



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 12:53 PM EDT

PDB ID : 7JXW  
Title : EGFR kinase (T790M/V948R) in complex with osimertinib and JBJ-09-063  
Authors : Beyett, T.S.; Eck, M.J.  
Deposited on : 2020-08-28  
Resolution : 2.50 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 : 2.23.1  
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) : 2.23.1

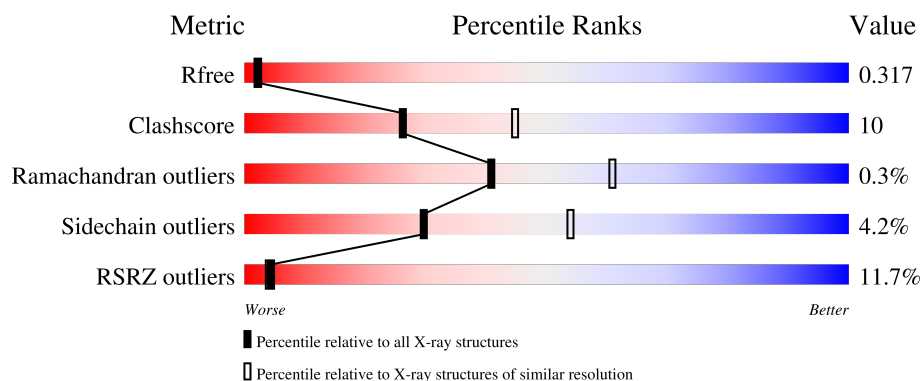
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	331	<div> <div>8%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>13%</div> </div>
1	B	331	<div> <div>6%</div> <div>67%</div> <div>19%</div> <div>•</div> <div>12%</div> </div>
1	C	331	<div> <div>14%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
1	D	331	<div> <div>14%</div> <div>67%</div> <div>19%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9737 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.

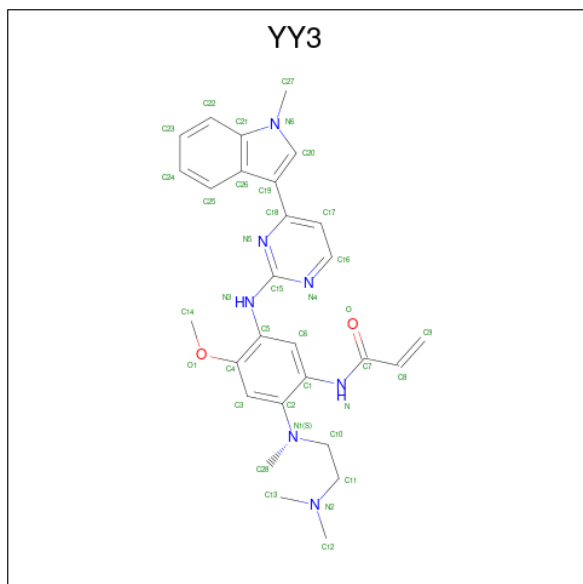
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	287	Total	C	N	O	S	0	1	0
			2323	1495	393	415	20			
1	A	288	Total	C	N	O	S	0	0	0
			2323	1494	394	416	19			
1	C	293	Total	C	N	O	S	0	1	0
			2369	1522	403	424	20			
1	B	291	Total	C	N	O	S	0	1	0
			2353	1511	400	422	20			

There are 20 discrepancies between the modelled and reference sequences:

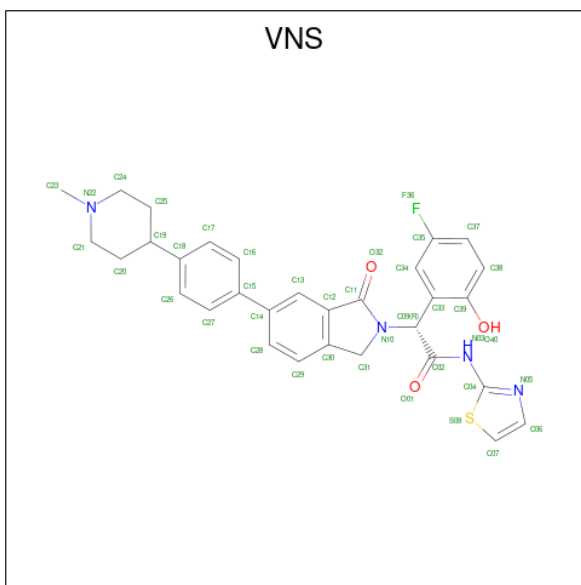
Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is N-(2-{[2-(dimethylamino)ethyl](methyl)amino}-4-methoxy-5-{[4-(1-methyl-1H-indol-3-yl)pyrimidin-2-yl]amino}phenyl)prop-2-enamide (three-letter code: YY3) (formula: C<sub>28</sub>H<sub>33</sub>N<sub>7</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			37	28	7	2		
2	A	1	Total	C	N	O	0	0
			37	28	7	2		
2	C	1	Total	C	N	O	0	0
			37	28	7	2		
2	B	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 3 is (2R)-2-(5-fluoro-2-hydroxyphenyl)-2-{6-[4-(1-methylpiperidin-4-yl)phenyl]-1-oxo-1,3-dihydro-2H-isoindol-2-yl}-N-(1,3-thiazol-2-yl)acetamide (three-letter code: VNS) (formula: C<sub>31</sub>H<sub>29</sub>FN<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	A	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	C	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	B	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0

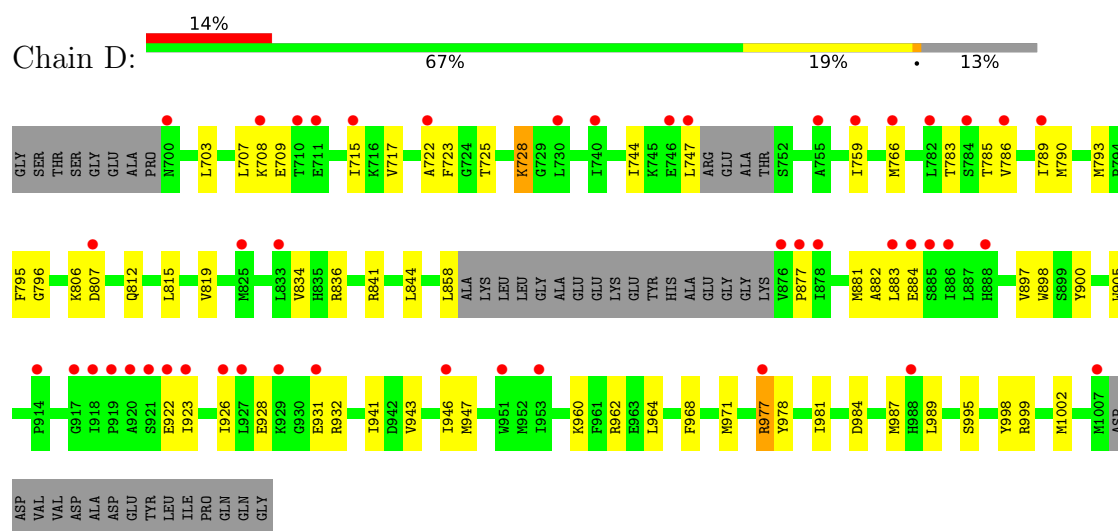
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	8	Total O 8 8	0	0
4	A	20	Total O 20 20	0	0
4	C	13	Total O 13 13	0	0
4	B	20	Total O 20 20	0	0

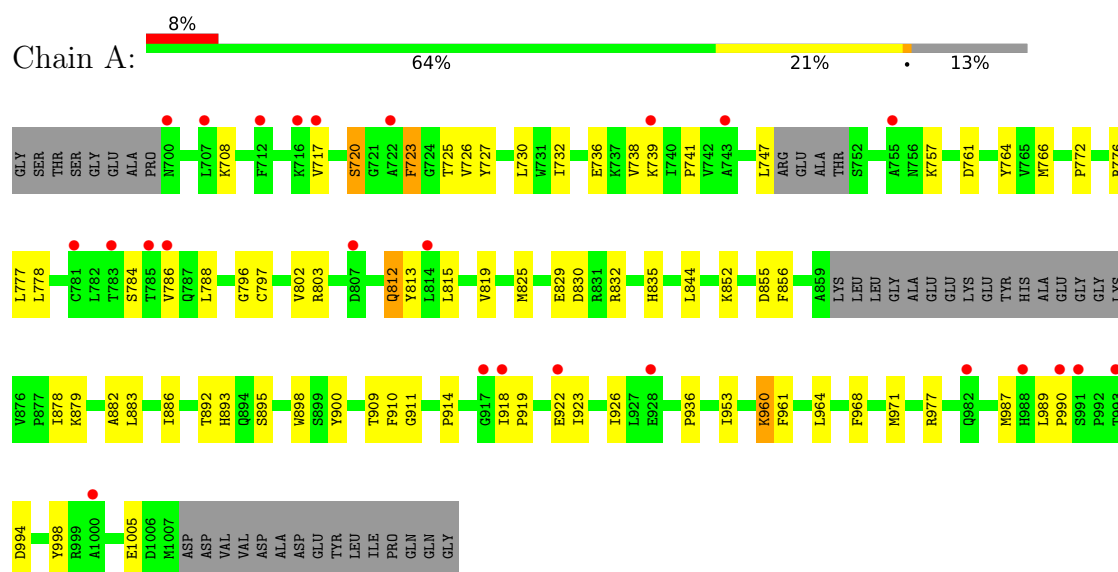
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Epidermal growth factor receptor

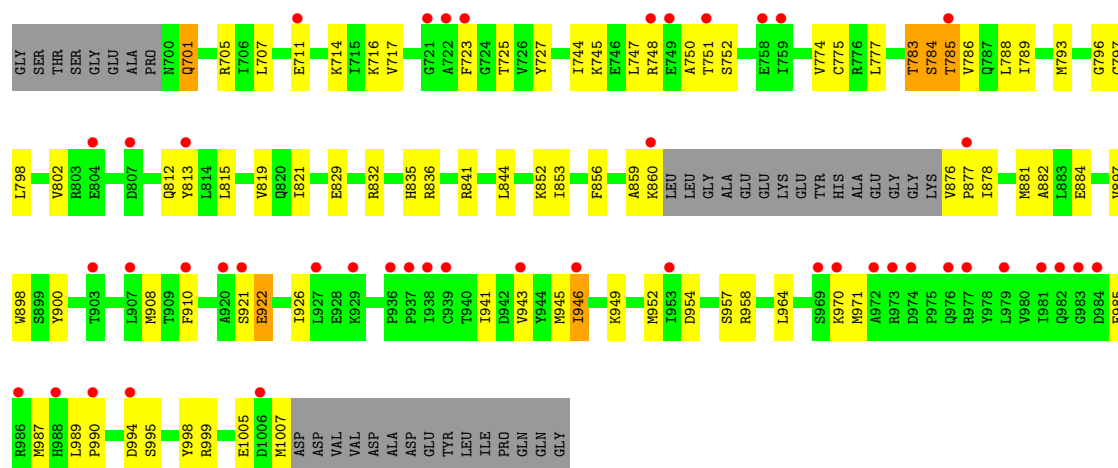


#### • Molecule 1: Epidermal growth factor receptor

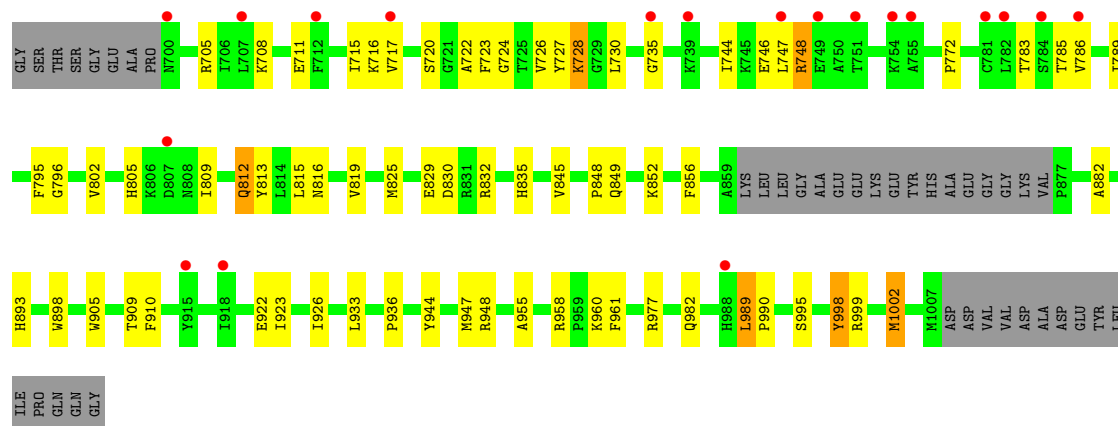


#### • Molecule 1: Epidermal growth factor receptor





● Molecule 1: Epidermal growth factor receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.25Å 73.06Å 119.07Å 90.00° 118.57° 90.00°	Depositor
Resolution (Å)	65.64 – 2.50 65.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (65.64-2.50) 97.7 (65.64-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.274 , 0.319 0.274 , 0.317	Depositor DCC
$R_{free}$ test set	2080 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	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 76.62 % 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 1.0027e-06. 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: VNS, YY3

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	0.49	0/2374	0.69	0/3209
1	B	0.53	0/2408	0.72	0/3254
1	C	0.48	0/2424	0.68	0/3276
1	D	0.44	0/2377	0.64	1/3212 (0.0%)
All	All	0.49	0/9583	0.68	1/12951 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	977	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2323	0	2364	51	0
1	B	2353	0	2397	57	0
1	C	2369	0	2418	53	0
1	D	2323	0	2368	47	0
2	A	37	0	32	4	0
2	B	37	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	37	0	31	5	0
2	D	37	0	32	3	0
3	A	40	0	0	1	0
3	B	40	0	0	0	0
3	C	40	0	0	2	0
3	D	40	0	0	3	0
4	A	20	0	0	2	0
4	B	20	0	0	3	0
4	C	13	0	0	1	0
4	D	8	0	0	4	0
All	All	9737	0	9674	202	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 10.

