



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 PM UTC

PDB ID : 7JXW / pdb_00007jxw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

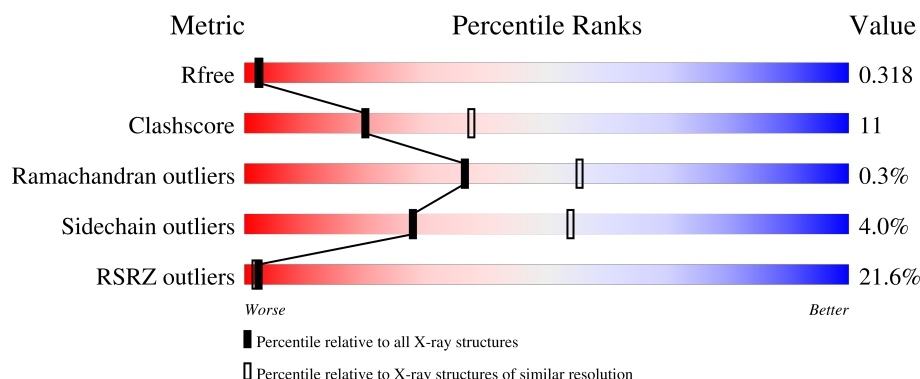
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	16% 63% 22% 13%
1	B	331	8% 65% 22% 12%
1	C	331	16% 63% 24% 11%
1	D	331	35% 65% 22% 13%

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
3	VNS	D	1302	-	X	-	-

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.

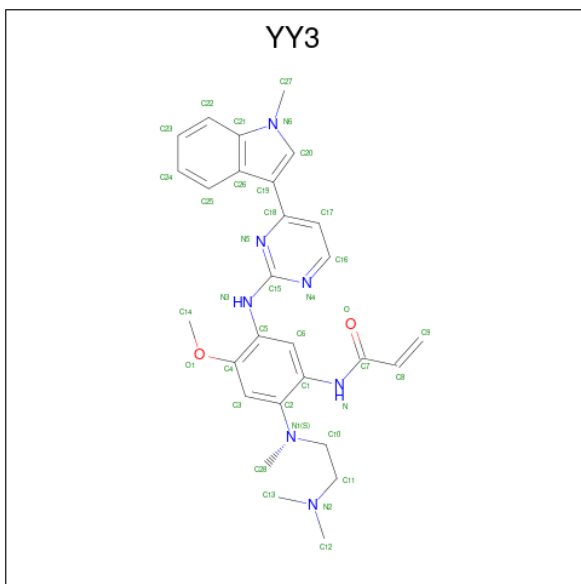
- Molecule 1 is a protein called Epidermal growth factor receptor.

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:

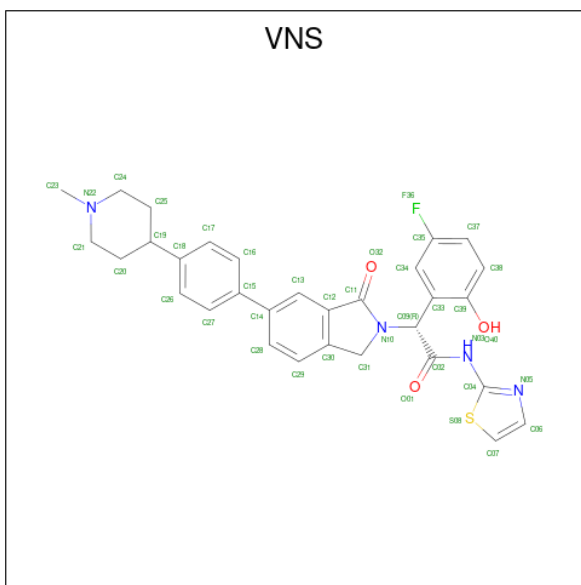
Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	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 (CCD ID: YY3) (formula: $C_{28}H_{33}N_7O_2$) (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 (CCD ID: VNS) (formula: $C_{31}H_{29}FN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



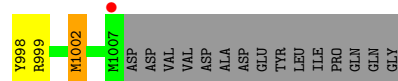
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	A	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	C	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0
3	B	1	Total 40	C 31	F 1	N 4	O 3	S 1	0	0

- 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

- 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, α , β , γ	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) 97.1 (65.64-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.274 , 0.319 0.275 , 0.318	Depositor DCC
R_{free} test set	2111 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9737	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/2374	0.71	0/3209
1	B	0.51	0/2408	0.76	0/3254
1	C	0.45	0/2424	0.68	0/3276
1	D	0.40	0/2377	0.62	0/3212
All	All	0.45	0/9583	0.69	0/12951

There are no bond length outliers.

There are no bond angle outliers.

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	55	0
1	B	2353	0	2397	60	0
1	C	2369	0	2418	58	0
1	D	2323	0	2368	54	0
2	A	37	0	32	3	0
2	B	37	0	32	3	0
2	C	37	0	31	4	0
2	D	37	0	32	4	0
3	A	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	220	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 11.

