



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:14 am BST

PDB ID : 2VX3  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



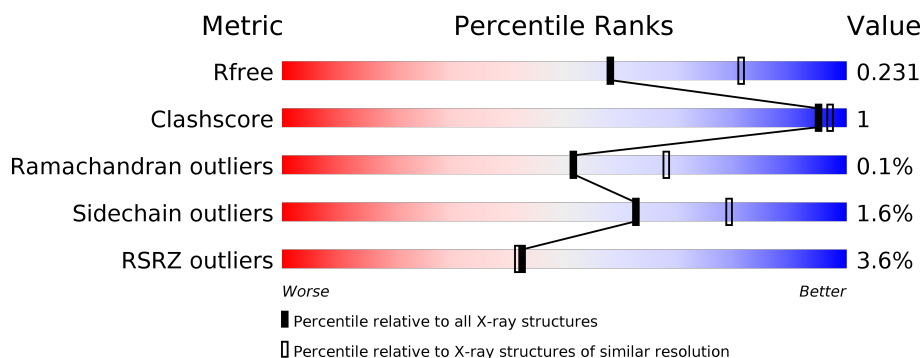
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 88%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">88%</span> </div> <div style="width: 9%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">9%</span> </div> </div>
1	B	382	<div> <div style="width: 2%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">2%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">85%</span> </div> <div style="width: 11%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">11%</span> </div> </div>
1	C	382	<div> <div style="width: 4%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">4%</span> </div> <div style="width: 86%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">86%</span> </div> <div style="width: 11%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">11%</span> </div> </div>
1	D	382	<div> <div style="width: 5%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">5%</span> </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">85%</span> </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">10%</span> </div> </div>



## 2 Entry composition

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

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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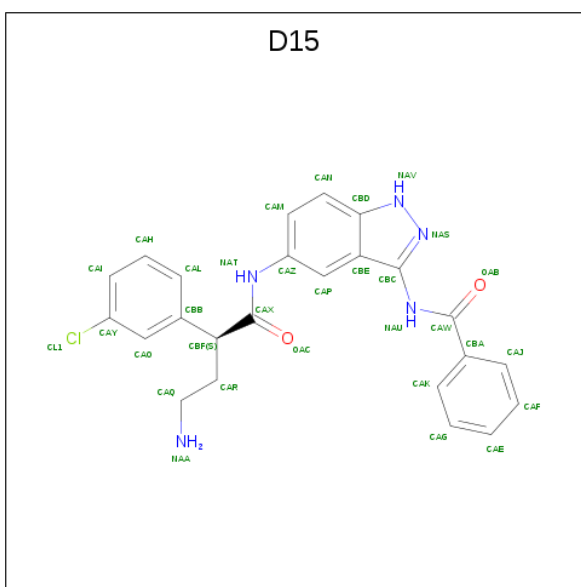


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Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASN	-	expression tag	UNP Q13627
C	121	LEU	-	expression tag	UNP Q13627
C	122	TYR	-	expression tag	UNP Q13627
C	123	PHE	-	expression tag	UNP Q13627
C	124	GLN	-	expression tag	UNP Q13627
C	125	SER	-	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 (three-letter code: D15) (formula: C<sub>24</sub>H<sub>22</sub>ClN<sub>5</sub>O<sub>2</sub>).





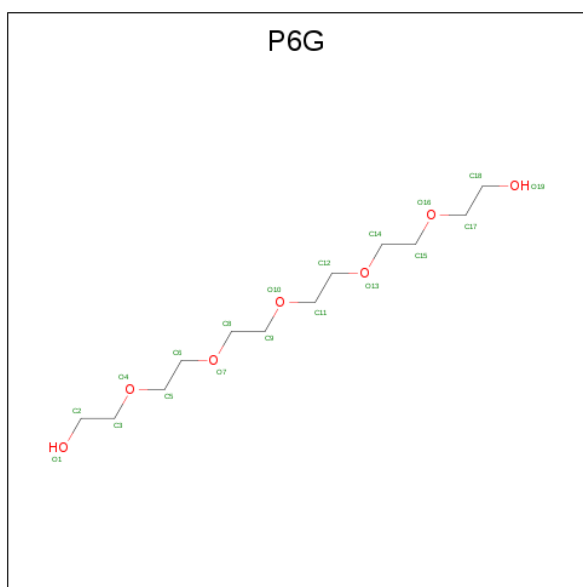
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 32	C 24	Cl 1	N 5	O 2	0	0
2	B	1	Total 32	C 24	Cl 1	N 5	O 2	0	0
2	C	1	Total 32	C 24	Cl 1	N 5	O 2	0	0
2	D	1	Total 32	C 24	Cl 1	N 5	O 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $\text{C}_{12}\text{H}_{26}\text{O}_7$ ).

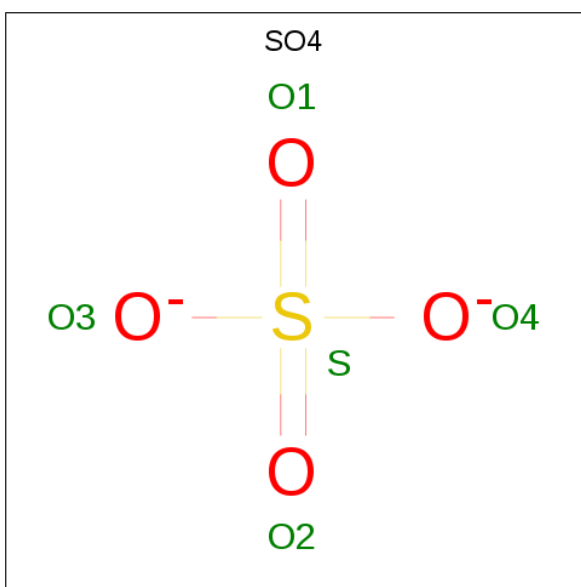




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 16	C 10	O 6	0	0
4	A	1	Total 13	C 8	O 5	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	B	1	Total 16	C 10	O 6	0	0
4	B	1	Total 13	C 8	O 5	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	C	1	Total 16	C 10	O 6	0	0
4	D	1	Total 16	C 10	O 6	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).





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.

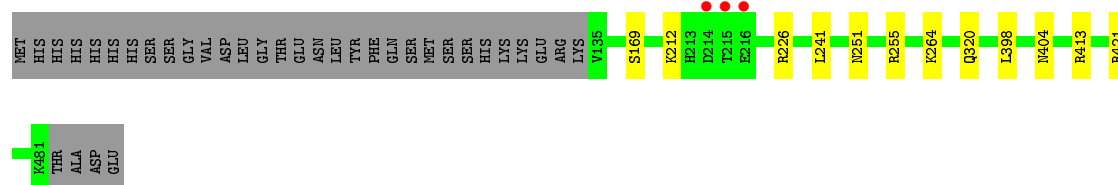
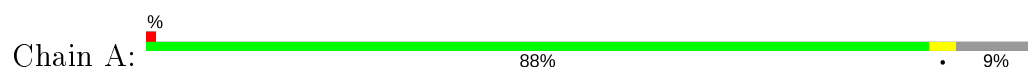
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	105	Total	O	0	0
			105	105		
6	B	52	Total	O	0	0
			52	52		
6	C	26	Total	O	0	0
			26	26		
6	D	22	Total	O	0	0
			22	22		



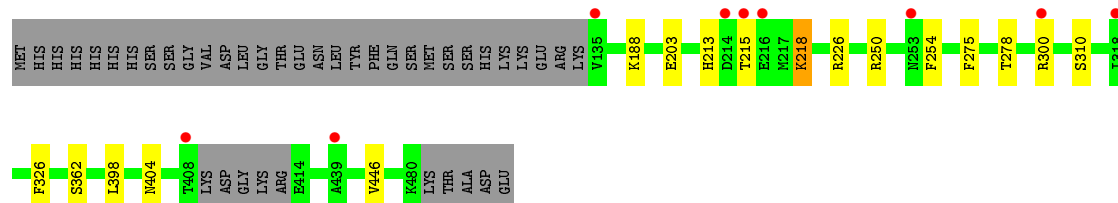
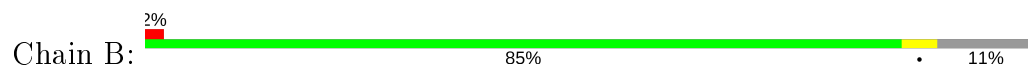
### 3 Residue-property plots [i](#)

