



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2022 – 02:05 PM EST

PDB ID : 7MDP  
Title : KRas G12C in complex with G-2897  
Authors : Oh, A.; Frank, Y.; Wang, W.  
Deposited on : 2021-04-05  
Resolution : 1.96 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 : 2.27  
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) : 2.27

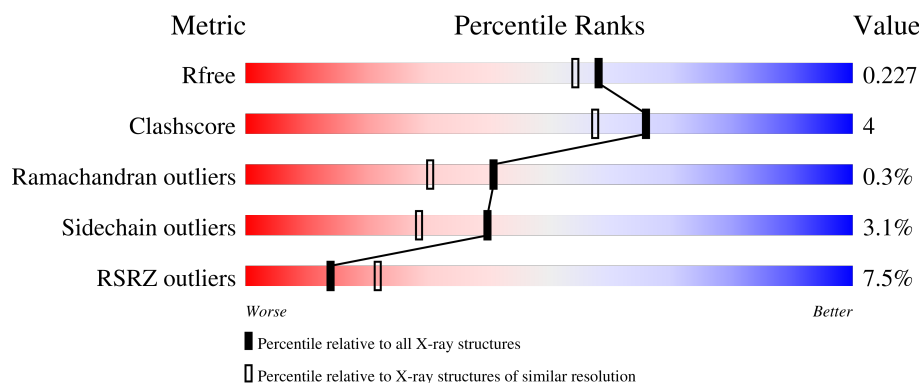
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	169	<div> <div>21%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
2	H	226	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
3	I	215	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	H	309	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4860 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1334	835	229	262	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	CYS	GLY	engineered mutation	UNP P01116-2

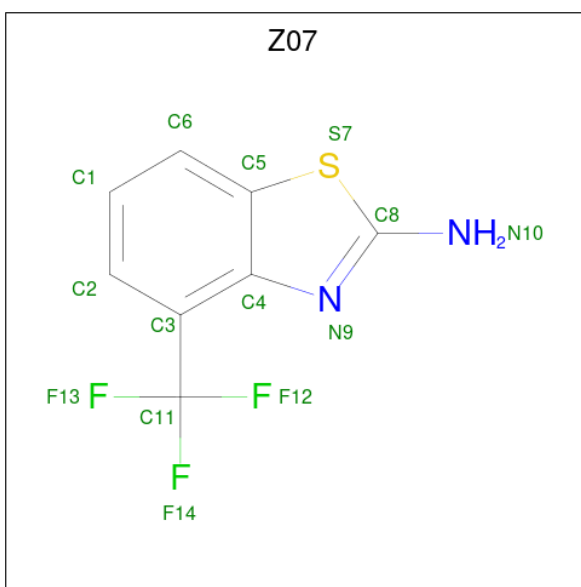
- Molecule 2 is a protein called IgG heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1664	1054	275	331	4			

- Molecule 3 is a protein called IgG light chain.

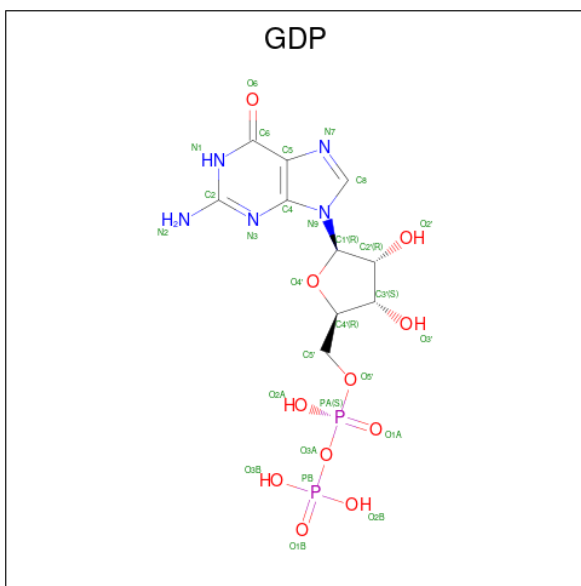
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	211	Total	C	N	O	S	0	0	0
			1581	990	269	318	4			

- Molecule 4 is 4-(trifluoromethyl)-1,3-benzothiazol-2-amine (three-letter code: Z07) (formula: C<sub>8</sub>H<sub>5</sub>F<sub>3</sub>N<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	S	0	0
			14	8	3	2	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

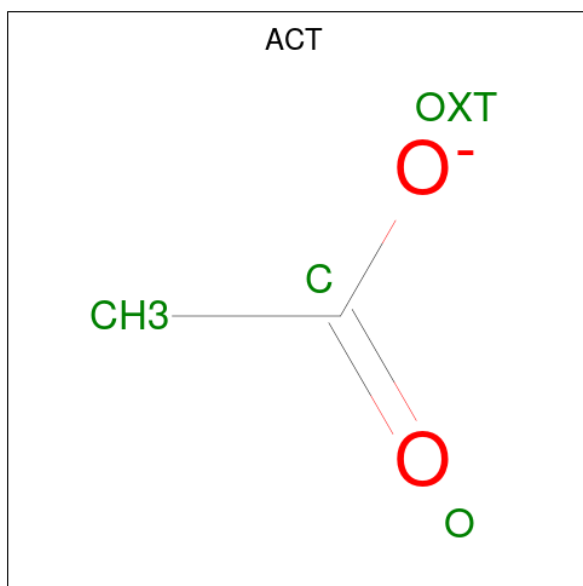


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

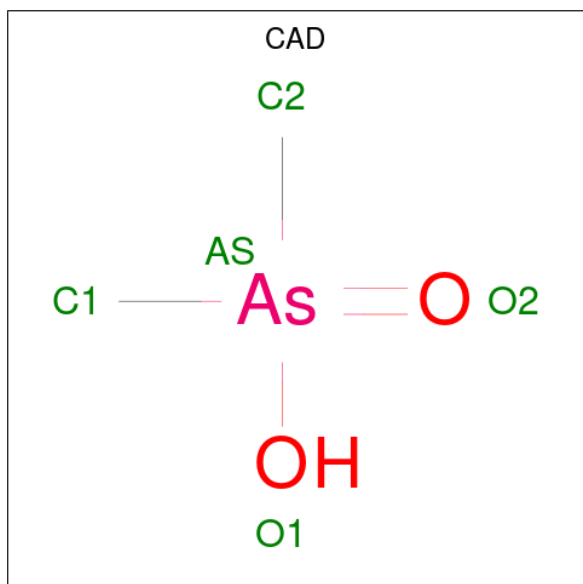
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