All (220) 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:766:MET:HE1	1:D:858:LEU:HD23	1.62	0.80
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:D:795:PHE:HE2	1:D:1002:MET:HE1	1.56	0.70
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:943:VAL:HG22	1:C:971:MET:HE1	1.77	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:C:783:THR:OG1	1:C:784:SER:N	2.30	0.61
1:B:716:LYS:HG2	1:B:717:VAL:H	1.65	0.60
1:C:949:LYS:HG2	1:C:952:MET:HE2	1.84	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:A:905:TRP:HB2	1:A:947:MET:HE3	1.85	0.58
1:D:949:LYS:HG2	1:D:952:MET:HE2	1.86	0.58
1:D:905:TRP:HB2	1:D:947:MET:HE3	1.85	0.58
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:C:716:LYS:HZ2	2:C:1301:YY3:H2	1.69	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:B:905:TRP:HB2	1:B:947:MET:HE3	1.87	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:C:905:TRP:HD1	1:C:947:MET:HE1	1.70	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:D:795:PHE:CE2	1:D:1002:MET:HE1	2.38	0.55
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:C:947:MET:HE3	1:C:951:TRP:CH2	2.43	0.53
1:A:968:PHE:HA	1:A:971:MET:HE3	1.91	0.53
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:C:793:MET:HE1	1:C:852:LYS:HD3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:THR:HG22	1:A:936:PRO:HB3	1.92	0.51
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.75	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
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:B:766:MET:HE1	1:B:857:GLY:HA3	1.95	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
2:D:1301:YY3:H25	2:D:1301:YY3:N5	2.29	0.48
1:A:766:MET:HE2	1:A:856:PHE:O	2.13	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:C:825:MET:HE1	1:C:835:HIS:HB2	1.96	0.47
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.15	0.47
1:D:946:ILE:HG21	1:D:968:PHE:CE1	2.49	0.47
1:A:793:MET:HE1	1:A:852:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:HIS:CD2	1:A:856:PHE:HB3	2.50	0.47
3:C:1302:VNS:S08	3:C:1302:VNS:O01	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:D:855:ASP:OD2	2:D:1301:YY3:H33	2.15	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:B:825:MET:HE1	1:B:835:HIS:HB2	1.97	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:C:1002:MET:HE2	1:C:1002:MET:HB3	1.56	0.45
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:D:1002:MET:HE2	1:D:1002:MET:HB3	1.58	0.45
1:C:717:VAL:HG11	1:B:830:ASP:HB3	1.98	0.45
1:D:904:VAL:HG13	1:D:908[B]:MET:HE3	1.99	0.45
1:D:892:THR:O	1:D:895:SER:OG	2.34	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:B:949:LYS:HG2	1:B:952:MET:HE2	1.99	0.44
1:C:714:LYS:HD2	1:C:727:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:788:LEU:C	1:A:789:ILE:HD12	2.44	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
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
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: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:A:747:LEU:HD12	1:A:786:VAL:HB	2.02	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:A:793:MET:HE1	1:A:852:LYS:CD	2.50	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:A:1002:MET:HB3	1:A:1002:MET:HE2	1.67	0.42
1:B:722:ALA:O	1:B:723:PHE:HB2	2.20	0.42
1:B:788:LEU:C	1:B:789:ILE:HD12	2.44	0.42
1:C:705:ARG:NH2	1:C:711:GLU:OE2	2.52	0.41
1:C:744:ILE:HG12	1:C:789:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:934:PRO:HB2	1:B:945:MET:HE1	2.02	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: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: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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/331 (85%)	269 (95%)	12 (4%)	1 (0%)	30	49
1	B	288/331 (87%)	280 (97%)	8 (3%)	0	100	100
1	C	290/331 (88%)	279 (96%)	10 (3%)	1 (0%)	36	55
1	D	282/331 (85%)	270 (96%)	11 (4%)	1 (0%)	30	49
All	All	1142/1324 (86%)	1098 (96%)	41 (4%)	3 (0%)	36	55

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%)	246 (95%)	12 (5%)	23	47
1	B	261/290 (90%)	254 (97%)	7 (3%)	39	67
1	C	263/290 (91%)	246 (94%)	17 (6%)	15	32
1	D	259/290 (89%)	253 (98%)	6 (2%)	44	72
All	All	1041/1160 (90%)	999 (96%)	42 (4%)	28	54

All (42) 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

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Mol	Chain	Res	Type
1	D	987	MET
1	A	720	SER
1	A	732	ILE
1	A	736	GLU
1	A	738	VAL
1	A	739	LYS
1	A	766	MET
1	A	784	SER
1	A	876	VAL
1	A	918	ILE
1	A	960	LYS
1	A	987	MET
1	A	1007	MET
1	C	701	GLN
1	C	723	PHE
1	C	748	ARG
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	947	MET
1	C	985	GLU
1	C	987	MET
1	C	1007	MET
1	B	720	SER
1	B	728	LYS
1	B	748	ARG
1	B	783	THR
1	B	977	ARG
1	B	989	LEU
1	B	1002	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	791	GLN

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Mol	Chain	Res	Type
1	D	988	HIS
1	A	700	ASN
1	A	773	HIS
1	A	812	GLN
1	A	849	GLN
1	C	849	GLN
1	C	988	HIS
1	B	812	GLN
1	B	816	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	VNS	D	1302	-	45,45,45	3.63	28 (62%)	61,65,65	4.58	32 (52%)
3	VNS	A	1302	-	45,45,45	3.48	32 (71%)	61,65,65	4.22	27 (44%)
2	YY3	A	1301	1	40,40,40	2.87	20 (50%)	56,56,56	2.76	18 (32%)
3	VNS	B	1302	-	45,45,45	2.85	22 (48%)	61,65,65	3.90	27 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YY3	D	1301	1	40,40,40	2.10	14 (35%)	56,56,56	2.12	16 (28%)
3	VNS	C	1302	-	45,45,45	3.41	25 (55%)	61,65,65	4.30	32 (52%)
2	YY3	C	1301	1	40,40,40	2.38	14 (35%)	56,56,56	2.48	20 (35%)
2	YY3	B	1301	1	40,40,40	2.46	16 (40%)	56,56,56	2.20	16 (28%)

