



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 01:56 pm BST

PDB ID : 9F3G / pdb\_00009f3g  
Title : Human carbonic anhydrase XII with 3-(cyclooctylamino)-2,6-difluoro-5-((4-hydroxybutyl)amino)-4-((3-hydroxypropyl)sulfonyl)benzenesulfonamide  
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Deposited on : 2024-04-25  
Resolution : 1.21 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.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

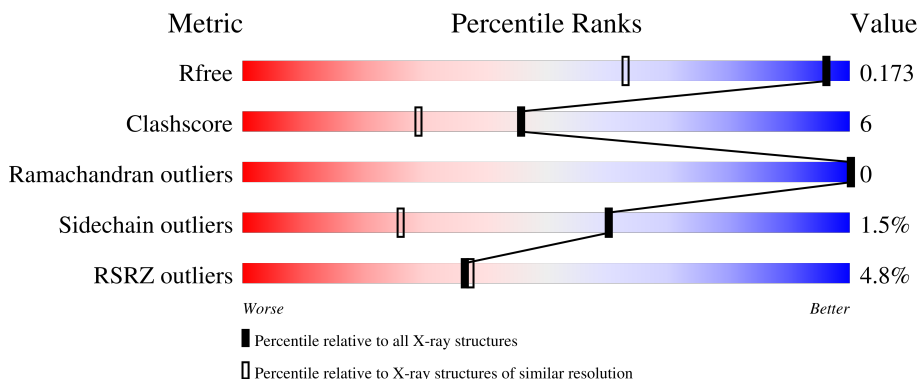
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1745 (1.24-1.20)
Clashscore	180529	1895 (1.24-1.20)
Ramachandran outliers	177936	1845 (1.24-1.20)
Sidechain outliers	177891	1844 (1.24-1.20)
RSRZ outliers	164620	1744 (1.24-1.20)

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	263	 4% 92% 8%
1	B	263	 4% 91% 8%
1	C	263	 7% 87% 12%
1	D	263	 4% 89% 10%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10167 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	18	0
			2218	1410	375	425	8			
1	B	262	Total	C	N	O	S	0	16	0
			2223	1410	377	428	8			
1	C	260	Total	C	N	O	S	3	11	0
			2171	1374	372	414	11			
1	D	262	Total	C	N	O	S	5	14	0
			2208	1403	372	425	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



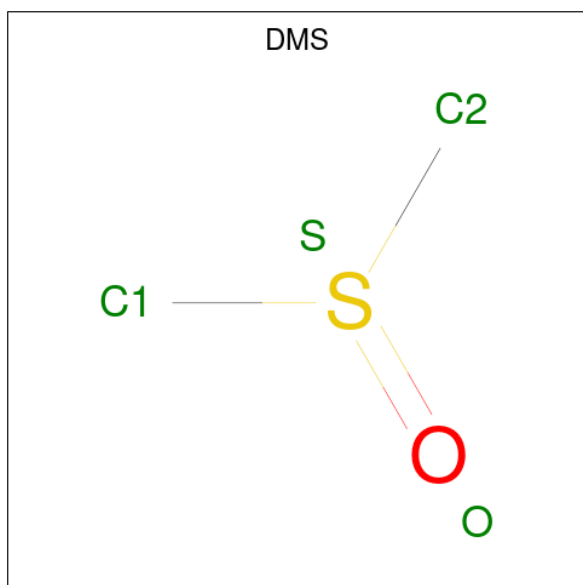
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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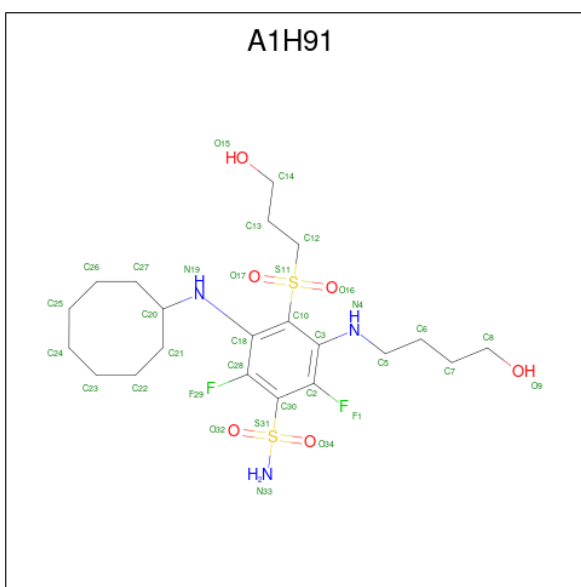
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 3-(cyclooctylamino)-2,6-bis(fluoranyl)-5-(4-oxidanylbutylamino)-4-[( { E } )-3-oxidanylprop-1-enyl]sulfonyl-benzenesulfonamide (CCD ID: A1H91) (formula: C<sub>21</sub>H<sub>35</sub>F<sub>2</sub>N<sub>3</sub>O<sub>6</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 34	C 21	F 2	N 3	O 6	S 2	0	0
5	B	1	Total 34	C 21	F 2	N 3	O 6	S 2	0	0
5	C	1	Total 34	C 21	F 2	N 3	O 6	S 2	0	0
5	D	1	Total 34	C 21	F 2	N 3	O 6	S 2	0	0

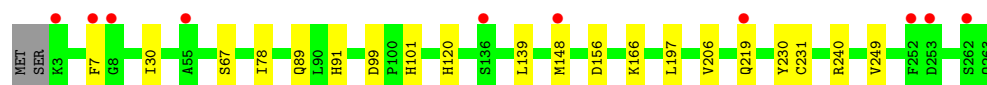
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	270	Total O 271 271	0	1
6	B	289	Total O 295 295	0	6
6	C	260	Total O 260 260	0	0
6	D	306	Total O 309 309	0	3

### 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.

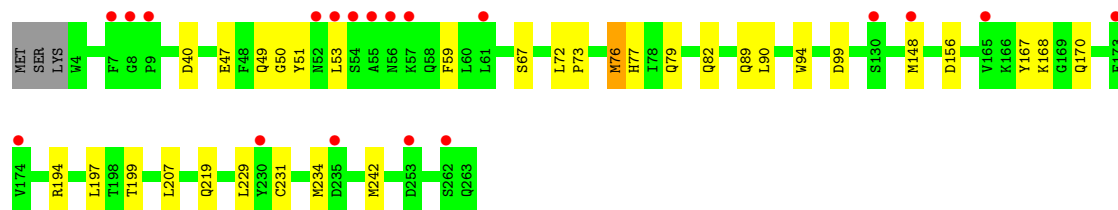
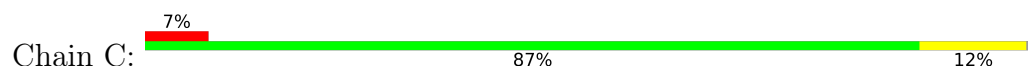
- Molecule 1: Carbonic anhydrase 12



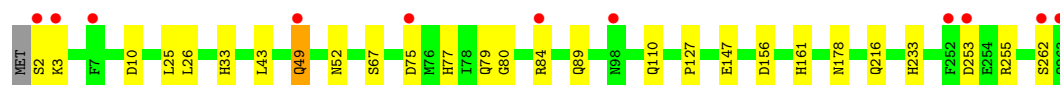
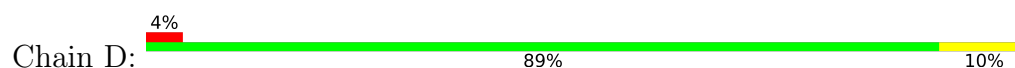
- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