All (202) 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:A:812:GLN:HG2	1:A:989:LEU:HG	1.54	0.89
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.63	0.80
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.63	0.78
1:A:977:ARG:HH12	1:B:926:ILE:HG21	1.53	0.73
1:B:716:LYS:HG2	1:B:717:VAL:N	2.05	0.71
1:B:812:GLN:HG2	1:B:989:LEU:HG	1.71	0.71
1:A:829:GLU:OE2	1:A:960:LYS:NZ	2.24	0.70
1:B:802:VAL:HG12	1:B:910:PHE:HA	1.74	0.69
1:B:744:ILE:HG12	1:B:789:ILE:HG13	1.75	0.67
1:C:852:LYS:NZ	1:C:1005:GLU:OE2	2.27	0.66
1:C:748:ARG:HH21	1:B:832:ARG:HD3	1.61	0.66
1:B:922:GLU:O	1:B:926:ILE:HG23	1.95	0.66
1:D:841:ARG:HH12	1:D:877:PRO:HB3	1.61	0.66
1:A:852:LYS:NZ	1:A:1005:GLU:OE2	2.30	0.65
1:A:812:GLN:HG2	1:A:989:LEU:CG	2.28	0.64
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.77	0.64
1:C:783:THR:OG1	1:C:784:SER:N	2.30	0.64
1:B:909:THR:HG22	1:B:936:PRO:HB3	1.79	0.64
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.33	0.63
1:C:796:GLY:HA2	2:C:1301:YY3:C6	2.28	0.63
1:A:813:TYR:OH	1:A:990:PRO:HD3	2.00	0.62
1:B:716:LYS:HG2	1:B:717:VAL:H	1.65	0.60
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ILE:O	1:A:926:ILE:HG12	2.02	0.59
1:D:900:TYR:CE2	1:D:964:LEU:HD13	2.39	0.57
1:C:922:GLU:O	1:C:926:ILE:HG23	2.04	0.57
1:A:977:ARG:NH1	1:B:926:ILE:HG21	2.19	0.57
1:B:735:GLY:N	4:B:1403:HOH:O	2.37	0.57
1:C:716:LYS:NZ	2:C:1301:YY3:H2	2.19	0.57
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.39	0.57
1:D:977:ARG:HH12	1:C:926:ILE:HB	1.69	0.56
1:D:725:THR:OG1	1:A:832:ARG:NH2	2.38	0.56
1:A:878:ILE:HD12	1:A:886:ILE:HG23	1.86	0.56
1:A:855:ASP:OD2	2:A:1301:YY3:H33	2.06	0.56
1:D:931:GLU:HG2	1:D:932:ARG:N	2.20	0.56
1:C:798:LEU:O	1:C:802:VAL:HG23	2.05	0.56
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.33	0.56
1:B:795:PHE:HB2	1:B:845:VAL:O	2.06	0.56
1:C:747:LEU:HD12	1:C:786:VAL:HB	1.88	0.56
1:C:841:ARG:HH12	1:C:877:PRO:HB3	1.71	0.55
1:C:829:GLU:O	1:C:832:ARG:N	2.29	0.55
1:C:745:LYS:NZ	3:C:1302:VNS:O32	2.34	0.54
1:A:815:LEU:O	1:A:819:VAL:HG23	2.08	0.54
1:A:772:PRO:O	1:A:852:LYS:HE3	2.08	0.54
1:C:707:LEU:HD12	1:C:789:ILE:HD13	1.89	0.54
1:B:923:ILE:O	1:B:926:ILE:HG12	2.09	0.53
1:A:990:PRO:HB2	1:A:994:ASP:HB2	1.91	0.53
1:D:707:LEU:HD12	1:D:789:ILE:HD13	1.91	0.53
1:D:977:ARG:HD2	1:D:978:TYR:CE2	2.44	0.53
1:D:923:ILE:O	1:D:926:ILE:HG12	2.09	0.52
1:B:829:GLU:OE2	1:B:960:LYS:NZ	2.42	0.52
1:D:995:SER:O	1:D:999:ARG:HG3	2.10	0.52
1:B:705:ARG:NH2	1:B:711:GLU:OE2	2.42	0.52
1:B:726:VAL:HG21	2:B:1301:YY3:C21	2.39	0.52
1:A:717:VAL:HG22	1:A:727:TYR:CE2	2.45	0.51
1:A:909:THR:HG22	1:A:936:PRO:HB3	1.92	0.51
1:A:900:TYR:CE2	1:A:964:LEU:HD13	2.46	0.51
1:A:922:GLU:O	1:A:926:ILE:HG23	2.09	0.51
1:B:802:VAL:CG1	1:B:910:PHE:HA	2.40	0.51
1:A:720:SER:HA	1:A:725:THR:HA	1.92	0.50
1:A:796:GLY:HA2	2:A:1301:YY3:C5	2.42	0.50
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.93	0.50
1:A:909:THR:CG2	1:A:936:PRO:HB3	2.42	0.49
1:C:836:ARG:NH2	4:C:1402:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:GLU:O	1:D:926:ILE:HG23	2.12	0.49
1:A:919:PRO:HD2	1:A:922:GLU:OE1	2.12	0.49
1:B:747:LEU:O	1:B:785:THR:HG23	2.12	0.49
1:A:825:MET:HB3	1:A:961:PHE:CE2	2.47	0.49
1:D:715:ILE:HG12	1:D:728:LYS:O	2.12	0.48
1:D:747:LEU:HD12	1:D:786:VAL:HB	1.95	0.48
1:D:928:GLU:O	4:D:1401:HOH:O	2.20	0.48
1:C:796:GLY:HA2	2:C:1301:YY3:C1	2.44	0.48
1:D:960:LYS:HG3	1:D:962:ARG:NH1	2.27	0.48
1:A:730:LEU:HD13	1:A:739:LYS:HB3	1.95	0.48
1:B:829:GLU:HA	1:B:893:HIS:NE2	2.29	0.48
1:C:748:ARG:NH2	1:B:832:ARG:HD3	2.27	0.48
1:C:943:VAL:HG22	1:C:971:MET:HE1	1.96	0.48
2:D:1301:YY3:N5	2:D:1301:YY3:H25	2.29	0.48
1:A:726:VAL:HG21	2:A:1301:YY3:C21	2.44	0.48
1:D:717:VAL:HG11	1:A:830:ASP:HB3	1.96	0.47
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.14	0.47
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.49	0.47
1:C:908[B]:MET:SD	1:C:943:VAL:HG11	2.54	0.47
1:B:849:GLN:HG2	1:B:990:PRO:HG3	1.96	0.47
1:D:796:GLY:HA2	2:D:1301:YY3:C6	2.44	0.47
1:C:725:THR:OG1	1:B:832:ARG:NH2	2.47	0.47
1:D:834:VAL:HG12	1:D:836:ARG:HG3	1.96	0.47
1:C:995:SER:O	1:C:999:ARG:HG3	2.15	0.47
1:A:717:VAL:HG22	1:A:727:TYR:CD2	2.50	0.47
1:D:793:MET:HG3	1:D:844:LEU:HD13	1.96	0.47
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.15	0.47
1:D:905:TRP:HB2	1:D:947:MET:HE3	1.96	0.47
1:D:946:ILE:HG21	1:D:968:PHE:CE1	2.49	0.47
1:A:835:HIS:CD2	1:A:856:PHE:HB3	2.50	0.47
3:C:1302:VNS:O01	3:C:1302:VNS:S08	2.72	0.47
1:B:715:ILE:HD11	1:B:728:LYS:HZ2	1.80	0.47
1:B:829:GLU:HA	1:B:893:HIS:CD2	2.50	0.47
1:C:954:ASP:OD2	1:C:957:SER:OG	2.28	0.47
1:A:953:ILE:HG22	1:B:982:GLN:OE1	2.15	0.46
1:A:892:THR:N	1:A:895:SER:OG	2.45	0.46
1:D:759:ILE:HG12	3:D:1302:VNS:C27	2.46	0.46
1:B:796:GLY:HA2	2:B:1301:YY3:C5	2.46	0.46
1:D:977:ARG:HH12	1:C:926:ILE:CB	2.29	0.45
1:B:989:LEU:HD13	1:B:990:PRO:HD2	1.98	0.45
1:D:795:PHE:HE2	1:D:1002:MET:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LYS:HD3	1:A:914:PRO:O	2.17	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.51	0.45
1:C:884:GLU:OE1	1:C:958:ARG:NH2	2.41	0.45
1:D:715:ILE:HD11	1:D:728:LYS:HE2	1.98	0.45
1:C:717:VAL:HG11	1:B:830:ASP:HB3	1.98	0.45
1:D:981:ILE:O	1:D:984:ASP:HB2	2.16	0.45
1:C:797:CYS:HA	1:C:844:LEU:HA	1.98	0.45
1:D:943:VAL:HG22	1:D:971:MET:SD	2.57	0.45
1:A:835:HIS:O	4:A:1401:HOH:O	2.21	0.45
1:B:815:LEU:O	1:B:819:VAL:HG23	2.16	0.45
1:C:774:VAL:HG12	1:C:775:CYS:O	2.16	0.44
1:B:717:VAL:HG22	1:B:727:TYR:CE1	2.52	0.44
1:D:884:GLU:N	4:D:1406:HOH:O	2.51	0.44
1:C:701:GLN:H	1:C:701:GLN:HG2	1.40	0.44
1:C:802:VAL:CG1	1:C:910:PHE:HA	2.48	0.44
1:B:723:PHE:O	1:B:748:ARG:N	2.44	0.44
1:C:949:LYS:HA	1:C:952:MET:HG3	2.00	0.44
1:B:989:LEU:HD22	1:B:990:PRO:HD2	2.00	0.44
1:D:815:LEU:O	1:D:819:VAL:HG23	2.18	0.44
2:A:1301:YY3:H5	2:A:1301:YY3:H10	1.81	0.44
1:C:750:ALA:HB2	1:C:785:THR:HG23	1.98	0.44
1:B:796:GLY:HA2	2:B:1301:YY3:C6	2.48	0.44
1:C:714:LYS:HD2	1:C:727:TYR:CD1	2.53	0.43
1:C:897:VAL:O	1:C:900:TYR:HB3	2.17	0.43
3:D:1302:VNS:S08	3:D:1302:VNS:O01	2.76	0.43
1:A:829:GLU:HA	1:A:893:HIS:CD2	2.53	0.43
1:A:829:GLU:HA	1:A:893:HIS:NE2	2.33	0.43
1:C:793:MET:HG3	1:C:844:LEU:HB3	2.00	0.43
1:D:747:LEU:HD11	3:D:1302:VNS:C16	2.48	0.43
1:A:803:ARG:CG	1:A:911:GLY:HA3	2.48	0.43
1:C:877:PRO:O	1:C:881:MET:HG3	2.19	0.43
1:B:816:ASN:OD1	4:B:1401:HOH:O	2.21	0.43
1:B:998:TYR:O	1:B:1002:MET:HG3	2.18	0.43
1:D:709:GLU:HG3	1:D:783:THR:HG21	2.00	0.43
1:B:1002:MET:HE3	1:B:1002:MET:HB3	1.80	0.43
2:D:1301:YY3:H25	2:D:1301:YY3:O	2.19	0.43
1:D:897:VAL:O	1:D:900:TYR:HB3	2.18	0.43
1:C:876:VAL:HG23	1:C:878:ILE:HG12	2.00	0.43
1:C:777:LEU:HD11	1:C:788:LEU:HB3	2.01	0.43
1:B:835:HIS:CD2	1:B:856:PHE:HB3	2.53	0.43
1:A:764:TYR:HB3	4:A:1406:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:ARG:HE	1:B:999:ARG:HB3	1.27	0.43
1:D:882:ALA:HA	1:D:898:TRP:CE2	2.53	0.42
1:C:900:TYR:CE2	1:C:964:LEU:HD13	2.54	0.42
1:A:708:LYS:HB3	1:A:708:LYS:HE2	1.84	0.42
1:C:821:ILE:HG23	1:C:853:ILE:HD11	2.01	0.42
1:A:968:PHE:HA	1:A:971:MET:HE3	2.02	0.42
1:C:802:VAL:HG12	1:C:910:PHE:HA	2.01	0.42
1:B:724:GLY:HA3	1:B:746:GLU:O	2.19	0.42
1:B:944:TYR:O	1:B:948:ARG:HG2	2.19	0.42
1:D:790:MET:HB2	4:D:1404:HOH:O	2.20	0.42
1:A:777:LEU:HD11	1:A:788:LEU:HB3	2.00	0.42
1:C:716:LYS:HZ3	2:C:1301:YY3:H2	1.84	0.42
1:A:747:LEU:HD12	1:A:786:VAL:HB	2.02	0.42
1:A:757:LYS:NZ	1:A:761:ASP:OD2	2.40	0.42
1:C:900:TYR:CD2	1:C:964:LEU:HD13	2.54	0.42
1:B:995:SER:O	1:B:999:ARG:HG3	2.20	0.42
1:D:841:ARG:NH1	1:D:877:PRO:HB3	2.31	0.42
1:B:722:ALA:O	1:B:723:PHE:HB2	2.20	0.42
1:D:747:LEU:HD23	1:D:747:LEU:HA	1.77	0.42
1:A:730:LEU:HD23	1:A:741:PRO:HA	2.02	0.42
1:A:855:ASP:HA	3:A:1302:VNS:C39	2.50	0.42
1:C:705:ARG:NH2	1:C:711:GLU:OE2	2.52	0.41
1:C:716:LYS:HZ2	2:C:1301:YY3:H2	1.84	0.41
1:C:744:ILE:HG12	1:C:789:ILE:HG13	2.01	0.41
1:C:815:LEU:O	1:C:819:VAL:HG23	2.20	0.41
1:D:999:ARG:HE	1:D:999:ARG:HB3	1.43	0.41
1:C:946:ILE:H	1:C:946:ILE:HG13	1.45	0.41
1:D:744:ILE:HG12	1:D:789:ILE:HG13	2.03	0.41
1:B:795:PHE:CZ	1:B:848:PRO:HD3	2.55	0.41
1:D:946:ILE:HG21	1:D:968:PHE:HE1	1.86	0.41
1:A:776:ARG:NH2	1:A:778:LEU:HD22	2.36	0.41
1:D:877:PRO:O	1:D:881:MET:HG3	2.19	0.41
1:B:715:ILE:HG21	1:B:730:LEU:HD12	2.02	0.41
1:A:803:ARG:HG2	1:A:911:GLY:HA3	2.03	0.41
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.86	0.41
1:B:955:ALA:HA	1:B:958:ARG:CZ	2.51	0.41
1:A:723:PHE:HB3	1:A:747:LEU:HD22	2.01	0.41
1:A:883:LEU:HD23	1:A:953:ILE:HG13	2.03	0.41
1:B:825:MET:HB3	1:B:961:PHE:CE2	2.56	0.41
1:D:708:LYS:HB3	1:D:708:LYS:HE2	1.76	0.41
1:D:766:MET:HE2	1:D:858:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:835:HIS:CD2	1:C:856:PHE:HB3	2.56	0.41
1:C:941:ILE:HD12	1:C:941:ILE:HA	1.93	0.41
1:B:960:LYS:HD2	4:B:1410:HOH:O	2.21	0.40
1:A:797:CYS:HA	1:A:844:LEU:HA	2.03	0.40
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.55	0.40
1:B:905:TRP:HD1	1:B:947:MET:CE	2.34	0.40
1:B:747:LEU:HD12	1:B:786:VAL:HB	2.04	0.40
1:B:772:PRO:O	1:B:852:LYS:HE3	2.22	0.40
1:B:805:HIS:O	1:B:809:ILE:HG13	2.22	0.40
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.56	0.40
1:D:703:LEU:HD23	1:D:703:LEU:HA	1.95	0.40
1:D:883:LEU:HB3	4:D:1406:HOH:O	2.20	0.40
1:D:941:ILE:HD12	1:D:941:ILE:HA	1.95	0.40
1:B:708:LYS:HB3	1:B:708:LYS:HE2	1.86	0.40
1:B:905:TRP:CZ2	1:B:933:LEU:HD22	2.57	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	282/331 (85%)	269 (95%)	12 (4%)	1 (0%)	34	54
1	B	288/331 (87%)	280 (97%)	8 (3%)	0	100	100
1	C	290/331 (88%)	279 (96%)	10 (3%)	1 (0%)	41	61
1	D	282/331 (85%)	270 (96%)	11 (4%)	1 (0%)	34	54
All	All	1142/1324 (86%)	1098 (96%)	41 (4%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	859	ALA
1	D	722	ALA
1	A	723	PHE