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	VNS	D	1302	-	-	7/24/46/46	0/6/6/6
3	VNS	A	1302	-	-	1/24/46/46	0/6/6/6
2	YY3	A	1301	1	-	5/25/25/25	0/4/4/4
3	VNS	B	1302	-	-	2/24/46/46	0/6/6/6
2	YY3	D	1301	1	-	7/25/25/25	0/4/4/4
3	VNS	C	1302	-	-	7/24/46/46	0/6/6/6
2	YY3	C	1301	1	-	6/25/25/25	0/4/4/4
2	YY3	B	1301	1	-	9/25/25/25	0/4/4/4

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1302	VNS	C09-C02	11.34	1.66	1.54
3	C	1302	VNS	C09-C02	10.63	1.65	1.54
3	A	1302	VNS	C09-C02	9.62	1.64	1.54
3	D	1302	VNS	C11-N10	9.53	1.45	1.36
2	A	1301	YY3	C7-N	9.44	1.53	1.35
3	A	1302	VNS	C11-N10	9.16	1.45	1.36
3	B	1302	VNS	C09-C02	8.44	1.63	1.54
3	C	1302	VNS	C11-N10	8.29	1.44	1.36
2	C	1301	YY3	C1-C2	7.74	1.49	1.40
3	B	1302	VNS	O01-C02	-7.43	1.09	1.23
3	D	1302	VNS	C04-S08	7.08	1.83	1.74
3	C	1302	VNS	C04-S08	6.90	1.83	1.74
3	B	1302	VNS	C11-N10	6.86	1.43	1.36
3	C	1302	VNS	C02-N03	6.51	1.48	1.36
3	A	1302	VNS	C02-N03	6.40	1.48	1.36
2	B	1301	YY3	C7-N	6.19	1.47	1.35
3	D	1302	VNS	C02-N03	6.03	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	VNS	O01-C02	-5.87	1.12	1.23
3	D	1302	VNS	C18-C19	5.22	1.62	1.52
3	B	1302	VNS	C02-N03	5.21	1.46	1.36
2	B	1301	YY3	C1-C2	4.98	1.46	1.40
2	C	1301	YY3	C10-C11	4.96	1.69	1.51
3	B	1302	VNS	C04-S08	4.92	1.80	1.74
3	D	1302	VNS	C15-C14	4.80	1.60	1.49
3	A	1302	VNS	C04-S08	4.70	1.80	1.74
3	A	1302	VNS	C04-N03	4.68	1.45	1.38
3	D	1302	VNS	O01-C02	-4.61	1.14	1.23
2	A	1301	YY3	C5-N3	4.57	1.52	1.39
3	C	1302	VNS	C15-C14	4.54	1.59	1.49
2	A	1301	YY3	O1-C4	4.53	1.44	1.37
2	A	1301	YY3	C1-N	4.50	1.50	1.41
2	C	1301	YY3	C2-N1	4.50	1.51	1.41
2	D	1301	YY3	O1-C4	4.48	1.44	1.37
2	B	1301	YY3	C2-N1	4.44	1.51	1.41
2	A	1301	YY3	C8-C7	4.25	1.54	1.48
2	C	1301	YY3	C11-N2	4.19	1.61	1.46
3	D	1302	VNS	C12-C11	4.12	1.55	1.48
3	C	1302	VNS	O01-C02	-4.10	1.15	1.23
3	A	1302	VNS	C39-C33	4.09	1.45	1.40
2	A	1301	YY3	C20-C19	4.03	1.41	1.37
3	A	1302	VNS	C15-C14	4.03	1.58	1.49
2	D	1301	YY3	C2-N1	4.01	1.50	1.41
2	A	1301	YY3	C6-C5	4.01	1.45	1.39
2	B	1301	YY3	C6-C1	3.95	1.45	1.39
3	C	1302	VNS	C18-C19	3.92	1.59	1.52
3	D	1302	VNS	C31-C30	3.90	1.55	1.50
3	D	1302	VNS	C27-C26	3.89	1.45	1.38
2	D	1301	YY3	C7-N	3.88	1.42	1.35
3	D	1302	VNS	C26-C18	3.82	1.45	1.39
2	C	1301	YY3	C10-N1	3.82	1.58	1.46
3	C	1302	VNS	C06-N05	3.79	1.45	1.38
2	A	1301	YY3	C6-C1	3.79	1.45	1.39
3	A	1302	VNS	C12-C11	3.76	1.54	1.48
3	D	1302	VNS	C04-N03	3.75	1.43	1.38
3	C	1302	VNS	C09-N10	3.70	1.51	1.46
2	C	1301	YY3	O1-C4	3.69	1.43	1.37
2	A	1301	YY3	C3-C2	3.69	1.45	1.39
2	B	1301	YY3	C12-N2	3.67	1.57	1.46
3	B	1302	VNS	C33-C09	3.66	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	VNS	C06-N05	3.66	1.44	1.38
3	C	1302	VNS	C17-C16	3.61	1.44	1.38
2	B	1301	YY3	C10-C11	3.55	1.64	1.51
3	C	1302	VNS	C12-C11	3.54	1.54	1.48
2	A	1301	YY3	C2-N1	3.53	1.49	1.41
2	D	1301	YY3	C20-C19	3.51	1.40	1.37
3	A	1302	VNS	C33-C09	3.48	1.56	1.52
3	A	1302	VNS	C18-C19	3.47	1.59	1.52
3	C	1302	VNS	C34-C35	3.47	1.43	1.37
3	C	1302	VNS	C27-C26	3.47	1.44	1.38
3	B	1302	VNS	C04-N03	3.38	1.43	1.38
3	C	1302	VNS	C29-C28	3.38	1.44	1.38
3	C	1302	VNS	C04-N05	3.32	1.36	1.31
2	D	1301	YY3	C15-N3	3.31	1.43	1.36
3	D	1302	VNS	C06-N05	3.23	1.44	1.38
2	B	1301	YY3	C11-N2	3.21	1.57	1.46
3	B	1302	VNS	C06-N05	3.21	1.44	1.38
3	A	1302	VNS	C25-C24	3.17	1.61	1.52
2	D	1301	YY3	C1-C2	3.16	1.44	1.40
3	D	1302	VNS	C29-C28	3.13	1.43	1.38
2	B	1301	YY3	C20-C19	3.12	1.40	1.37