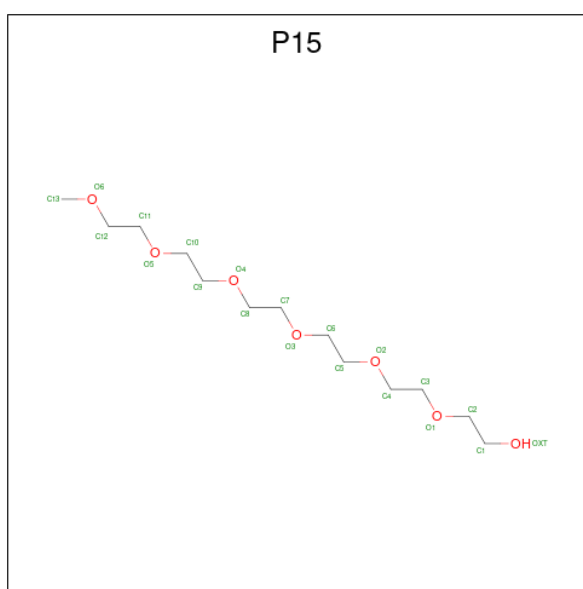
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CACODYLIC ACID (three-letter code: CAD) (formula:  $C_2H_7AsO_2$ ).



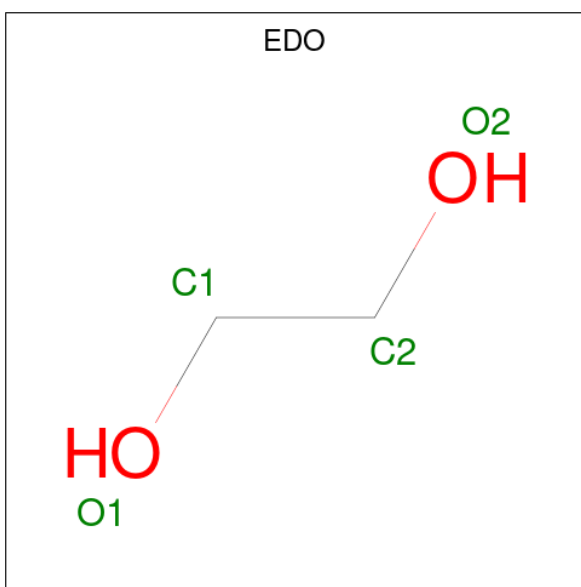
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	As	C	O	0	0
			5	1	2	2		
8	H	1	Total	As	C	O	0	0
			5	1	2	2		
8	H	1	Total	As	C	O	0	0
			5	1	2	2		
8	I	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 9 is 2,5,8,11,14,17-HEXAOXANONADECAN-19-OL (three-letter code: P15) (formula:  $C_{13}H_{28}O_7$ ).



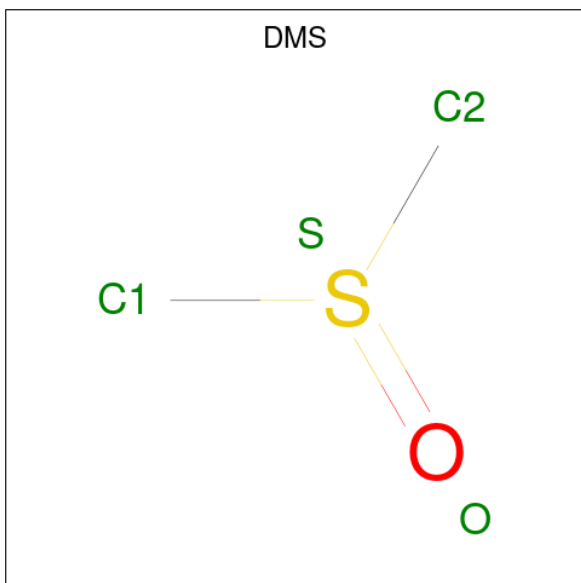
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			12	8	4		
9	H	1	Total	C	O	0	0
			12	8	4		
9	H	1	Total	C	O	0	0
			12	8	4		
9	I	1	Total	C	O	0	0
			11	7	4		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			4	2	2		
10	H	1	Total	C	O	0	0
			4	2	2		
10	I	1	Total	C	O	0	0
			4	2	2		
10	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	I	1	Total	C	O	S	0	0
			4	2	1	1		

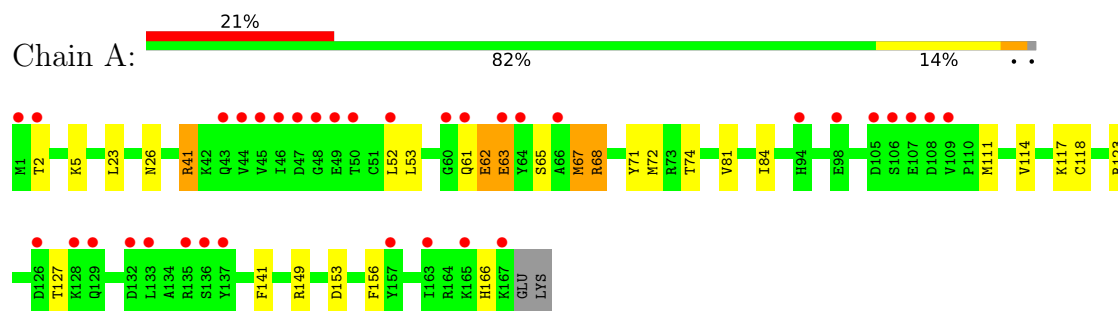
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	7	Total	O	0	0
			7	7		
12	H	68	Total	O	0	0
			68	68		
12	I	68	Total	O	0	0
			68	68		

