU	-	expression tag	UNP Q13627
D	122	TYR	-	expression tag	UNP Q13627
D	123	PHE	-	expression tag	UNP Q13627
D	124	GLN	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is N-(5-{{(2S)-4-amino-2-(3-chlorophenyl)butanoyl}amino}-1H-indazol-3-yl)benzamide (CCD ID: D15) (formula: C₂₄H₂₂ClN₅O₂).

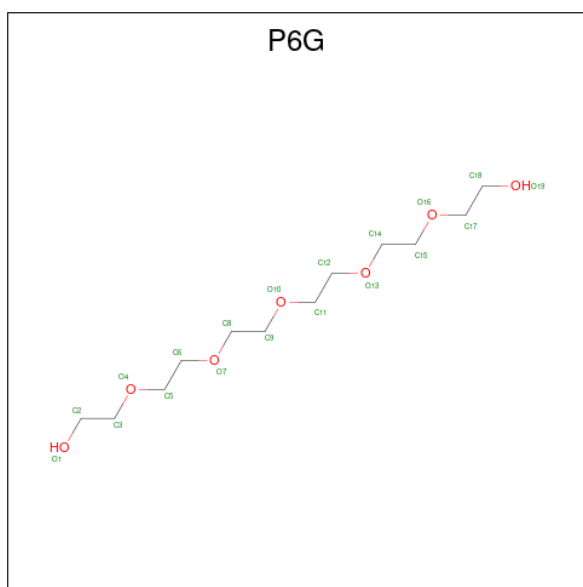


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	32	24	1	5	2	0	0
2	B	1	32	24	1	5	2	0	0
2	C	1	32	24	1	5	2	0	0
2	D	1	32	24	1	5	2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

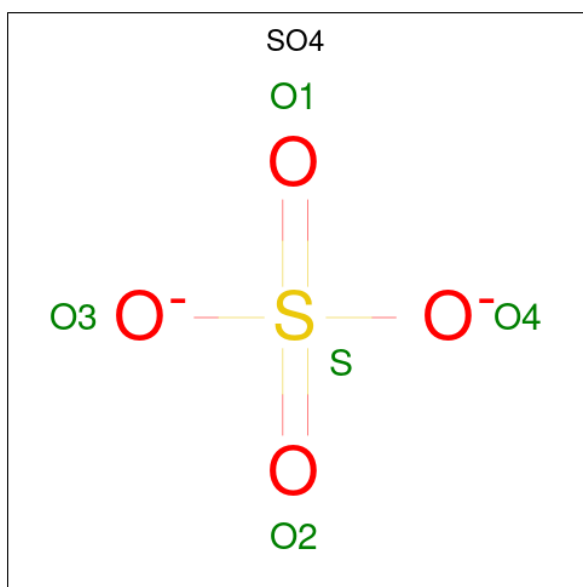
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	3	3	3	0	0

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			16	10	6		

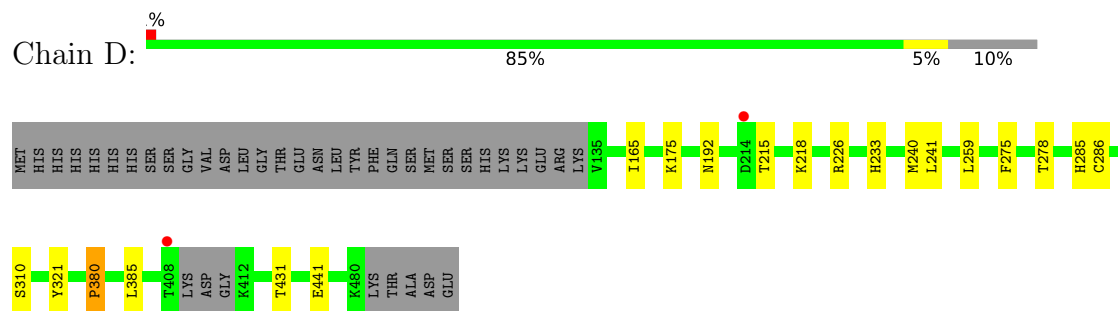
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	105	Total	O	0	0
			105	105		
6	B	52	Total	O	0	0
			52	52		
6	C	26	Total	O	0	0
			26	26		
6	D	22	Total	O	0	0
			22	22		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.20Å 65.11Å 140.28Å 90.00° 115.44° 90.00°	Depositor
Resolution (Å)	26.00 – 2.40 26.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.00-2.40) 99.8 (26.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.185 , 0.230 0.188 , 0.231	Depositor DCC
R_{free} test set	1799 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11571	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, D15, PTR, SO4, P6G

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	0.96	1/2887 (0.0%)	0.92	4/3895 (0.1%)
1	B	0.86	0/2811	0.89	1/3797 (0.0%)
1	C	0.80	0/2772	0.87	0/3745
1	D	0.81	0/2826	0.84	2/3816 (0.1%)
All	All	0.86	1/11296 (0.0%)	0.88	7/15253 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	ILE	CA-CB	6.02	1.61	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ASP	N-CA-C	7.49	119.08	111.07
1	A	213	HIS	CA-C-N	5.83	128.01	120.44
1	A	213	HIS	C-N-CA	5.83	128.01	120.44
1	D	380	PRO	O-C-N	5.61	123.78	121.15
1	B	417	PRO	O-C-N	5.34	123.77	121.31
1	D	215	THR	N-CA-C	5.33	117.70	110.35
1	A	171	GLY	N-CA-C	5.08	116.90	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	HIS	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	2828	0	2803	3	0
1	B	2760	0	2733	9	0
1	C	2726	0	2662	5	0
1	D	2772	0	2731	9	0
2	A	32	0	22	3	0
2	B	32	0	22	2	0
2	C	32	0	22	2	0
2	D	32	0	22	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	36	0	47	0	0
4	B	36	0	47	0	0
4	C	16	0	21	1	0
4	D	16	0	21	1	0
5	A	5	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
5	D	5	0	0	0	0
6	A	105	0	0	1	0
6	B	52	0	0	1	0
6	C	26	0	0	0	0
6	D	22	0	0	0	0
All	All	11571	0	11153	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (31) 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:275:PHE:O	1:B:278:THR:HG23	1.74	0.88
1:B:398:LEU:HD11	1:B:404:ASN:ND2	1.97	0.79
1:D:275:PHE:O	1:D:278:THR:HG23	1.83	0.78
2:B:600:D15:OAC	2:B:600:D15:HAP	1.85	0.73
2:A:600:D15:HAP	2:A:600:D15:OAC	1.99	0.60
1:B:398:LEU:HD11	1:B:404:ASN:HD22	1.65	0.59
4:C:700:P6G:O1	4:C:700:P6G:O16	2.23	0.56
2:A:600:D15:OAC	2:A:600:D15:CAP	2.56	0.53
1:D:380:PRO:HD2	1:D:385:LEU:HD11	1.91	0.53
1:D:240:MET:HE3	1:D:241:LEU:O	2.09	0.52
1:D:285:HIS:O	1:D:286:CYS:HB2	2.10	0.52
1:A:398:LEU:HD11	1:A:404:ASN:ND2	2.25	0.51
1:B:326:PHE:CD1	1:B:362:SER:HA	2.47	0.50
1:B:215:THR:O	1:B:218:LYS:HG2	2.12	0.49
1:B:188:LYS:NZ	1:B:203:GLU:OE2	2.49	0.46
1:B:250:ARG:HG2	1:B:254:PHE:CZ	2.51	0.46
2:B:600:D15:OAC	2:B:600:D15:CAP	2.49	0.45
1:C:292:ASN:OD1	2:C:600:D15:NAA	2.46	0.45
1:D:240:MET:HE2	4:D:700:P6G:H52	2.00	0.43
1:A:241:LEU:O	2:A:600:D15:HAK	2.19	0.42
1:C:204:VAL:O	1:C:205:ARG:C	2.61	0.42
1:D:165:ILE:HG21	1:D:175:LYS:HB2	2.01	0.42
1:C:334:LEU:HB3	1:C:388:ALA:HB1	2.01	0.41
1:D:259:LEU:HD12	1:D:259:LEU:HA	1.90	0.41
1:C:241:LEU:O	2:C:600:D15:HAK	2.21	0.41
1:B:446:VAL:HG23	6:B:2045:HOH:O	2.20	0.41
1:A:264:LYS:NZ	6:A:2030:HOH:O	2.39	0.41
1:D:165:ILE:HG21	1:D:165:ILE:HD13	1.84	0.41
1:D:192:ASN:HB2	1:D:233:HIS:CE1	2.56	0.41
1:C:275:PHE:O	1:C:278:THR:HG23	2.20	0.41
1:B:217:MET:C	1:B:219:TYR:N	2.80	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	A	346/382 (91%)	330 (95%)	16 (5%)	0	100	100
1	B	337/382 (88%)	318 (94%)	19 (6%)	0	100	100
1	C	330/382 (86%)	315 (96%)	14 (4%)	1 (0%)	36	50
1	D	340/382 (89%)	325 (96%)	15 (4%)	0	100	100
All	All	1353/1528 (88%)	1288 (95%)	64 (5%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	LYS