2	A	1301	YY3	C10-C11	3.12	1.63	1.51
2	B	1301	YY3	C8-C7	3.12	1.53	1.48
3	D	1302	VNS	C13-C12	3.10	1.44	1.39
3	D	1302	VNS	C09-N10	3.06	1.50	1.46
3	A	1302	VNS	C29-C28	3.05	1.43	1.38
2	A	1301	YY3	C15-N3	3.04	1.42	1.36
3	A	1302	VNS	C26-C18	3.03	1.43	1.39
3	A	1302	VNS	C17-C16	3.02	1.43	1.38
3	B	1302	VNS	C15-C14	3.02	1.56	1.49
3	C	1302	VNS	C06-C07	3.00	1.41	1.34
3	D	1302	VNS	C34-C35	2.98	1.42	1.37
3	A	1302	VNS	C37-C35	2.97	1.43	1.37
2	D	1301	YY3	C5-N3	2.96	1.48	1.39
3	D	1302	VNS	C04-N05	2.95	1.36	1.31
3	A	1302	VNS	C04-N05	2.94	1.36	1.31
3	B	1302	VNS	C31-N10	2.94	1.50	1.47
2	D	1301	YY3	C10-C11	2.93	1.62	1.51
3	A	1302	VNS	C34-C35	2.93	1.42	1.37
3	A	1302	VNS	C27-C26	2.92	1.43	1.38
3	C	1302	VNS	C31-C30	2.91	1.54	1.50
3	A	1302	VNS	C31-N10	2.90	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	VNS	C13-C12	2.88	1.44	1.39
3	D	1302	VNS	C17-C16	2.85	1.43	1.38
2	B	1301	YY3	C21-N6	2.85	1.42	1.38
3	A	1302	VNS	C06-C07	2.84	1.40	1.34
3	B	1302	VNS	C27-C26	2.79	1.43	1.38
3	C	1302	VNS	C28-C14	2.78	1.44	1.39
3	D	1302	VNS	C13-C14	2.77	1.44	1.39
2	A	1301	YY3	C11-N2	2.77	1.56	1.46
2	C	1301	YY3	C5-N3	2.76	1.47	1.39
3	D	1302	VNS	C31-N10	2.74	1.50	1.47
3	D	1302	VNS	C33-C09	2.73	1.55	1.52
3	A	1302	VNS	C09-N10	2.72	1.50	1.46
2	B	1301	YY3	C6-C5	2.69	1.43	1.39
2	D	1301	YY3	C11-N2	2.64	1.55	1.46
3	C	1302	VNS	C37-C35	2.62	1.42	1.37
2	C	1301	YY3	C7-N	2.62	1.40	1.35
3	C	1302	VNS	C31-N10	2.61	1.49	1.47
3	A	1302	VNS	C21-N22	2.59	1.52	1.46
2	B	1301	YY3	C1-N	2.59	1.46	1.41
3	C	1302	VNS	C04-N03	2.59	1.42	1.38
3	B	1302	VNS	F36-C35	-2.57	1.30	1.36
2	B	1301	YY3	O1-C4	2.56	1.41	1.37
2	B	1301	YY3	C13-N2	2.55	1.54	1.46
3	B	1302	VNS	C29-C28	2.54	1.42	1.38
2	A	1301	YY3	C17-C16	2.54	1.43	1.38
2	D	1301	YY3	C10-N1	2.54	1.54	1.46
2	D	1301	YY3	C13-N2	2.49	1.53	1.46
2	B	1301	YY3	C3-C2	2.49	1.43	1.39
3	C	1302	VNS	C13-C12	2.48	1.43	1.39
2	A	1301	YY3	C1-C2	2.48	1.43	1.40
2	C	1301	YY3	C28-N1	2.47	1.50	1.46
2	A	1301	YY3	C10-N1	2.45	1.54	1.46
3	D	1302	VNS	C37-C35	2.45	1.41	1.37
2	A	1301	YY3	C3-C4	2.44	1.43	1.38
2	D	1301	YY3	C15-N4	2.44	1.38	1.34
2	C	1301	YY3	C20-C19	2.43	1.39	1.37
3	B	1302	VNS	C04-N05	2.40	1.35	1.31
3	D	1302	VNS	C28-C14	2.39	1.44	1.39
3	C	1302	VNS	C17-C18	2.39	1.42	1.39
3	B	1302	VNS	C17-C16	2.38	1.42	1.38
3	D	1302	VNS	C25-C19	2.38	1.59	1.53
3	B	1302	VNS	C31-C30	2.36	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	VNS	C39-C33	2.34	1.42	1.40
3	A	1302	VNS	C29-C30	2.34	1.43	1.39
3	B	1302	VNS	C34-C35	2.33	1.41	1.37
3	A	1302	VNS	C13-C14	2.33	1.43	1.39
3	A	1302	VNS	C17-C18	2.32	1.42	1.39
2	D	1301	YY3	C3-C2	2.32	1.43	1.39
3	D	1302	VNS	C29-C30	2.30	1.43	1.39
2	C	1301	YY3	C15-N3	2.29	1.41	1.36
3	A	1302	VNS	C28-C14	2.27	1.43	1.39
3	D	1302	VNS	C27-C15	2.26	1.43	1.39
2	C	1301	YY3	C1-N	2.23	1.46	1.41
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	D	1302	VNS	C06-C07	2.19	1.39	1.34
2	A	1301	YY3	C28-N1	2.19	1.49	1.46
3	B	1302	VNS	C18-C19	2.18	1.56	1.52
3	A	1302	VNS	C24-N22	2.18	1.51	1.46
3	B	1302	VNS	C26-C18	2.13	1.42	1.39
3	A	1302	VNS	C31-C30	2.12	1.53	1.50
2	C	1301	YY3	C23-C24	2.12	1.42	1.38
2	A	1301	YY3	C13-N2	2.10	1.52	1.46
2	B	1301	YY3	C18-C19	-2.08	1.44	1.48
3	B	1302	VNS	C28-C14	2.07	1.43	1.39
3	B	1302	VNS	C09-N10	2.06	1.49	1.46
3	C	1302	VNS	C20-C21	2.04	1.57	1.52
2	C	1301	YY3	C15-N4	2.04	1.37	1.34
2	D	1301	YY3	C17-C16	2.02	1.42	1.38
2	A	1301	YY3	C18-C19	-2.00	1.44	1.48