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

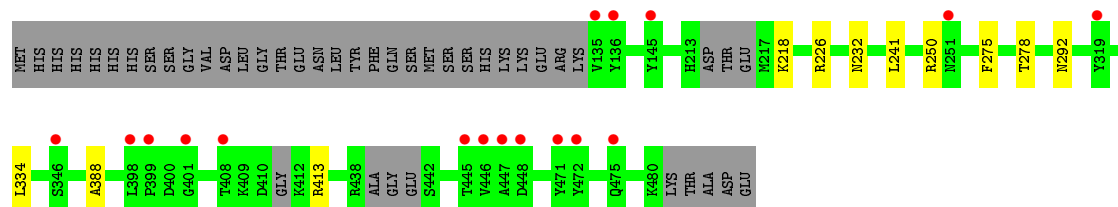
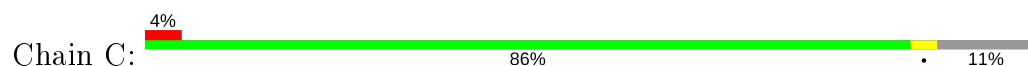
- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION- REGULATED KINASE 1A



- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION- REGULATED KINASE 1A

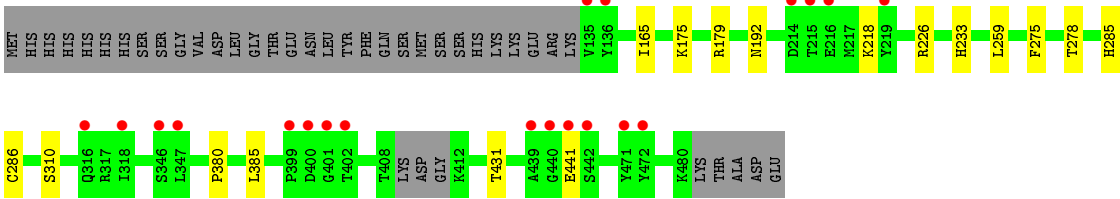
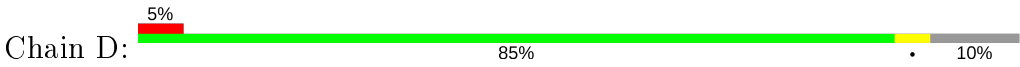


- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION- REGULATED KINASE 1A



- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION- REGULATED KINASE 1A







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.20Å 65.11Å 140.28Å 90.00° 115.44° 90.00°	Depositor
Resolution (Å)	26.00 – 2.40 25.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.00-2.40) 99.9 (25.96-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.39Å)	Xtriage
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 <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.74	0/2887	0.75	2/3895 (0.1%)
1	B	0.67	0/2811	0.71	0/3797
1	C	0.66	0/2772	0.71	1/3745 (0.0%)
1	D	0.65	0/2826	0.72	1/3816 (0.0%)
All	All	0.68	0/11296	0.72	4/15253 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	421	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	413	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	226	ARG	NE-CZ-NH1	-5.07	117.77	120.30

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 ⓘ

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	8	0
1	C	2726	0	2662	4	0
1	D	2772	0	2731	7	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	0	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	27	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 (27) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:D15:HAP	2:B:600:D15:OAC	1.85	0.73
2:A:600:D15:OAC	2:A:600:D15:HAP	1.99	0.60
1:B:398:LEU:HD11	1:B:404:ASN:HD22	1.65	0.59
4:C:700:P6G:O16	4:C:700:P6G:O1	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: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:CAP	2:B:600:D15:OAC	2.49	0.45
1:C:292:ASN:OD1	2:C:600:D15:NAA	2.46	0.45
1:A:241:LEU:O	2:A:600:D15:HAK	2.19	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:HD13	1:D:165:ILE:HG21	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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	346/382 (91%)	330 (95%)	16 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	337/382 (88%)	318 (94%)	19 (6%)	0	100	100
1	C	330/382 (86%)	315 (96%)	14 (4%)	1 (0%)	41	55
1	D	340/382 (89%)	325 (96%)	15 (4%)	0	100	100
All	All	1353/1528 (88%)	1288 (95%)	64 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/339 (89%)	295 (98%)	6 (2%)	55	74
1	B	292/339 (86%)	288 (99%)	4 (1%)	67	82
1	C	284/339 (84%)	281 (99%)	3 (1%)	73	87
1	D	289/339 (85%)	283 (98%)	6 (2%)	53	72
All	All	1166/1356 (86%)	1147 (98%)	19 (2%)	62	79

All (19) 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	251	ASN
1	A	255	ARG
1	A	320	GLN
1	B	218	LYS
1	B	226	ARG
1	B	300	ARG
1	B	310	SER

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	ASN
1	B	251	ASN
1	B	404	ASN
1	C	198	ASN
1	D	425	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.95	2 (13%)	19,22,24	1.24	3 (15%)
1	PTR	A	321	1	15,16,17	2.04	1 (6%)	19,22,24	1.43	4 (21%)
1	PTR	D	321	1	15,16,17	2.04	2 (13%)	19,22,24	1.30	3 (15%)
1	PTR	C	321	1	15,16,17	1.95	1 (6%)	19,22,24	1.32	3 (15%)



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	A	321	1	-	1/10/11/13	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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	PTR	OH-CZ	-7.29	1.24	1.40
1	C	321	PTR	OH-CZ	-6.98	1.24	1.40
1	B	321	PTR	OH-CZ	-6.74	1.25	1.40
1	D	321	PTR	OH-CZ	-6.46	1.26	1.40
1	D	321	PTR	P-OH	2.87	1.63	1.59
1	B	321	PTR	P-OH	2.23	1.62	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	PTR	O3P-P-OH	3.66	116.70	105.24
1	A	321	PTR	P-OH-CZ	3.45	134.81	123.75
1	C	321	PTR	P-OH-CZ	3.33	134.43	123.75
1	D	321	PTR	P-OH-CZ	2.97	133.29	123.75
1	B	321	PTR	O3P-P-O2P	2.77	118.22	107.64
1	A	321	PTR	O3P-P-O2P	2.65	117.78	107.64
1	B	321	PTR	O2P-P-OH	2.59	113.35	105.24
1	B	321	PTR	P-OH-CZ	2.54	131.88	123.75
1	C	321	PTR	O3P-P-OH	2.51	113.10	105.24
1	A	321	PTR	CB-CA-C	2.50	116.16	111.47
1	C	321	PTR	O3P-P-O2P	2.36	116.67	107.64
1	A	321	PTR	O3P-P-OH	2.17	112.03	105.24
1	D	321	PTR	CG-CB-CA	2.04	118.23	114.10

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 carbohydrates 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	1484	-	4,4,4	0.16	0	6,6,6	0.73	0
4	P6G	B	701	-	12,12,18	0.53	0	11,11,17	0.42	0
5	SO4	A	1483	-	4,4,4	0.24	0	6,6,6	0.55	0
2	D15	C	600	-	33,35,35	1.72	4 (12%)	38,48,48	1.99	9 (23%)
2	D15	A	600	-	33,35,35	1.73	5 (15%)	38,48,48	2.30	12 (31%)
4	P6G	A	702	-	6,6,18	0.45	0	5,5,17	0.30	0
2	D15	D	600	-	33,35,35	1.77	3 (9%)	38,48,48	1.89	9 (23%)
5	SO4	D	1482	-	4,4,4	0.15	0	6,6,6	0.39	0
2	D15	B	600	-	33,35,35	1.69	6 (18%)	38,48,48	2.43	9 (23%)
4	P6G	B	702	-	6,6,18	0.46	0	5,5,17	0.29	0
5	SO4	B	1482	-	4,4,4	0.38	0	6,6,6	0.32	0
4	P6G	A	700	-	15,15,18	0.62	0	14,14,17	0.30	0
4	P6G	D	700	-	15,15,18	0.53	0	14,14,17	0.37	0
4	P6G	C	700	-	15,15,18	0.69	0	14,14,17	0.61	0
5	SO4	C	1483	-	4,4,4	0.13	0	6,6,6	0.27	0
5	SO4	C	1484	-	4,4,4	0.20	0	6,6,6	0.42	0
4	P6G	A	701	-	12,12,18	0.50	0	11,11,17	0.84	0
5	SO4	B	1483	-	4,4,4	0.21	0	6,6,6	0.62	0
4	P6G	B	700	-	15,15,18	0.61	0	14,14,17	0.26	0
5	SO4	C	1482	-	4,4,4	0.20	0	6,6,6	0.24	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
4	P6G	B	701	-	-	1/10/10/16	-
2	D15	C	600	-	-	4/21/23/23	0/4/4/4
2	D15	A	600	-	-	3/21/23/23	0/4/4/4
4	P6G	A	702	-	-	1/4/4/16	-
2	D15	D	600	-	-	4/21/23/23	0/4/4/4
2	D15	B	600	-	-	4/21/23/23	0/4/4/4
4	P6G	B	702	-	-	2/4/4/16	-
4	P6G	B	700	-	-	3/13/13/16	-
4	P6G	A	700	-	-	5/13/13/16	-
4	P6G	D	700	-	-	3/13/13/16	-
4	P6G	C	700	-	-	8/13/13/16	-
4	P6G	A	701	-	-	3/10/10/16	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	D15	NAV-NAS	-7.60	1.23	1.37
2	C	600	D15	NAV-NAS	-7.42	1.23	1.37
2	A	600	D15	NAV-NAS	-6.89	1.24	1.37
2	B	600	D15	NAV-NAS	-6.52	1.25	1.37
2	D	600	D15	CBF-CAX	3.45	1.57	1.53
2	A	600	D15	CAP-CAZ	3.37	1.44	1.37
2	C	600	D15	CBA-CAW	3.12	1.56	1.50
2	B	600	D15	CAR-CBF	-2.91	1.49	1.53
2	A	600	D15	CBA-CAW	2.89	1.56	1.50
2	D	600	D15	CAP-CAZ	2.77	1.43	1.37
2	C	600	D15	CAZ-NAT	-2.69	1.36	1.41
2	B	600	D15	CAO-CAY	2.68	1.42	1.38
2	B	600	D15	CAP-CAZ	2.53	1.43	1.37
2	A	600	D15	CAZ-NAT	-2.33	1.36	1.41
2	C	600	D15	CAP-CAZ	2.25	1.42	1.37
2	B	600	D15	CBC-NAU	-2.23	1.32	1.36
2	B	600	D15	CAN-CBD	-2.17	1.38	1.41
2	A	600	D15	CAR-CBF	-2.08	1.51	1.53