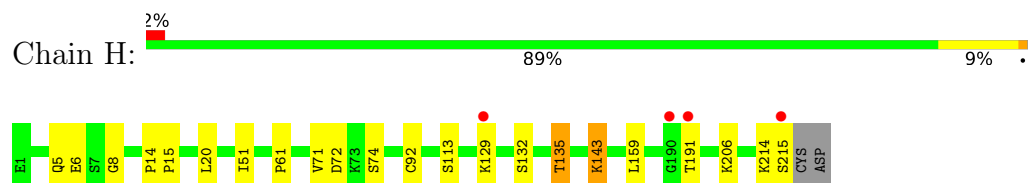
### 3 Residue-property plots [i](#)

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

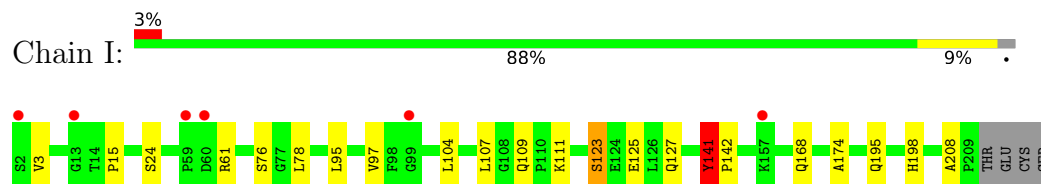
- Molecule 1: Isoform 2B of GTPase KRas



- Molecule 2: IgG heavy chain



- Molecule 3: IgG light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.37Å 68.92Å 100.54Å 90.00° 114.29° 90.00°	Depositor
Resolution (Å)	37.90 – 1.96 37.90 – 1.96	Depositor EDS
% Data completeness (in resolution range)	57.9 (37.90-1.96) 60.2 (37.90-1.96)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, $R_{free}$	0.195 , 0.229 0.192 , 0.227	Depositor DCC
$R_{free}$ test set	2053 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, GDP, ACT, CAD, MG, P15, EDO, Z07

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	0.30	0/1355	0.48	0/1828
2	H	0.39	0/1710	0.56	0/2338
3	I	0.36	0/1622	0.56	1/2215 (0.0%)
All	All	0.35	0/4687	0.54	1/6381 (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
2	H	0	1
3	I	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	141	TYR	C-N-CD	-5.20	109.17	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	14	PRO	Peptide
3	I	141	TYR	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	1334	0	1314	16	0
2	H	1664	0	1632	11	0
3	I	1581	0	1531	13	0
4	A	14	0	0	1	0
5	A	28	0	12	1	0
6	A	1	0	0	0	0
7	A	4	0	3	0	0
7	H	4	0	3	0	0
8	H	15	0	0	0	0
8	I	5	0	0	0	0
9	H	36	0	42	2	0
9	I	11	0	12	0	0
10	H	8	0	12	0	0
10	I	8	0	12	0	0
11	I	4	0	6	0	0
12	A	7	0	0	0	0
12	H	68	0	0	0	0
12	I	68	0	0	1	0
All	All	4860	0	4579	37	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 4.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.83	0.61
3:I:109:GLN:HB2	3:I:141:TYR:CE2	2.37	0.59
2:H:132:SER:HB2	2:H:135:THR:HG22	1.85	0.59
1:A:84:ILE:HD13	1:A:123:ARG:HB3	1.86	0.58
3:I:123:SER:O	3:I:127:GLN:HG2	2.05	0.57
3:I:3:VAL:HB	3:I:97:VAL:HB	1.88	0.56
1:A:23:LEU:HD22	1:A:156:PHE:CG	2.41	0.54
2:H:5:GLN:HB2	9:H:304:P15:H71	1.91	0.52
2:H:61:PRO:HG3	3:I:95:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:OD1	1:A:149:ARG:NH1	2.48	0.47
2:H:51:ILE:HD13	2:H:71:VAL:HG23	1.97	0.47
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.57	0.45
3:I:195:GLN:NE2	12:I:408:HOH:O	2.50	0.45
1:A:127:THR:HG23	1:A:141:PHE:HE2	1.82	0.45
3:I:15:PRO:HD3	3:I:107:LEU:O	2.17	0.44
1:A:111:MET:HE3	1:A:111:MET:HB3	1.79	0.44
3:I:141:TYR:O	3:I:198:HIS:NE2	2.51	0.44
2:H:206:LYS:HD3	9:H:308:P15:H111	2.00	0.43
1:A:62:GLU:HG3	4:A:201:Z07:F14	2.08	0.43
2:H:159:LEU:HD12	2:H:159:LEU:HA	1.80	0.43
3:I:78:LEU:HD11	3:I:104:LEU:HD21	2.00	0.43
2:H:143:LYS:NZ	3:I:125:GLU:OE2	2.41	0.43
1:A:117:LYS:HG2	5:A:202:GDP:C5	2.54	0.42
1:A:61:GLN:O	1:A:63:GLU:N	2.47	0.42
3:I:168:GLN:OE1	3:I:174:ALA:HB2	2.20	0.42
1:A:149:ARG:NH2	1:A:153:ASP:OD1	2.53	0.42
1:A:5:LYS:HD2	1:A:74:THR:HG22	2.00	0.42
2:H:72:ASP:OD1	2:H:74:SER:OG	2.32	0.42
1:A:81:VAL:HG22	1:A:114:VAL:HB	2.03	0.41
1:A:41:ARG:HA	1:A:53:LEU:O	2.21	0.41
1:A:52:LEU:HA	1:A:52:LEU:HD12	1.78	0.41
3:I:61:ARG:HB2	3:I:76:SER:O	2.21	0.41
3:I:111:LYS:H	3:I:111:LYS:HG2	1.66	0.40
1:A:67:MET:O	1:A:71:TYR:HB2	2.21	0.40
1:A:166:HIS:ND1	1:A:166:HIS:O	2.54	0.40
1:A:68:ARG:O	1:A:72:MET:HG2	2.22	0.40
2:H:129:LYS:NZ	3:I:208:ALA:H	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/169 (98%)	158 (96%)	7 (4%)	0	100	100
2	H	222/226 (98%)	212 (96%)	9 (4%)	1 (0%)	29	17
3	I	209/215 (97%)	201 (96%)	7 (3%)	1 (0%)	29	17
All	All	596/610 (98%)	571 (96%)	23 (4%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	15	PRO
3	I	142	PRO