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	VNS	C31-N10-C11	-20.11	104.67	113.15
3	C	1302	VNS	C31-N10-C11	-19.80	104.80	113.15
3	D	1302	VNS	C31-N10-C11	-19.74	104.83	113.15
3	A	1302	VNS	C31-N10-C11	-18.34	105.42	113.15
2	A	1301	YY3	C8-C7-N	14.44	123.64	113.84
2	C	1301	YY3	C8-C7-N	11.46	121.62	113.84
2	B	1301	YY3	C8-C7-N	10.64	121.06	113.84
3	B	1302	VNS	C12-C11-N10	10.41	113.04	106.42
3	D	1302	VNS	C30-C31-N10	10.39	107.84	102.31
3	C	1302	VNS	C30-C31-N10	10.31	107.79	102.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	VNS	C30-C31-N10	10.12	107.69	102.31
2	D	1301	YY3	C8-C7-N	9.55	120.33	113.84
3	D	1302	VNS	C24-C25-C19	9.47	122.08	111.00
3	C	1302	VNS	C12-C11-N10	9.38	112.39	106.42
3	D	1302	VNS	C12-C11-N10	9.35	112.36	106.42
3	A	1302	VNS	C20-C21-N22	8.77	122.51	111.20
3	B	1302	VNS	C30-C31-N10	8.67	106.92	102.31
3	C	1302	VNS	C21-C20-C19	8.21	120.61	111.00
3	A	1302	VNS	C21-C20-C19	8.17	120.56	111.00
3	D	1302	VNS	C21-C20-C19	8.13	120.52	111.00
3	C	1302	VNS	O32-C11-N10	-8.07	118.92	125.34
3	A	1302	VNS	C24-C25-C19	7.94	120.29	111.00
3	D	1302	VNS	O32-C11-N10	-7.69	119.23	125.34
3	D	1302	VNS	C24-N22-C21	7.68	121.76	109.54
3	D	1302	VNS	C30-C12-C11	-7.66	104.78	108.94
3	D	1302	VNS	C20-C21-N22	7.63	121.04	111.20
3	A	1302	VNS	C12-C11-N10	7.55	111.22	106.42
3	C	1302	VNS	C30-C12-C11	-7.49	104.88	108.94
3	A	1302	VNS	C25-C24-N22	7.07	120.32	111.20
3	B	1302	VNS	O32-C11-N10	-6.82	119.92	125.34
3	C	1302	VNS	C20-C21-N22	6.76	119.92	111.20
3	A	1302	VNS	C30-C12-C11	-6.53	105.40	108.94
3	A	1302	VNS	C20-C19-C18	-6.43	97.45	112.67
3	A	1302	VNS	O32-C11-N10	-6.41	120.25	125.34
3	C	1302	VNS	C24-C25-C19	5.92	117.92	111.00
2	C	1301	YY3	C1-C2-N1	5.56	129.46	118.29
3	B	1302	VNS	C30-C12-C11	-5.39	106.01	108.94
3	D	1302	VNS	C25-C24-N22	5.37	118.13	111.20
3	A	1302	VNS	N03-C04-N05	5.32	131.27	121.19
3	C	1302	VNS	C26-C18-C17	-5.22	111.83	118.30
3	D	1302	VNS	C26-C18-C17	-5.20	111.86	118.30
3	C	1302	VNS	N03-C04-N05	5.05	130.75	121.19
3	B	1302	VNS	N03-C04-N05	5.03	130.72	121.19
3	D	1302	VNS	N03-C04-N05	5.01	130.69	121.19
2	A	1301	YY3	O-C7-C8	-4.86	115.41	122.70
3	A	1302	VNS	C24-N22-C21	4.59	116.85	109.54
2	A	1301	YY3	C21-C26-C19	4.50	109.41	106.83
3	C	1302	VNS	C24-N22-C21	4.45	116.63	109.54
3	B	1302	VNS	C21-C20-C19	4.37	116.11	111.00
2	A	1301	YY3	C6-C5-C4	-4.32	113.88	118.95
3	C	1302	VNS	C16-C15-C14	4.26	128.60	121.25
2	C	1301	YY3	C3-C2-C1	-4.14	114.18	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	VNS	C20-C19-C18	-4.09	102.98	112.67
3	D	1302	VNS	C33-C09-C02	-3.98	103.05	112.87
2	A	1301	YY3	C18-N5-C15	3.98	119.89	116.87
3	B	1302	VNS	C31-N10-C09	3.90	127.48	123.84
2	C	1301	YY3	O1-C4-C5	3.86	119.62	114.81
3	A	1302	VNS	C26-C18-C17	-3.84	113.54	118.30
2	B	1301	YY3	C3-C2-C1	-3.80	114.64	119.95
3	A	1302	VNS	C07-S08-C04	3.79	94.42	90.07
2	B	1301	YY3	C1-C2-N1	3.76	125.86	118.29