- Molecule 1: Carbonic anhydrase 12



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.50Å 74.12Å 91.63Å 90.00° 108.83° 90.00°	Depositor
Resolution (Å)	86.73 – 1.21 86.73 – 1.21	Depositor EDS
% Data completeness (in resolution range)	97.1 (86.73-1.21) 97.3 (86.73-1.21)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.21Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.137 , 0.168 0.149 , 0.173	Depositor DCC
$R_{free}$ test set	29926 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7214e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, DMS, EDO, A1H91

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	0.59	1/2305 (0.0%)	0.89	0/3132
1	B	0.58	0/2301	0.90	2/3130 (0.1%)
1	C	0.59	0/2240	0.93	2/3045 (0.1%)
1	D	0.61	1/2286 (0.0%)	0.88	1/3108 (0.0%)
All	All	0.59	2/9132 (0.0%)	0.90	5/12415 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLN	N-CA	5.96	1.53	1.46
1	D	161	HIS	CE1-NE2	5.22	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	ASP	CA-CB-CG	8.27	120.87	112.60
1	B	75	ASP	CA-CB-CG	7.81	120.41	112.60
1	C	59	PHE	CA-CB-CG	-5.89	107.91	113.80
1	C	40	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	59	PHE	CA-CB-CG	-5.18	108.62	113.80

There are no chirality outliers.

There are no planarity outliers.

### 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	2218	0	2120	17	0
1	B	2223	0	2103	20	0
1	C	2171	0	2054	43	0
1	D	2208	0	2086	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	18	0	0
3	B	20	0	30	0	0
3	C	12	0	18	0	0
3	D	20	0	30	4	0
4	A	4	0	6	1	0
4	D	4	0	6	2	0
5	A	34	0	0	3	0
5	B	34	0	0	1	0
5	C	34	0	0	4	0
5	D	34	0	0	1	0
6	A	271	0	0	2	0
6	B	295	0	0	3	0
6	C	260	0	0	0	0
6	D	309	0	0	3	0
All	All	10167	0	8471	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (100) 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:C:148[B]:MET:HE2	1:C:219[B]:GLN:CG	1.34	1.57
1:C:148[B]:MET:CE	1:C:219[B]:GLN:HG3	1.12	1.53
1:C:148[B]:MET:CE	1:C:219[B]:GLN:CG	1.85	1.48
1:C:94:TRP:CZ2	1:C:242[B]:MET:HE3	1.77	1.20
1:C:148[B]:MET:HE1	1:C:219[B]:GLN:CG	1.71	1.12
1:C:94:TRP:CH2	1:C:242[B]:MET:HE3	1.86	1.09
1:A:166:LYS:HE2	1:A:230[A]:TYR:HE1	1.08	1.05
1:C:148[B]:MET:CE	1:C:219[B]:GLN:HG2	1.89	1.03
1:A:166:LYS:HE2	1:A:230[A]:TYR:CE1	1.95	1.00
1:B:77[A]:HIS:CD2	1:B:84:ARG:HD2	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201[A]:PRO:HG2	1:B:203[A]:ASN:OD1	1.61	0.99
1:C:94:TRP:CZ2	1:C:242[B]:MET:CE	2.51	0.92
1:C:53:LEU:HD21	1:C:76[B]:MET:CE	2.02	0.89
1:A:7:PHE:HZ	1:A:240:ARG:HD2	1.36	0.89
1:C:94:TRP:CH2	1:C:242[B]:MET:CE	2.57	0.86
1:C:148[B]:MET:HE1	1:C:219[B]:GLN:HG2	1.55	0.85
1:A:7:PHE:CZ	1:A:240:ARG:HD2	2.17	0.79
1:C:53:LEU:HD21	1:C:76[B]:MET:HE2	1.66	0.78
1:C:148[B]:MET:HE2	1:C:219[B]:GLN:CB	2.14	0.77
1:C:229:LEU:HD12	1:C:242[B]:MET:CE	2.15	0.76
1:D:77[B]:HIS:CD2	1:D:84:ARG:HD2	2.23	0.74
1:C:67:SER:HB2	5:C:305:A1H91:C8	2.18	0.73
1:C:94:TRP:HZ2	1:C:242[B]:MET:CE	2.01	0.72
1:C:168:LYS:HB2	1:C:231[B]:CYS:O	1.93	0.68
1:A:89[B]:GLN:NE2	1:A:91:HIS:HD1	1.92	0.67
1:C:197:LEU:HD22	5:C:305:A1H91:F29	1.85	0.66
1:C:229:LEU:HD12	1:C:242[B]:MET:HE2	1.79	0.65
1:C:53:LEU:HD21	1:C:76[B]:MET:HE1	1.79	0.65
1:A:166:LYS:CE	1:A:230[A]:TYR:HE1	1.98	0.64
1:C:51:TYR:CD1	1:C:76[B]:MET:HG3	2.33	0.64
1:B:110[B]:GLN:O	1:B:110[B]:GLN:HG3	1.97	0.64
1:C:229:LEU:HD12	1:C:242[B]:MET:HE1	1.79	0.63
1:B:47[A]:GLU:HB2	1:B:79:GLN:HB3	1.81	0.62
1:C:94:TRP:HH2	1:C:242[B]:MET:CE	2.12	0.62
1:B:26:LEU:CD2	1:B:255:ARG:HD3	2.30	0.61