### 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	258/290 (89%)	247 (96%)	11 (4%)	29	53
1	B	261/290 (90%)	252 (97%)	9 (3%)	37	63
1	C	263/290 (91%)	246 (94%)	17 (6%)	17	33
1	D	259/290 (89%)	252 (97%)	7 (3%)	44	71
All	All	1041/1160 (90%)	997 (96%)	44 (4%)	30	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	723	PHE
1	D	728	LYS
1	D	785	THR
1	D	806	LYS
1	D	807	ASP
1	D	987	MET
1	D	998	TYR
1	A	720	SER
1	A	732	ILE
1	A	736	GLU
1	A	738	VAL
1	A	766	MET
1	A	784	SER
1	A	812	GLN
1	A	918	ILE
1	A	960	LYS
1	A	987	MET
1	A	998	TYR
1	C	701	GLN

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Mol	Chain	Res	Type
1	C	723	PHE
1	C	751	THR
1	C	752	SER
1	C	783	THR
1	C	784	SER
1	C	785	THR
1	C	860	LYS
1	C	921	SER
1	C	922	GLU
1	C	945	MET
1	C	946	ILE
1	C	970	LYS
1	C	985	GLU
1	C	987	MET
1	C	998	TYR
1	C	1007	MET
1	B	720	SER
1	B	728	LYS
1	B	748	ARG
1	B	783	THR
1	B	812	GLN
1	B	977	ARG
1	B	989	LEU
1	B	998	TYR
1	B	1002	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	773	HIS
1	B	812	GLN
1	B	816	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	YY3	B	1301	1	38,40,40	2.49	14 (36%)	50,56,56	2.17	12 (24%)
3	VNS	B	1302	-	43,45,45	2.72	18 (41%)	54,65,65	4.40	24 (44%)
2	YY3	C	1301	1	38,40,40	2.41	13 (34%)	50,56,56	2.53	17 (34%)
3	VNS	D	1302	-	43,45,45	3.43	24 (55%)	54,65,65	5.16	31 (57%)
3	VNS	C	1302	-	43,45,45	3.17	21 (48%)	54,65,65	4.90	27 (50%)
2	YY3	D	1301	1	38,40,40	2.12	13 (34%)	50,56,56	2.10	11 (22%)
3	VNS	A	1302	-	43,45,45	3.37	28 (65%)	54,65,65	4.75	24 (44%)
2	YY3	A	1301	1	38,40,40	2.99	20 (52%)	50,56,56	2.73	12 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YY3	B	1301	1	-	9/21/25/25	0/4/4/4
3	VNS	B	1302	-	-	2/22/46/46	0/6/6/6
2	YY3	C	1301	1	-	6/21/25/25	0/4/4/4
3	VNS	D	1302	-	-	6/22/46/46	0/6/6/6
3	VNS	C	1302	-	-	6/22/46/46	0/6/6/6
2	YY3	D	1301	1	-	7/21/25/25	0/4/4/4
3	VNS	A	1302	-	-	4/22/46/46	0/6/6/6
2	YY3	A	1301	1	-	5/21/25/25	0/4/4/4

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1302	VNS	C09-C02	11.17	1.66	1.54
3	C	1302	VNS	C09-C02	10.47	1.65	1.54
2	A	1301	YY3	C7-N	10.31	1.53	1.35
3	D	1302	VNS	C11-N10	9.64	1.45	1.36
3	A	1302	VNS	C09-C02	9.49	1.64	1.54
3	A	1302	VNS	C11-N10	9.27	1.45	1.36
3	C	1302	VNS	C11-N10	8.39	1.44	1.36
3	B	1302	VNS	C09-C02	8.33	1.63	1.54
2	C	1301	YY3	C1-C2	7.48	1.49	1.40
3	B	1302	VNS	O01-C02	-7.17	1.09	1.23
3	B	1302	VNS	C11-N10	6.95	1.43	1.36
2	B	1301	YY3	C7-N	6.76	1.47	1.35
3	A	1302	VNS	O01-C02	-5.66	1.12	1.23
3	C	1302	VNS	C02-N03	5.63	1.48	1.35
3	A	1302	VNS	C02-N03	5.55	1.48	1.35
3	D	1302	VNS	C02-N03	5.24	1.47	1.35
3	D	1302	VNS	C18-C19	5.11	1.62	1.52
2	C	1301	YY3	C10-C11	5.01	1.69	1.51
3	A	1302	VNS	C04-N03	4.83	1.45	1.36
2	B	1301	YY3	C1-C2	4.80	1.46	1.40
2	A	1301	YY3	C1-N	4.64	1.50	1.41
2	A	1301	YY3	O1-C4	4.62	1.44	1.37
3	B	1302	VNS	C02-N03	4.59	1.46	1.35
3	D	1302	VNS	C15-C14	4.58	1.60	1.49
2	D	1301	YY3	O1-C4	4.56	1.44	1.37
2	A	1301	YY3	C5-N3	4.53	1.52	1.39
3	D	1302	VNS	O01-C02	-4.45	1.14	1.23
3	B	1302	VNS	C31-N10	4.39	1.50	1.46
3	A	1302	VNS	C31-N10	4.35	1.50	1.46
3	C	1302	VNS	C15-C14	4.34	1.59	1.49
2	C	1301	YY3	C2-N1	4.33	1.51	1.41
2	B	1301	YY3	C2-N1	4.28	1.51	1.41
2	D	1301	YY3	C7-N	4.24	1.42	1.35
2	C	1301	YY3	C11-N2	4.13	1.61	1.46
3	A	1302	VNS	C39-C33	4.12	1.45	1.40
3	D	1302	VNS	C31-N10	4.11	1.50	1.46
3	D	1302	VNS	C12-C11	4.08	1.55	1.48
2	A	1301	YY3	C6-C5	4.05	1.45	1.39
2	A	1301	YY3	C8-C7	4.03	1.54	1.48
3	C	1302	VNS	C09-N10	4.03	1.51	1.46
3	D	1302	VNS	C04-N03	4.03	1.43	1.36
2	B	1301	YY3	C6-C1	3.99	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1302	VNS	O01-C02	-3.96	1.15	1.23
3	C	1302	VNS	C31-N10	3.92	1.49	1.46
2	B	1301	YY3	C19-C18	-3.89	1.44	1.49
2	D	1301	YY3	C2-N1	3.86	1.50	1.41
3	A	1302	VNS	C15-C14	3.85	1.58	1.49
3	C	1302	VNS	C18-C19	3.84	1.59	1.52
2	A	1301	YY3	C6-C1	3.83	1.45	1.39
3	D	1302	VNS	C31-C30	3.81	1.55	1.50
3	D	1302	VNS	C26-C18	3.78	1.45	1.39
2	A	1301	YY3	C19-C18	-3.77	1.44	1.49
2	C	1301	YY3	O1-C4	3.76	1.43	1.37
3	A	1302	VNS	C12-C11	3.73	1.54	1.48
3	B	1302	VNS	C04-N03	3.71	1.43	1.36
2	A	1301	YY3	C3-C2	3.67	1.45	1.39
2	B	1301	YY3	C12-N2	3.65	1.57	1.46
2	C	1301	YY3	C10-N1	3.64	1.58	1.46
2	B	1301	YY3	C10-C11	3.58	1.64	1.51
2	D	1301	YY3	C19-C18	-3.55	1.44	1.49
3	C	1302	VNS	C12-C11	3.50	1.54	1.48
3	D	1302	VNS	C27-C26	3.48	1.45	1.38
3	C	1302	VNS	C34-C35	3.44	1.43	1.37
2	D	1301	YY3	C15-N3	3.40	1.43	1.36
3	A	1302	VNS	C18-C19	3.40	1.59	1.52
2	A	1301	YY3	C2-N1	3.39	1.49	1.41
3	B	1302	VNS	C33-C09	3.36	1.56	1.52
3	D	1302	VNS	C09-N10	3.34	1.50	1.46
3	C	1302	VNS	C17-C16	3.23	1.44	1.38
3	A	1302	VNS	C33-C09	3.19	1.56	1.52
2	B	1301	YY3	C11-N2	3.18	1.57	1.46
2	A	1301	YY3	C10-C11	3.16	1.63	1.51
2	A	1301	YY3	C15-N3	3.12	1.42	1.36
3	C	1302	VNS	C27-C26	3.11	1.44	1.38
3	D	1302	VNS	C13-C12	3.09	1.44	1.39
3	A	1302	VNS	C25-C24	3.08	1.61	1.52
2	D	1301	YY3	C1-C2	3.04	1.44	1.40
3	C	1302	VNS	C29-C28	3.03	1.44	1.38
3	C	1302	VNS	C04-N03	3.02	1.42	1.36
3	A	1302	VNS	C26-C18	3.01	1.43	1.39
3	A	1302	VNS	C37-C35	3.00	1.43	1.37
3	A	1302	VNS	C09-N10	2.98	1.50	1.46
2	B	1301	YY3	C8-C7	2.97	1.53	1.48
2	D	1301	YY3	C10-C11	2.96	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1302	VNS	C34-C35	2.96	1.42	1.37
2	D	1301	YY3	C5-N3	2.94	1.48	1.39
3	A	1302	VNS	C34-C35	2.91	1.42	1.37
3	A	1302	VNS	C21-N22	2.90	1.52	1.46
3	B	1302	VNS	C15-C14	2.89	1.56	1.49
3	A	1302	VNS	C13-C12	2.87	1.44	1.39
2	C	1301	YY3	C7-N	2.86	1.40	1.35
3	C	1302	VNS	C31-C30	2.85	1.54	1.50
3	D	1302	VNS	C29-C28	2.82	1.43	1.38
3	D	1302	VNS	C13-C14	2.78	1.44	1.39
2	C	1301	YY3	C5-N3	2.74	1.47	1.39
2	A	1301	YY3	C11-N2	2.74	1.56	1.46
3	A	1302	VNS	C29-C28	2.74	1.43	1.38
3	A	1302	VNS	C17-C16	2.72	1.43	1.38
2	B	1301	YY3	C6-C5	2.72	1.43	1.39
2	B	1301	YY3	C1-N	2.66	1.46	1.41
3	C	1302	VNS	C37-C35	2.65	1.42	1.37
3	C	1302	VNS	C28-C14	2.64	1.44	1.39
3	A	1302	VNS	C27-C26	2.63	1.43	1.38
2	D	1301	YY3	C11-N2	2.61	1.55	1.46
2	B	1301	YY3	O1-C4	2.61	1.41	1.37
3	D	1302	VNS	C17-C16	2.56	1.43	1.38
3	B	1302	VNS	F36-C35	-2.56	1.30	1.36
2	B	1301	YY3	C13-N2	2.54	1.54	1.46
3	B	1302	VNS	C27-C26	2.51	1.43	1.38
3	D	1302	VNS	C33-C09	2.51	1.55	1.52
2	D	1301	YY3	C13-N2	2.48	1.53	1.46
3	D	1302	VNS	C37-C35	2.48	1.41	1.37
2	B	1301	YY3	C3-C2	2.48	1.43	1.39
3	C	1302	VNS	C13-C12	2.47	1.43	1.39
2	D	1301	YY3	C15-N4	2.44	1.38	1.34
3	A	1302	VNS	C24-N22	2.44	1.51	1.46
2	A	1301	YY3	C17-C16	2.41	1.43	1.38
2	D	1301	YY3	C10-N1	2.41	1.54	1.46
3	C	1302	VNS	C17-C18	2.39	1.42	1.39
2	A	1301	YY3	C1-C2	2.38	1.43	1.40
3	B	1302	VNS	C39-C33	2.37	1.42	1.40
2	C	1301	YY3	C15-N3	2.35	1.41	1.36
3	A	1302	VNS	C13-C14	2.33	1.43	1.39
2	C	1301	YY3	C28-N1	2.33	1.50	1.46
2	A	1301	YY3	C10-N1	2.33	1.54	1.46
3	A	1302	VNS	C17-C18	2.32	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	VNS	C31-C30	2.32	1.53	1.50
3	B	1302	VNS	C34-C35	2.32	1.41	1.37
2	A	1301	YY3	C3-C4	2.32	1.43	1.38
2	D	1301	YY3	C3-C2	2.31	1.43	1.39
2	C	1301	YY3	C1-N	2.30	1.46	1.41
3	B	1302	VNS	C29-C28	2.29	1.42	1.38
3	D	1302	VNS	C28-C14	2.28	1.44	1.39
3	B	1302	VNS	C09-N10	2.27	1.49	1.46
3	D	1302	VNS	C25-C19	2.25	1.59	1.53
3	A	1302	VNS	C29-C30	2.25	1.43	1.39
2	C	1301	YY3	C19-C18	-2.23	1.46	1.49
3	D	1302	VNS	C29-C30	2.22	1.43	1.39
3	C	1302	VNS	C26-C18	2.22	1.42	1.39
3	A	1302	VNS	F36-C35	-2.20	1.31	1.36
3	C	1302	VNS	C21-N22	2.18	1.51	1.46
2	A	1301	YY3	C20-C19	2.17	1.41	1.38
3	A	1302	VNS	C28-C14	2.17	1.43	1.39
3	D	1302	VNS	C27-C15	2.16	1.43	1.39
3	B	1302	VNS	C17-C16	2.14	1.42	1.38
3	B	1302	VNS	C18-C19	2.13	1.56	1.52
3	B	1302	VNS	C26-C18	2.13	1.42	1.39
3	A	1302	VNS	C31-C30	2.09	1.53	1.50
2	A	1301	YY3	C13-N2	2.09	1.52	1.46
2	A	1301	YY3	C28-N1	2.06	1.49	1.46
2	C	1301	YY3	C15-N4	2.05	1.37	1.34