All (39) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	D15	OAC-CAX-CBF	-7.04	115.73	122.46
2	A	600	D15	OAC-CAX-CBF	-6.37	116.37	122.46
2	B	600	D15	CAO-CAY-CL1	5.89	126.52	119.15
2	D	600	D15	OAC-CAX-CBF	-5.62	117.08	122.46
2	B	600	D15	CAI-CAY-CL1	-5.60	110.59	119.35
2	C	600	D15	OAC-CAX-CBF	-5.44	117.26	122.46
2	C	600	D15	CAO-CAY-CL1	4.84	125.20	119.15
2	B	600	D15	CAL-CBB-CBF	-4.78	112.20	120.93
2	C	600	D15	CAL-CBB-CBF	-4.70	112.33	120.93
2	A	600	D15	CAP-CBE-CBC	4.69	141.38	132.74
2	A	600	D15	CAL-CBB-CBF	-4.28	113.11	120.93
2	C	600	D15	CAI-CAY-CL1	-4.06	113.01	119.35
2	A	600	D15	CAO-CAY-CL1	4.05	124.21	119.15
2	A	600	D15	CAI-CAY-CL1	-3.99	113.11	119.35
2	D	600	D15	CAP-CBE-CBC	3.93	139.97	132.74
2	B	600	D15	CAO-CBB-CBF	3.89	127.38	120.35
2	A	600	D15	CAZ-NAT-CAX	-3.88	118.12	127.40
2	B	600	D15	CAZ-NAT-CAX	-3.86	118.16	127.40
2	B	600	D15	CAP-CBE-CBC	3.85	139.83	132.74
2	D	600	D15	CAL-CBB-CAO	3.83	123.17	118.76
2	A	600	D15	CBC-CBE-CBD	-3.77	101.45	106.59
2	B	600	D15	CBC-CBE-CBD	-3.70	101.55	106.59
2	C	600	D15	CAO-CBB-CBF	3.69	127.01	120.35
2	D	600	D15	CAL-CBB-CBF	-3.61	114.33	120.93
2	D	600	D15	CBC-CBE-CBD	-3.35	102.02	106.59
2	C	600	D15	CAZ-NAT-CAX	-3.14	119.89	127.40
2	A	600	D15	CAY-CAO-CBB	-3.08	115.36	119.42
2	C	600	D15	CBB-CBF-CAX	2.93	116.25	109.78
2	D	600	D15	CAO-CAY-CL1	2.90	122.77	119.15
2	B	600	D15	CAY-CAO-CBB	-2.88	115.62	119.42
2	A	600	D15	CAO-CBB-CBF	2.86	125.51	120.35
2	D	600	D15	CAZ-NAT-CAX	-2.83	120.62	127.40
2	C	600	D15	CAP-CBE-CBC	2.69	137.70	132.74
2	C	600	D15	CBC-CBE-CBD	-2.55	103.11	106.59
2	A	600	D15	CAM-CAN-CBD	2.47	123.94	120.84
2	D	600	D15	CAY-CAO-CBB	-2.41	116.24	119.42
2	A	600	D15	CAL-CBB-CAO	2.27	121.38	118.76
2	D	600	D15	CAM-CAZ-CAP	-2.14	116.12	119.33
2	A	600	D15	CAL-CAH-CAI	-2.00	117.40	120.25

There are no chirality outliers.

All (41) torsion outliers are listed below:



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

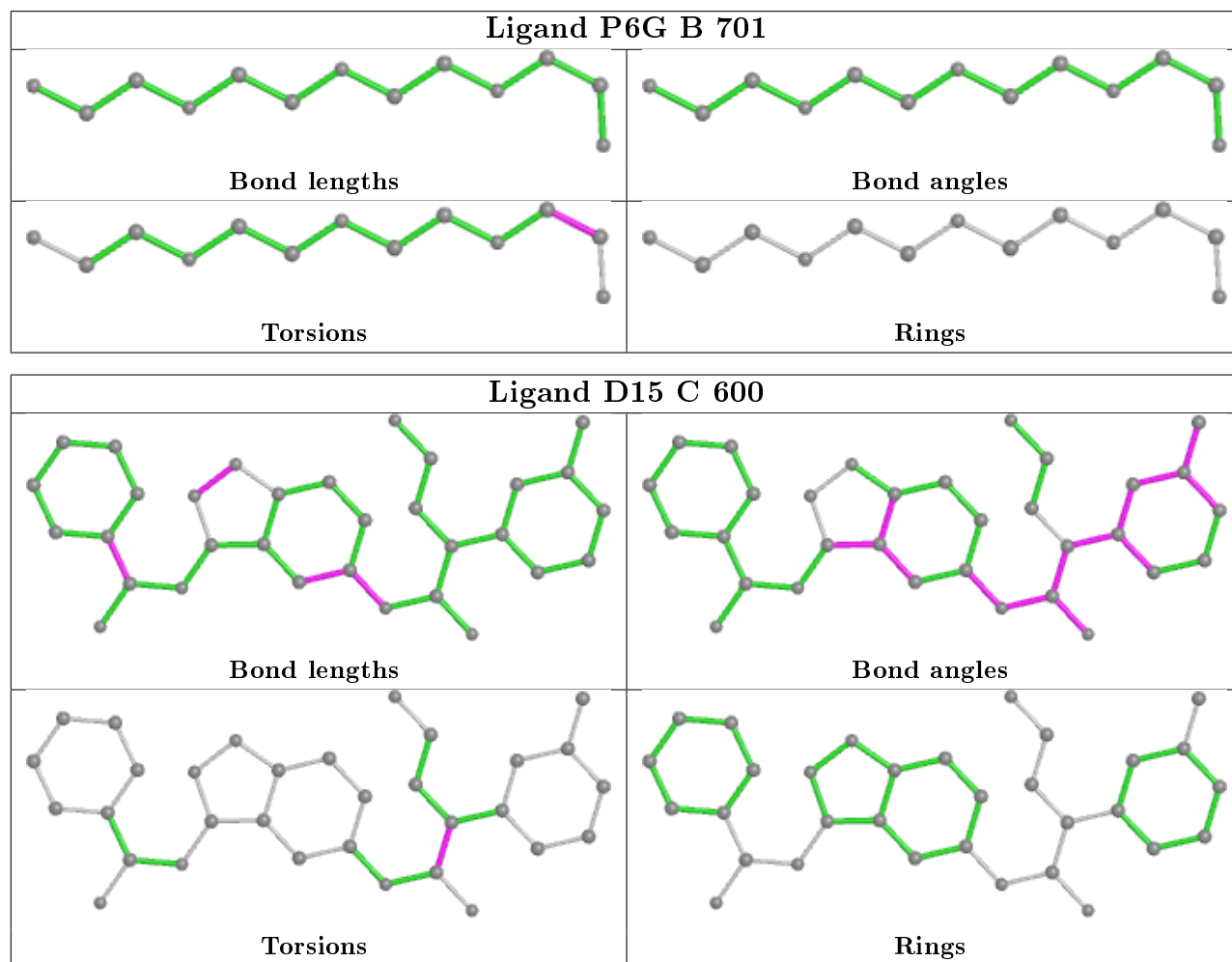
There are no ring outliers.