1:D:253:ASP:CB	6:D:401:HOH:O	2.48	0.61
1:D:2:SER:HB3	1:D:10:ASP:OD2	2.02	0.59
1:D:127:PRO:HA	3:D:306:EDO:H12	1.83	0.59
1:B:26:LEU:HD23	1:B:255:ARG:HD3	1.85	0.58
1:A:231[A]:CYS:SG	1:A:240:ARG:HB2	2.43	0.58
1:B:137:GLU:HG2	1:B:194:ARG:HH12	1.69	0.57
1:D:147[A]:GLU:HG3	1:D:216:GLN:HG2	1.87	0.55
1:C:148[B]:MET:HE1	1:C:219[B]:GLN:CD	2.31	0.55
1:C:199:THR:HG21	5:C:305:A1H91:C5	2.36	0.54
1:C:73:PRO:HD2	1:C:76[B]:MET:HE3	1.91	0.53
1:C:148[B]:MET:HE2	1:C:219[B]:GLN:HG3	0.53	0.52
1:C:49:GLN:OE1	1:C:77:HIS:NE2	2.42	0.52
1:B:180[A]:GLU:HG3	1:B:183:LEU:HD12	1.90	0.52
1:B:255:ARG:HD2	6:B:526:HOH:O	2.09	0.52
1:C:99:ASP:OD1	1:D:33:HIS:HE1	1.94	0.51
1:C:94:TRP:HZ2	1:C:242[B]:MET:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:HB2	5:A:306:A1H91:O9	2.11	0.50
1:C:148[B]:MET:HE2	1:C:219[B]:GLN:HA	1.92	0.50
1:A:197[B]:LEU:HD13	5:A:306:A1H91:C27	2.42	0.48
1:D:43:LEU:HA	3:D:302:EDO:H12	1.95	0.48
1:B:252:PHE:HD1	1:B:252:PHE:HA	1.55	0.48
1:B:252:PHE:CE2	1:B:257:VAL:HG23	2.49	0.48
1:A:30:ILE:HA	1:A:249[B]:VAL:HG13	1.96	0.48
1:D:233:HIS:CG	4:D:307:DMS:H13	2.49	0.47
1:B:253:ASP:O	1:B:254:GLU:HB2	2.15	0.47
1:A:139:LEU:HD12	1:A:197[A]:LEU:HD21	1.96	0.47
1:B:77[A]:HIS:CD2	1:B:84:ARG:CD	2.85	0.47
1:C:51:TYR:CD1	1:C:76[B]:MET:CG	2.98	0.47
1:B:252:PHE:CZ	1:B:257:VAL:HG23	2.49	0.47
1:D:233:HIS:ND1	4:D:307:DMS:H22	2.30	0.47
1:D:49:GLN:HE22	1:D:79:GLN:HG3	1.80	0.46
1:A:7:PHE:HZ	1:A:240:ARG:HH11	1.62	0.46
1:C:47:GLU:HB2	1:C:79[A]:GLN:HB3	1.96	0.46
1:A:7:PHE:CE2	6:A:564:HOH:O	2.69	0.46
1:C:148[B]:MET:HE2	1:C:219[B]:GLN:CA	2.46	0.46
1:C:170:GLN:HE22	1:C:234:MET:HE3	1.81	0.45
1:A:197[A]:LEU:HD22	1:A:206:VAL:HG23	1.98	0.45
1:D:67:SER:HB2	5:D:308:A1H91:O9	2.16	0.45
1:C:194:ARG:HD3	1:C:207:LEU:CD1	2.46	0.45
1:C:50:GLY:O	1:C:76[A]:MET:HG3	2.17	0.44
1:C:229:LEU:CD1	1:C:242[B]:MET:HE1	2.45	0.44
1:A:78[A]:ILE:HG13	1:A:120:HIS:CD2	2.53	0.44
1:D:26:LEU:HD22	1:D:255:ARG:HD3	2.00	0.44
5:A:306:A1H91:N33	5:A:306:A1H91:F1	2.40	0.44
1:C:72:LEU:HD13	1:C:76[A]:MET:HE1	1.99	0.44
1:B:67:SER:HB2	5:B:307:A1H91:O9	2.18	0.43
1:D:80:GLY:O	3:D:302:EDO:H21	2.18	0.43
1:A:99:ASP:OD1	1:A:101:HIS:HD2	2.02	0.43
1:A:139:LEU:CD1	1:A:197[A]:LEU:HD21	2.48	0.43
1:B:180[B]:GLU:CD	6:B:401:HOH:O	2.62	0.43
1:C:167:TYR:CD1	1:C:234:MET:HA	2.54	0.43
1:D:127:PRO:C	3:D:306:EDO:H12	2.44	0.43
5:C:305:A1H91:F1	5:C:305:A1H91:N33	2.42	0.42
4:A:305:DMS:H22	6:A:629:HOH:O	2.19	0.42
1:B:134[A]:ASN:OD1	1:B:203[A]:ASN:ND2	2.52	0.42
1:C:194:ARG:HD3	1:C:207:LEU:HD13	2.02	0.42
1:C:53:LEU:HD11	1:C:76[B]:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110[B]:GLN:HE21	1:D:110[B]:GLN:HB3	1.63	0.42
1:D:233:HIS:HE1	6:D:658:HOH:O	2.03	0.42
1:B:255:ARG:CD	6:B:526:HOH:O	2.69	0.41
1:D:25:LEU:HB3	6:D:401:HOH:O	2.19	0.41
1:C:90:LEU:C	1:C:90:LEU:HD12	2.45	0.41
1:D:52:ASN:HA	1:D:178:ASN:HA	2.02	0.40
1:B:26:LEU:HD22	1:B:255:ARG:HD3	2.03	0.40
1:B:137:GLU:CG	1:B:194:ARG:HH12	2.34	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	276/263 (105%)	272 (99%)	4 (1%)	0	100	100
1	B	276/263 (105%)	271 (98%)	5 (2%)	0	100	100
1	C	269/263 (102%)	262 (97%)	7 (3%)	0	100	100
1	D	274/263 (104%)	267 (97%)	7 (3%)	0	100	100
All	All	1095/1052 (104%)	1072 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	251/235 (107%)	249 (99%)	2 (1%)	79	53
1	B	250/235 (106%)	247 (99%)	3 (1%)	67	33
1	C	243/235 (103%)	238 (98%)	5 (2%)	48	12
1	D	248/235 (106%)	243 (98%)	5 (2%)	50	14
All	All	992/940 (106%)	977 (98%)	15 (2%)	60	26