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	301/339 (89%)	293 (97%)	8 (3%)	39	62
1	B	292/339 (86%)	286 (98%)	6 (2%)	47	69
1	C	284/339 (84%)	281 (99%)	3 (1%)	65	82
1	D	289/339 (85%)	283 (98%)	6 (2%)	47	69
All	All	1166/1356 (86%)	1143 (98%)	23 (2%)	50	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	SER
1	A	212	LYS
1	A	226	ARG
1	A	236	LEU
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	255	ARG
1	A	320	GLN
1	A	465	LYS
1	B	218	LYS
1	B	226	ARG
1	B	232	ASN
1	B	300	ARG
1	B	310	SER
1	B	465	LYS
1	C	232	ASN
1	C	250	ARG
1	C	413	ARG
1	D	218	LYS
1	D	226[A]	ARG
1	D	226[B]	ARG
1	D	310	SER
1	D	431	THR
1	D	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	383	HIS
1	A	425	ASN
1	B	172	GLN
1	B	198	ASN
1	B	201	GLN
1	B	232	ASN
1	B	297	ASN
1	C	198	ASN
1	C	201	GLN
1	C	251	ASN
1	C	316	GLN
1	C	475	GLN
1	D	182	GLN
1	D	383	HIS
1	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](#)

4 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	PTR	B	321	1	15,16,17	1.93	1 (6%)	17,22,24	1.24	3 (17%)
1	PTR	D	321	1	15,16,17	2.01	2 (13%)	17,22,24	1.28	2 (11%)
1	PTR	C	321	1	15,16,17	1.97	1 (6%)	17,22,24	1.28	3 (17%)
1	PTR	A	321	1	15,16,17	2.05	1 (6%)	17,22,24	1.28	3 (17%)

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	PTR	B	321	1	-	0/10/11/13	0/1/1/1
1	PTR	D	321	1	-	0/10/11/13	0/1/1/1
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	PTR	OH-CZ	-7.36	1.24	1.40
1	C	321	PTR	OH-CZ	-7.05	1.24	1.40
1	B	321	PTR	OH-CZ	-6.81	1.25	1.40
1	D	321	PTR	OH-CZ	-6.53	1.26	1.40
1	D	321	PTR	P-OH	2.14	1.63	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	PTR	O3P-P-OH	3.85	116.70	105.32
1	A	321	PTR	P-OH-CZ	3.07	134.81	123.88
1	C	321	PTR	P-OH-CZ	2.96	134.43	123.88
1	B	321	PTR	O3P-P-O2P	2.78	118.22	107.80
1	B	321	PTR	O2P-P-OH	2.72	113.35	105.32
1	A	321	PTR	O3P-P-O2P	2.66	117.78	107.80
1	D	321	PTR	P-OH-CZ	2.64	133.29	123.88
1	C	321	PTR	O3P-P-OH	2.63	113.10	105.32
1	C	321	PTR	O3P-P-O2P	2.36	116.67	107.80
1	A	321	PTR	O3P-P-OH	2.27	112.03	105.32
1	B	321	PTR	P-OH-CZ	2.25	131.88	123.88

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	O-C-CA-CB
1	C	321	PTR	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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
5	SO4	B	1483	-	4,4,4	0.33	0	6,6,6	0.49	0
5	SO4	D	1482	-	4,4,4	0.26	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	1482	-	4,4,4	0.31	0	6,6,6	0.27	0
4	P6G	A	701	-	12,12,18	0.51	0	11,11,17	0.83	0
4	P6G	B	702	-	6,6,18	0.46	0	5,5,17	0.29	0
4	P6G	A	700	-	15,15,18	0.62	0	14,14,17	0.30	0
4	P6G	A	702	-	6,6,18	0.45	0	5,5,17	0.30	0
4	P6G	B	700	-	15,15,18	0.62	0	14,14,17	0.26	0
2	D15	A	600	-	35,35,35	1.68	9 (25%)	42,48,48	2.72	17 (40%)
4	P6G	D	700	-	15,15,18	0.53	0	14,14,17	0.37	0
2	D15	B	600	-	35,35,35	1.66	7 (20%)	42,48,48	2.72	13 (30%)
2	D15	D	600	-	35,35,35	1.69	6 (17%)	42,48,48	2.31	13 (30%)
4	P6G	C	700	-	15,15,18	0.69	0	14,14,17	0.61	0
5	SO4	B	1482	-	4,4,4	0.48	0	6,6,6	0.26	0
5	SO4	B	1484	-	4,4,4	0.28	0	6,6,6	0.68	0
5	SO4	C	1483	-	4,4,4	0.24	0	6,6,6	0.27	0
5	SO4	A	1483	-	4,4,4	0.32	0	6,6,6	0.57	0
4	P6G	B	701	-	12,12,18	0.53	0	11,11,17	0.41	0
5	SO4	C	1484	-	4,4,4	0.31	0	6,6,6	0.44	0
2	D15	C	600	-	35,35,35	1.61	4 (11%)	42,48,48	2.18	11 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P6G	A	700	-	-	5/13/13/16	-
4	P6G	A	702	-	-	1/4/4/16	-
2	D15	A	600	-	-	4/23/23/23	0/4/4/4
4	P6G	D	700	-	-	3/13/13/16	-
2	D15	B	600	-	-	4/23/23/23	0/4/4/4
4	P6G	A	701	-	-	3/10/10/16	-
4	P6G	B	702	-	-	2/4/4/16	-
4	P6G	B	701	-	-	1/10/10/16	-
2	D15	D	600	-	-	5/23/23/23	0/4/4/4
4	P6G	B	700	-	-	3/13/13/16	-
4	P6G	C	700	-	-	8/13/13/16	-
2	D15	C	600	-	-	5/23/23/23	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	D15	NAV-NAS	-5.58	1.23	1.36
2	C	600	D15	NAV-NAS	-5.44	1.23	1.36
2	A	600	D15	NAV-NAS	-5.02	1.24	1.36
2	B	600	D15	NAV-NAS	-4.72	1.25	1.36
2	C	600	D15	CBE-CBC	-3.96	1.41	1.47
2	B	600	D15	CBE-CBC	-3.94	1.41	1.47
2	D	600	D15	CBF-CAX	3.80	1.57	1.53
2	D	600	D15	CBE-CBC	-3.64	1.42	1.47
2	A	600	D15	CBE-CBC	-3.39	1.42	1.47
2	A	600	D15	CAP-CAZ	3.31	1.44	1.39
2	B	600	D15	CAW-NAU	-2.99	1.32	1.37
2	C	600	D15	CBA-CAW	2.96	1.56	1.50
2	B	600	D15	CAR-CBF	-2.92	1.49	1.54
2	A	600	D15	CBA-CAW	2.73	1.56	1.50
2	B	600	D15	CAO-CAY	2.72	1.42	1.38
2	C	600	D15	CAZ-NAT	-2.70	1.36	1.41
2	B	600	D15	CBC-NAU	-2.60	1.32	1.39
2	D	600	D15	CAP-CAZ	2.50	1.43	1.39
2	A	600	D15	CAW-NAU	-2.50	1.33	1.37
2	D	600	D15	CAW-NAU	-2.47	1.33	1.37
2	A	600	D15	CAZ-NAT	-2.34	1.36	1.41
2	A	600	D15	CBC-NAU	-2.20	1.33	1.39
2	A	600	D15	CAR-CBF	-2.20	1.51	1.54
2	B	600	D15	CAP-CAZ	2.18	1.43	1.39
2	A	600	D15	CAP-CBE	2.15	1.43	1.39
2	D	600	D15	CAR-CBF	-2.04	1.51	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	D15	CAP-CBE-CBC	9.39	141.38	130.55
2	D	600	D15	CAP-CBE-CBC	8.17	139.97	130.55
2	B	600	D15	CAP-CBE-CBC	8.05	139.83	130.55
2	B	600	D15	OAC-CAX-CBF	-7.20	115.73	122.31
2	A	600	D15	OAC-CAX-CBF	-6.50	116.37	122.31
2	C	600	D15	CAP-CBE-CBC	6.20	137.70	130.55
2	B	600	D15	CAI-CAY-CL1	-5.94	110.59	119.36
2	B	600	D15	CAO-CAY-CL1	5.86	126.52	119.17
2	D	600	D15	OAC-CAX-CBF	-5.72	117.08	122.31
2	C	600	D15	OAC-CAX-CBF	-5.53	117.26	122.31
2	C	600	D15	CAO-CAY-CL1	4.81	125.20	119.17
2	B	600	D15	CAL-CBB-CBF	-4.78	112.20	120.90
2	C	600	D15	CAL-CBB-CBF	-4.70	112.33	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	D15	CAI-CAY-CL1	-4.30	113.01	119.36
2	A	600	D15	CAL-CBB-CBF	-4.28	113.11	120.90
2	A	600	D15	CAI-CAY-CL1	-4.23	113.11	119.36
2	A	600	D15	CAZ-NAT-CAX	-4.05	118.12	127.37
2	B	600	D15	CAZ-NAT-CAX	-4.03	118.16	127.37
2	A	600	D15	CAO-CAY-CL1	4.02	124.21	119.17
2	B	600	D15	CAO-CBB-CBF	3.95	127.38	120.44
2	D	600	D15	CAL-CBB-CAO	3.83	123.17	118.74
2	C	600	D15	CAO-CBB-CBF	3.75	127.01	120.44
2	A	600	D15	CBE-CBD-NAV	3.62	109.19	106.59
2	D	600	D15	CAL-CBB-CBF	-3.61	114.33	120.90
2	A	600	D15	CAY-CAO-CBB	-3.41	115.36	119.43
2	C	600	D15	CAZ-NAT-CAX	-3.28	119.89	127.37
2	B	600	D15	CAY-CAO-CBB	-3.19	115.62	119.43
2	B	600	D15	CBE-CBD-NAV	3.10	108.82	106.59
2	A	600	D15	CAN-CBD-CBE	-3.00	119.29	122.19
2	A	600	D15	CBD-NAV-NAS	-2.98	109.69	111.90
2	D	600	D15	CAZ-NAT-CAX	-2.96	120.62	127.37
2	D	600	D15	CAM-CAZ-CAP	-2.93	116.12	119.66
2	C	600	D15	CBB-CBF-CAX	2.90	116.25	109.50
2	A	600	D15	CAO-CBB-CBF	2.89	125.51	120.44
2	D	600	D15	CAO-CAY-CL1	2.87	122.77	119.17
2	B	600	D15	CAN-CBD-CBE	-2.82	119.46	122.19
2	D	600	D15	CAY-CAO-CBB	-2.67	116.24	119.43
2	D	600	D15	CBE-CBC-NAU	2.64	134.58	123.07
2	D	600	D15	CAR-CBF-CBB	-2.55	108.80	113.10
2	B	600	D15	CBD-NAV-NAS	-2.45	110.08	111.90
2	D	600	D15	CBE-CBD-NAV	2.32	108.25	106.59
2	A	600	D15	CAP-CBE-CBD	-2.30	117.15	119.39
2	D	600	D15	CBD-NAV-NAS	-2.29	110.20	111.90
2	A	600	D15	CAG-CAE-CAF	-2.28	116.74	119.87
2	A	600	D15	CAL-CBB-CAO	2.28	121.38	118.74
2	A	600	D15	CAM-CAN-CBD	2.26	123.94	119.57
2	A	600	D15	CAL-CAH-CAI	-2.21	117.40	120.24
2	B	600	D15	CAM-CAZ-CAP	-2.14	117.06	119.66
2	C	600	D15	CBD-NAV-NAS	-2.11	110.33	111.90
2	A	600	D15	CBE-CBC-NAU	2.11	132.24	123.07
2	B	600	D15	CBE-CBC-NAU	2.08	132.12	123.07
2	C	600	D15	CAG-CAK-CBA	2.07	122.40	120.36
2	C	600	D15	CBE-CBC-NAU	2.05	131.99	123.07
2	D	600	D15	CAI-CAY-CL1	-2.00	116.40	119.36