### 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	148/150 (99%)	140 (95%)	8 (5%)	22	10
2	H	192/194 (99%)	186 (97%)	6 (3%)	40	28
3	I	176/180 (98%)	174 (99%)	2 (1%)	73	71
All	All	516/524 (98%)	500 (97%)	16 (3%)	40	28

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	41	ARG
1	A	62	GLU
1	A	63	GLU
1	A	65	SER
1	A	67	MET
1	A	68	ARG
1	A	118	CYS
2	H	113	SER
2	H	135	THR
2	H	143	LYS

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Mol	Chain	Res	Type
2	H	191	THR
2	H	214	LYS
2	H	215	SER
3	I	24	SER
3	I	123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z  > 2$
10	EDO	I	301	-	3,3,3	0.46	0	2,2,2	0.32	0
10	EDO	H	305	-	3,3,3	0.44	0	2,2,2	0.47	0
9	P15	H	306	-	11,11,19	0.59	0	10,10,18	0.47	0
8	CAD	I	303	-	1,4,4	9.26	1 (100%)	2,6,6	1.12	0
11	DMS	I	304	-	3,3,3	0.71	0	3,3,3	0.71	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	EDO	H	309	-	3,3,3	0.58	0	2,2,2	0.98	0
4	Z07	A	201	-	11,15,15	1.47	4 (36%)	15,23,23	2.13	3 (20%)
9	P15	H	308	-	11,11,19	0.64	0	10,10,18	0.21	0
7	ACT	A	204	-	1,3,3	6.92	1 (100%)	0,3,3	-	-
9	P15	H	304	-	11,11,19	0.57	0	10,10,18	0.31	0
10	EDO	I	302	-	3,3,3	0.47	0	2,2,2	0.29	0
8	CAD	H	303	-	1,4,4	9.35	1 (100%)	2,6,6	1.13	0
9	P15	I	305	-	10,10,19	0.47	0	9,9,18	0.32	0
8	CAD	H	301	-	1,4,4	9.50	1 (100%)	2,6,6	1.03	0
5	GDP	A	202	6	24,30,30	1.17	2 (8%)	31,47,47	1.93	9 (29%)
7	ACT	H	307	-	1,3,3	7.64	1 (100%)	0,3,3	-	-
8	CAD	H	302	-	1,4,4	9.59	1 (100%)	2,6,6	1.13	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
10	EDO	I	301	-	-	0/1/1/1	-
10	EDO	H	305	-	-	0/1/1/1	-
4	Z07	A	201	-	-	6/6/6/6	0/2/2/2
9	P15	H	308	-	-	5/9/9/17	-
9	P15	H	304	-	-	4/9/9/17	-
10	EDO	I	302	-	-	1/1/1/1	-
9	P15	I	305	-	-	2/8/8/17	-
9	P15	H	306	-	-	2/9/9/17	-
5	GDP	A	202	6	-	5/12/32/32	0/3/3/3
10	EDO	H	309	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	302	CAD	O1-AS	9.59	1.94	1.70
8	H	301	CAD	O1-AS	9.50	1.94	1.70
8	H	303	CAD	O1-AS	9.35	1.94	1.70
8	I	303	CAD	O1-AS	9.26	1.93	1.70
7	H	307	ACT	CH3-C	7.64	1.58	1.48
7	A	204	ACT	CH3-C	6.92	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	202	GDP	C5-C6	3.92	1.48	1.41
4	A	201	Z07	C3-C4	-2.69	1.40	1.43
5	A	202	GDP	C5-C4	2.46	1.47	1.40
4	A	201	Z07	F13-C11	2.22	1.40	1.32
4	A	201	Z07	F12-C11	2.13	1.40	1.32
4	A	201	Z07	F14-C11	2.02	1.40	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	Z07	F14-C11-C3	-5.92	106.18	112.32
5	A	202	GDP	C2-N3-C4	4.52	120.52	115.36
5	A	202	GDP	C5-C6-N1	-4.03	117.91	123.43
5	A	202	GDP	C2-N1-C6	4.00	122.28	115.93
5	A	202	GDP	PA-O3A-PB	-3.91	119.39	132.83
5	A	202	GDP	C4-C5-C6	-3.44	117.52	120.80
5	A	202	GDP	N3-C2-N1	-3.16	123.01	127.22
4	A	201	Z07	C4-C5-S7	-3.11	107.57	112.46
4	A	201	Z07	F12-C11-C3	-3.08	109.12	112.32
5	A	202	GDP	C4-C5-N7	-2.44	106.85	109.40
5	A	202	GDP	C3'-C2'-C1'	2.24	104.35	100.98
5	A	202	GDP	O2B-PB-O3A	2.09	111.65	104.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	Z07	F12-C11-C3-C4
4	A	201	Z07	F13-C11-C3-C4
4	A	201	Z07	F14-C11-C3-C4
5	A	202	GDP	C5'-O5'-PA-O1A
9	H	308	P15	O5-C10-C9-O4
9	H	308	P15	O3-C7-C8-O4
9	H	308	P15	O2-C5-C6-O3
4	A	201	Z07	F13-C11-C3-C2
4	A	201	Z07	F12-C11-C3-C2
4	A	201	Z07	F14-C11-C3-C2
9	H	306	P15	O5-C10-C9-O4
10	H	309	EDO	O1-C1-C2-O2
9	H	308	P15	C8-C7-O3-C6
9	I	305	P15	O2-C5-C6-O3
9	H	304	P15	C8-C7-O3-C6