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

Mol	Chain	Res	Type
1	A	148	MET
1	A	156	ASP
1	B	89	GLN
1	B	156	ASP
1	B	252	PHE
1	C	76[A]	MET
1	C	76[B]	MET
1	C	82	GLN
1	C	89	GLN
1	C	156	ASP
1	D	3	LYS
1	D	49	GLN
1	D	89	GLN
1	D	156	ASP
1	D	262	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	79	GLN
1	A	110	GLN
1	B	96	ASN
1	B	111	HIS
1	B	244	ASN
1	B	250	GLN
1	C	13	ASN
1	C	82	GLN
1	C	170	GLN
1	C	250	GLN
1	D	13	ASN

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Mol	Chain	Res	Type
1	D	233	HIS
1	D	250	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	$\# Z  > 2$
3	EDO	C	303	-	3,3,3	0.37	0	2,2,2	0.85	0
3	EDO	B	302	-	3,3,3	0.35	0	2,2,2	0.67	0
3	EDO	C	302	-	3,3,3	0.07	0	2,2,2	0.06	0
3	EDO	D	303	-	3,3,3	0.11	0	2,2,2	0.48	0
5	A1H91	B	307	2	32,35,35	1.34	5 (15%)	41,49,49	1.61	9 (21%)
3	EDO	D	302	-	3,3,3	0.10	0	2,2,2	0.29	0
4	DMS	A	305	-	3,3,3	0.19	0	3,3,3	0.13	0
3	EDO	A	303	-	3,3,3	0.11	0	2,2,2	0.17	0
3	EDO	B	306	-	3,3,3	0.74	0	2,2,2	0.23	0
3	EDO	A	302	-	3,3,3	0.26	0	2,2,2	0.58	0
3	EDO	C	304	-	3,3,3	0.11	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1H91	A	306	2	32,35,35	1.28	4 (12%)	41,49,49	1.63	10 (24%)
3	EDO	D	304	-	3,3,3	0.04	0	2,2,2	0.35	0
4	DMS	D	307	-	3,3,3	0.33	0	3,3,3	0.03	0
5	A1H91	C	305	2	32,35,35	1.37	6 (18%)	41,49,49	1.76	14 (34%)
3	EDO	B	305	-	3,3,3	0.26	0	2,2,2	0.73	0
3	EDO	B	304	-	3,3,3	0.18	0	2,2,2	0.76	0
3	EDO	A	304	-	3,3,3	0.06	0	2,2,2	0.36	0
3	EDO	B	303	-	3,3,3	0.08	0	2,2,2	0.26	0
3	EDO	D	306	-	3,3,3	0.07	0	2,2,2	0.81	0
5	A1H91	D	308	2	32,35,35	1.22	3 (9%)	41,49,49	1.86	10 (24%)
3	EDO	D	305	-	3,3,3	0.32	0	2,2,2	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	303	-	-	0/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
5	A1H91	B	307	2	-	9/27/37/37	0/2/2/2
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	C	304	-	-	0/1/1/1	-
5	A1H91	A	306	2	-	7/27/37/37	0/2/2/2
3	EDO	D	304	-	-	1/1/1/1	-
5	A1H91	C	305	2	-	13/27/37/37	0/2/2/2
3	EDO	B	305	-	-	0/1/1/1	-
3	EDO	B	304	-	-	0/1/1/1	-
3	EDO	A	304	-	-	1/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	D	306	-	-	1/1/1/1	-
5	A1H91	D	308	2	-	9/27/37/37	0/2/2/2
3	EDO	D	305	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	307	A1H91	S31-N33	3.87	1.68	1.60
5	C	305	A1H91	S31-N33	3.74	1.67	1.60
5	D	308	A1H91	C30-S31	-3.56	1.73	1.79
5	A	306	A1H91	S31-N33	3.54	1.67	1.60
5	D	308	A1H91	S31-N33	3.46	1.67	1.60
5	C	305	A1H91	C20-N19	3.06	1.53	1.46
5	C	305	A1H91	C30-S31	-3.03	1.74	1.79
5	D	308	A1H91	C20-N19	2.98	1.53	1.46
5	B	307	A1H91	C20-N19	2.89	1.53	1.46
5	B	307	A1H91	C30-S31	-2.89	1.74	1.79
5	A	306	A1H91	C20-N19	2.81	1.53	1.46
5	C	305	A1H91	C18-C28	2.67	1.43	1.39
5	A	306	A1H91	C18-C28	2.59	1.43	1.39
5	B	307	A1H91	C18-C28	2.39	1.43	1.39
5	A	306	A1H91	C30-S31	-2.32	1.75	1.79
5	C	305	A1H91	C12-S11	2.08	1.82	1.77
5	C	305	A1H91	C3-C2	2.03	1.42	1.39
5	B	307	A1H91	C3-C2	2.01	1.42	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	308	A1H91	C28-C30-C2	5.84	120.77	116.67
5	B	307	A1H91	C28-C30-C2	4.58	119.88	116.67
5	C	305	A1H91	C13-C12-S11	3.89	126.28	113.33
5	C	305	A1H91	C28-C30-C2	3.70	119.27	116.67
5	D	308	A1H91	C2-C3-C10	3.55	122.34	116.14
5	A	306	A1H91	C13-C12-S11	3.34	124.47	113.33
5	D	308	A1H91	C26-C27-C20	3.27	128.92	116.21
5	A	306	A1H91	C28-C30-C2	3.26	118.95	116.67
5	D	308	A1H91	C6-C5-N4	-3.13	103.06	111.49
5	B	307	A1H91	C26-C27-C20	3.11	128.30	116.21
5	C	305	A1H91	C25-C26-C27	3.08	130.85	117.44
5	C	305	A1H91	C6-C5-N4	-3.07	103.23	111.49
5	B	307	A1H91	C13-C12-S11	3.01	123.37	113.33
5	A	306	A1H91	C2-C3-C10	3.01	121.39	116.14
5	C	305	A1H91	O32-S31-O34	2.94	123.59	118.76
5	A	306	A1H91	C26-C27-C20	2.93	127.58	116.21
5	B	307	A1H91	C25-C26-C27	2.73	129.35	117.44
5	D	308	A1H91	O34-S31-C30	2.66	111.25	107.30
5	B	307	A1H91	C2-C3-C10	2.65	120.75	116.14
5	D	308	A1H91	C2-C3-N4	-2.56	114.30	122.55
5	B	307	A1H91	O32-S31-N33	-2.55	103.59	107.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	305	A1H91	C22-C21-C20	2.53	126.02	116.21
5	B	307	A1H91	C12-C13-C14	2.48	120.41	111.83
5	D	308	A1H91	C25-C26-C27	2.45	128.14	117.44
5	B	307	A1H91	O32-S31-O34	2.44	122.77	118.76
5	C	305	A1H91	C2-C3-C10	2.44	120.39	116.14
5	A	306	A1H91	F29-C28-C30	-2.43	116.15	120.70
5	A	306	A1H91	O32-S31-N33	-2.43	103.76	107.36
5	C	305	A1H91	C26-C27-C20	2.43	125.64	116.21
5	D	308	A1H91	O32-S31-O34	2.42	122.74	118.76
5	C	305	A1H91	C12-S11-C10	2.40	118.10	108.15
5	C	305	A1H91	C12-C13-C14	2.38	120.06	111.83
5	A	306	A1H91	C5-N4-C3	-2.37	109.82	121.23
5	A	306	A1H91	C12-C13-C14	2.37	120.03	111.83
5	A	306	A1H91	O32-S31-C30	2.32	110.75	107.30
5	C	305	A1H91	O32-S31-N33	-2.22	104.07	107.36
5	C	305	A1H91	O34-S31-N33	-2.22	104.07	107.36
5	C	305	A1H91	F29-C28-C30	-2.11	116.75	120.70
5	C	305	A1H91	C24-C25-C26	2.09	128.41	117.47
5	D	308	A1H91	O32-S31-C30	-2.09	104.19	107.30
5	D	308	A1H91	O32-S31-N33	-2.08	104.28	107.36
5	B	307	A1H91	F29-C28-C30	-2.07	116.82	120.70
5	A	306	A1H91	C25-C26-C27	2.03	126.29	117.44

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	306	A1H91	S11-C12-C13-C14
5	A	306	A1H91	C2-C30-S31-O34
5	A	306	A1H91	C2-C30-S31-N33
5	A	306	A1H91	C2-C3-N4-C5
5	B	307	A1H91	C2-C30-S31-O34
5	B	307	A1H91	C2-C30-S31-N33
5	B	307	A1H91	C10-C18-N19-C20
5	B	307	A1H91	C2-C3-N4-C5
5	C	305	A1H91	S11-C12-C13-C14
5	C	305	A1H91	C2-C30-S31-O34
5	C	305	A1H91	C28-C30-S31-O34
5	C	305	A1H91	C28-C30-S31-O32
5	C	305	A1H91	C2-C30-S31-N33
5	C	305	A1H91	C2-C3-N4-C5
5	D	308	A1H91	C2-C30-S31-N33

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Mol	Chain	Res	Type	Atoms
5	D	308	A1H91	C10-C18-N19-C20
5	D	308	A1H91	N4-C5-C6-C7
5	D	308	A1H91	C28-C30-S31-N33
5	D	308	A1H91	C2-C3-N4-C5
3	A	304	EDO	O1-C1-C2-O2
5	A	306	A1H91	C6-C7-C8-O9
5	A	306	A1H91	C6-C5-N4-C3
3	D	306	EDO	O1-C1-C2-O2
5	C	305	A1H91	C18-C10-S11-O16
5	C	305	A1H91	C27-C20-N19-C18
5	C	305	A1H91	C21-C20-N19-C18
3	A	302	EDO	O1-C1-C2-O2
5	A	306	A1H91	C28-C30-S31-O34
5	C	305	A1H91	C2-C30-S31-O32
5	D	308	A1H91	C2-C30-S31-O34
5	C	305	A1H91	N4-C5-C6-C7
5	B	307	A1H91	N4-C5-C6-C7
3	B	302	EDO	O1-C1-C2-O2
3	B	306	EDO	O1-C1-C2-O2
3	D	305	EDO	O1-C1-C2-O2
5	C	305	A1H91	C6-C7-C8-O9
5	D	308	A1H91	C6-C7-C8-O9
3	D	304	EDO	O1-C1-C2-O2
5	B	307	A1H91	C28-C18-N19-C20
5	D	308	A1H91	C28-C18-N19-C20
5	B	307	A1H91	C6-C5-N4-C3
5	B	307	A1H91	C6-C7-C8-O9
5	B	307	A1H91	C28-C30-S31-N33
5	C	305	A1H91	C28-C30-S31-N33
5	D	308	A1H91	C5-C6-C7-C8

There are no ring outliers.