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	D15	CAQ-CAR-CBF-CAX
2	C	600	D15	OAC-CAX-CBF-CBB
4	B	701	P6G	O1-C2-C3-O4
4	A	700	P6G	O10-C11-C12-O13
4	C	700	P6G	O10-C11-C12-O13
4	B	700	P6G	O1-C2-C3-O4
4	B	702	P6G	O1-C2-C3-O4
4	A	700	P6G	O1-C2-C3-O4
4	A	701	P6G	O4-C5-C6-O7
4	C	700	P6G	O13-C14-C15-O16
4	A	700	P6G	O7-C8-C9-O10
4	C	700	P6G	O4-C5-C6-O7
4	A	701	P6G	O10-C11-C12-O13
4	C	700	P6G	O7-C8-C9-O10
2	A	600	D15	CAQ-CAR-CBF-CAX
2	C	600	D15	NAT-CAX-CBF-CBB
4	A	702	P6G	C6-C5-O4-C3
4	C	700	P6G	C11-C12-O13-C14
4	D	700	P6G	C2-C3-O4-C5
2	A	600	D15	NAS-CBC-NAU-CAW
2	C	600	D15	NAS-CBC-NAU-CAW
2	D	600	D15	NAS-CBC-NAU-CAW
4	A	700	P6G	C15-C14-O13-C12
4	A	701	P6G	O1-C2-C3-O4
4	C	700	P6G	C15-C14-O13-C12
2	A	600	D15	OAC-CAX-CBF-CAR
2	B	600	D15	OAC-CAX-CBF-CAR
2	C	600	D15	OAC-CAX-CBF-CAR
2	D	600	D15	OAC-CAX-CBF-CAR
2	A	600	D15	NAT-CAX-CBF-CAR
2	B	600	D15	NAT-CAX-CBF-CAR
2	C	600	D15	NAT-CAX-CBF-CAR
2	D	600	D15	NAT-CAX-CBF-CAR
2	D	600	D15	NAT-CAX-CBF-CBB
2	B	600	D15	CAQ-CAR-CBF-CBB
4	D	700	P6G	O4-C5-C6-O7
4	D	700	P6G	O13-C14-C15-O16
4	B	700	P6G	C2-C3-O4-C5
4	A	700	P6G	C2-C3-O4-C5
2	D	600	D15	NAA-CAQ-CAR-CBF
4	C	700	P6G	C2-C3-O4-C5
4	B	702	P6G	O4-C5-C6-O7

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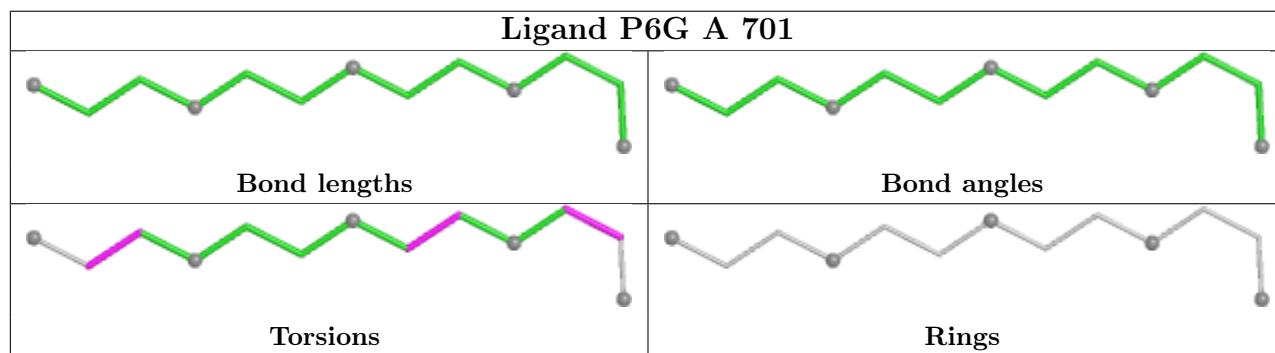
Mol	Chain	Res	Type	Atoms
4	C	700	P6G	C12-C11-O10-C9
4	B	700	P6G	O10-C11-C12-O13