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	VNS	C31-N10-C11	-20.53	104.67	113.12
3	C	1302	VNS	C31-N10-C11	-20.21	104.80	113.12
3	D	1302	VNS	C31-N10-C11	-20.15	104.83	113.12
3	A	1302	VNS	C31-N10-C11	-18.71	105.42	113.12
3	D	1302	VNS	C30-C31-N10	16.98	107.84	102.18
3	C	1302	VNS	C30-C31-N10	16.85	107.79	102.18
3	A	1302	VNS	C30-C31-N10	16.55	107.69	102.18
2	A	1301	YY3	C8-C7-N	14.88	123.64	113.84
3	B	1302	VNS	C30-C31-N10	14.23	106.92	102.18
2	C	1301	YY3	C8-C7-N	11.81	121.62	113.84
3	B	1302	VNS	C12-C11-N10	11.19	113.04	106.44
2	B	1301	YY3	C8-C7-N	10.96	121.06	113.84
3	C	1302	VNS	C12-C11-N10	10.07	112.39	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1302	VNS	C12-C11-N10	10.04	112.36	106.44
2	D	1301	YY3	C8-C7-N	9.84	120.33	113.84
3	D	1302	VNS	C24-C25-C19	9.33	122.08	111.04
3	D	1302	VNS	C24-N22-C21	8.75	121.76	109.52
3	C	1302	VNS	O32-C11-N10	-8.42	118.92	125.24
3	A	1302	VNS	C20-C21-N22	8.42	122.51	111.22
3	A	1302	VNS	C12-C11-N10	8.10	111.22	106.44
3	C	1302	VNS	C21-C20-C19	8.09	120.61	111.04
3	A	1302	VNS	C21-C20-C19	8.05	120.56	111.04
3	D	1302	VNS	O32-C11-N10	-8.02	119.23	125.24
3	D	1302	VNS	C21-C20-C19	8.01	120.52	111.04
3	A	1302	VNS	C24-C25-C19	7.82	120.29	111.04
3	D	1302	VNS	C30-C12-C11	-7.76	104.78	108.94
3	C	1302	VNS	C30-C12-C11	-7.58	104.88	108.94
3	D	1302	VNS	C20-C21-N22	7.32	121.04	111.22
3	B	1302	VNS	O32-C11-N10	-7.10	119.92	125.24
3	A	1302	VNS	C25-C24-N22	6.79	120.32	111.22
3	A	1302	VNS	O32-C11-N10	-6.66	120.25	125.24
3	A	1302	VNS	C30-C12-C11	-6.61	105.40	108.94
3	A	1302	VNS	C20-C19-C18	-6.54	97.45	112.79
3	C	1302	VNS	C20-C21-N22	6.49	119.92	111.22
3	C	1302	VNS	C24-C25-C19	5.82	117.92	111.04
3	B	1302	VNS	C30-C12-C11	-5.46	106.01	108.94
3	A	1302	VNS	C24-N22-C21	5.24	116.85	109.52
3	C	1302	VNS	C26-C18-C17	-5.18	111.83	118.29
3	D	1302	VNS	C26-C18-C17	-5.15	111.86	118.29
3	D	1302	VNS	C25-C24-N22	5.15	118.13	111.22
3	C	1302	VNS	C24-N22-C21	5.08	116.63	109.52
2	A	1301	YY3	O-C7-C8	-4.57	115.41	122.72
3	B	1302	VNS	C21-C20-C19	4.29	116.11	111.04
3	B	1302	VNS	C20-C19-C18	-4.19	102.98	112.79
3	C	1302	VNS	C16-C15-C14	4.18	128.60	121.36
2	A	1301	YY3	C6-C5-C4	-4.17	113.88	118.91
2	C	1301	YY3	C3-C2-C1	-3.97	114.18	120.04
2	C	1301	YY3	O1-C4-C5	3.93	119.62	114.80
2	A	1301	YY3	C18-N5-C15	3.88	119.89	116.69
3	B	1302	VNS	C31-N10-C09	3.87	127.48	123.86
3	A	1302	VNS	C26-C18-C17	-3.81	113.54	118.29
3	B	1302	VNS	C26-C18-C17	-3.68	113.71	118.29
2	B	1301	YY3	C3-C2-C1	-3.66	114.64	120.04
3	B	1302	VNS	C24-N22-C21	3.62	114.58	109.52
2	D	1301	YY3	O1-C4-C5	3.59	119.20	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	YY3	C6-C5-C4	-3.57	114.59	118.91
2	C	1301	YY3	O-C7-N	-3.57	118.96	123.05
3	D	1302	VNS	C33-C34-C35	3.53	123.18	118.59
3	B	1302	VNS	C24-C25-C19	3.50	115.18	111.04
2	D	1301	YY3	N4-C15-N5	-3.50	123.23	126.55
3	D	1302	VNS	C37-C35-C34	-3.46	118.80	123.29
2	C	1301	YY3	C6-C5-C4	-3.46	114.73	118.91
2	A	1301	YY3	C2-C3-C4	3.43	125.22	117.91
2	D	1301	YY3	C3-C2-C1	-3.42	115.00	120.04
2	C	1301	YY3	C3-C2-N1	-3.40	116.34	120.93
3	D	1302	VNS	C20-C19-C18	-3.39	104.84	112.79
2	D	1301	YY3	O-C7-C8	-3.38	117.31	122.72
3	C	1302	VNS	C28-C14-C13	-3.38	113.38	118.16
3	C	1302	VNS	C31-N10-C09	3.36	127.00	123.86
3	D	1302	VNS	C28-C14-C13	-3.34	113.44	118.16
2	A	1301	YY3	N4-C15-N5	-3.30	123.42	126.55
3	D	1302	VNS	C13-C12-C11	3.29	134.87	129.36
3	D	1302	VNS	C16-C17-C18	3.27	124.49	121.20
3	D	1302	VNS	C31-N10-C09	3.24	126.89	123.86
3	A	1302	VNS	C25-C19-C20	3.24	116.32	109.56
2	C	1301	YY3	C2-C3-C4	3.23	124.80	117.91
3	A	1302	VNS	C23-N22-C24	-3.20	105.87	110.66
3	C	1302	VNS	C27-C15-C16	-3.18	111.25	117.59
2	C	1301	YY3	O1-C4-C3	-3.18	118.65	124.12
3	A	1302	VNS	C13-C12-C11	3.17	134.66	129.36
3	B	1302	VNS	C23-N22-C21	-3.14	105.96	110.66
2	A	1301	YY3	C3-C2-C1	-3.13	115.42	120.04
3	D	1302	VNS	C27-C15-C16	-3.13	111.36	117.59
3	C	1302	VNS	C27-C26-C18	3.11	124.33	121.20
3	C	1302	VNS	C04-N03-C02	-3.05	122.23	129.02
3	C	1302	VNS	O01-C02-C09	-3.04	116.90	120.97
2	B	1301	YY3	C6-C5-C4	-3.03	115.25	118.91
2	B	1301	YY3	C25-C26-C19	-3.02	131.32	135.63
2	C	1301	YY3	C18-C19-C26	3.02	129.80	123.90
3	B	1302	VNS	C23-N22-C24	-3.01	106.16	110.66
2	C	1301	YY3	C4-C5-N3	2.96	123.99	117.78
3	A	1302	VNS	C28-C14-C13	-2.96	113.98	118.16
3	B	1302	VNS	C33-C34-C35	2.94	122.40	118.59
3	C	1302	VNS	C37-C35-C34	-2.92	119.49	123.29
2	D	1301	YY3	C2-C3-C4	2.91	124.12	117.91
3	C	1302	VNS	C20-C19-C18	-2.89	106.02	112.79
3	D	1302	VNS	C17-C16-C15	2.87	125.26	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	VNS	O01-C02-C09	-2.84	117.17	120.97
2	B	1301	YY3	C2-C3-C4	2.83	123.95	117.91
3	D	1302	VNS	C04-N03-C02	-2.83	122.72	129.02
2	B	1301	YY3	O-C7-C8	-2.81	118.23	122.72
3	C	1302	VNS	C29-C30-C12	-2.79	117.78	120.31
2	D	1301	YY3	C25-C26-C19	-2.74	131.72	135.63
2	D	1301	YY3	C4-C5-N3	2.73	123.51	117.78
3	B	1302	VNS	C29-C30-C12	-2.72	117.85	120.31
3	B	1302	VNS	C28-C14-C15	2.71	126.06	121.36
2	D	1301	YY3	O1-C4-C3	-2.71	119.45	124.12
2	C	1301	YY3	C2-C1-N	2.67	123.58	118.58
3	C	1302	VNS	C13-C12-C11	2.63	133.76	129.36
3	B	1302	VNS	C20-C21-N22	2.62	114.74	111.22
2	C	1301	YY3	N4-C15-N5	-2.61	124.07	126.55
3	D	1302	VNS	C26-C18-C19	2.60	127.86	121.11
2	A	1301	YY3	C12-N2-C13	-2.55	103.15	109.73
3	D	1302	VNS	C29-C30-C12	-2.54	118.00	120.31
2	A	1301	YY3	C6-C1-C2	-2.51	117.03	119.67
3	C	1302	VNS	C17-C16-C15	2.51	124.75	121.13
2	C	1301	YY3	C19-C18-N5	2.51	119.43	116.14
2	A	1301	YY3	C25-C26-C19	-2.50	132.07	135.63
3	D	1302	VNS	C23-N22-C21	2.47	114.35	110.66
3	B	1302	VNS	C28-C14-C13	-2.45	114.70	118.16
3	B	1302	VNS	C25-C19-C18	2.45	118.54	112.79
3	B	1302	VNS	C37-C35-C34	-2.43	120.13	123.29
3	B	1302	VNS	C27-C15-C16	-2.43	112.74	117.59
3	D	1302	VNS	C23-N22-C24	-2.43	107.03	110.66
3	B	1302	VNS	C17-C16-C15	2.39	124.58	121.13
3	A	1302	VNS	C29-C30-C12	-2.38	118.16	120.31
2	A	1301	YY3	C16-C17-C18	-2.37	114.98	117.22
3	D	1302	VNS	C25-C19-C20	2.37	114.50	109.56
3	B	1302	VNS	O01-C02-C09	-2.34	117.84	120.97
2	B	1301	YY3	C16-C17-C18	-2.33	115.02	117.22
2	B	1301	YY3	N4-C15-N5	-2.31	124.36	126.55
3	D	1302	VNS	O01-C02-C09	-2.30	117.88	120.97
3	D	1302	VNS	C25-C19-C18	2.30	118.18	112.79
2	C	1301	YY3	C11-C10-N1	2.29	115.96	112.31
2	A	1301	YY3	O1-C4-C5	2.28	117.60	114.80
3	A	1302	VNS	C23-N22-C21	-2.25	107.29	110.66
3	C	1302	VNS	C25-C24-N22	2.24	114.23	111.22
3	C	1302	VNS	C16-C17-C18	2.24	123.45	121.20
3	C	1302	VNS	C34-C33-C09	2.24	123.93	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	YY3	C3-C4-C5	2.24	123.22	120.54
3	A	1302	VNS	C27-C26-C18	2.23	123.44	121.20
2	C	1301	YY3	C1-N-C7	-2.19	122.09	127.15
3	C	1302	VNS	C26-C27-C15	2.19	124.28	121.13
2	B	1301	YY3	C6-C5-N3	2.16	125.54	121.05
2	D	1301	YY3	C11-C10-N1	2.16	115.76	112.31
3	D	1302	VNS	C26-C27-C15	2.15	124.23	121.13
3	A	1302	VNS	C17-C16-C15	2.13	124.20	121.13
3	D	1302	VNS	C16-C15-C14	2.11	125.01	121.36
2	B	1301	YY3	C16-N4-C15	2.11	117.32	115.45
3	C	1302	VNS	C33-C34-C35	2.11	121.33	118.59
3	A	1302	VNS	C33-C34-C35	2.11	121.33	118.59
3	A	1302	VNS	C37-C35-C34	-2.09	120.58	123.29
3	A	1302	VNS	C27-C15-C16	-2.08	113.44	117.59
2	C	1301	YY3	O-C7-C8	-2.07	119.40	122.72
2	B	1301	YY3	O-C7-N	-2.04	120.71	123.05
2	C	1301	YY3	C17-C18-C19	-2.03	118.41	121.04
3	D	1302	VNS	C13-C14-C15	2.03	124.21	120.86
3	B	1302	VNS	C31-C30-C29	2.00	132.80	128.85