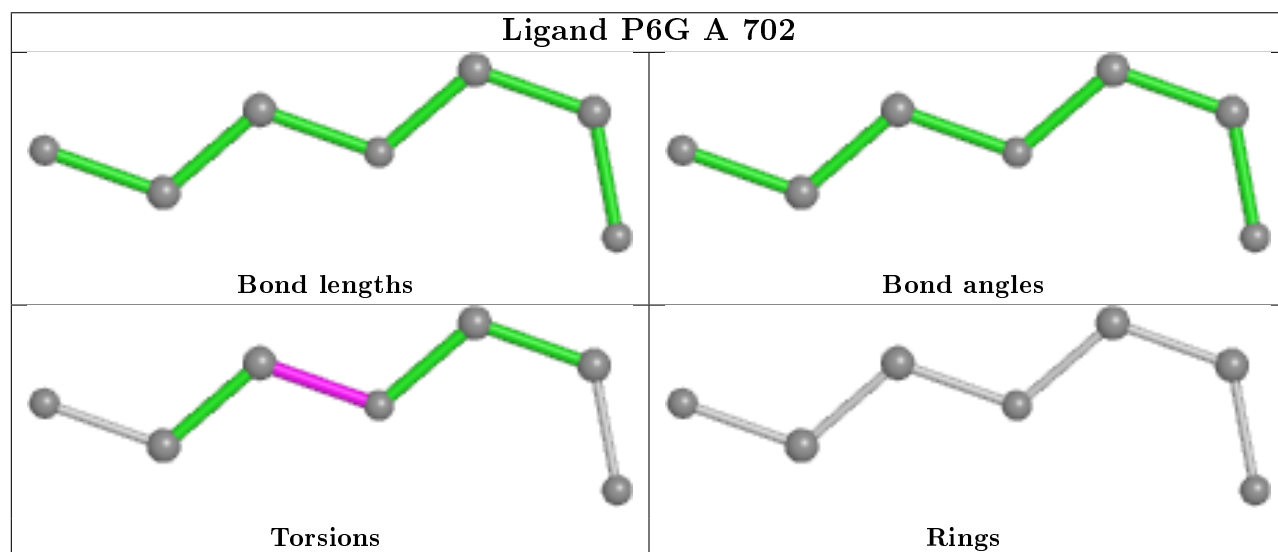
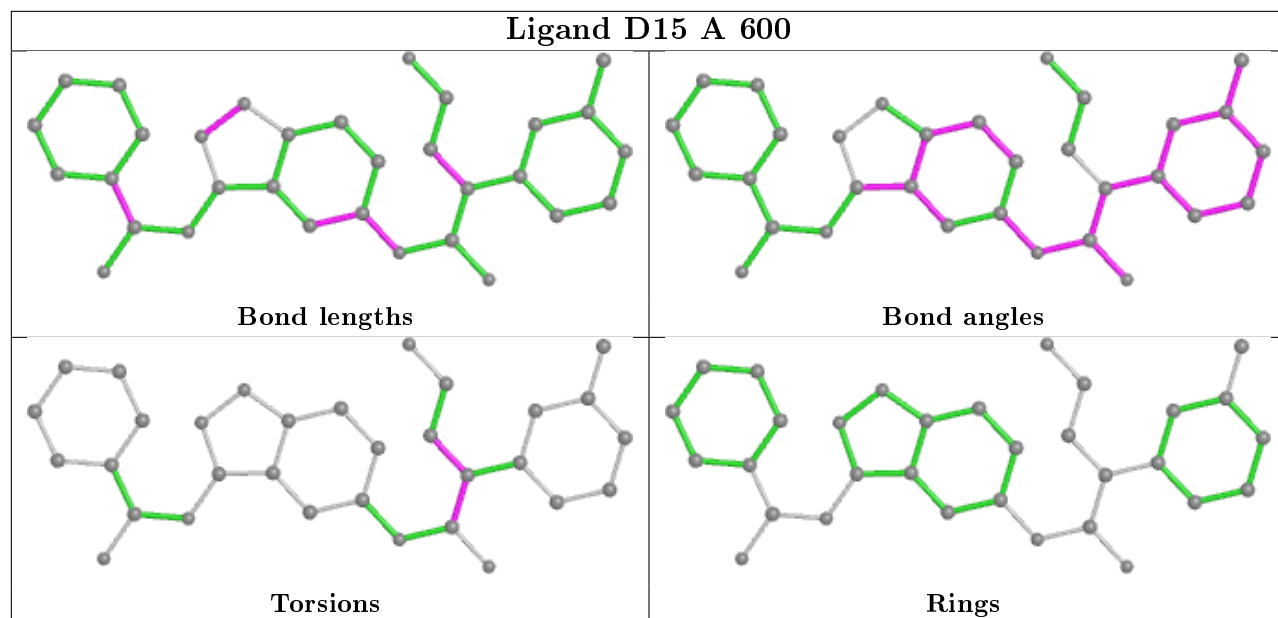
4 monomers are involved in 8 short contacts:

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

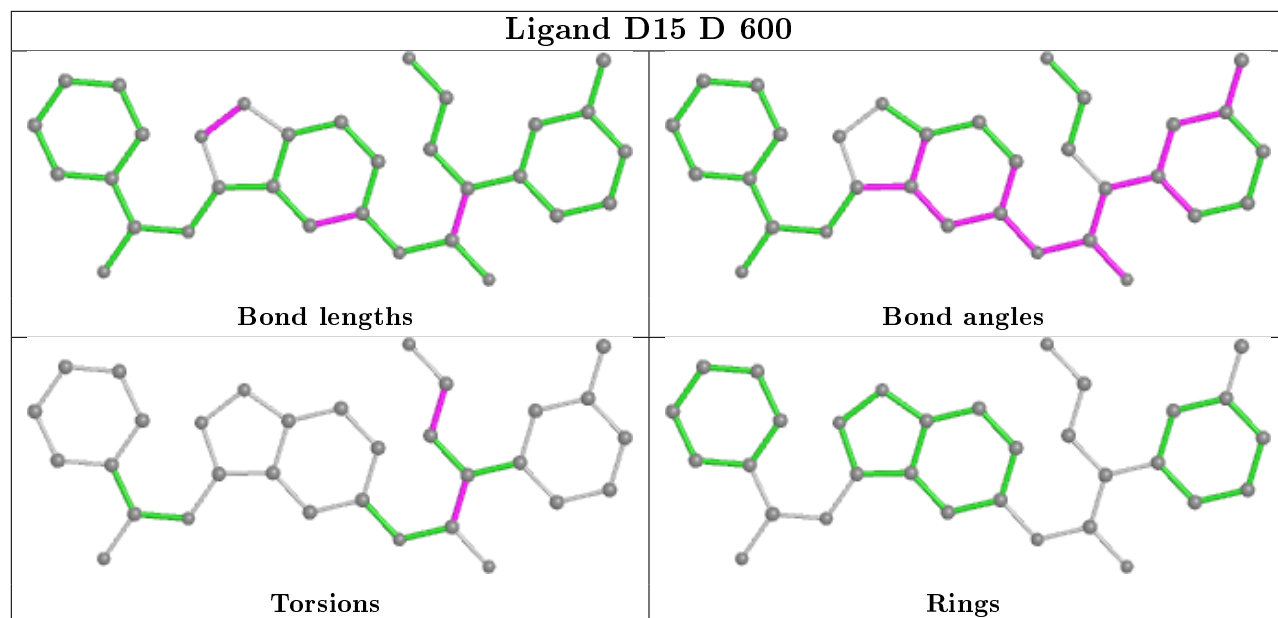




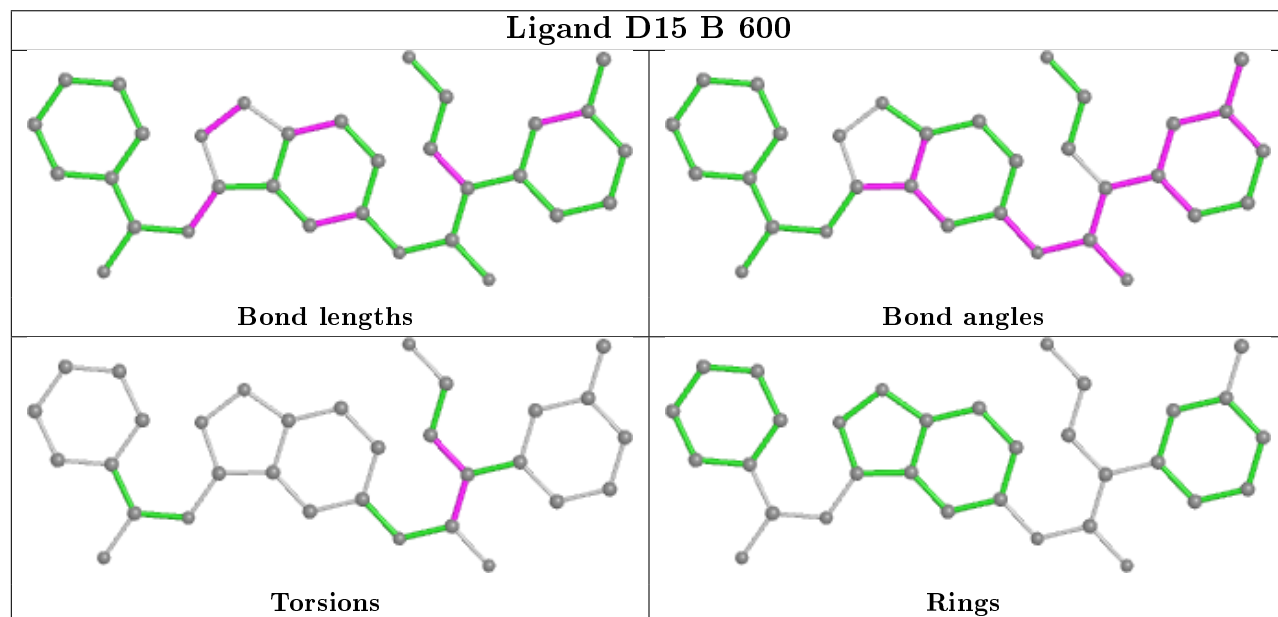




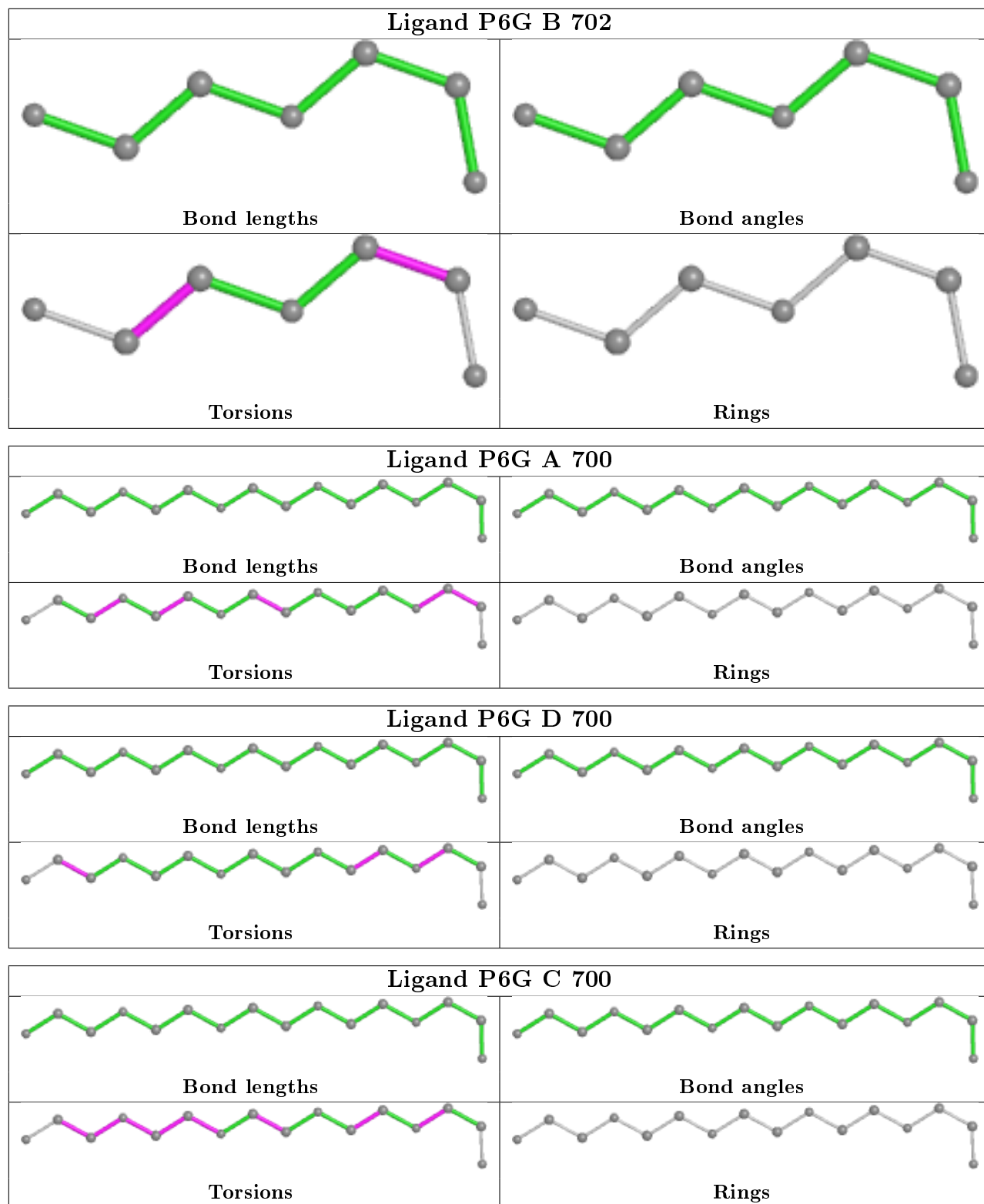
## Ligand D15 D 600



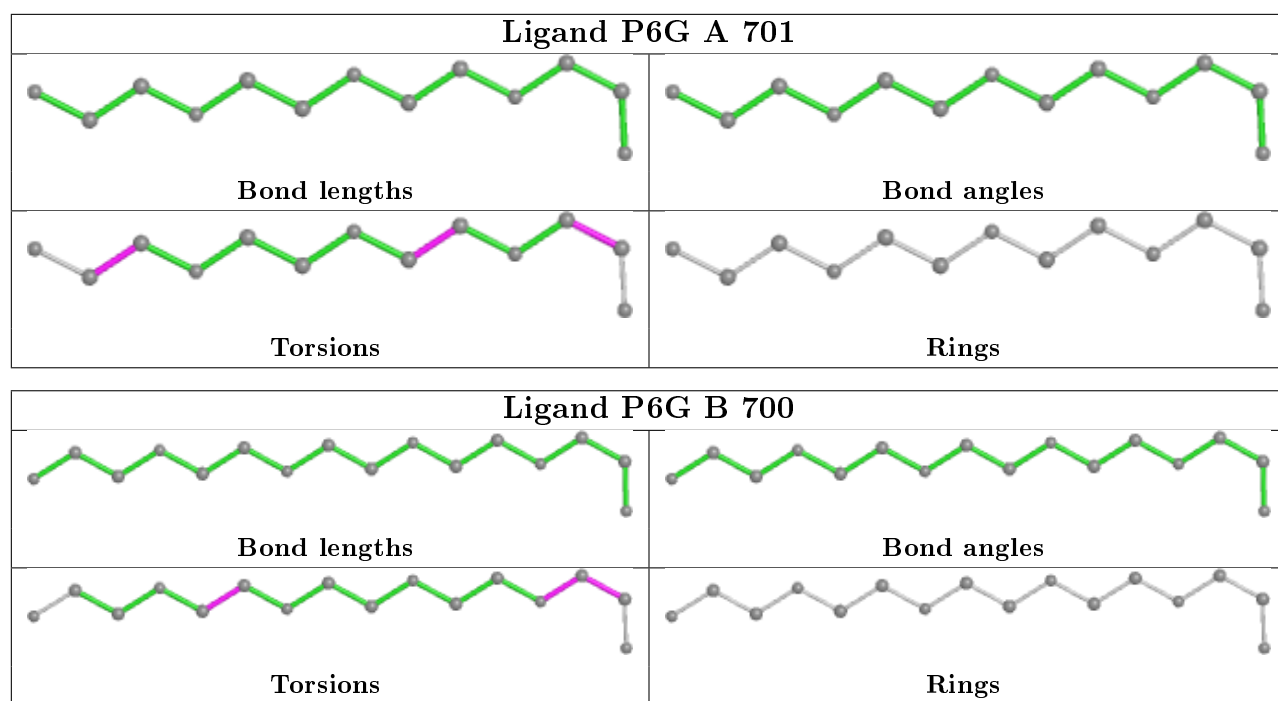
## Ligand D15 B 600











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	346/382 (90%)	-0.34	3 (0%) 84 82	21, 29, 43, 59	0
1	B	340/382 (89%)	-0.27	9 (2%) 56 54	19, 30, 43, 62	0
1	C	338/382 (88%)	-0.07	17 (5%) 28 27	21, 30, 43, 54	0
1	D	342/382 (89%)	-0.09	20 (5%) 23 22	21, 30, 43, 86	0
All	All	1366/1528 (89%)	-0.19	49 (3%) 42 42	19, 30, 43, 86	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	440	GLY	7.1
1	A	215	THR	5.8
1	B	215	THR	5.0
1	B	214	ASP	4.7
1	D	399	PRO	4.2
1	D	214	ASP	4.2
1	D	401	GLY	4.0
1	D	136	TYR	3.9
1	C	399	PRO	3.8
1	C	471	TYR	3.7
1	D	439	ALA	3.7
1	B	135	VAL	3.5
1	C	446	VAL	3.4
1	D	442	SER	3.3
1	C	472	TYR	3.3
1	C	135	VAL	3.3
1	B	318	ILE	3.2
1	B	439	ALA	3.0
1	C	475	GLN	3.0
1	D	347	LEU	3.0
1	C	136	TYR	3.0