2	D	1301	YY3	C6-C5-C4	-3.71	114.59	118.95
3	B	1302	VNS	C26-C18-C17	-3.71	113.71	118.30
2	D	1301	YY3	C21-C26-C19	3.63	108.91	106.83
3	C	1302	VNS	C27-C15-C16	-3.59	111.25	117.68
2	D	1301	YY3	O-C7-C8	-3.59	117.31	122.70
2	C	1301	YY3	C6-C5-C4	-3.59	114.73	118.95
3	B	1302	VNS	C24-C25-C19	3.57	115.18	111.00
2	A	1301	YY3	C1-C2-N1	3.57	125.46	118.29
2	D	1301	YY3	C3-C2-C1	-3.55	115.00	119.95
3	D	1302	VNS	C27-C15-C16	-3.53	111.36	117.68
3	D	1302	VNS	C33-C34-C35	3.53	123.18	118.57
2	D	1301	YY3	O1-C4-C5	3.53	119.20	114.81
3	C	1302	VNS	C28-C14-C13	-3.52	113.38	118.23
3	D	1302	VNS	S08-C04-N05	-3.50	108.00	114.59
3	D	1302	VNS	C28-C14-C13	-3.48	113.44	118.23
2	B	1301	YY3	C21-C26-C19	3.45	108.81	106.83
2	A	1301	YY3	C2-C3-C4	3.40	125.22	118.01
3	C	1302	VNS	C31-N10-C09	3.39	127.00	123.84
3	D	1302	VNS	C37-C35-C34	-3.36	118.80	123.23
3	A	1302	VNS	S08-C04-N05	-3.36	108.26	114.59
3	D	1302	VNS	C16-C17-C18	3.31	124.49	121.18
3	D	1302	VNS	C20-C19-C18	-3.31	104.84	112.67
2	D	1301	YY3	N4-C15-N5	-3.30	123.23	126.42
3	B	1302	VNS	S08-C04-N05	-3.30	108.37	114.59
2	A	1301	YY3	C16-C17-C18	-3.30	114.98	117.02
3	D	1302	VNS	C31-N10-C09	3.27	126.89	123.84
2	A	1301	YY3	C3-C2-C1	-3.25	115.42	119.95
2	B	1301	YY3	C16-C17-C18	-3.24	115.02	117.02
3	D	1302	VNS	C17-C16-C15	3.23	125.26	121.12
2	C	1301	YY3	C26-C19-C20	-3.21	104.35	106.02
2	C	1301	YY3	C2-C3-C4	3.21	124.80	118.01
3	D	1302	VNS	C13-C12-C11	3.19	134.87	129.39
3	B	1302	VNS	C24-N22-C21	3.17	114.58	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	YY3	O-C7-N	-3.15	118.96	123.11
2	C	1301	YY3	O1-C4-C3	-3.15	118.65	124.08
3	C	1302	VNS	C27-C26-C18	3.15	124.33	121.18
2	B	1301	YY3	C6-C5-C4	-3.15	115.25	118.95
2	A	1301	YY3	N4-C15-N5	-3.10	123.42	126.42
3	A	1302	VNS	C28-C14-C13	-3.09	113.98	118.23
2	A	1301	YY3	C26-C21-N6	-3.08	106.03	107.91
2	D	1301	YY3	C1-C2-N1	3.08	124.47	118.29
3	B	1302	VNS	C07-S08-C04	3.07	93.59	90.07
3	A	1302	VNS	C13-C12-C11	3.07	134.66	129.39
3	A	1302	VNS	C25-C19-C20	3.05	116.32	109.68
2	B	1301	YY3	O-C7-C8	-2.98	118.23	122.70
3	C	1302	VNS	O01-C02-C09	-2.95	116.90	120.95
3	B	1302	VNS	C33-C34-C35	2.94	122.40	118.57
2	C	1301	YY3	C3-C2-N1	-2.93	116.34	120.90
2	D	1301	YY3	C2-C3-C4	2.88	124.12	118.01
2	B	1301	YY3	C26-C21-N6	-2.88	106.16	107.91
3	C	1302	VNS	C29-C30-C12	-2.85	117.78	120.28
2	A	1301	YY3	C19-C20-N6	-2.84	108.88	110.95
3	C	1302	VNS	C37-C35-C34	-2.83	119.49	123.23
3	C	1302	VNS	C17-C16-C15	2.82	124.75	121.12
3	C	1302	VNS	C20-C19-C18	-2.81	106.02	112.67
2	B	1301	YY3	C2-C3-C4	2.81	123.95	118.01
3	B	1302	VNS	C28-C14-C15	2.78	126.06	121.25
3	B	1302	VNS	C29-C30-C12	-2.78	117.85	120.28
3	A	1302	VNS	O01-C02-C09	-2.76	117.17	120.95
3	B	1302	VNS	C27-C15-C16	-2.76	112.74	117.68
3	B	1302	VNS	C20-C21-N22	2.75	114.74	111.20
3	D	1302	VNS	C07-S08-C04	2.74	93.21	90.07
2	D	1301	YY3	C26-C21-N6	-2.71	106.26	107.91
2	C	1301	YY3	C2-C1-N	2.70	123.58	118.61