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1301	YY3	C10-C11-N2-C13
2	D	1301	YY3	C11-C10-N1-C28
2	D	1301	YY3	N-C7-C8-C9
2	D	1301	YY3	O-C7-C8-C9
2	A	1301	YY3	C1-C2-N1-C10
2	A	1301	YY3	N-C7-C8-C9
2	A	1301	YY3	O-C7-C8-C9
2	C	1301	YY3	N-C7-C8-C9
2	C	1301	YY3	O-C7-C8-C9
2	B	1301	YY3	N-C7-C8-C9
2	B	1301	YY3	O-C7-C8-C9
2	A	1301	YY3	C10-C11-N2-C12
2	A	1301	YY3	N1-C10-C11-N2
2	B	1301	YY3	C1-C2-N1-C10
3	D	1302	VNS	C28-C14-C15-C27
2	B	1301	YY3	N1-C10-C11-N2
2	D	1301	YY3	C10-C11-N2-C12
2	B	1301	YY3	C5-C4-O1-C14

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Mol	Chain	Res	Type	Atoms
3	C	1302	VNS	C17-C18-C19-C25
3	D	1302	VNS	C13-C14-C15-C27
2	B	1301	YY3	C10-C11-N2-C13
2	B	1301	YY3	C10-C11-N2-C12
2	B	1301	YY3	C3-C4-O1-C14
2	D	1301	YY3	C1-C2-N1-C28
3	C	1302	VNS	C26-C18-C19-C25
2	C	1301	YY3	C6-C1-N-C7
2	D	1301	YY3	C3-C2-N1-C28
2	C	1301	YY3	C3-C2-N1-C28
2	B	1301	YY3	C3-C2-N1-C10
3	C	1302	VNS	C02-C09-C33-C39
3	D	1302	VNS	C17-C18-C19-C20
2	C	1301	YY3	C2-C1-N-C7
3	D	1302	VNS	C26-C18-C19-C20
3	D	1302	VNS	C33-C09-N10-C31
3	A	1302	VNS	C33-C09-N10-C31
3	C	1302	VNS	C33-C09-N10-C31
3	B	1302	VNS	C33-C09-N10-C31
3	C	1302	VNS	C28-C14-C15-C27
3	D	1302	VNS	C28-C14-C15-C16
2	C	1301	YY3	N1-C10-C11-N2
3	A	1302	VNS	C02-C09-C33-C34
3	C	1302	VNS	C02-C09-C33-C34
3	A	1302	VNS	C02-C09-N10-C31
3	B	1302	VNS	C02-C09-N10-C31
3	A	1302	VNS	C02-C09-C33-C39

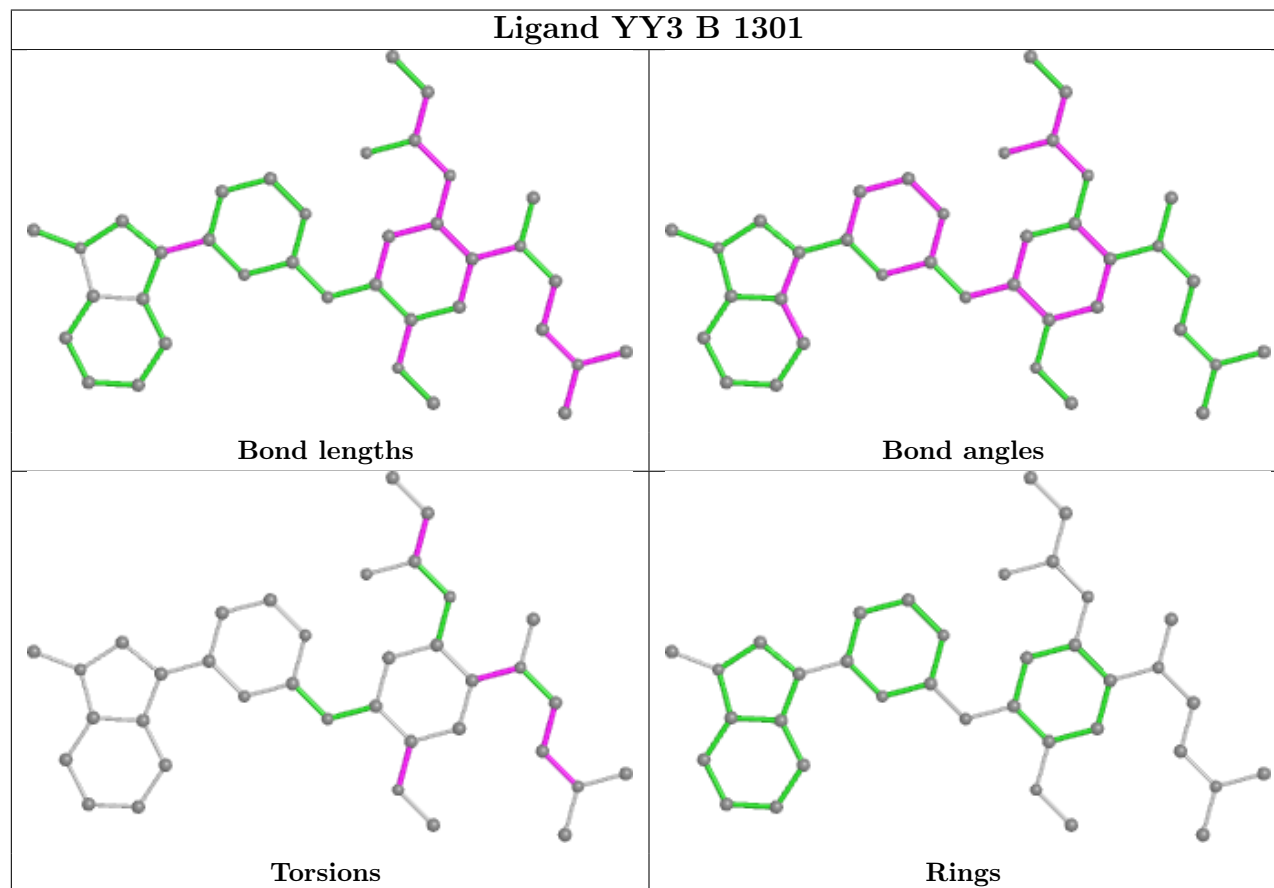
There are no ring outliers.

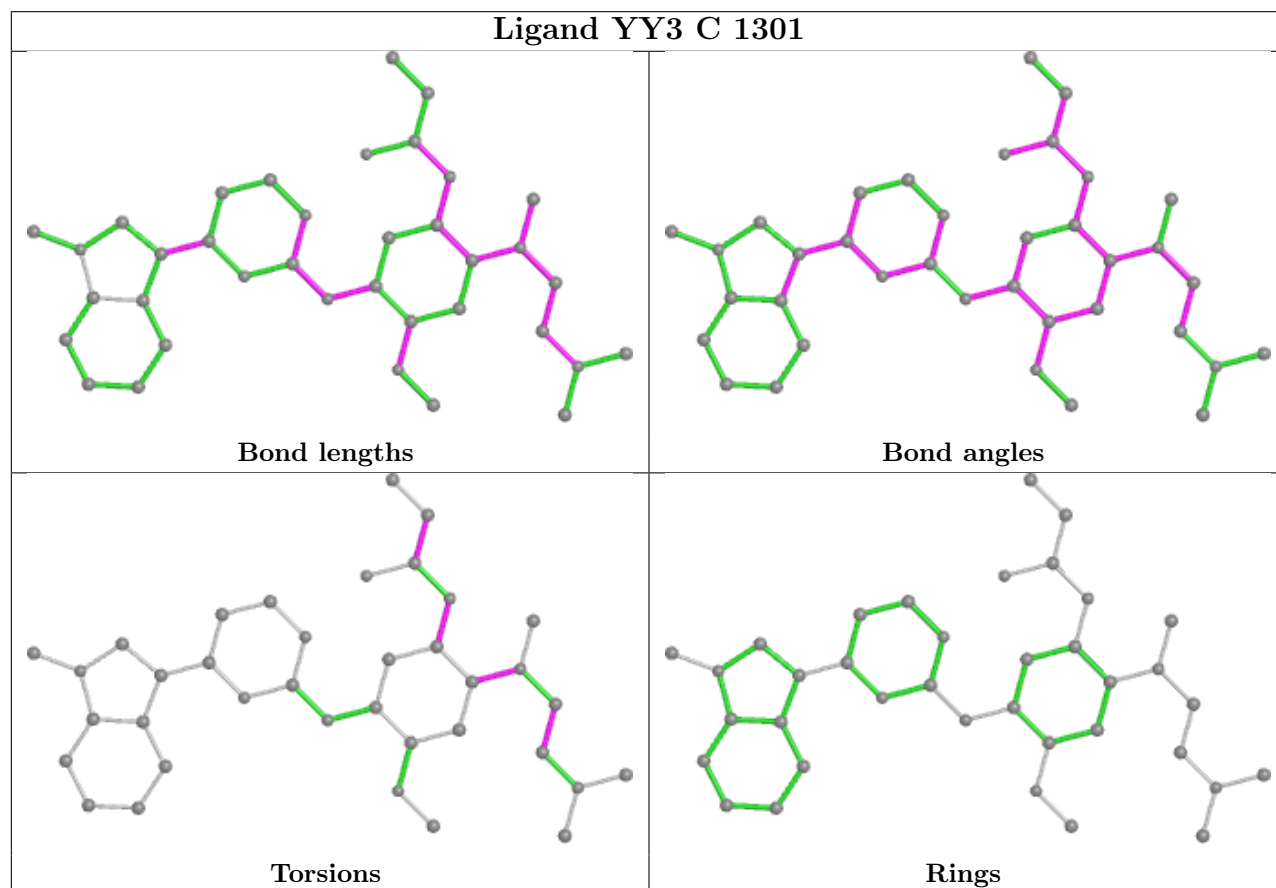
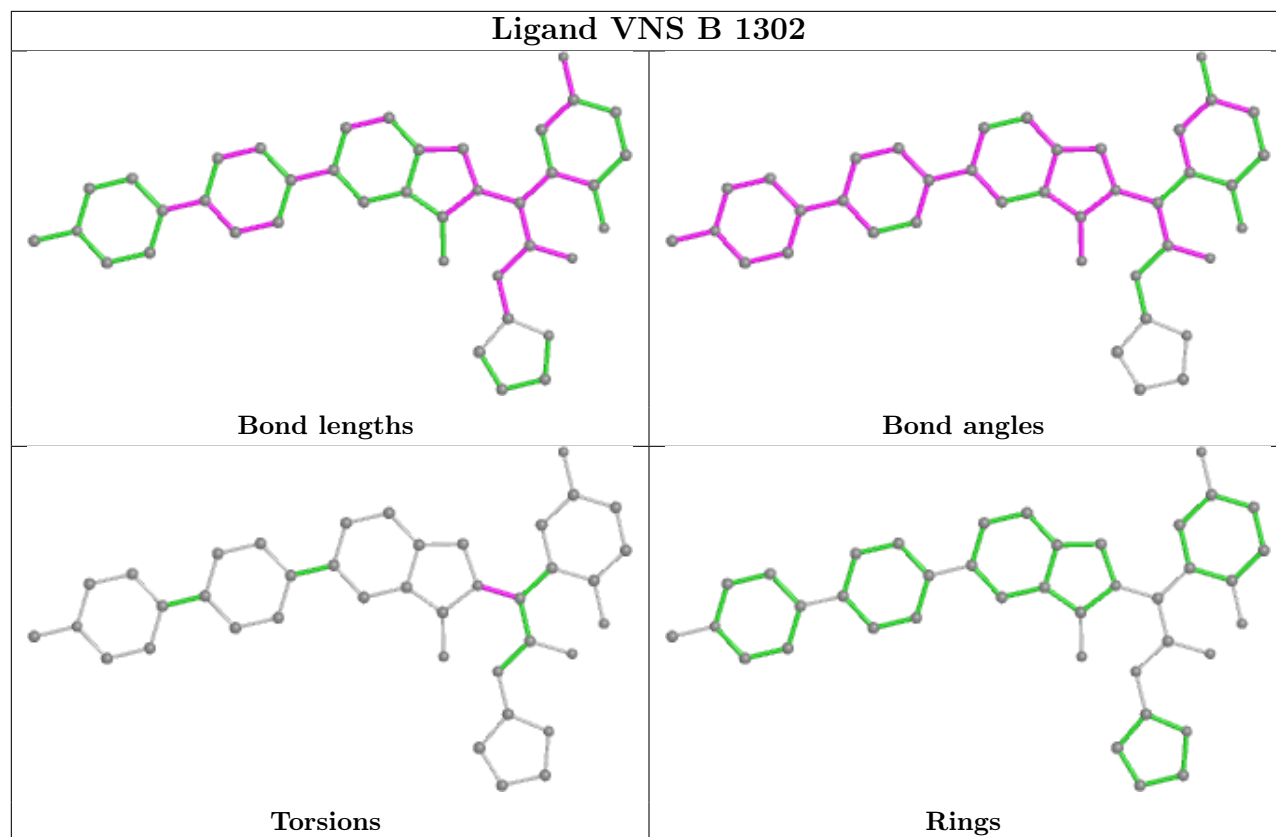
7 monomers are involved in 21 short contacts:

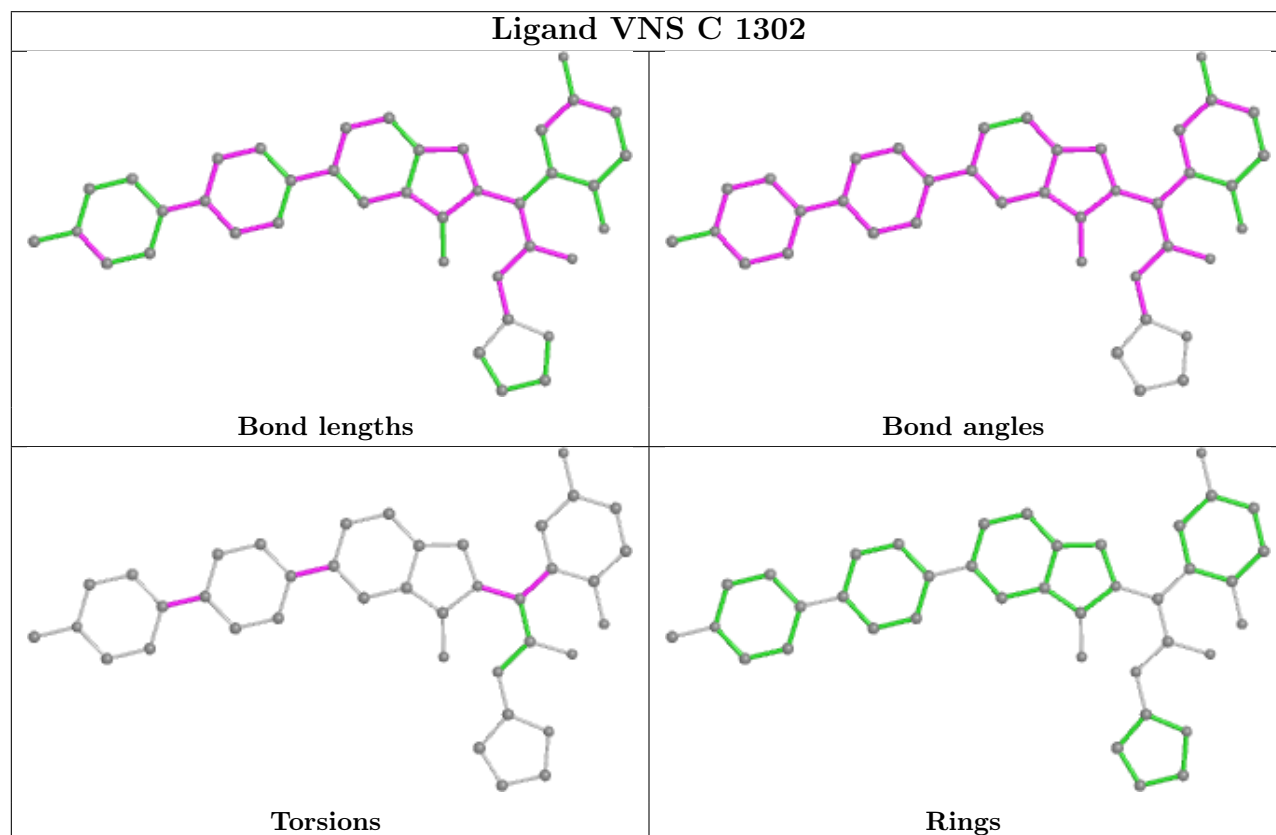
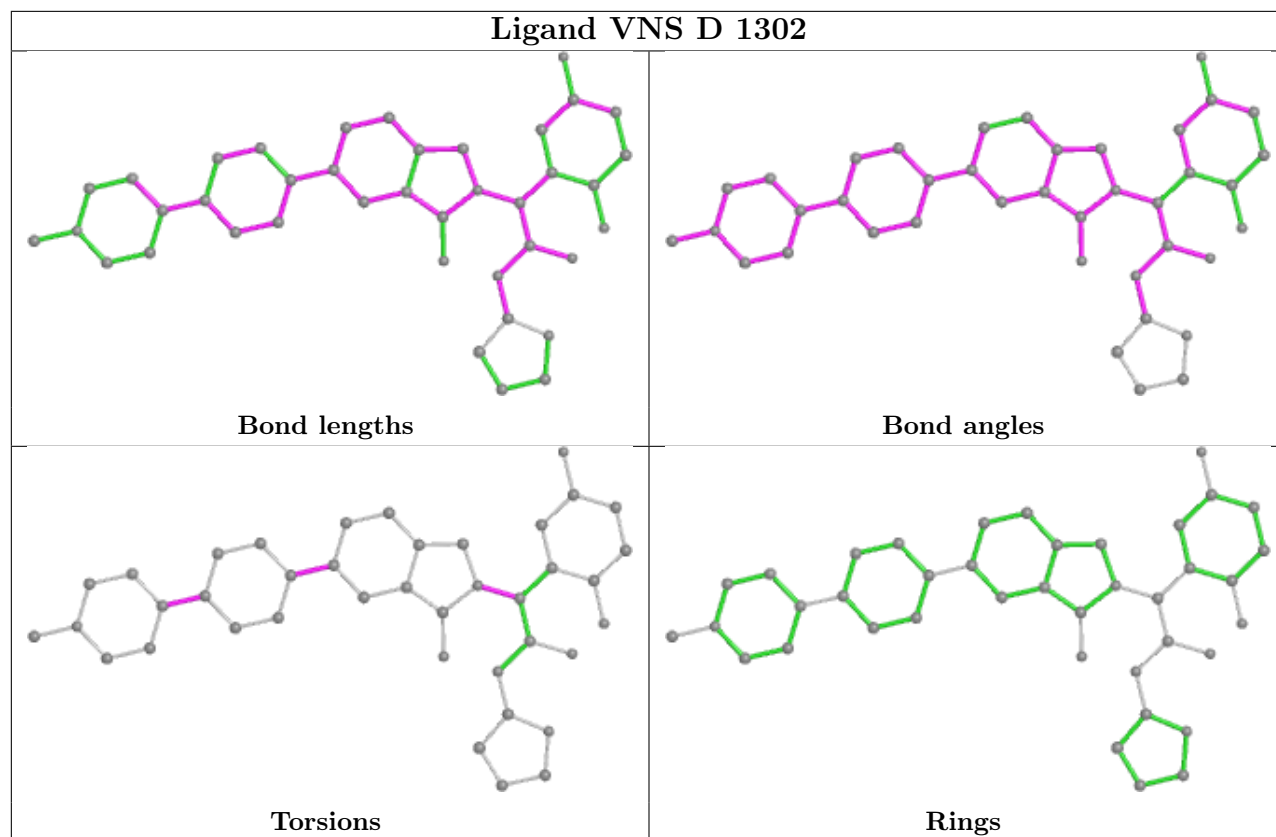
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	YY3	3	0
2	C	1301	YY3	5	0
3	D	1302	VNS	3	0
3	C	1302	VNS	2	0
2	D	1301	YY3	3	0
3	A	1302	VNS	1	0
2	A	1301	YY3	4	0

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

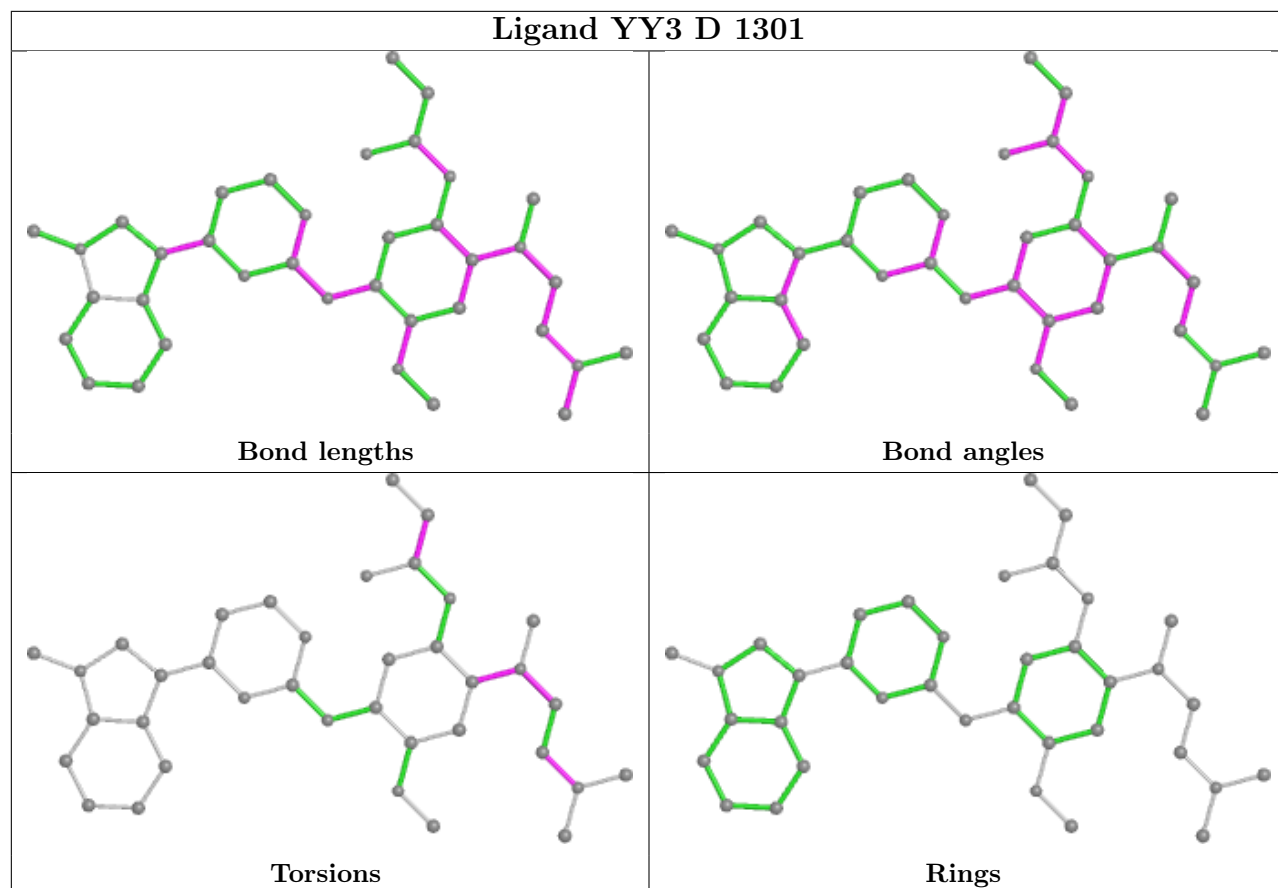
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