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	D	318	ILE	2.8
1	C	398	LEU	2.7
1	A	214	ASP	2.7
1	B	216	GLU	2.7
1	B	408	THR	2.6
1	C	408	THR	2.6
1	D	215	THR	2.5
1	D	346	SER	2.4
1	C	447	ALA	2.4
1	D	400	ASP	2.4
1	D	316	GLN	2.4
1	D	402	THR	2.3
1	C	401	GLY	2.3
1	D	216	GLU	2.2
1	D	219	TYR	2.2
1	C	346	SER	2.2
1	D	471	TYR	2.2
1	C	445	THR	2.1
1	C	319	TYR	2.1
1	D	441	GLU	2.1
1	C	448	ASP	2.1
1	C	145	TYR	2.1
1	C	251	ASN	2.1
1	B	253	ASN	2.0
1	D	135	VAL	2.0
1	B	300	ARG	2.0
1	A	216	GLU	2.0
1	D	472	TYR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PTR	D	321	16/17	0.91	0.27	37,47,60,61	0
1	PTR	C	321	16/17	0.91	0.18	34,45,59,60	0
1	PTR	B	321	16/17	0.93	0.24	37,47,60,62	0
1	PTR	A	321	16/17	0.96	0.13	34,44,57,58	0



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CL	D	1484	1/1	0.77	0.12	85,85,85,85	0
4	P6G	B	700	16/19	0.87	0.17	64,75,77,79	0
4	P6G	C	700	16/19	0.89	0.21	47,66,83,85	0
4	P6G	A	700	16/19	0.92	0.19	62,72,76,78	0
3	CL	D	1483	1/1	0.92	0.08	75,75,75,75	0
5	SO4	B	1483	5/5	0.92	0.28	72,76,98,100	0
4	P6G	A	702	7/19	0.93	0.18	55,55,64,70	0
5	SO4	C	1484	5/5	0.94	0.22	83,87,96,104	0
4	P6G	B	702	7/19	0.95	0.16	67,80,83,85	0
4	P6G	D	700	16/19	0.95	0.11	37,46,64,64	0
2	D15	C	600	32/32	0.95	0.11	40,55,67,73	0
3	CL	C	1485	1/1	0.95	0.08	75,75,75,75	0
2	D15	D	600	32/32	0.95	0.11	31,50,61,65	0
3	CL	B	1485	1/1	0.95	0.07	59,59,59,59	0
4	P6G	A	701	13/19	0.95	0.13	32,46,55,65	0
4	P6G	B	701	13/19	0.95	0.11	33,44,50,52	0
2	D15	A	600	32/32	0.96	0.10	29,36,50,64	0
5	SO4	B	1482	5/5	0.96	0.25	65,66,88,91	0
5	SO4	C	1483	5/5	0.96	0.34	99,106,109,112	0
5	SO4	C	1482	5/5	0.97	0.14	75,86,88,92	0
5	SO4	B	1484	5/5	0.97	0.17	65,66,72,81	0
2	D15	B	600	32/32	0.97	0.10	25,40,55,55	0
5	SO4	A	1483	5/5	0.98	0.10	54,57,60,61	0
5	SO4	D	1482	5/5	0.98	0.19	55,69,82,90	0
3	CL	C	620	1/1	0.98	0.09	61,61,61,61	0
3	CL	A	620	1/1	0.98	0.07	45,45,45,45	0
3	CL	B	620	1/1	0.98	0.09	47,47,47,47	0
3	CL	D	620	1/1	0.99	0.09	56,56,56,56	0

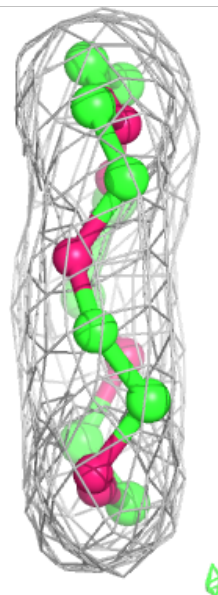
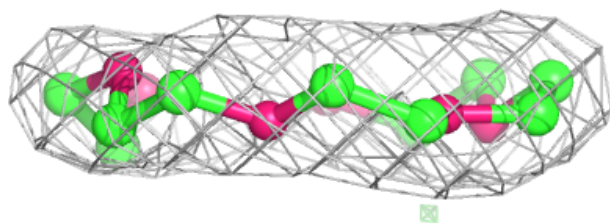
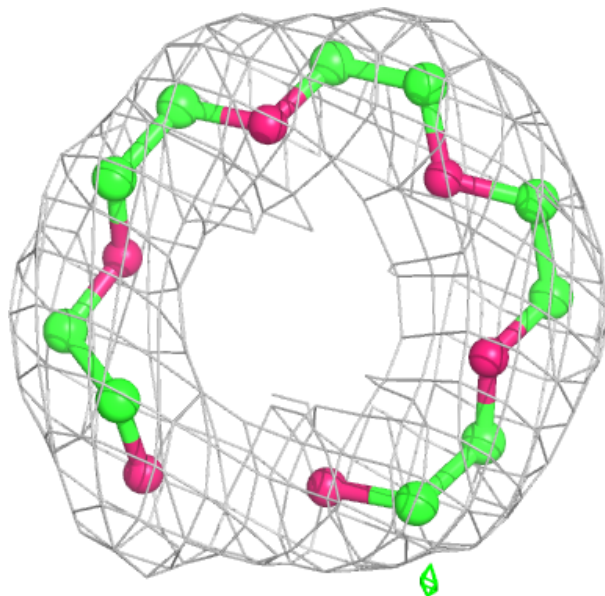
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.

**Electron density around P6G B 700:**

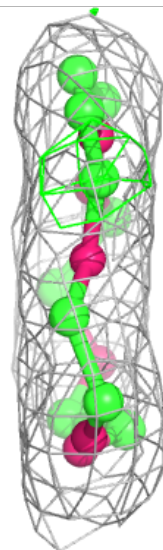
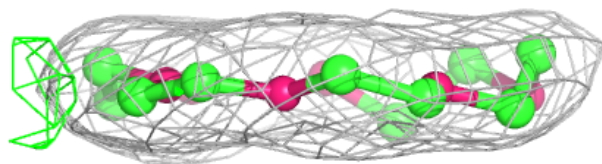
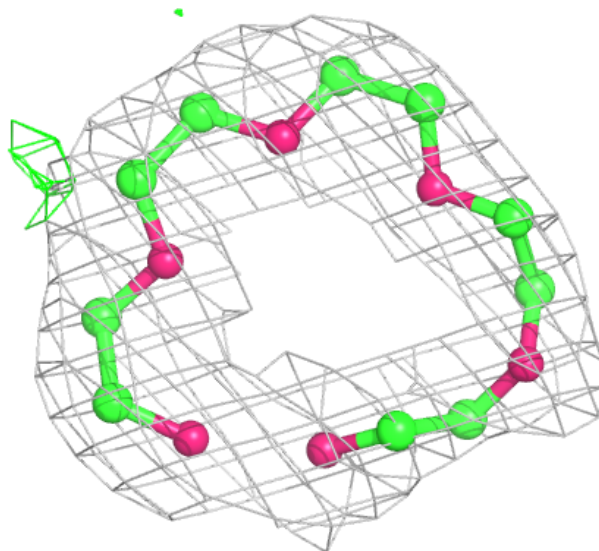
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around P6G C 700:**

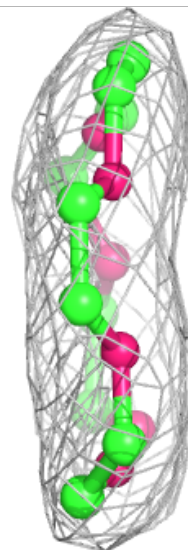
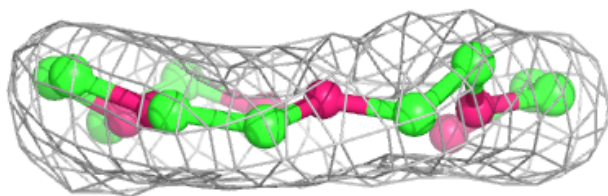
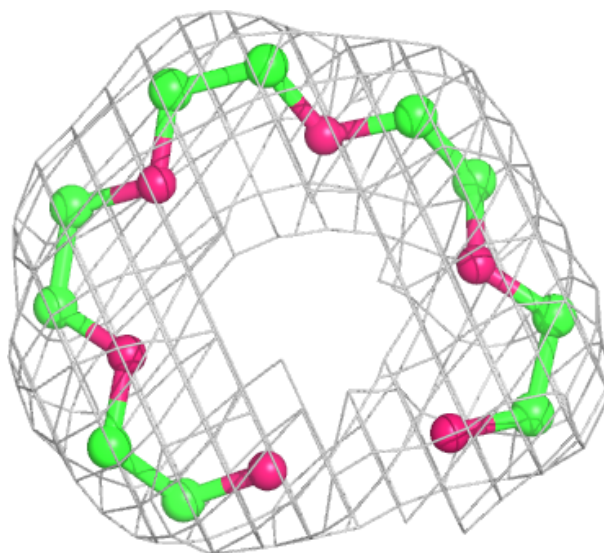
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around P6G A 700:**