3	B	1302	VNS	C17-C16-C15	2.69	124.58	121.12
2	D	1301	YY3	O1-C4-C3	-2.68	119.45	124.08
3	D	1302	VNS	C26-C18-C19	2.67	127.86	121.09
2	C	1301	YY3	C4-C5-N3	2.64	123.99	118.10
3	D	1302	VNS	C29-C30-C12	-2.60	118.00	120.28
2	B	1301	YY3	C22-C21-N6	2.57	133.41	129.91
3	B	1302	VNS	C28-C14-C13	-2.57	114.70	118.23
2	A	1301	YY3	C12-N2-C13	-2.56	103.15	109.72
3	C	1302	VNS	C13-C12-C11	2.55	133.76	129.39
2	A	1301	YY3	C6-C1-C2	-2.53	117.03	119.80
3	C	1302	VNS	S08-C04-N05	-2.51	109.86	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	YY3	C27-N6-C21	-2.51	123.36	125.69
2	A	1301	YY3	C21-N6-C20	2.50	110.35	108.54
3	A	1302	VNS	C23-N22-C24	-2.50	105.87	110.63
3	B	1302	VNS	C25-C19-C18	2.48	118.54	112.67
2	C	1301	YY3	C26-C19-C18	2.47	129.80	126.36
3	C	1302	VNS	C26-C27-C15	2.46	124.28	121.12
2	C	1301	YY3	C26-C21-N6	-2.45	106.42	107.91
3	B	1302	VNS	C23-N22-C21	-2.45	105.96	110.63
2	C	1301	YY3	N4-C15-N5	-2.43	124.07	126.42
3	A	1302	VNS	C29-C30-C12	-2.43	118.16	120.28
3	C	1302	VNS	C33-C09-C02	-2.43	106.89	112.87
3	D	1302	VNS	C26-C27-C15	2.42	124.23	121.12
2	D	1301	YY3	C4-C5-N3	2.42	123.51	118.10
3	A	1302	VNS	C17-C16-C15	2.40	124.20	121.12
3	A	1302	VNS	C27-C15-C16	-2.37	113.44	117.68
3	C	1302	VNS	C25-C24-N22	2.35	114.23	111.20
3	B	1302	VNS	C23-N22-C24	-2.35	106.16	110.63
3	B	1302	VNS	C37-C35-C34	-2.35	120.13	123.23
3	D	1302	VNS	C25-C19-C18	2.32	118.18	112.67
2	D	1301	YY3	C19-C20-N6	-2.28	109.29	110.95
2	B	1301	YY3	C27-N6-C20	-2.28	123.30	125.70
3	C	1302	VNS	C16-C17-C18	2.27	123.45	121.18
2	B	1301	YY3	C16-N4-C15	2.27	117.32	115.42
3	B	1302	VNS	O01-C02-C09	-2.27	117.84	120.95
3	A	1302	VNS	C27-C26-C18	2.27	123.44	121.18
3	D	1302	VNS	O01-C02-C09	-2.24	117.88	120.95
2	A	1301	YY3	O1-C4-C5	2.24	117.60	114.81
2	C	1301	YY3	C21-N6-C20	2.22	110.15	108.54
3	D	1302	VNS	C25-C19-C20	2.22	114.50	109.68
3	C	1302	VNS	S08-C04-N03	-2.21	119.35	123.29
2	C	1301	YY3	O-C7-C8	-2.20	119.40	122.70
2	D	1301	YY3	C16-C17-C18	-2.18	115.67	117.02
3	D	1302	VNS	C16-C15-C14	2.18	125.01	121.25
2	B	1301	YY3	C3-C4-C5	2.17	123.22	120.54
2	D	1301	YY3	C22-C21-N6	2.16	132.86	129.91
2	C	1301	YY3	C11-C10-N1	2.16	115.96	112.41
2	B	1301	YY3	C6-C5-N3	2.15	125.54	121.12
2	B	1301	YY3	N4-C15-N5	-2.14	124.36	126.42
2	C	1301	YY3	C21-C26-C19	2.12	108.05	106.83
3	C	1302	VNS	C33-C34-C35	2.11	121.33	118.57
3	A	1302	VNS	C33-C34-C35	2.11	121.33	118.57
3	A	1302	VNS	C06-N05-C04	2.10	114.51	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	YY3	C9-C8-C7	2.07	124.50	122.22
3	C	1302	VNS	C29-C28-C14	2.05	123.76	121.12
3	C	1302	VNS	C17-C18-C19	2.05	126.29	121.09
2	A	1301	YY3	C5-C6-C1	2.04	127.11	121.64
2	D	1301	YY3	C11-C10-N1	2.04	115.76	112.41
3	B	1302	VNS	C38-C39-C33	2.03	122.19	120.40
3	C	1302	VNS	C07-S08-C04	2.03	92.40	90.07
2	C	1301	YY3	C1-N-C7	-2.01	122.09	126.88
3	D	1302	VNS	C13-C14-C15	2.01	124.21	120.84
3	A	1302	VNS	C37-C35-C34	-2.01	120.58	123.23