8 monomers are involved in 16 short contacts:

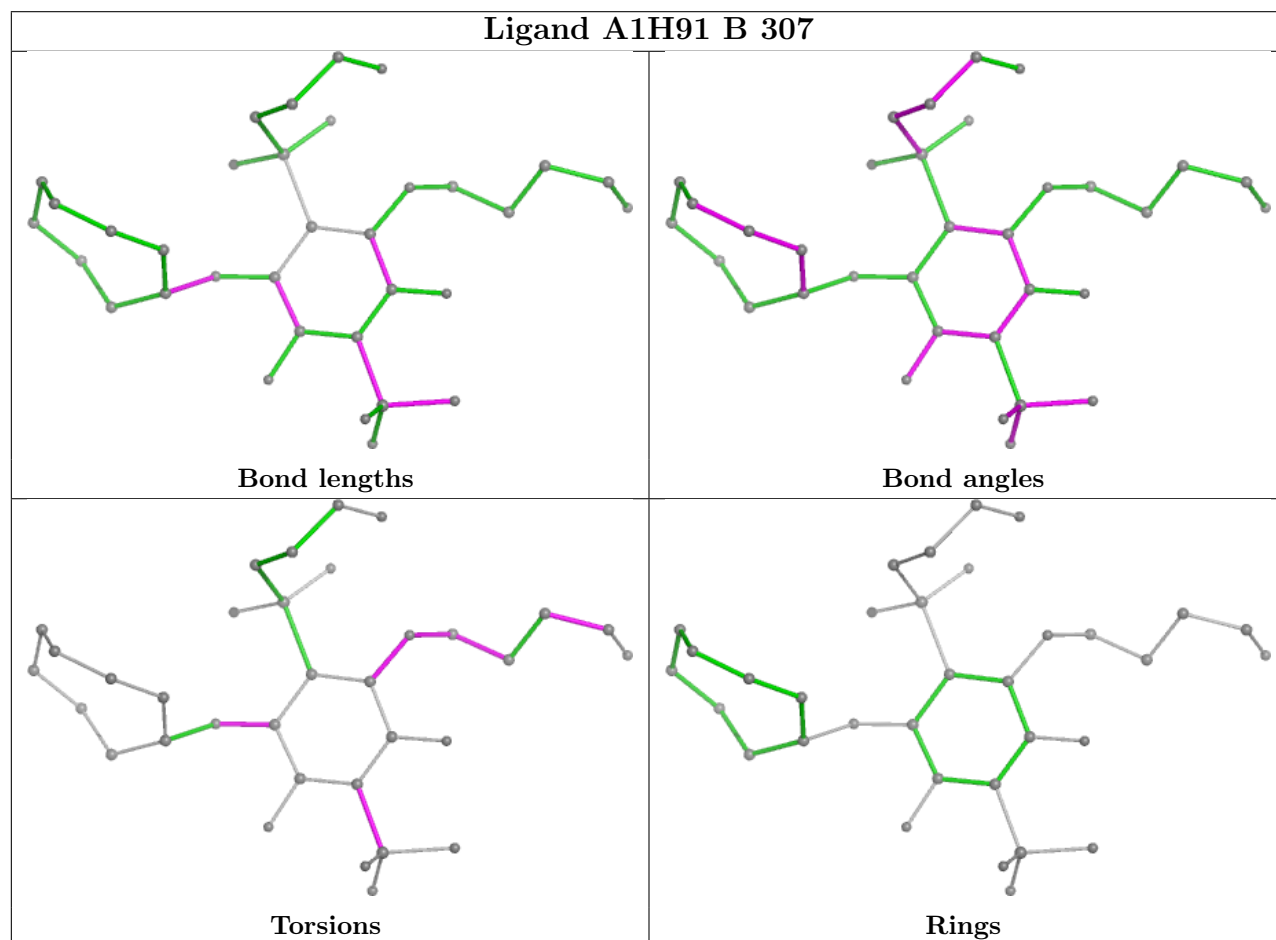
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	307	A1H91	1	0
3	D	302	EDO	2	0
4	A	305	DMS	1	0
5	A	306	A1H91	3	0
4	D	307	DMS	2	0
5	C	305	A1H91	4	0
3	D	306	EDO	2	0

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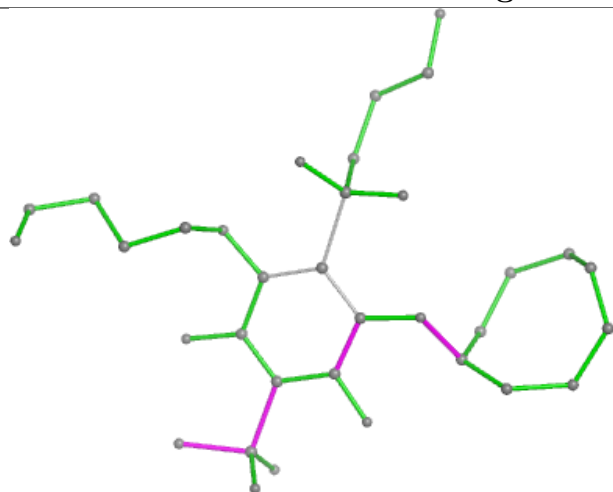
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	308	A1H91	1	0

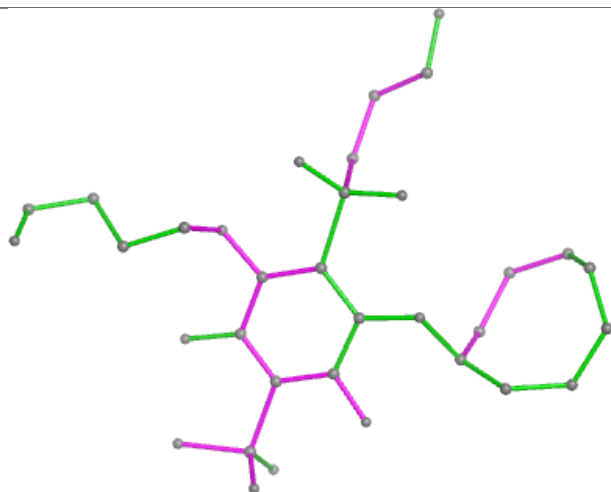
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