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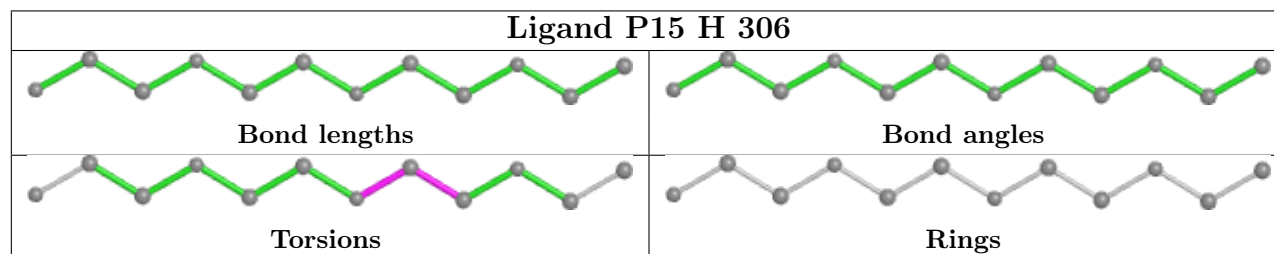
Mol	Chain	Res	Type	Atoms
9	H	304	P15	C10-C9-O4-C8
5	A	202	GDP	C5'-O5'-PA-O3A
5	A	202	GDP	C5'-O5'-PA-O2A
9	I	305	P15	O3-C7-C8-O4
9	H	308	P15	C12-C11-O5-C10
5	A	202	GDP	O4'-C4'-C5'-O5'
10	I	302	EDO	O1-C1-C2-O2
9	H	306	P15	C10-C9-O4-C8
9	H	304	P15	C9-C10-O5-C11
9	H	304	P15	O5-C10-C9-O4
5	A	202	GDP	C3'-C4'-C5'-O5'

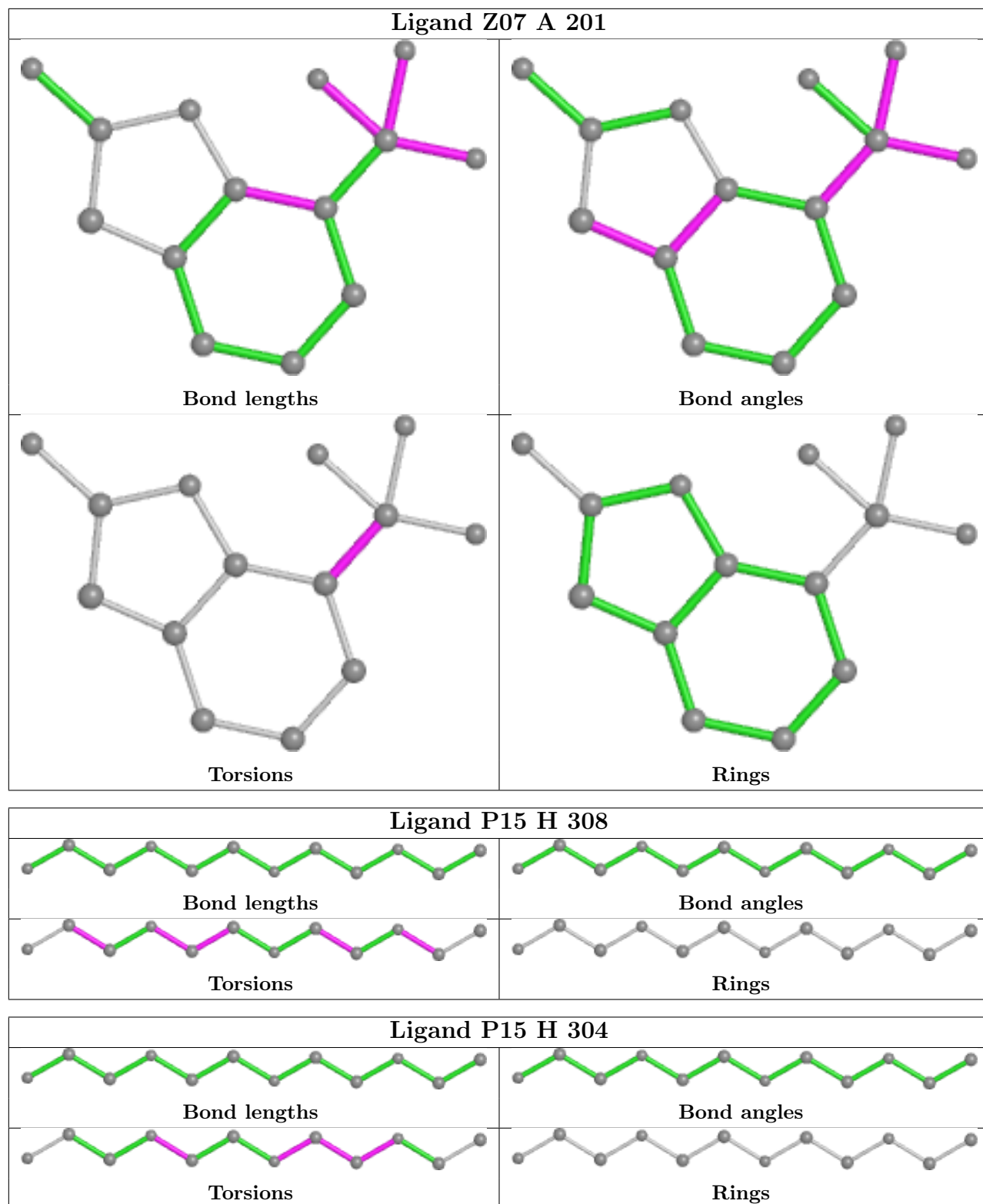
There are no ring outliers.