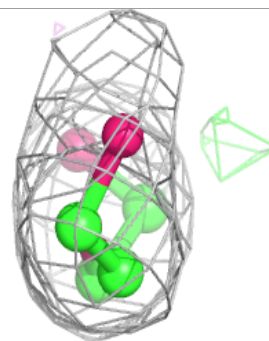
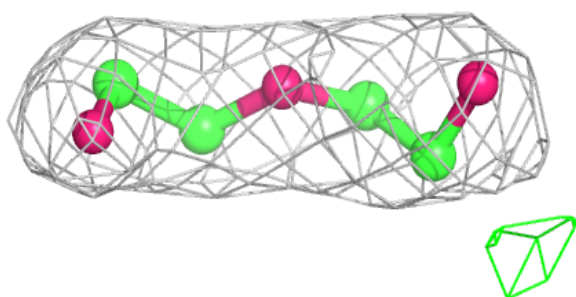
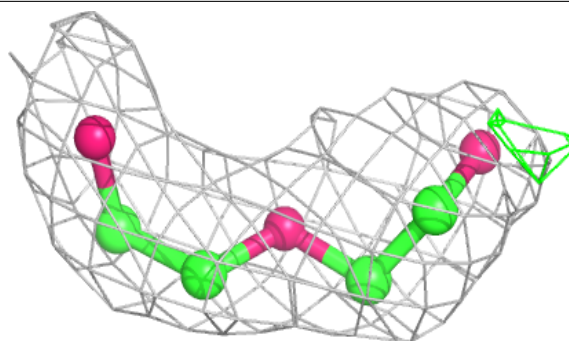
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



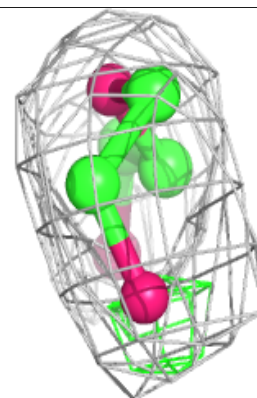
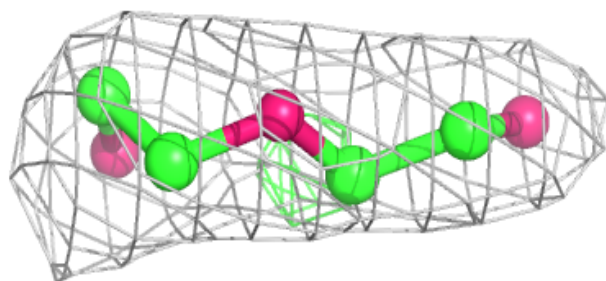
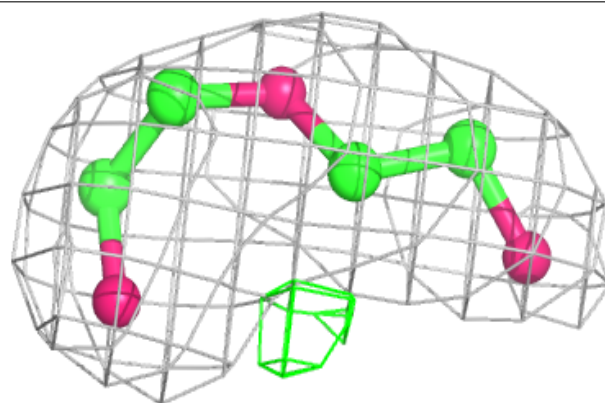


**Electron density around P6G A 702:**

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and green (positive)

**Electron density around P6G B 702:**

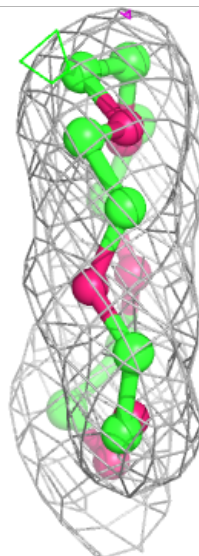
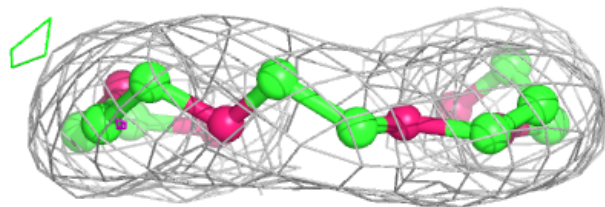
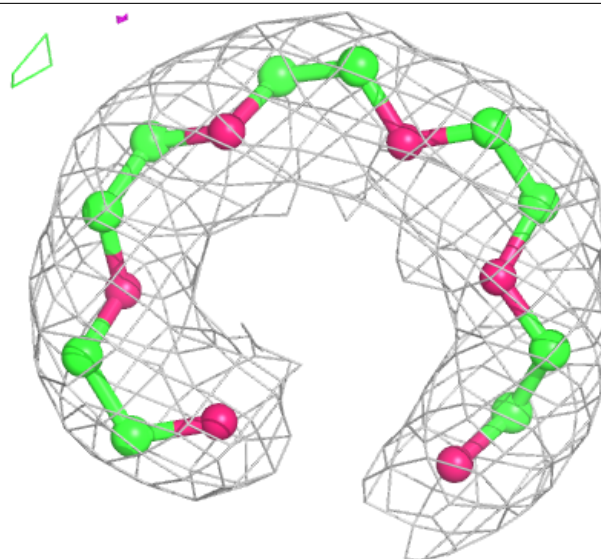
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and green (positive)





**Electron density around P6G D 700:**

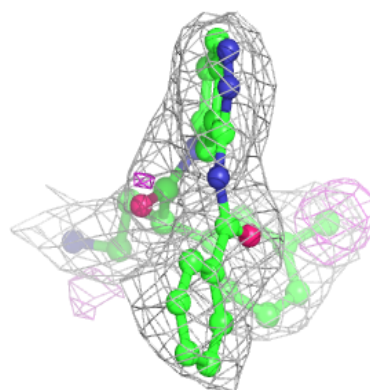
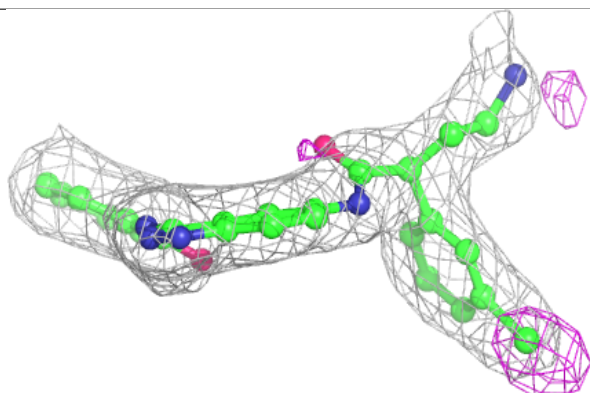
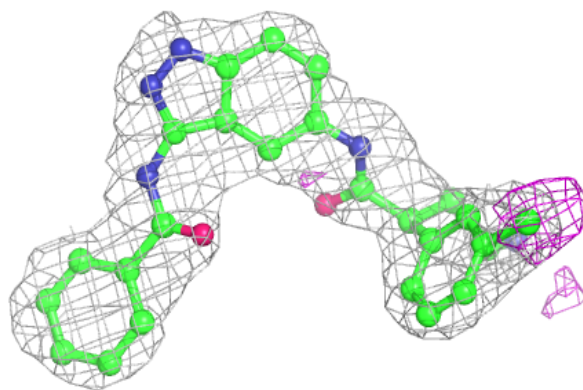
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