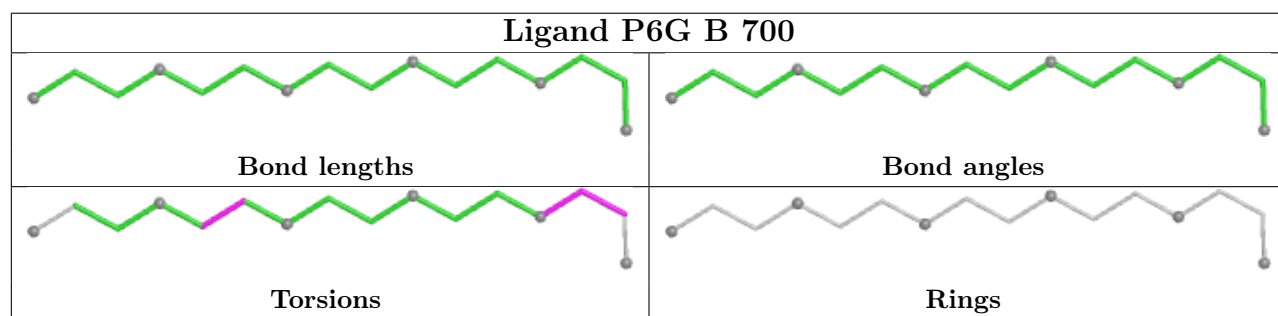
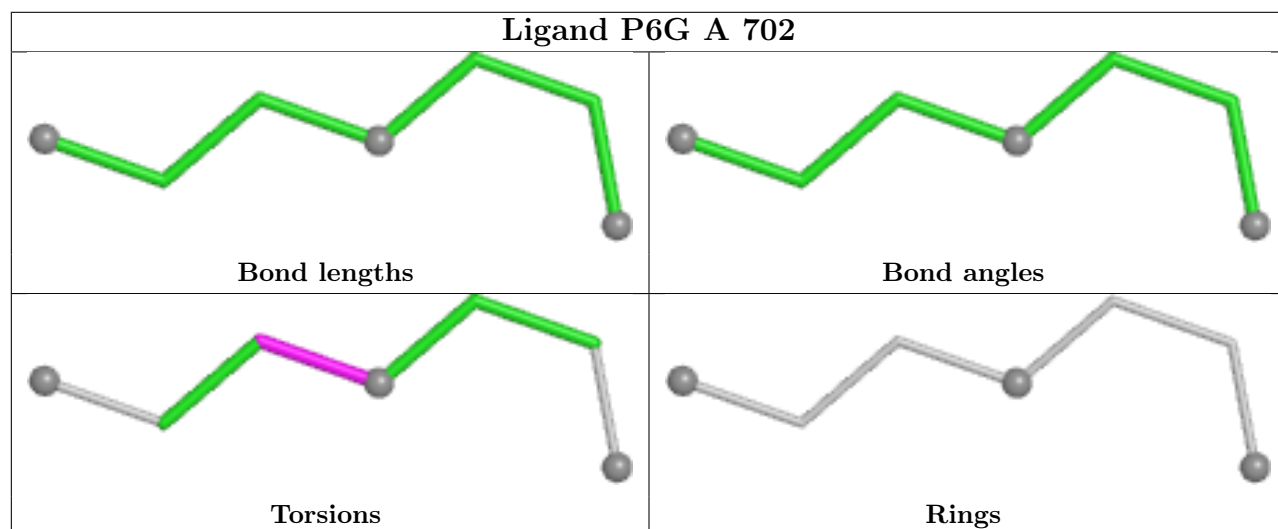
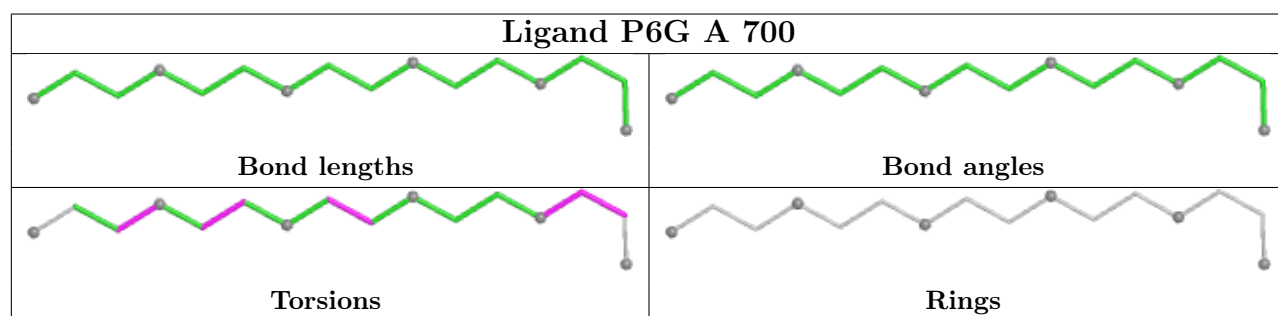
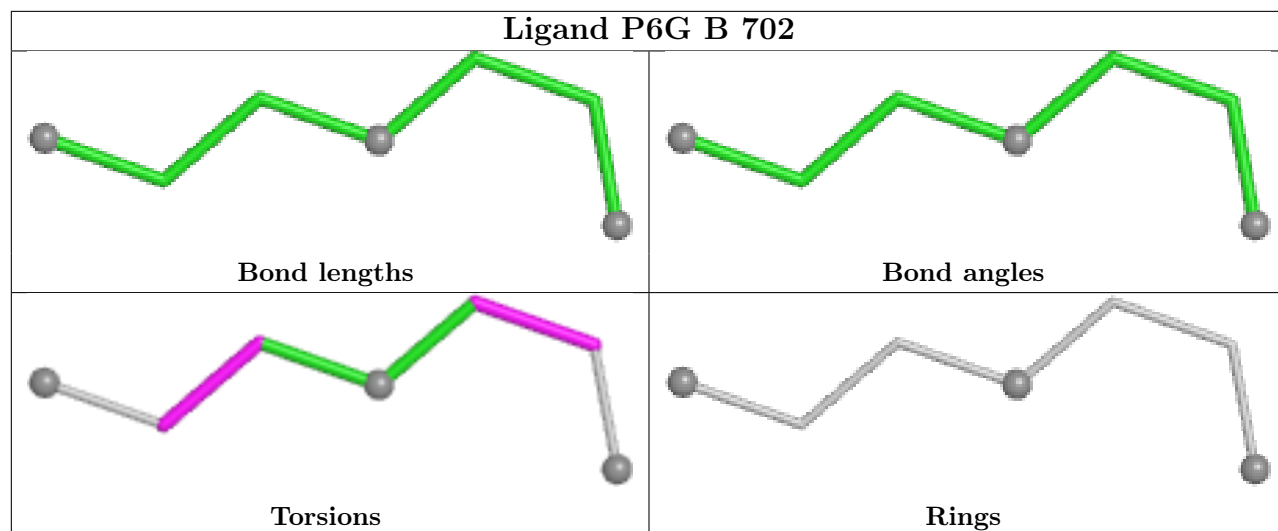
There are no ring outliers.

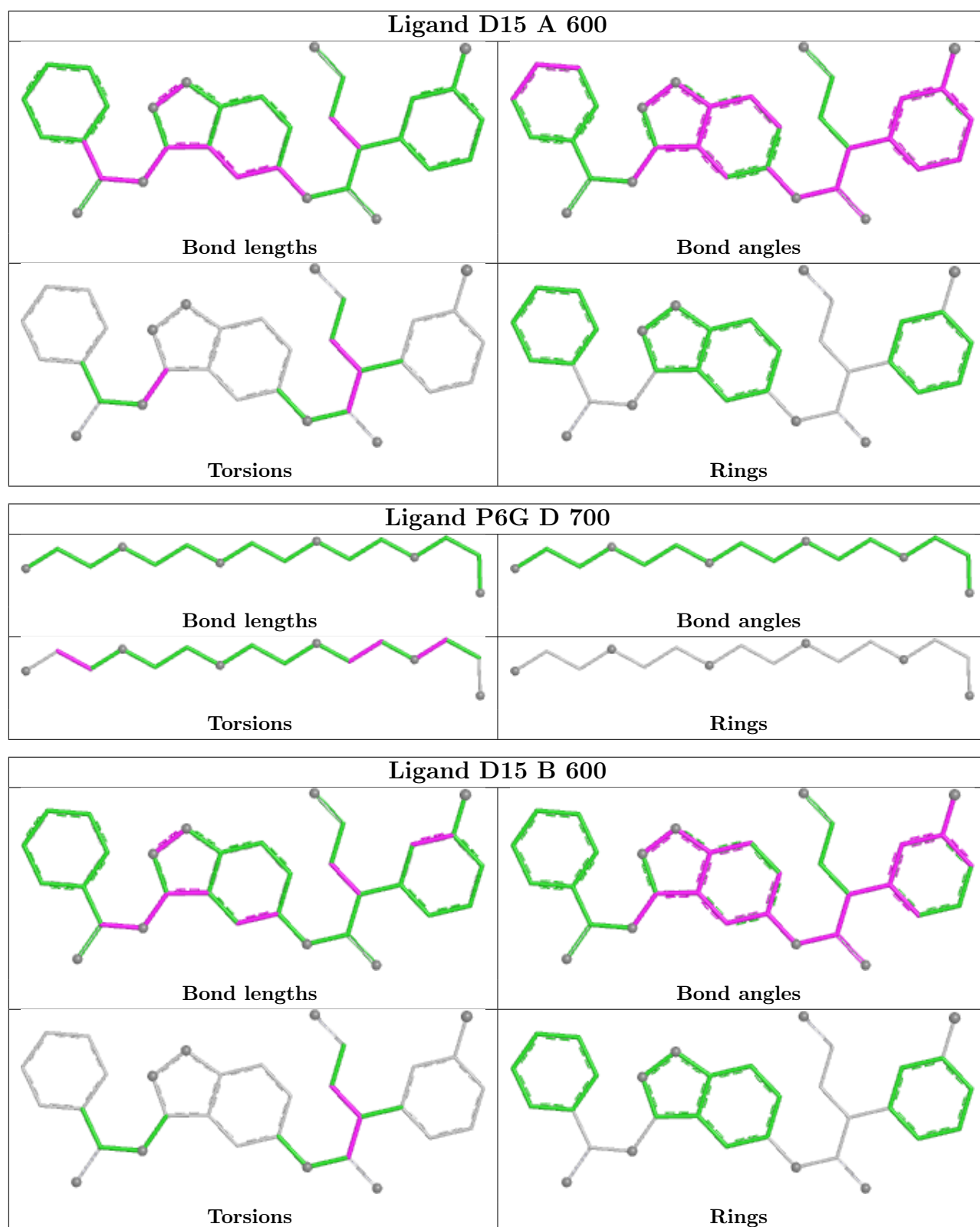
5 monomers are involved in 9 short contacts:

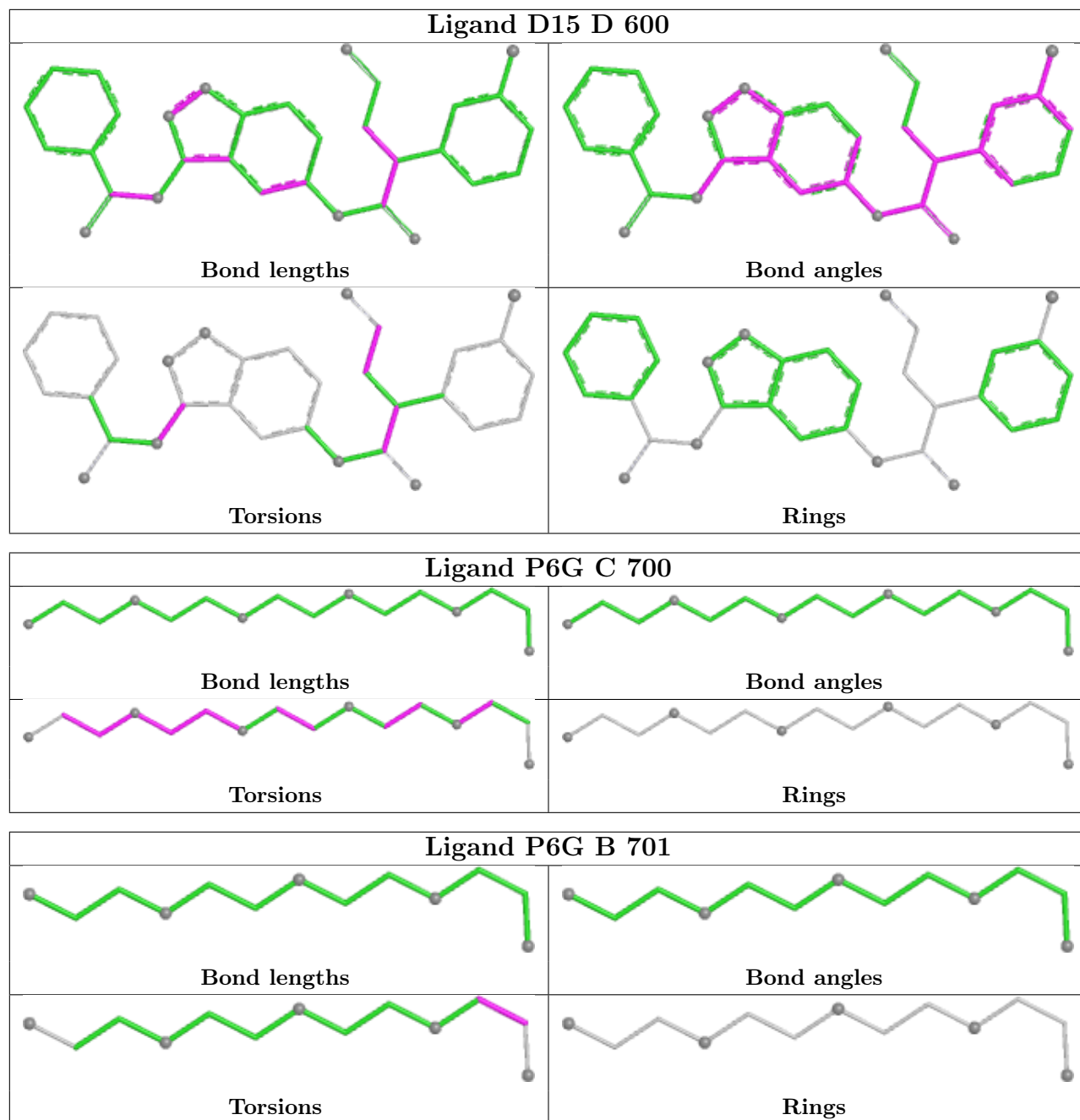
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	D15	3	0
4	D	700	P6G	1	0
2	B	600	D15	2	0
4	C	700	P6G	1	0
2	C	600	D15	2	0

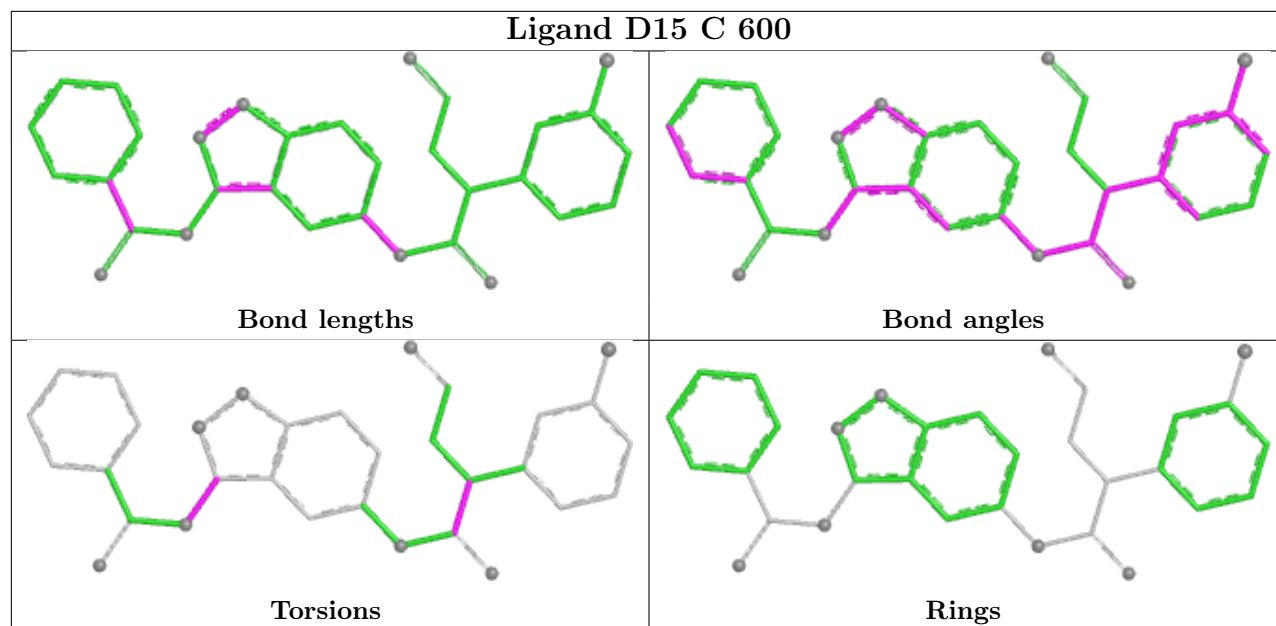
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/382 (90%)	-0.60	3 (0%) 81 78	19, 29, 43, 59	2 (0%)
1	B	340/382 (89%)	-0.46	4 (1%) 76 73	17, 30, 43, 62	1 (0%)
1	C	338/382 (88%)	-0.24	3 (0%) 81 78	21, 30, 43, 54	0
1	D	342/382 (89%)	-0.40	2 (0%) 85 83	16, 30, 42, 86	2 (0%)
All	All	1366/1528 (89%)	-0.43	12 (0%) 81 78	16, 30, 43, 86	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	ASP	4.4
1	B	216	GLU	4.0
1	D	408	THR	3.9
1	A	215	THR	3.4
1	B	214	ASP	2.9
1	B	215	THR	2.8
1	C	217	MET	2.5
1	C	442	SER	2.5
1	A	213	HIS	2.4
1	C	219	TYR	2.4
1	B	253	ASN	2.3
1	A	409	LYS	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PTR	B	321	16/17	0.90	0.12	37,47,60,62	0
1	PTR	D	321	16/17	0.91	0.11	37,47,60,61	0
1	PTR	C	321	16/17	0.92	0.09	34,45,59,60	0
1	PTR	A	321	16/17	0.95	0.09	34,44,57,58	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.