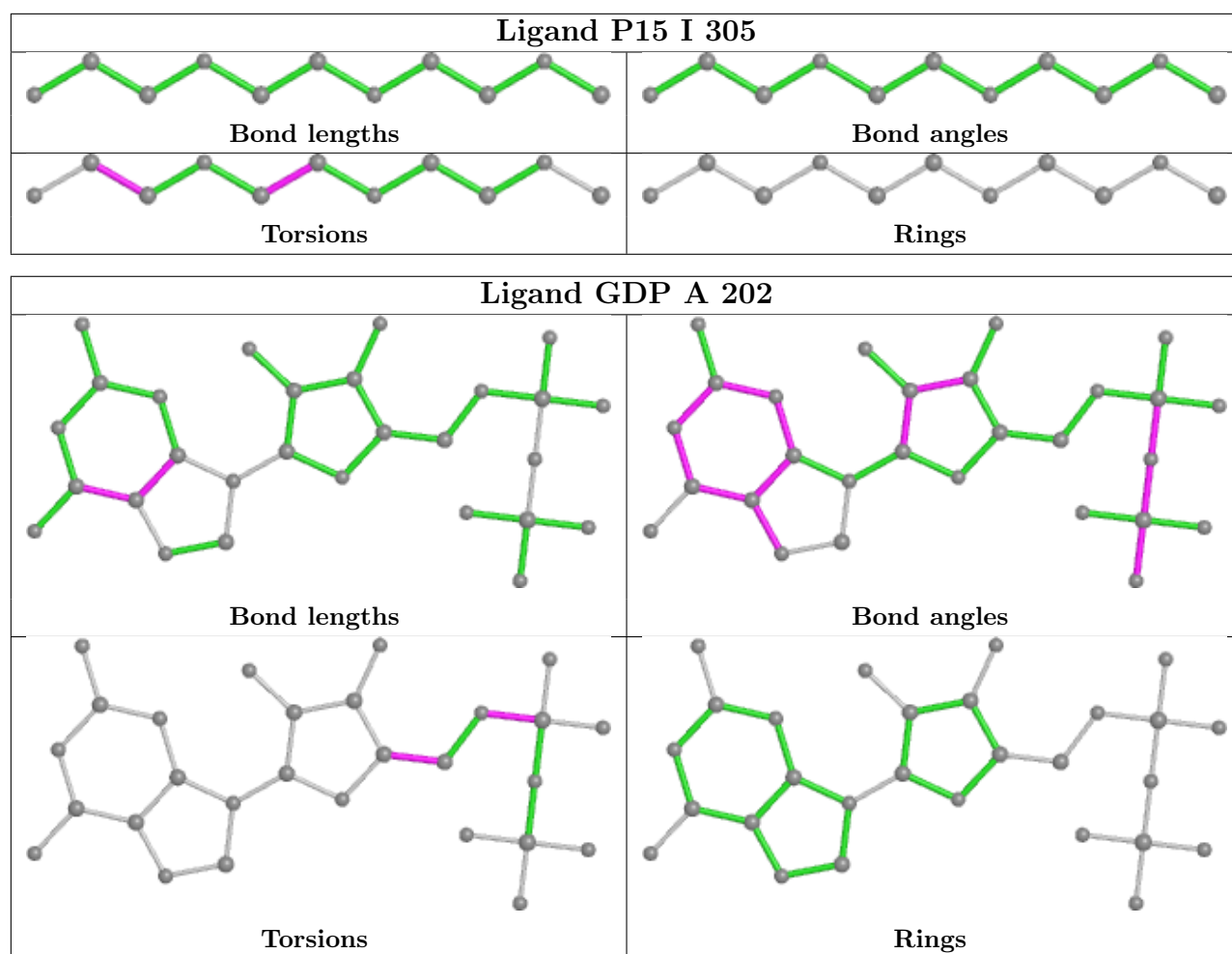
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	Z07	1	0
9	H	308	P15	1	0
9	H	304	P15	1	0
5	A	202	GDP	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.







## 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	167/169 (98%)	1.11	35 (20%) <b>1</b> <b>1</b>	56, 83, 122, 145	0
2	H	224/226 (99%)	0.02	4 (1%) 68 76	26, 40, 66, 83	0
3	I	211/215 (98%)	0.05	6 (2%) 53 62	26, 45, 70, 80	0
All	All	602/610 (98%)	0.34	45 (7%) <b>14</b> <b>22</b>	26, 50, 104, 145	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.1
1	A	64	TYR	10.3
1	A	45	VAL	5.0
1	A	165	LYS	4.9
1	A	107	GLU	4.7
1	A	128	LYS	4.5
1	A	105	ASP	4.3
1	A	46	ILE	4.3
1	A	66	ALA	4.2
1	A	136	SER	4.1
1	A	167	LYS	4.0
1	A	50	THR	3.7
2	H	191	THR	3.7
1	A	137	TYR	3.4
1	A	94	HIS	3.3
1	A	61	GLN	3.2
1	A	108	ASP	3.2
3	I	2	SER	3.1
1	A	44	VAL	3.1
1	A	135	ARG	3.1
1	A	63	GLU	2.9
3	I	60	ASP	2.8
1	A	49	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	2.7
2	H	215	SER	2.6
2	H	190	GLY	2.6
1	A	157	TYR	2.5
1	A	129	GLN	2.5
1	A	133	LEU	2.5
3	I	59	PRO	2.5
3	I	157	LYS	2.3
3	I	13	GLY	2.3
1	A	47	ASP	2.3
1	A	60	GLY	2.2
3	I	99	GLY	2.2
1	A	106	SER	2.2
1	A	132	ASP	2.2
1	A	98	GLU	2.1
1	A	109	VAL	2.1
1	A	48	GLY	2.1
1	A	43	GLN	2.1
1	A	2	THR	2.1
1	A	163	ILE	2.1
2	H	129	LYS	2.0
1	A	126	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
10	EDO	H	309	4/4	0.18	1.00	130,131,132,133	0