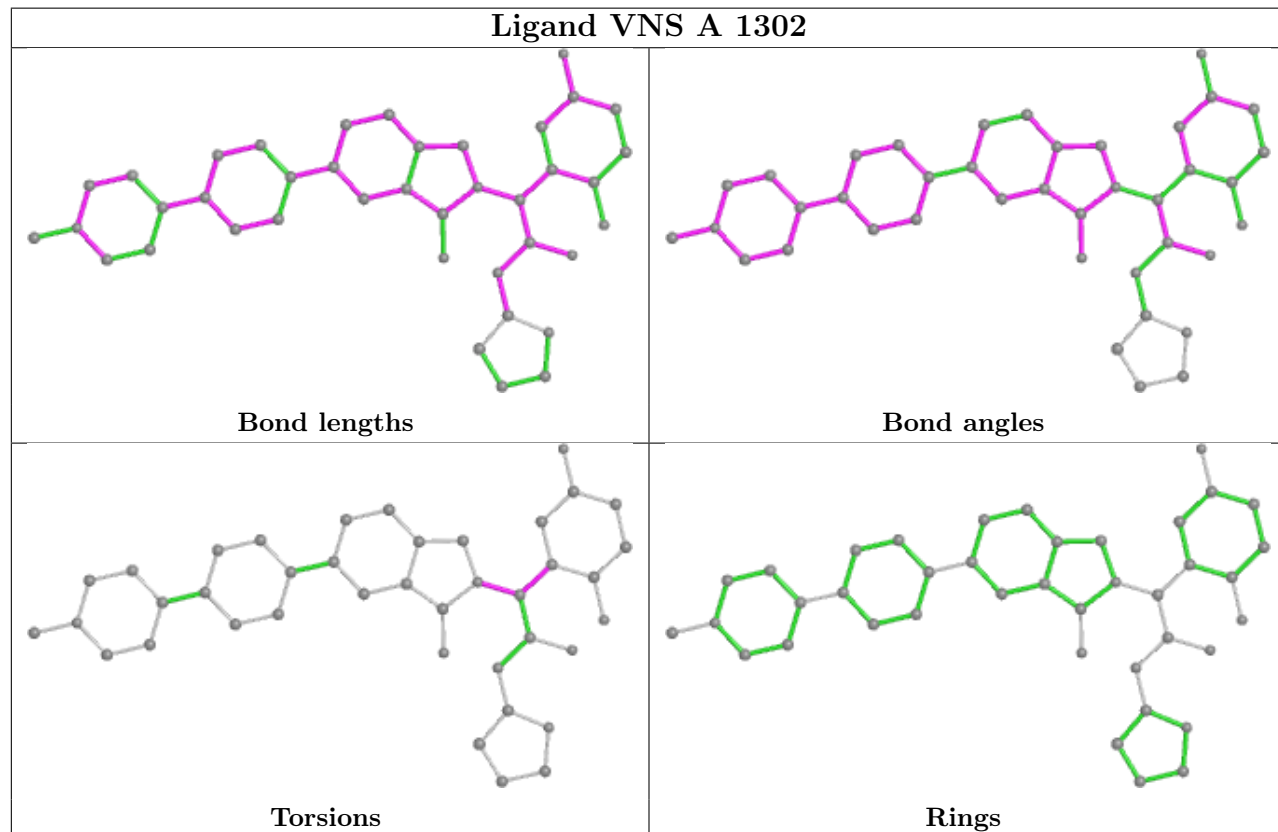


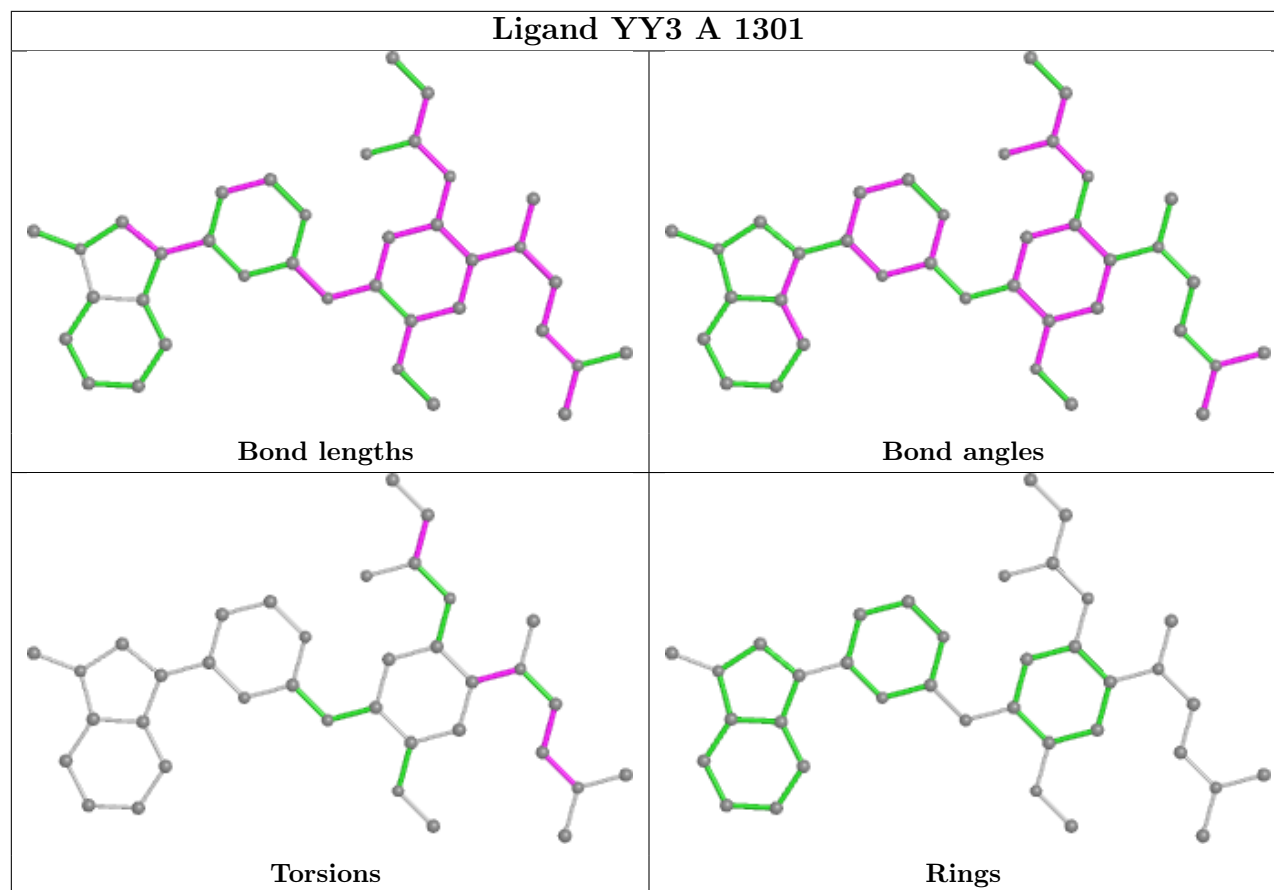


## Ligand YY3 D 1301



## Ligand VNS A 1302





## 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	288/331 (87%)	0.71	25 (8%)	10 10	37, 65, 99, 117	0
1	B	291/331 (87%)	0.38	19 (6%)	18 19	22, 53, 98, 114	0
1	C	293/331 (88%)	0.90	46 (15%)	2 1	35, 69, 113, 141	0
1	D	287/331 (86%)	1.14	46 (16%)	1 1	52, 86, 129, 144	0
All	All	1159/1324 (87%)	0.78	136 (11%)	4 4	22, 69, 114, 144	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	946	ILE	7.3
1	B	807	ASP	5.8
1	D	782	LEU	5.7
1	C	860	LYS	5.2
1	A	807	ASP	5.2
1	A	786	VAL	5.0
1	C	938	ILE	4.9
1	C	749	GLU	4.8
1	C	907	LEU	4.8
1	C	979	LEU	4.7
1	D	722	ALA	4.7
1	D	927	LEU	4.7
1	C	981	ILE	4.6
1	D	886	ILE	4.4
1	B	700	ASN	4.3
1	C	759	ILE	4.3
1	A	716	LYS	4.3
1	C	972	ALA	4.3
1	D	786	VAL	4.2
1	A	785	THR	4.2
1	C	813	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	982	GLN	4.0
1	C	943	VAL	4.0
1	D	746	GLU	3.9
1	B	755	ALA	3.8
1	B	751	THR	3.8
1	A	918	ILE	3.7
1	A	755	ALA	3.6
1	C	984	ASP	3.6
1	C	937	PRO	3.5
1	C	877	PRO	3.5
1	B	781	CYS	3.5
1	A	783	THR	3.4
1	D	878	ILE	3.4
1	C	986	ARG	3.4
1	B	782	LEU	3.4
1	D	789	ILE	3.4
1	D	883	LEU	3.4
1	C	920	ALA	3.4
1	C	748	ARG	3.3
1	A	722	ALA	3.3
1	C	807	ASP	3.3
1	D	920	ALA	3.2
1	A	712	PHE	3.2
1	B	988	HIS	3.2
1	D	929	LYS	3.2
1	B	707	LEU	3.2
1	D	747	LEU	3.1
1	C	722	ALA	3.1
1	B	918	ILE	3.1
1	C	990	PRO	3.0
1	A	781	CYS	3.0
1	D	876	VAL	3.0
1	B	717	VAL	3.0
1	D	931	GLU	3.0
1	D	926	ILE	3.0
1	D	977	ARG	2.9
1	A	717	VAL	2.9
1	D	700	ASN	2.9
1	C	758	GLU	2.9
1	C	953	ILE	2.9
1	C	988	HIS	2.8
1	D	807	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	754	LYS	2.8
1	C	903	THR	2.8
1	C	804	GLU	2.8
1	A	739	LYS	2.7
1	D	877	PRO	2.7
1	A	988	HIS	2.7
1	C	977	ARG	2.7
1	C	785	THR	2.7
1	B	712	PHE	2.7
1	D	711	GLU	2.7
1	C	929	LYS	2.7
1	D	953	ILE	2.7
1	D	922	GLU	2.6
1	D	784	SER	2.6
1	C	921	SER	2.6
1	D	918	ILE	2.6
1	A	707	LEU	2.5
1	A	922	GLU	2.5
1	C	927	LEU	2.5
1	D	755	ALA	2.5
1	A	917	GLY	2.5
1	C	721	GLY	2.5
1	D	946	ILE	2.5
1	C	723	PHE	2.5
1	D	919	PRO	2.5
1	A	993	THR	2.5
1	D	951	TRP	2.5
1	C	976	GLN	2.4
1	C	910	PHE	2.4
1	D	766	MET	2.4
1	D	759	ILE	2.4
1	A	700	ASN	2.4
1	C	1006	ASP	2.4
1	C	751	THR	2.4
1	D	833	LEU	2.4
1	B	784	SER	2.4
1	C	973	ARG	2.4
1	C	939	CYS	2.3
1	B	786	VAL	2.3
1	D	715	ILE	2.3
1	D	740	ILE	2.3
1	A	991	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	888	HIS	2.3
1	B	915	TYR	2.3
1	B	749	GLU	2.3
1	D	923	ILE	2.3
1	D	1007	MET	2.3
1	D	884	GLU	2.2
1	D	885	SER	2.2
1	A	990	PRO	2.2
1	C	994	ASP	2.2
1	C	936	PRO	2.2
1	D	730	LEU	2.2
1	A	982	GLN	2.1
1	B	747	LEU	2.1
1	C	983	GLY	2.1
1	A	814	LEU	2.1
1	C	711	GLU	2.1
1	D	708	LYS	2.1
1	D	988	HIS	2.1
1	B	735	GLY	2.1
1	A	743	ALA	2.1
1	D	917	GLY	2.1
1	C	974	ASP	2.1
1	A	928	GLU	2.1
1	C	970	LYS	2.1
1	D	825	MET	2.0
1	A	1000	ALA	2.0
1	D	710	THR	2.0
1	D	921	SER	2.0
1	C	969	SER	2.0
1	B	739	LYS	2.0
1	D	914	PRO	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](#)

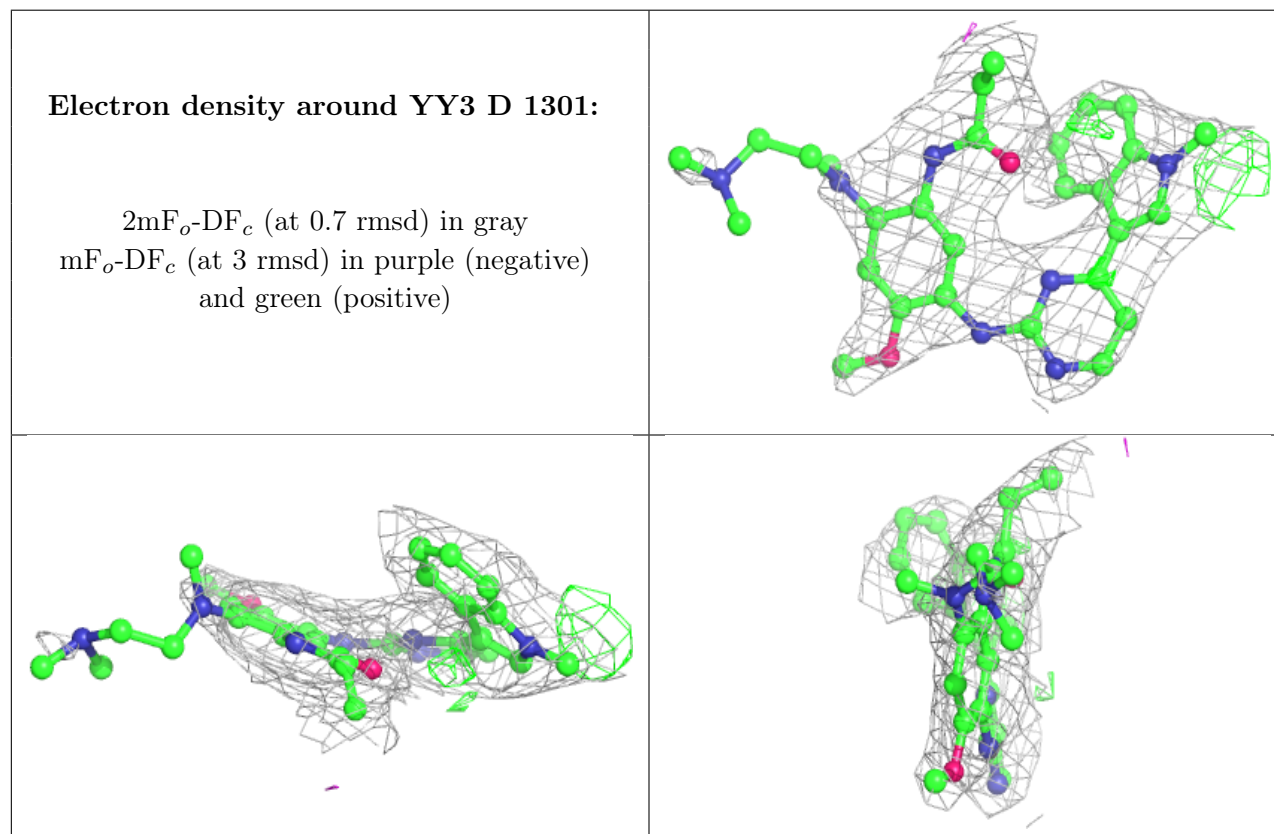
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