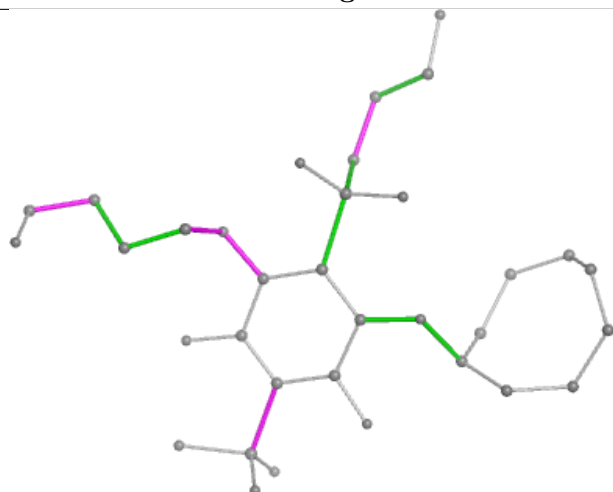
## Ligand A1H91 A 306



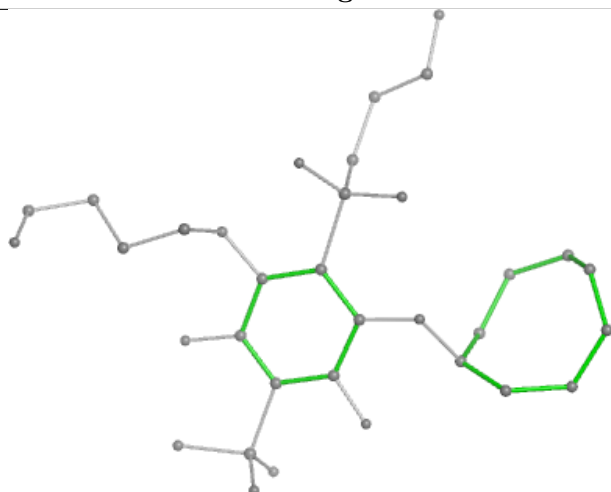
Bond lengths



Bond angles

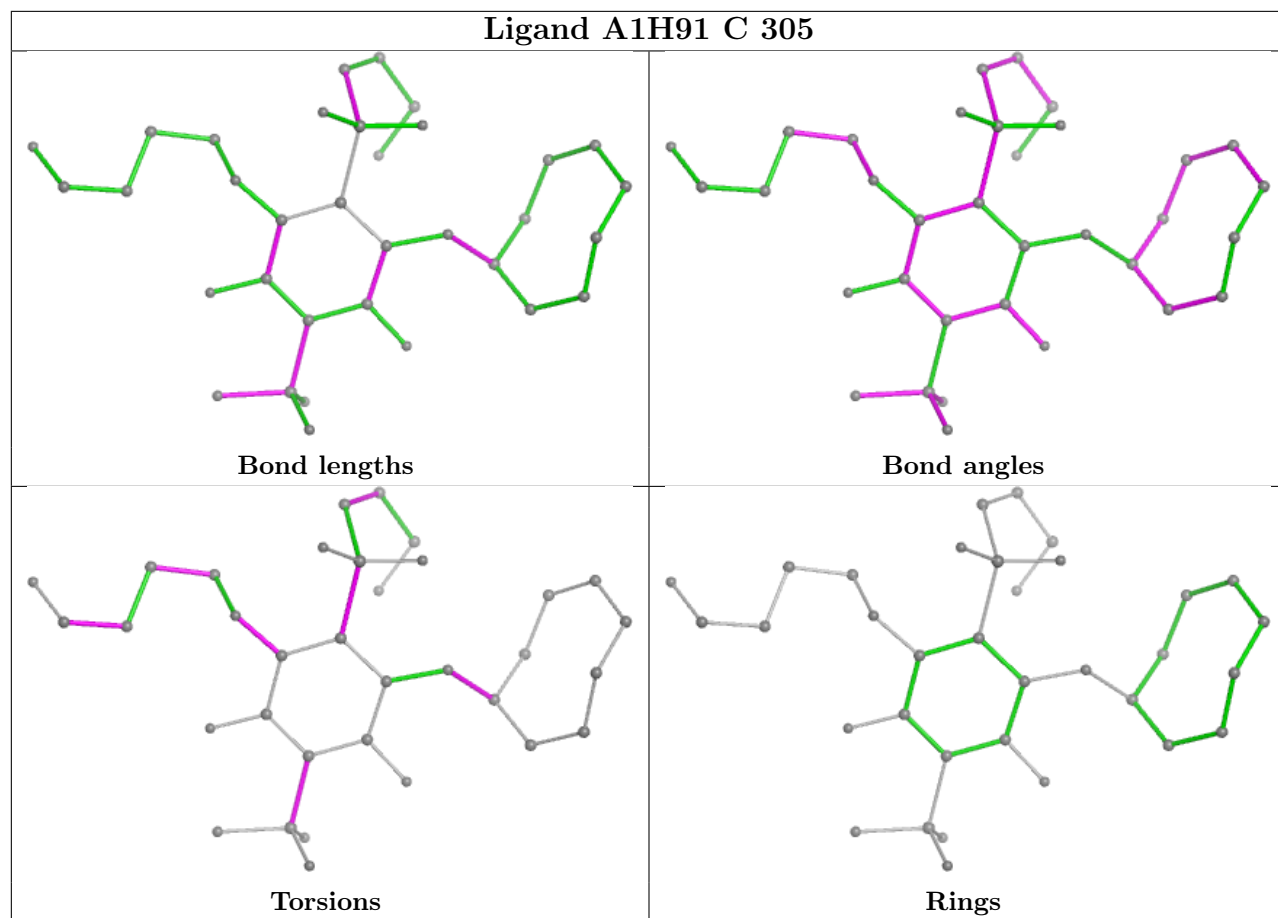


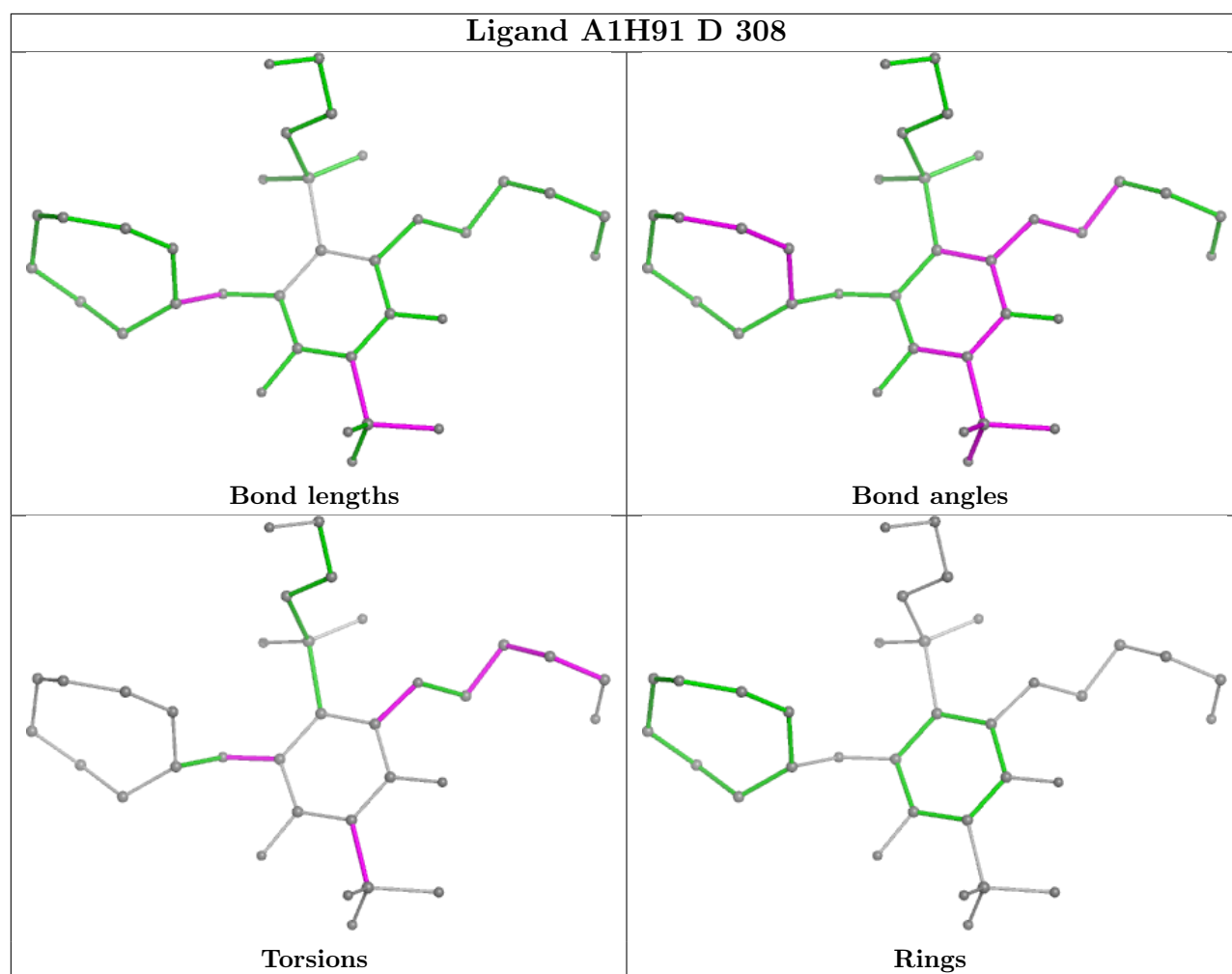
Torsions



Rings

## Ligand A1H91 C 305





## 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	261/263 (99%)	0.20	10 (3%) 44 45	7, 20, 35, 68	18 (6%)
1	B	262/263 (99%)	0.06	10 (3%) 44 45	8, 17, 34, 60	16 (6%)
1	C	260/263 (98%)	0.54	19 (7%) 22 21	8, 22, 38, 71	14 (5%)
1	D	262/263 (99%)	-0.03	11 (4%) 41 42	8, 17, 31, 52	15 (5%)
All	All	1045/1052 (99%)	0.19	50 (4%) 36 37	7, 18, 35, 71	63 (6%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	9.5
1	C	235	ASP	8.3
1	C	55	ALA	6.0
1	C	7	PHE	5.9
1	D	252[A]	PHE	5.7
1	A	7	PHE	4.6
1	C	230	TYR	4.4
1	D	263	GLN	4.4
1	C	148[A]	MET	3.9
1	D	2	SER	3.8
1	C	262	SER	3.6
1	C	173	PHE	3.5
1	C	57	LYS	3.5
1	B	81	LEU	3.4
1	C	56	ASN	3.3
1	B	2	SER	3.3
1	D	262	SER	3.1
1	C	54[A]	SER	3.1
1	C	61	LEU	2.9
1	A	253	ASP	2.8
1	B	255	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	137	GLU	2.7
1	D	253	ASP	2.6
1	B	7	PHE	2.6
1	D	98	ASN	2.5
1	C	165	VAL	2.5
1	D	49	GLN	2.4
1	A	148	MET	2.4
1	A	262[A]	SER	2.4
1	C	253	ASP	2.3
1	C	174	VAL	2.3
1	A	3	LYS	2.3
1	D	7	PHE	2.2
1	B	80	GLY	2.2
1	D	3	LYS	2.2
1	A	219	GLN	2.2
1	B	253	ASP	2.2
1	B	3	LYS	2.2
1	A	55	ALA	2.2
1	C	52	ASN	2.1
1	B	164	HIS	2.1
1	D	84	ARG	2.1
1	C	8	GLY	2.1
1	C	130	SER	2.1
1	A	8	GLY	2.1