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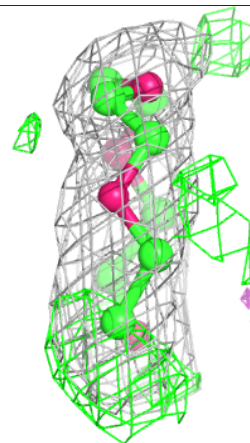
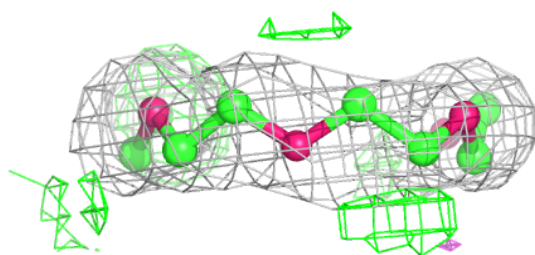
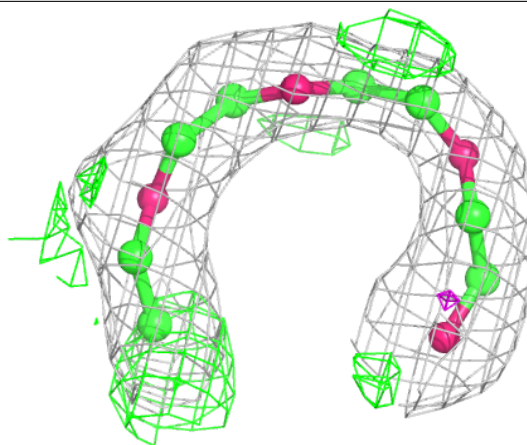
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	P15	H	308	12/20	0.71	0.16	41,61,71,72	0
6	MG	A	203	1/1	0.74	0.39	86,86,86,86	0
8	CAD	H	302	5/5	0.74	0.23	161,163,163,164	0
9	P15	H	304	12/20	0.77	0.24	75,79,85,86	0
9	P15	H	306	12/20	0.77	0.17	52,65,74,75	0
7	ACT	A	204	4/4	0.79	0.25	80,83,84,87	0
10	EDO	I	301	4/4	0.80	0.14	63,64,64,67	0
4	Z07	A	201	14/14	0.81	0.17	90,97,105,107	14
7	ACT	H	307	4/4	0.83	0.27	81,83,84,85	0
9	P15	I	305	11/20	0.85	0.28	72,75,85,86	0
11	DMS	I	304	4/4	0.85	0.27	88,90,93,94	0
10	EDO	H	305	4/4	0.90	0.36	72,75,80,83	0
8	CAD	H	301	5/5	0.91	0.43	143,146,146,148	0
8	CAD	H	303	5/5	0.92	0.38	158,158,160,160	0
10	EDO	I	302	4/4	0.93	0.13	52,53,53,53	0
5	GDP	A	202	28/28	0.95	0.12	58,66,75,78	0
8	CAD	I	303	5/5	0.96	0.18	120,122,125,126	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.



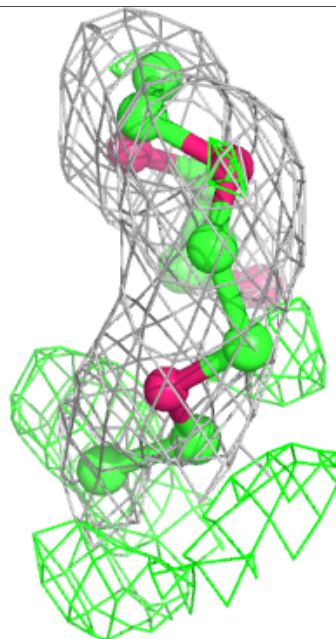
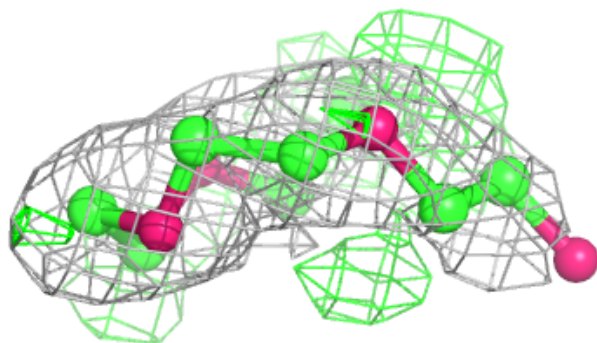
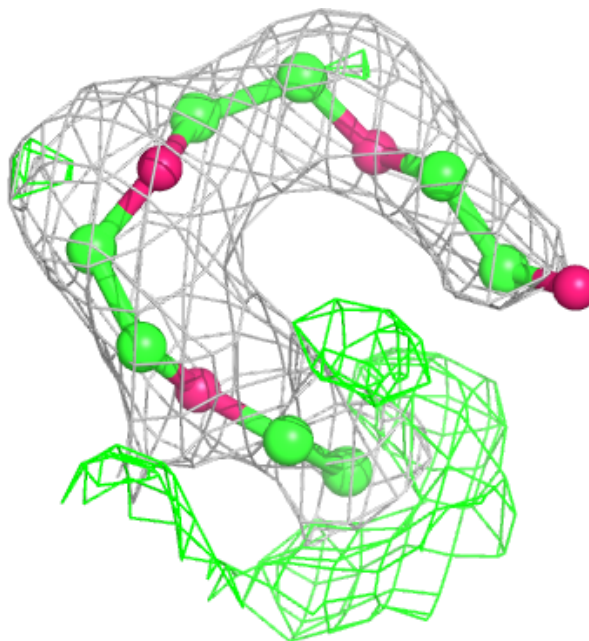
**Electron density around P15 H 308:**

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



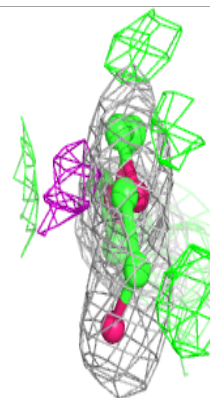
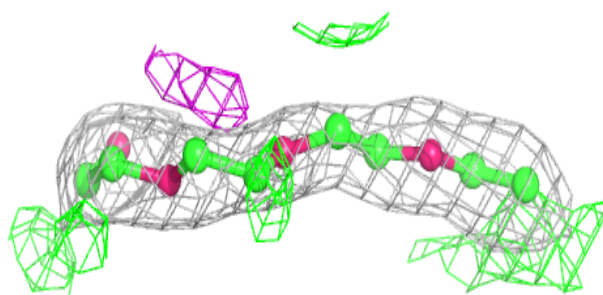
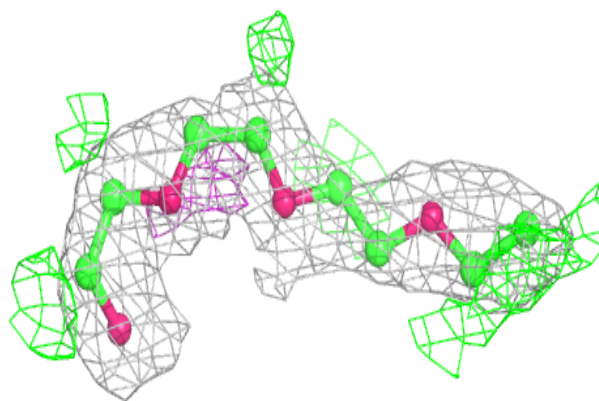
**Electron density around P15 H 304:**