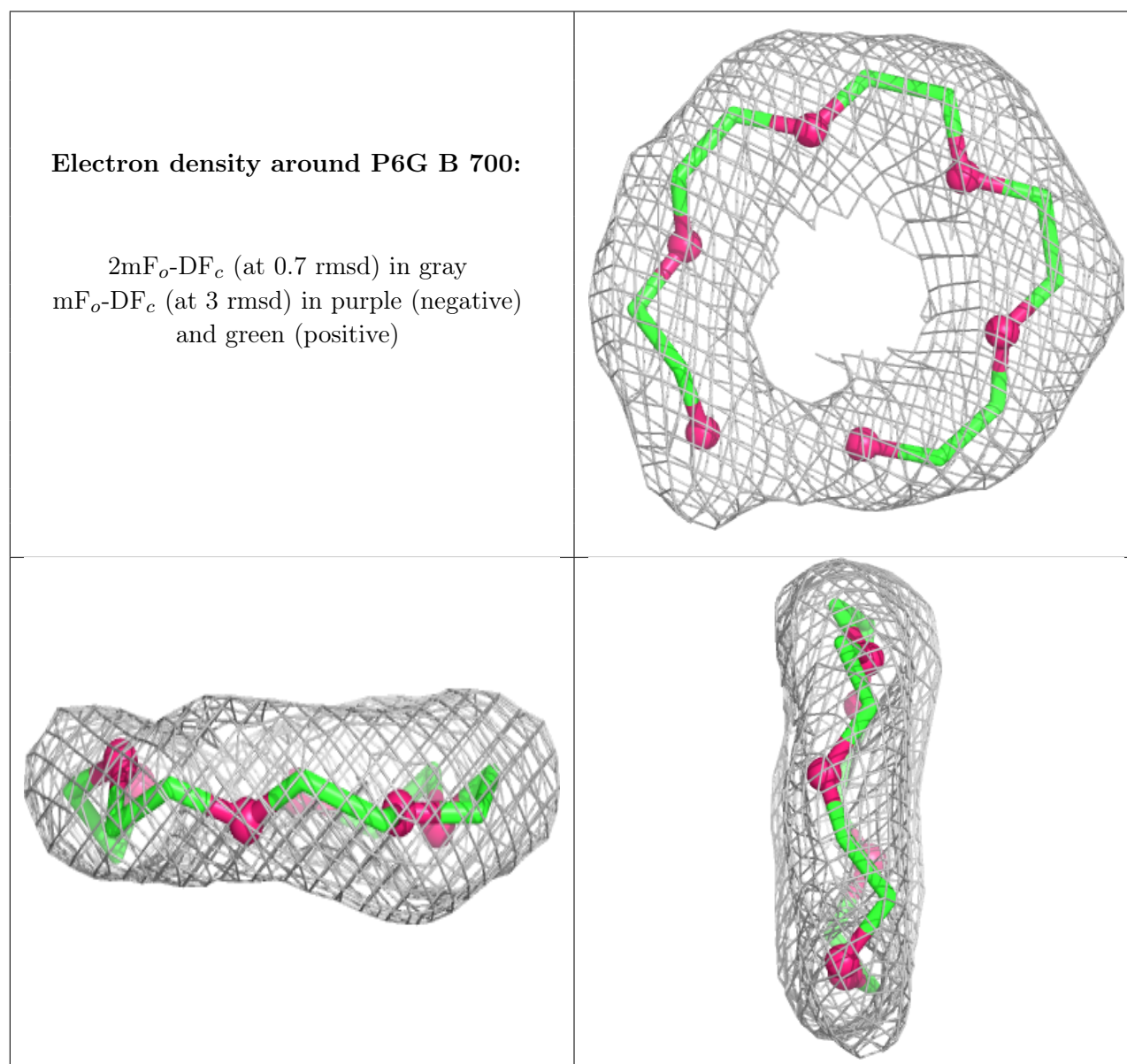
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	1483	5/5	0.75	0.10	99,106,109,112	0
3	CL	D	1484	1/1	0.82	0.13	85,85,85,85	0
5	SO4	C	1484	5/5	0.83	0.13	83,87,96,104	0
5	SO4	B	1483	5/5	0.85	0.13	72,76,98,100	0
4	P6G	B	700	16/19	0.89	0.13	64,75,77,79	0
4	P6G	B	702	7/19	0.89	0.13	67,80,83,85	0
5	SO4	B	1482	5/5	0.89	0.21	65,66,88,91	0
4	P6G	C	700	16/19	0.90	0.10	47,66,83,85	0
2	D15	C	600	32/32	0.92	0.10	40,55,67,73	0
5	SO4	C	1482	5/5	0.92	0.15	75,86,88,92	0
4	P6G	A	702	7/19	0.92	0.10	55,55,64,70	0
3	CL	D	1483	1/1	0.92	0.15	75,75,75,75	0
4	P6G	B	701	13/19	0.93	0.08	33,44,50,52	0
4	P6G	A	700	16/19	0.93	0.11	62,72,76,78	0
5	SO4	B	1484	5/5	0.94	0.11	65,66,72,81	0
2	D15	A	600	32/32	0.94	0.08	29,36,50,64	0
4	P6G	A	701	13/19	0.94	0.09	32,46,55,65	0
2	D15	D	600	32/32	0.94	0.08	31,50,61,65	0
5	SO4	D	1482	5/5	0.94	0.15	55,69,82,90	0
5	SO4	A	1483	5/5	0.95	0.12	54,57,60,61	0
2	D15	B	600	32/32	0.96	0.07	25,40,55,55	0
4	P6G	D	700	16/19	0.96	0.07	37,46,64,64	0
3	CL	B	620	1/1	0.96	0.13	47,47,47,47	0
3	CL	C	620	1/1	0.96	0.14	61,61,61,61	0
3	CL	C	1485	1/1	0.96	0.12	75,75,75,75	0

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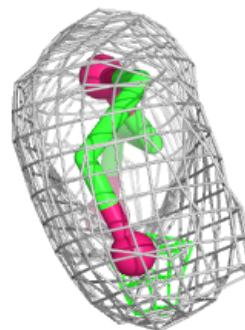
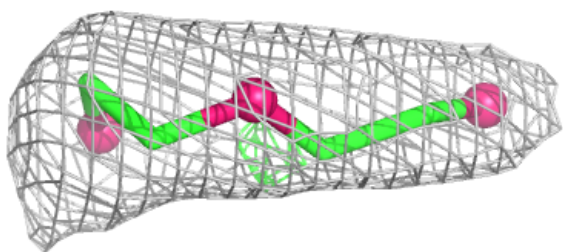
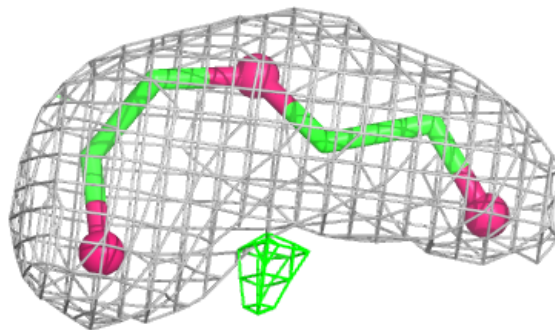
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	620	1/1	0.97	0.12	45,45,45,45	0
3	CL	B	1485	1/1	0.97	0.08	59,59,59,59	0
3	CL	D	620	1/1	0.97	0.17	56,56,56,56	0

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.



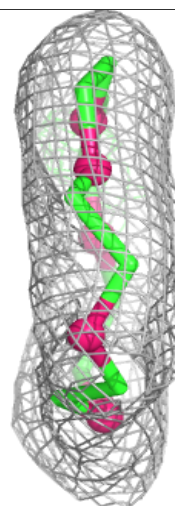
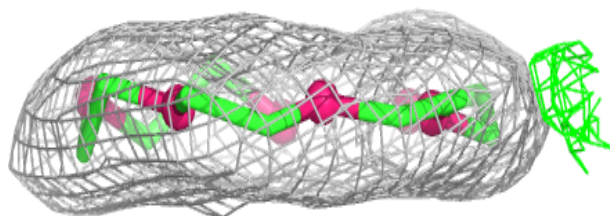
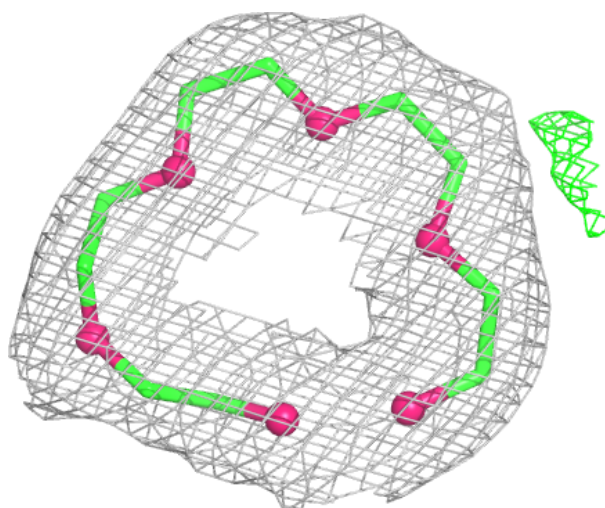
Electron density around P6G B 702:

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



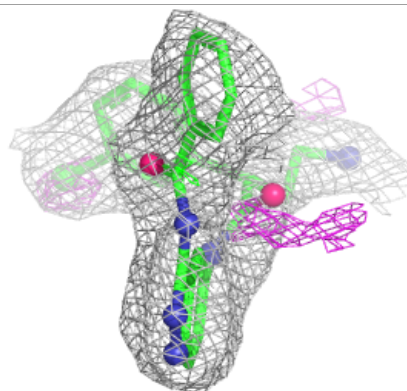
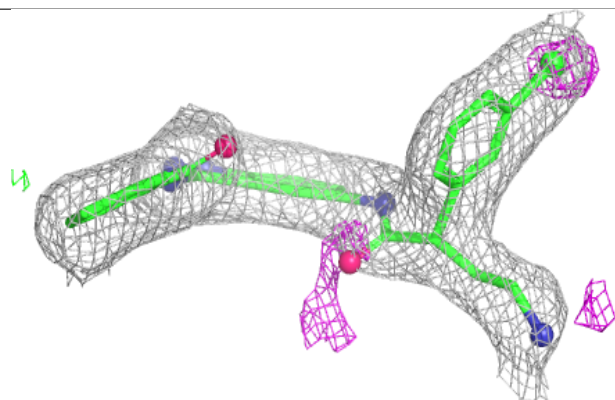
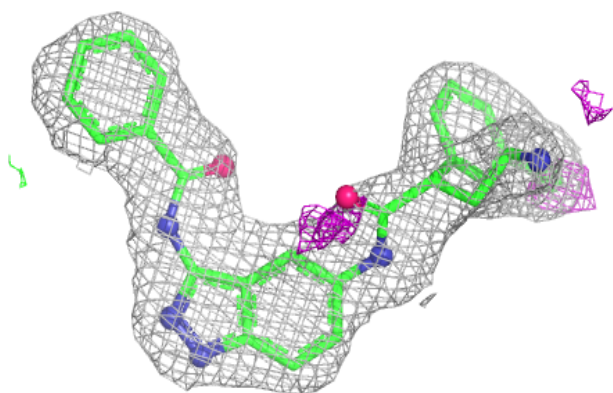
Electron density around P6G C 700:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