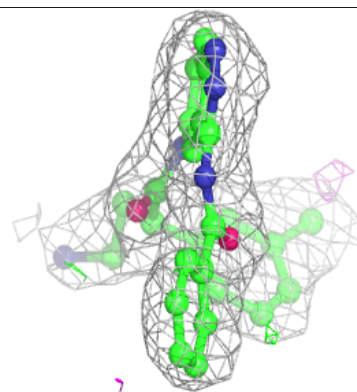
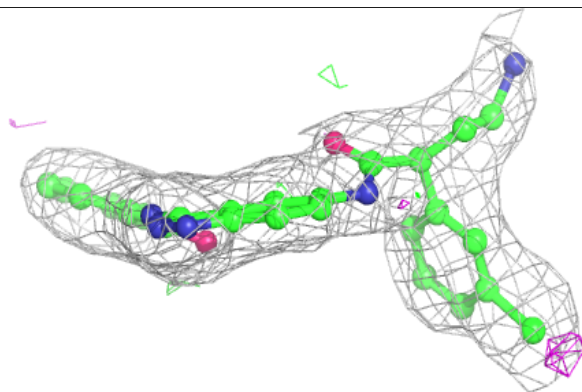
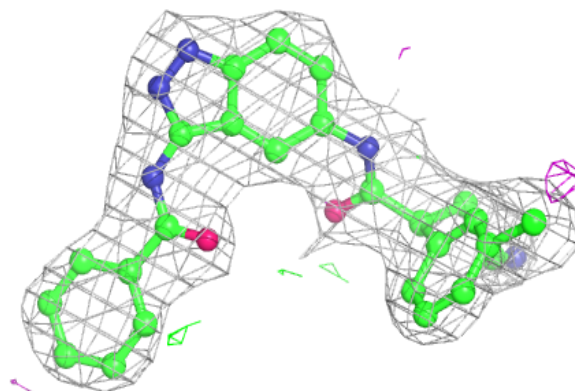


**Electron density around D15 C 600:**

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

**Electron density around D15 D 600:**

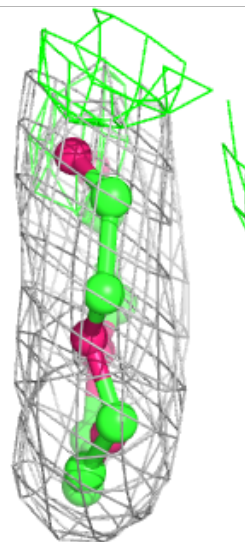
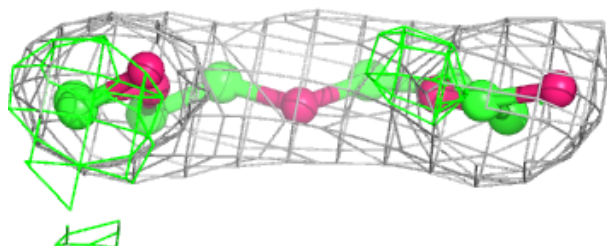
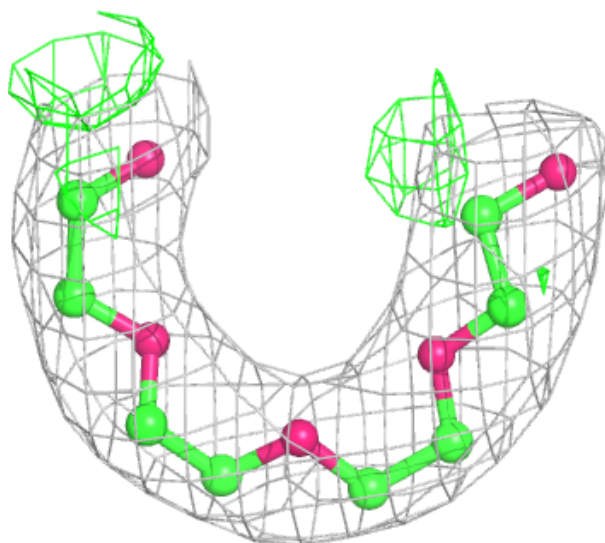
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and green (positive)





**Electron density around P6G A 701:**

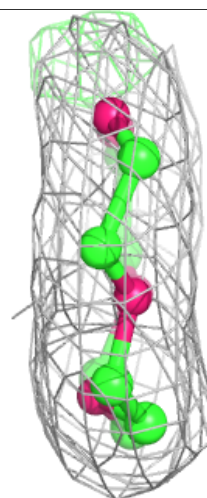
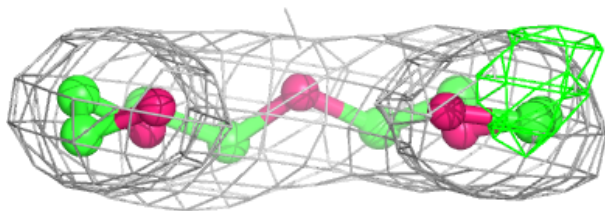
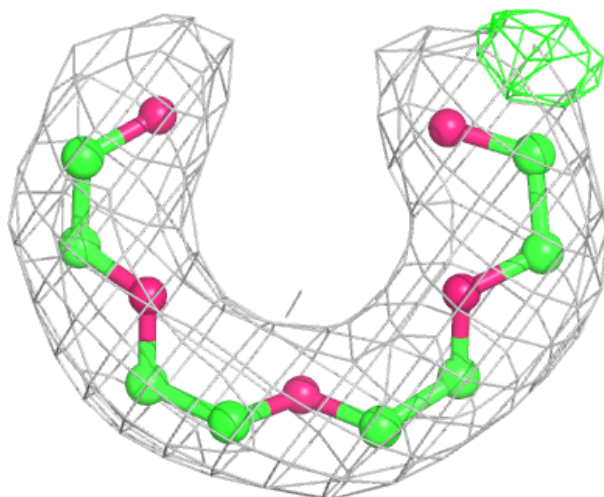
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around P6G B 701:**

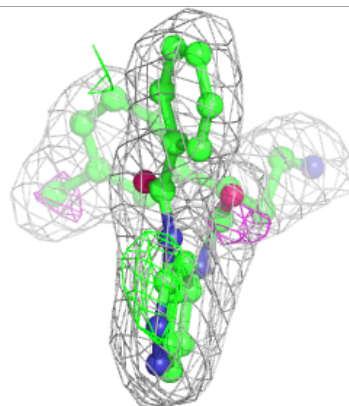
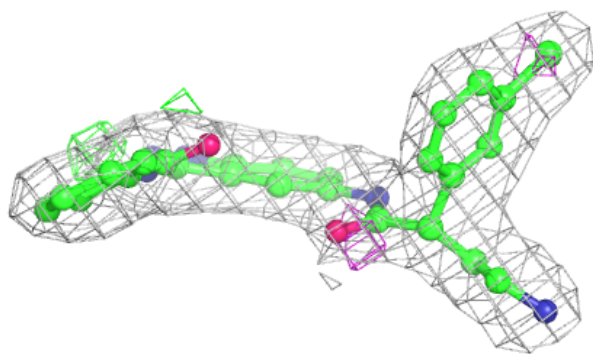
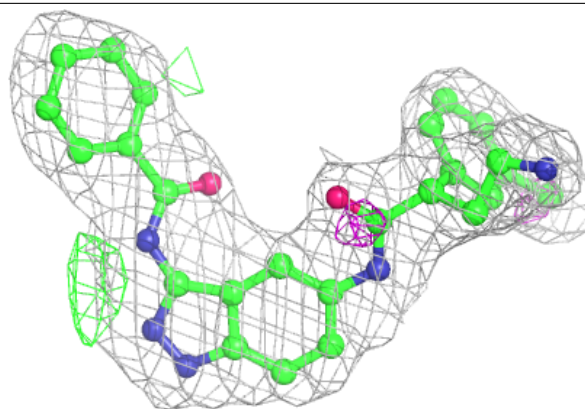
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



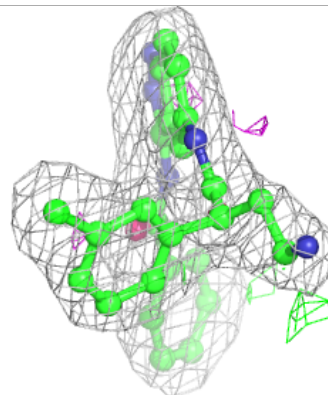
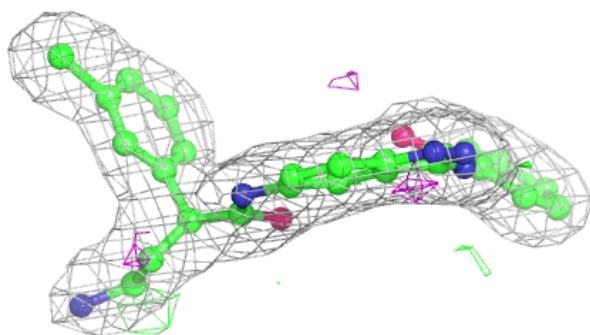
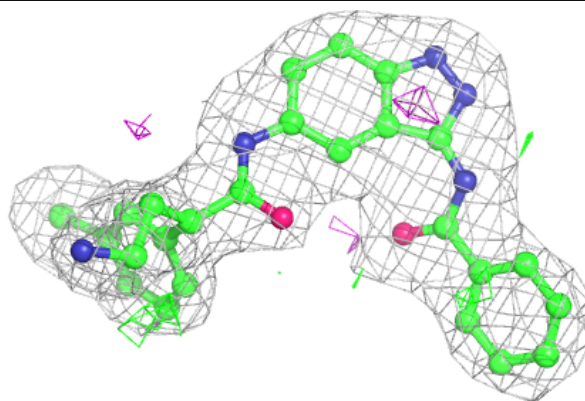


**Electron density around D15 A 600:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.