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



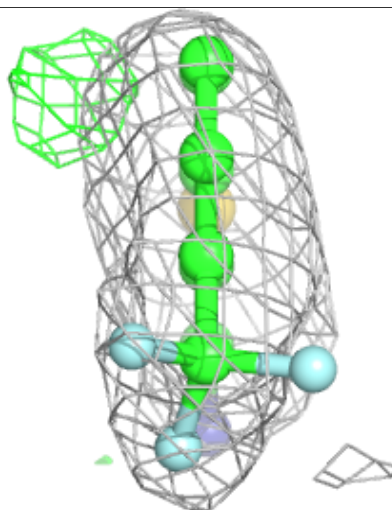
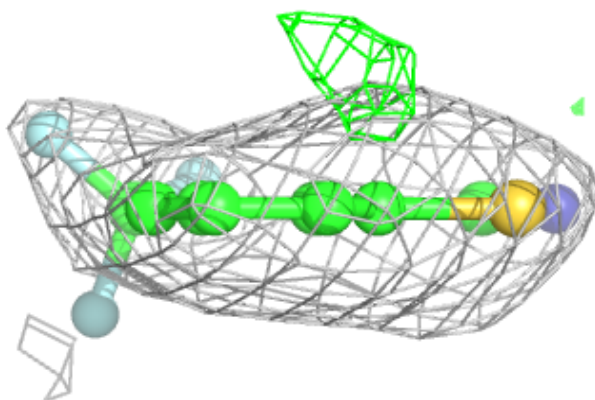
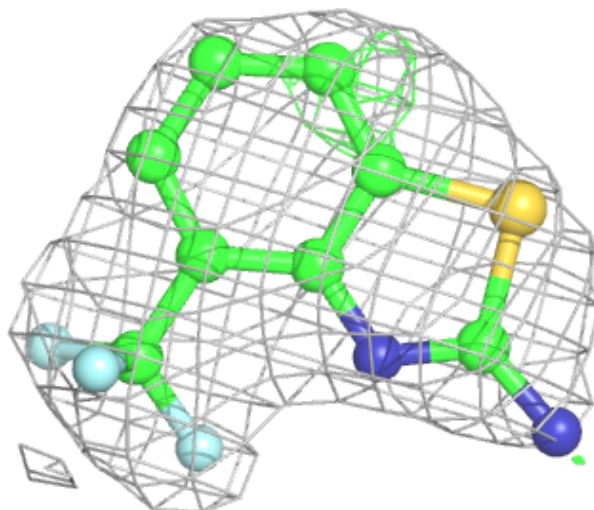
**Electron density around P15 H 306:**

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



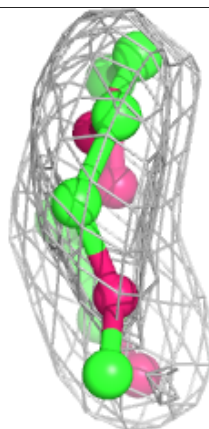
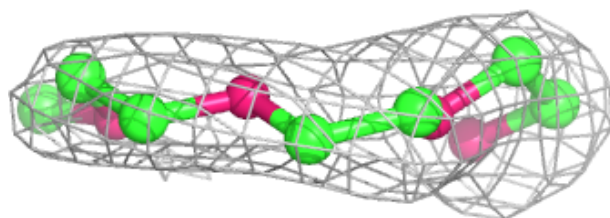
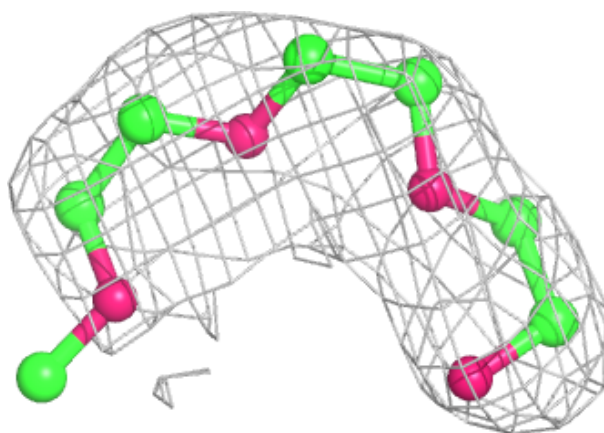
**Electron density around Z07 A 201:**

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



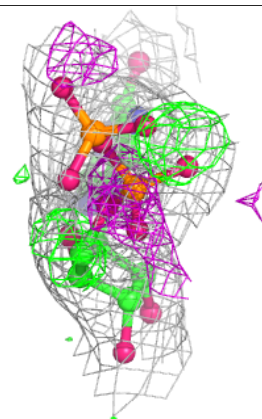
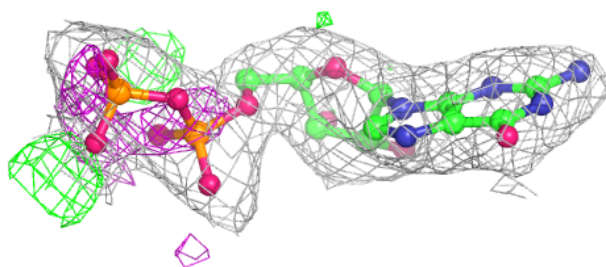
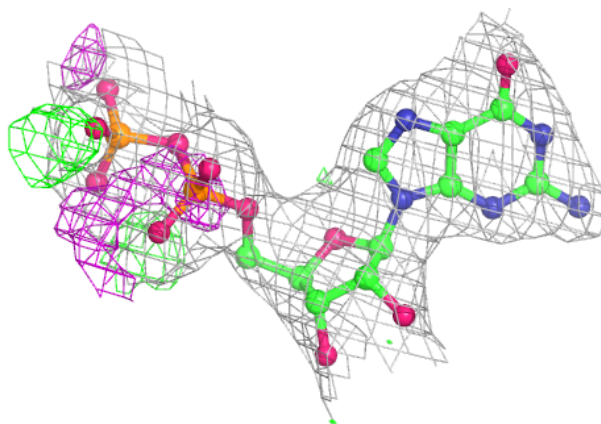
**Electron density around P15 I 305:**

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



**Electron density around GDP A 202:**

$2mF_o-DF_c$  (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.