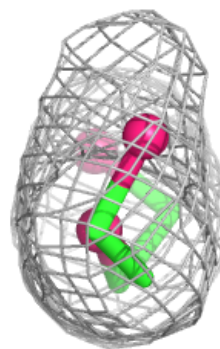
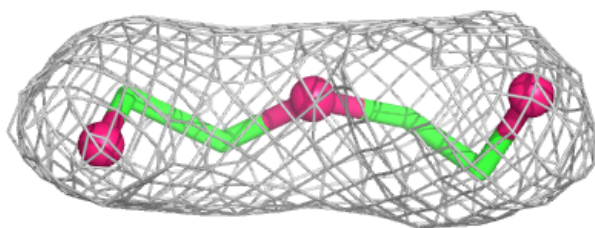
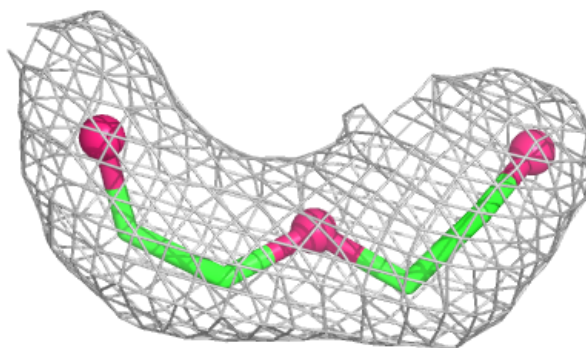


Electron density around D15 C 600:

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and green (positive)

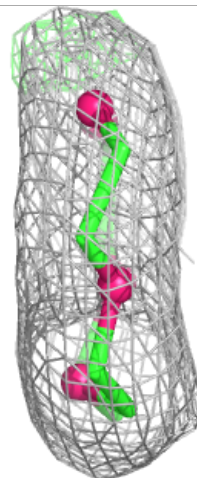
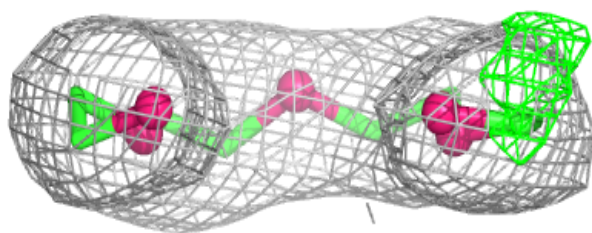
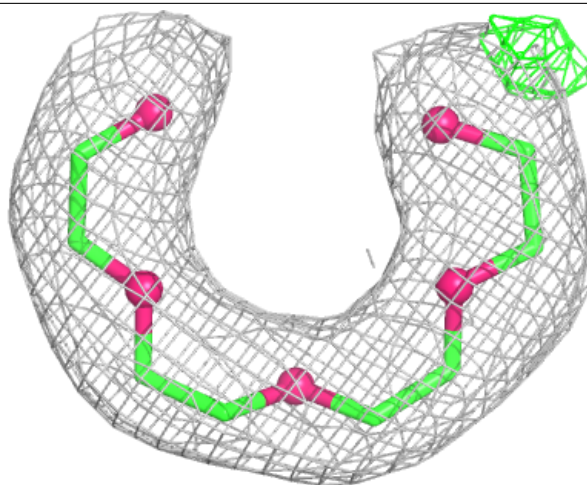
**Electron density around P6G A 702:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



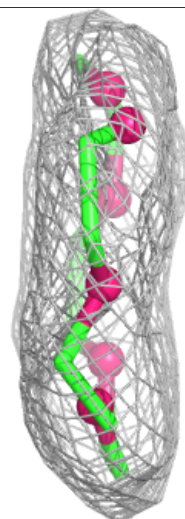
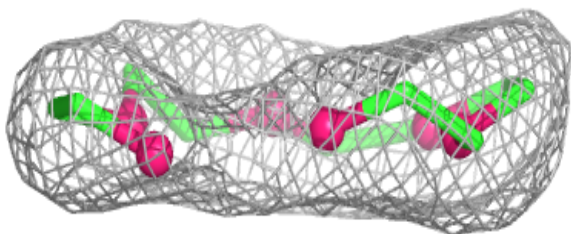
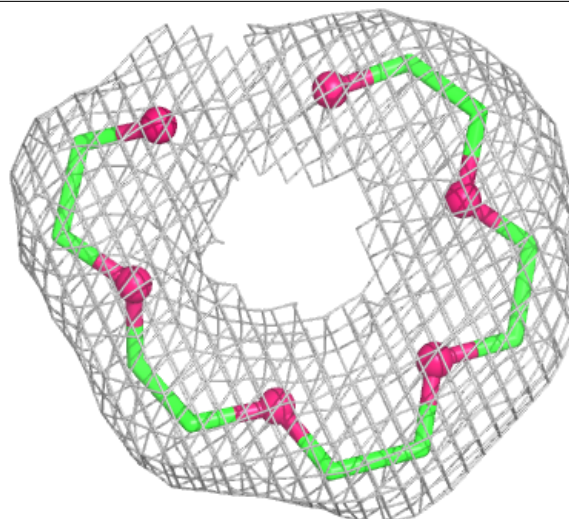
Electron density around P6G B 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



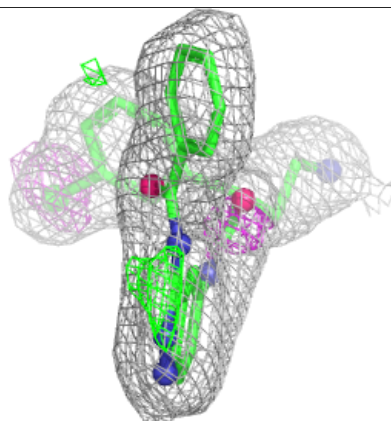
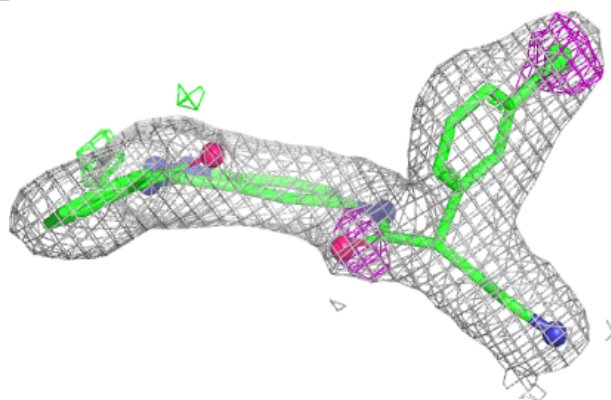
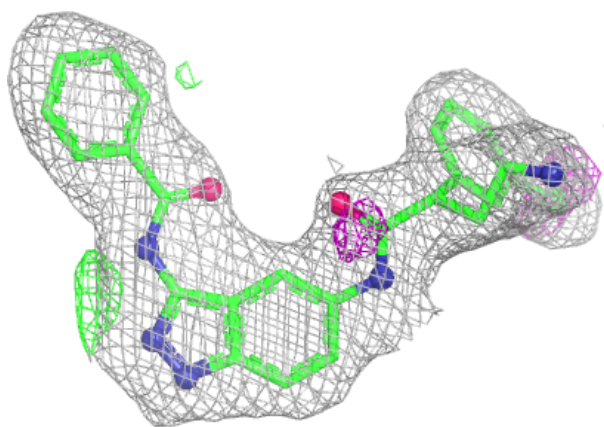
Electron density around P6G A 700:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



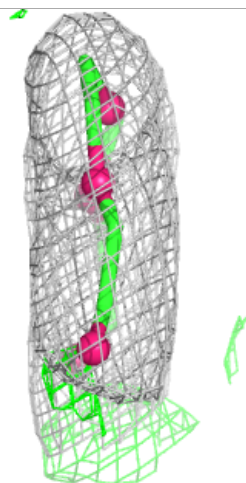
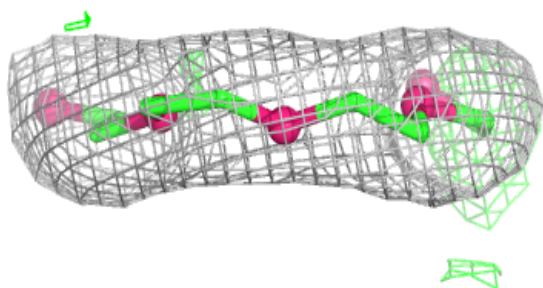
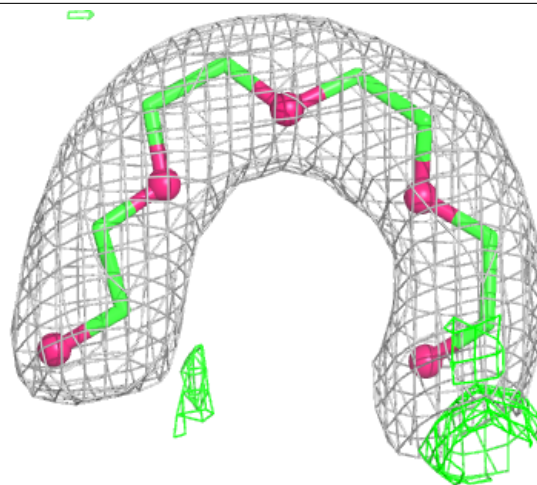
Electron density around D15 A 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