1	A	252	PHE	2.0
1	C	9	PRO	2.0
1	A	136	SER	2.0
1	D	75	ASP	2.0
1	C	53	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

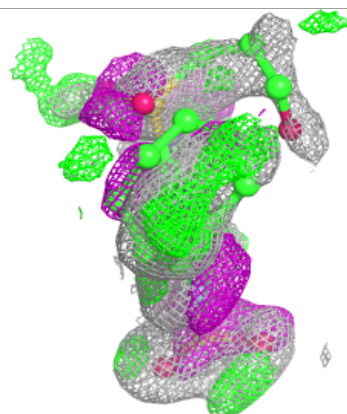
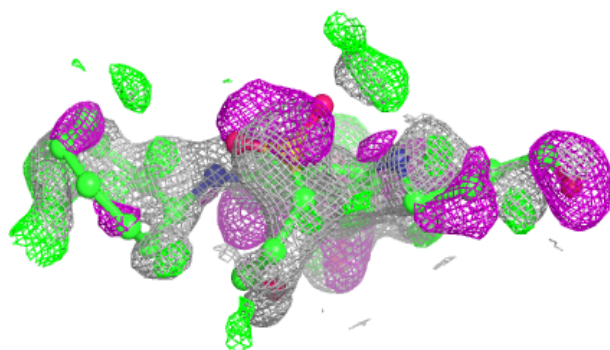
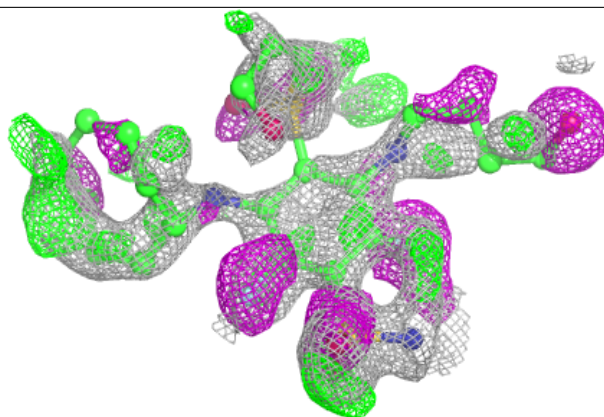
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	DMS	D	307	4/4	0.56	0.22	58,70,79,99	0
3	EDO	A	304	4/4	0.72	0.22	41,48,53,56	0
3	EDO	B	306	4/4	0.74	0.18	61,75,79,83	0
3	EDO	D	302	4/4	0.75	0.17	30,33,34,40	0
3	EDO	D	304	4/4	0.79	0.19	24,34,38,57	0
5	A1H91	C	305	34/34	0.79	0.22	22,42,72,76	0
5	A1H91	B	307	34/34	0.81	0.21	15,32,49,53	0
3	EDO	B	303	4/4	0.81	0.17	30,43,46,49	0
3	EDO	C	304	4/4	0.83	0.15	28,36,37,55	0
3	EDO	A	303	4/4	0.84	0.14	35,44,58,63	0
5	A1H91	A	306	34/34	0.84	0.20	22,41,64,65	0
3	EDO	B	304	4/4	0.85	0.15	28,48,59,73	0
3	EDO	D	306	4/4	0.86	0.13	27,35,37,42	0
4	DMS	A	305	4/4	0.87	0.15	59,81,89,91	0
3	EDO	C	302	4/4	0.89	0.11	23,28,30,31	0
5	A1H91	D	308	34/34	0.90	0.16	16,32,58,64	0
3	EDO	A	302	4/4	0.91	0.11	34,40,42,42	0
3	EDO	D	305	4/4	0.91	0.12	31,35,44,47	0
3	EDO	B	302	4/4	0.91	0.11	29,38,45,50	0
3	EDO	C	303	4/4	0.92	0.11	26,26,28,32	0
3	EDO	B	305	4/4	0.94	0.09	22,27,28,31	0
3	EDO	D	303	4/4	0.95	0.07	38,40,44,53	0
2	ZN	C	301	1/1	1.00	0.01	15,15,15,15	0
2	ZN	D	301	1/1	1.00	0.01	12,12,12,12	0
2	ZN	A	301	1/1	1.00	0.01	13,13,13,13	0
2	ZN	B	301	1/1	1.00	0.01	11,11,11,11	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.