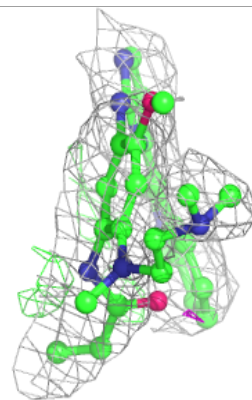
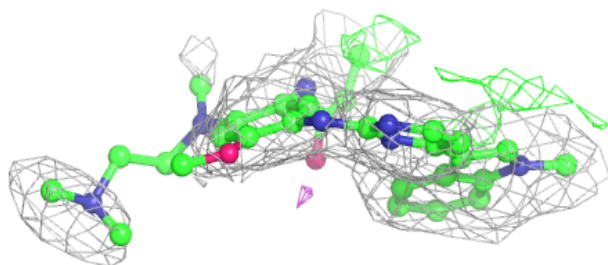
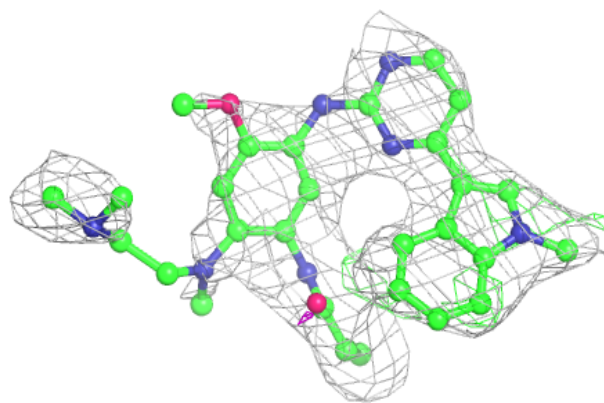
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	YY3	D	1301	37/37	0.85	0.26	46,69,88,90	0
2	YY3	C	1301	37/37	0.85	0.25	38,62,89,91	0
2	YY3	A	1301	37/37	0.89	0.22	34,53,77,81	0
3	VNS	D	1302	40/40	0.90	0.27	32,65,86,115	0
3	VNS	C	1302	40/40	0.90	0.23	24,42,80,84	0
3	VNS	A	1302	40/40	0.91	0.22	29,49,80,109	0
3	VNS	B	1302	40/40	0.91	0.22	18,45,76,92	0
2	YY3	B	1301	37/37	0.93	0.18	27,43,66,71	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.

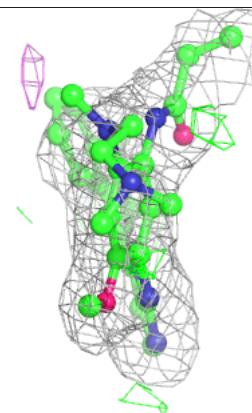
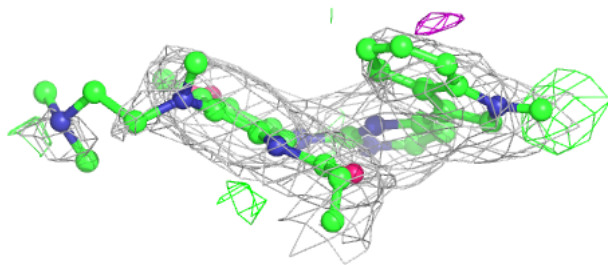
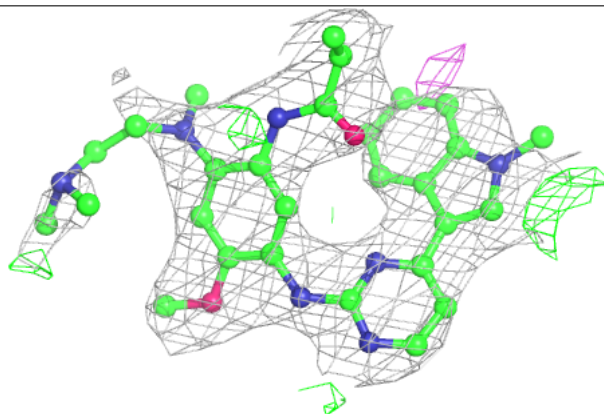


**Electron density around YY3 C 1301:**

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

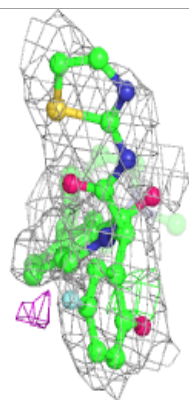
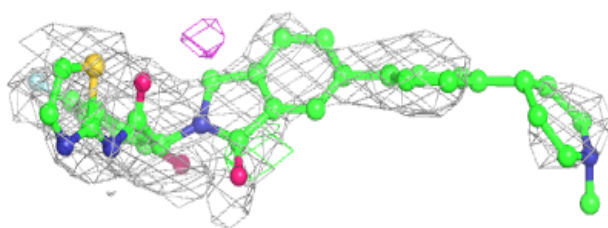
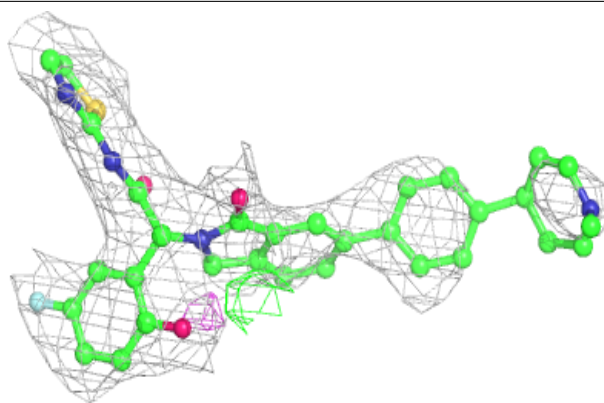
**Electron density around YY3 A 1301:**

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

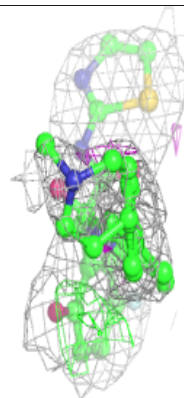
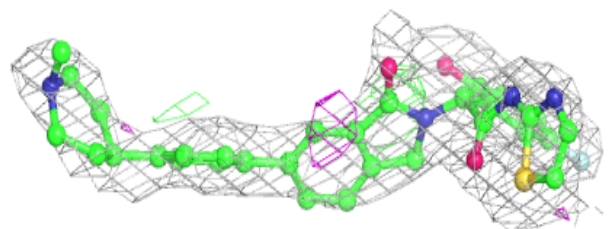
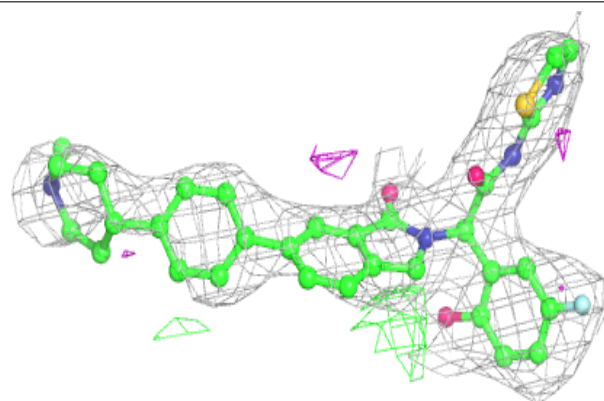


**Electron density around VNS D 1302:**

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

**Electron density around VNS C 1302:**

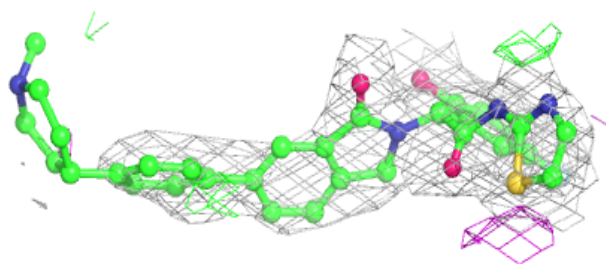
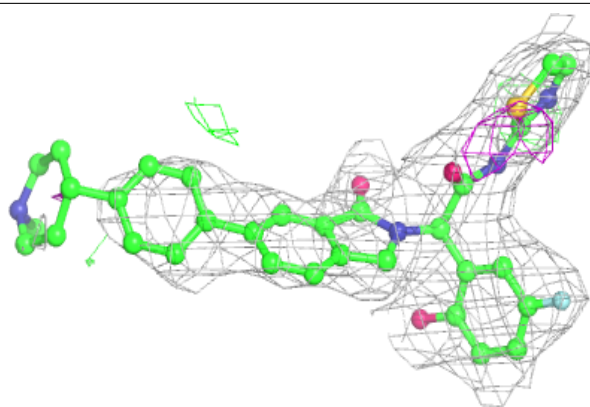
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



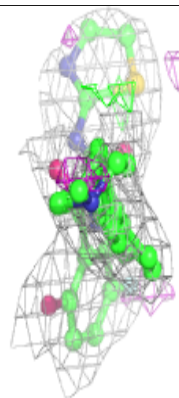
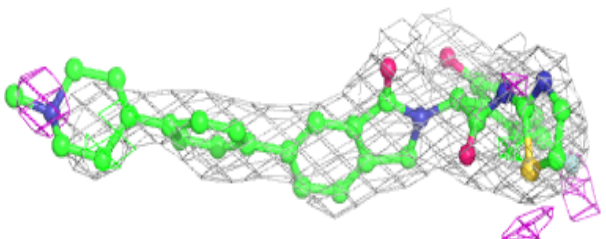
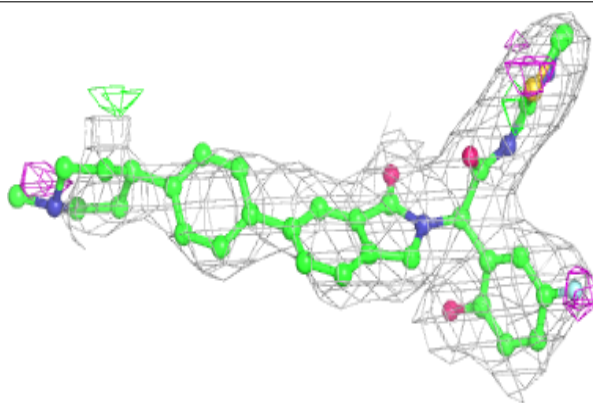


**Electron density around VNS A 1302:**

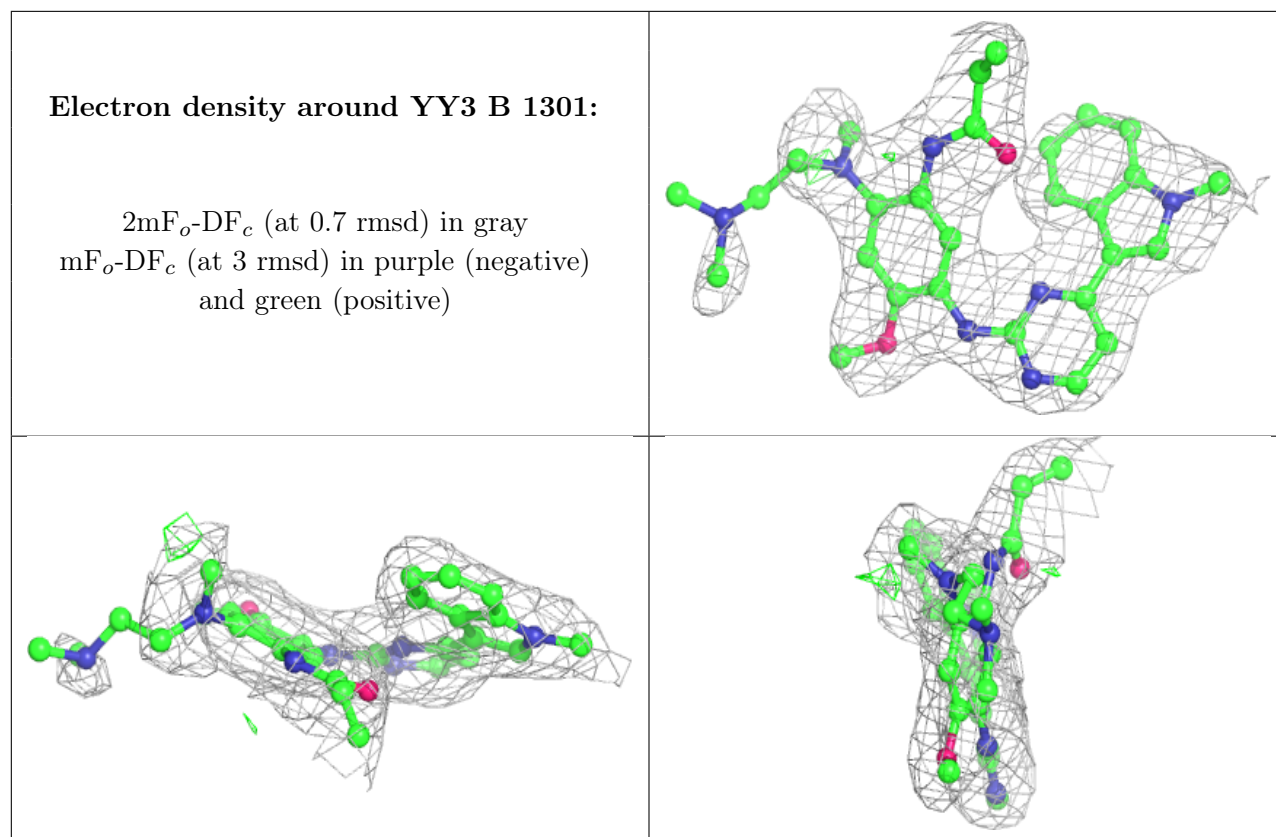
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around VNS B 1302:**

$2mF_o-DF_c$  (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.