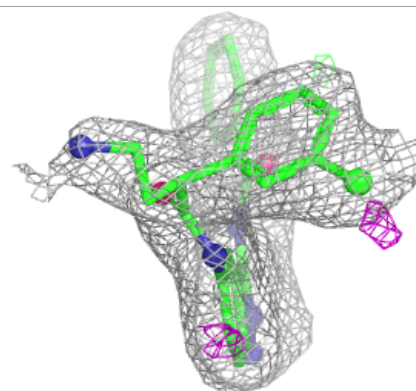
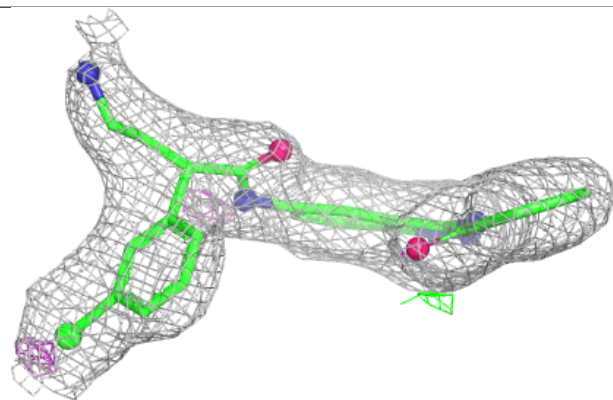
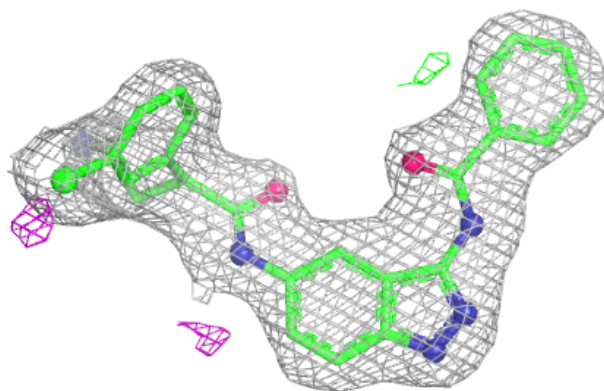
Electron density around P6G A 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

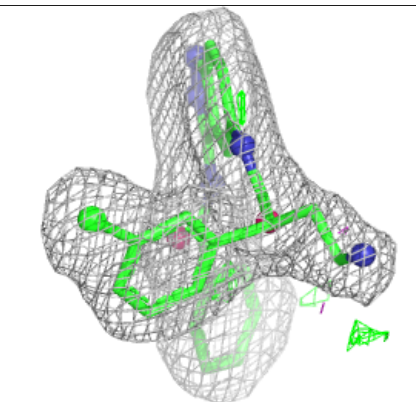
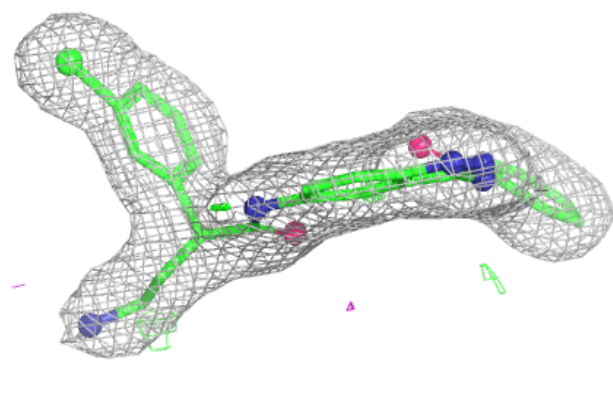
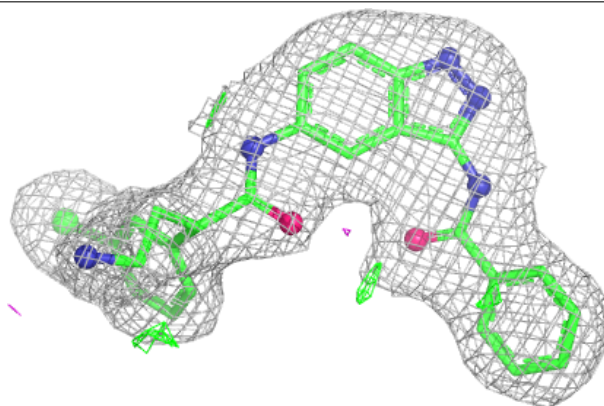


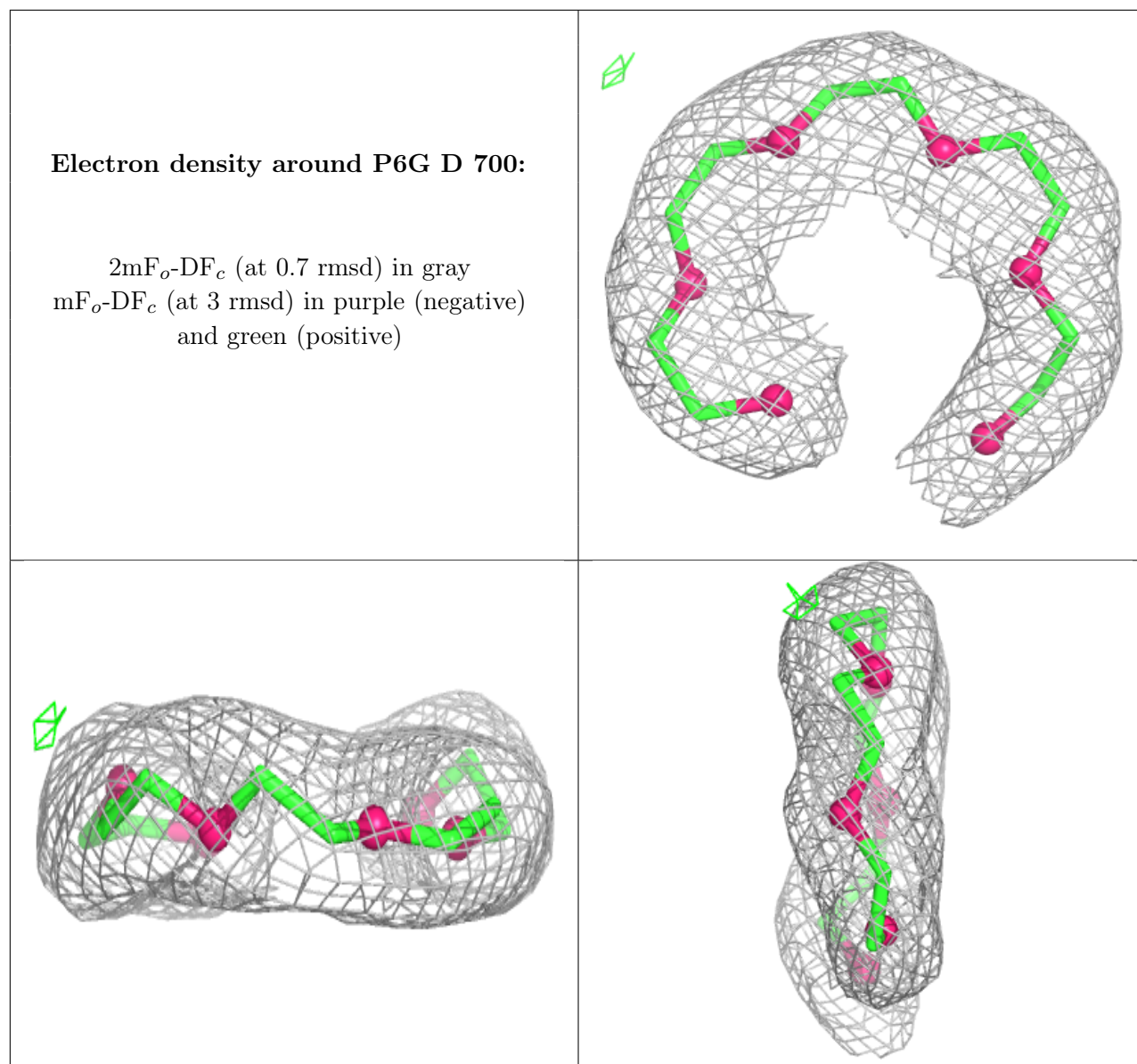
Electron density around D15 D 600:

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

**Electron density around D15 B 600:**

$2mF_o-DF_c$ (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.