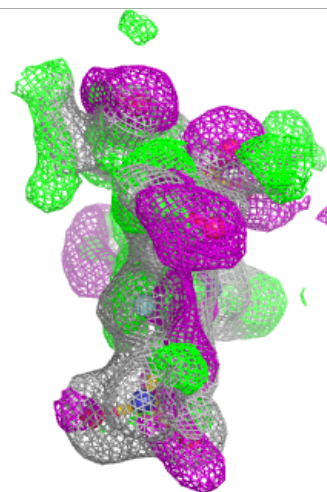
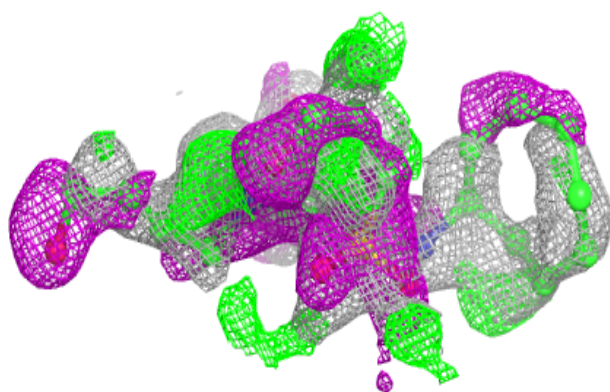
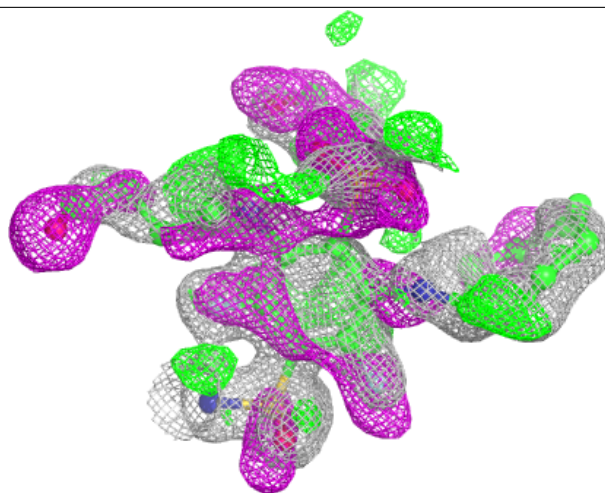
**Electron density around A1H91 C 305:**

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



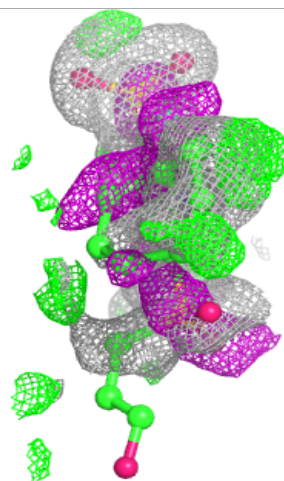
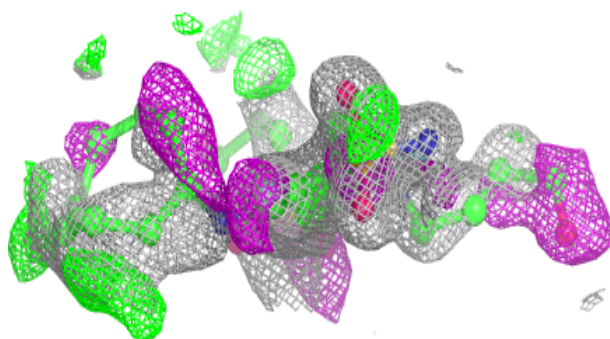
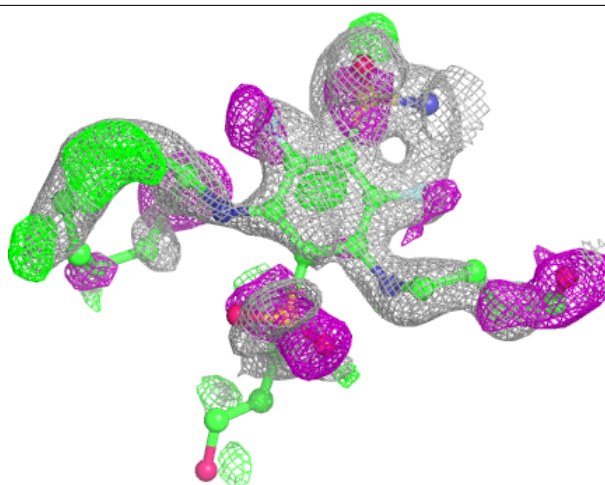
**Electron density around A1H91 B 307:**

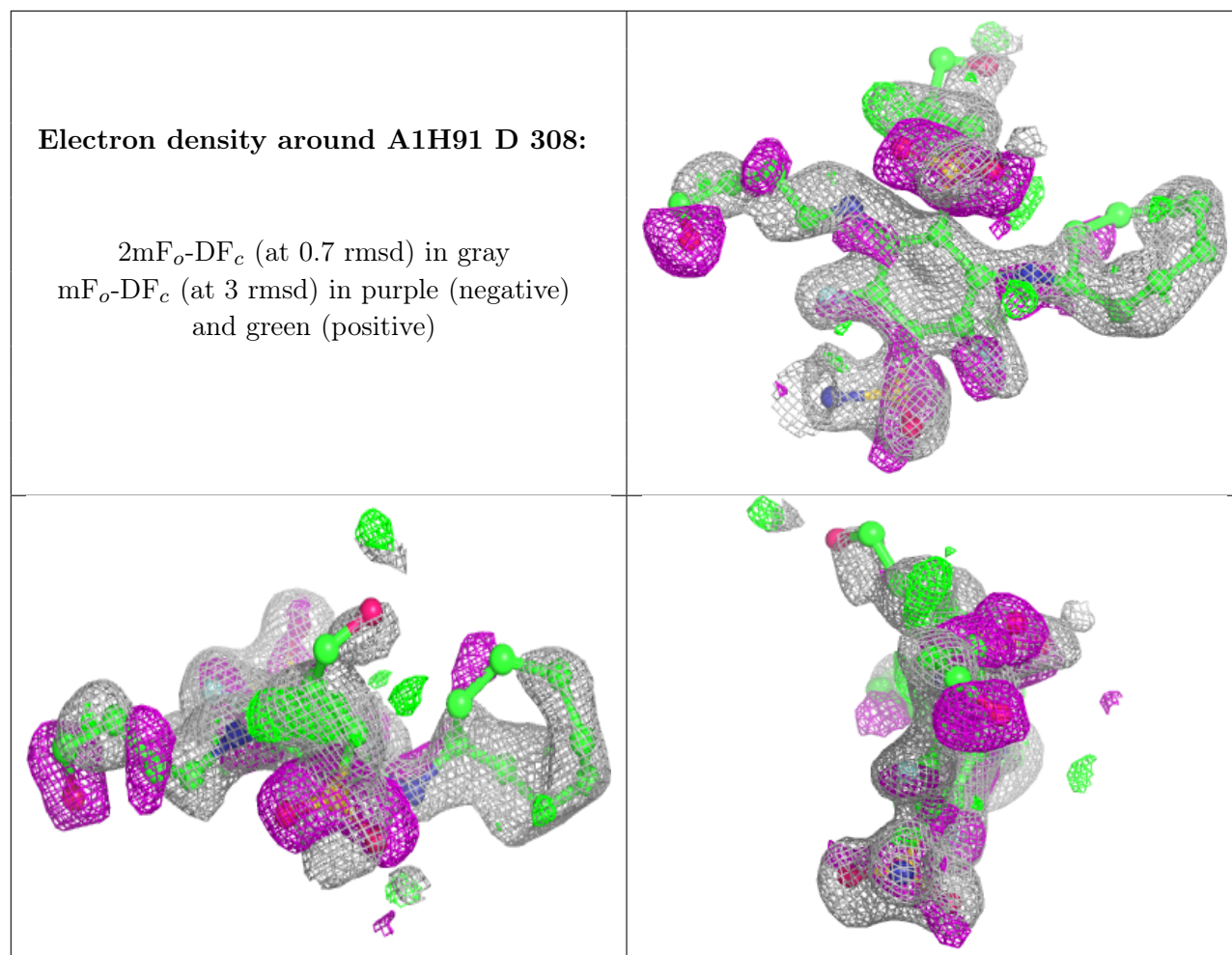
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1H91 A 306:**

$2mF_o-DF_c$  (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.