There are no chirality outliers.

All (44) 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	B	1302	VNS	S08-C04-N03-C02
3	D	1302	VNS	C28-C14-C15-C27
2	D	1301	YY3	C10-C11-N2-C12
2	B	1301	YY3	N1-C10-C11-N2
2	D	1301	YY3	C1-C2-N1-C28
3	C	1302	VNS	C17-C18-C19-C25
2	B	1301	YY3	C10-C11-N2-C12
2	B	1301	YY3	C5-C4-O1-C14
2	B	1301	YY3	C10-C11-N2-C13
2	D	1301	YY3	C3-C2-N1-C28
2	B	1301	YY3	C3-C2-N1-C10
2	B	1301	YY3	C3-C4-O1-C14
3	C	1302	VNS	C26-C18-C19-C25

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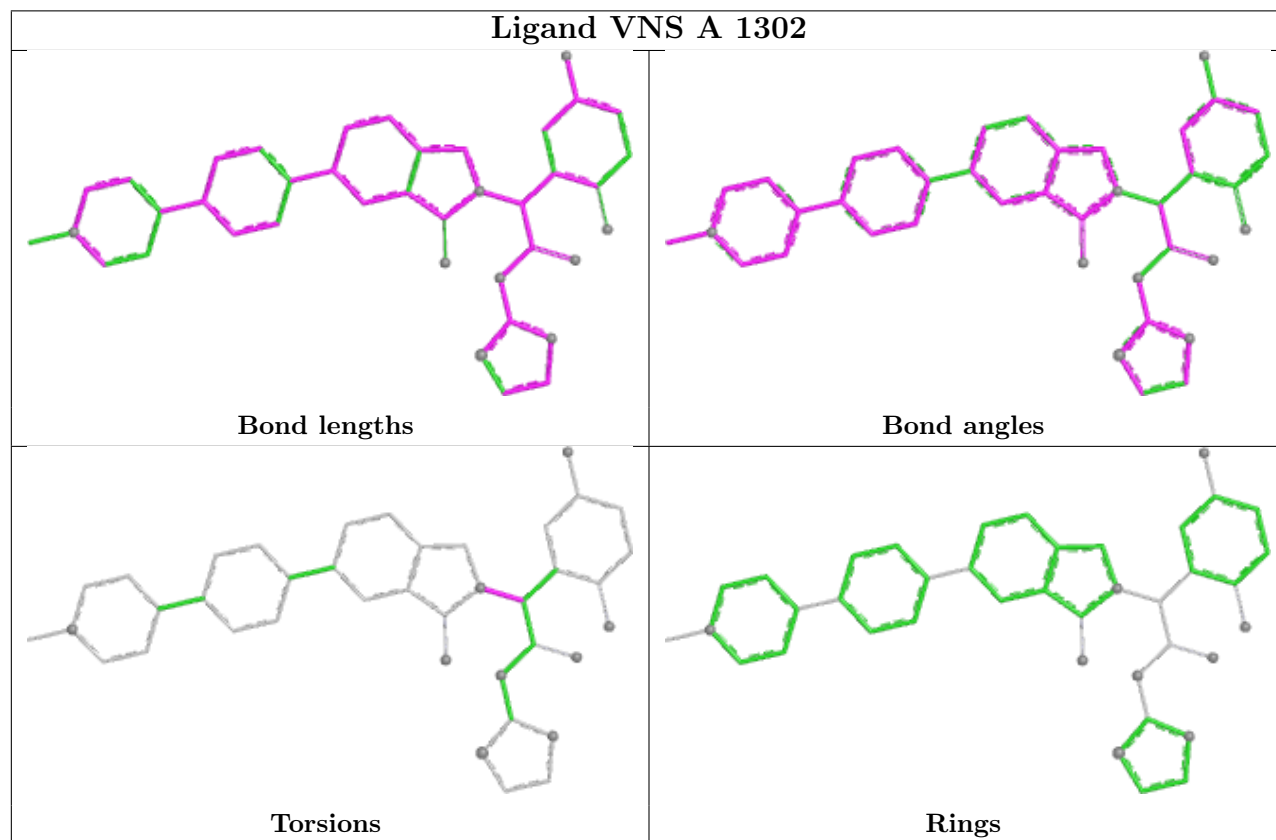
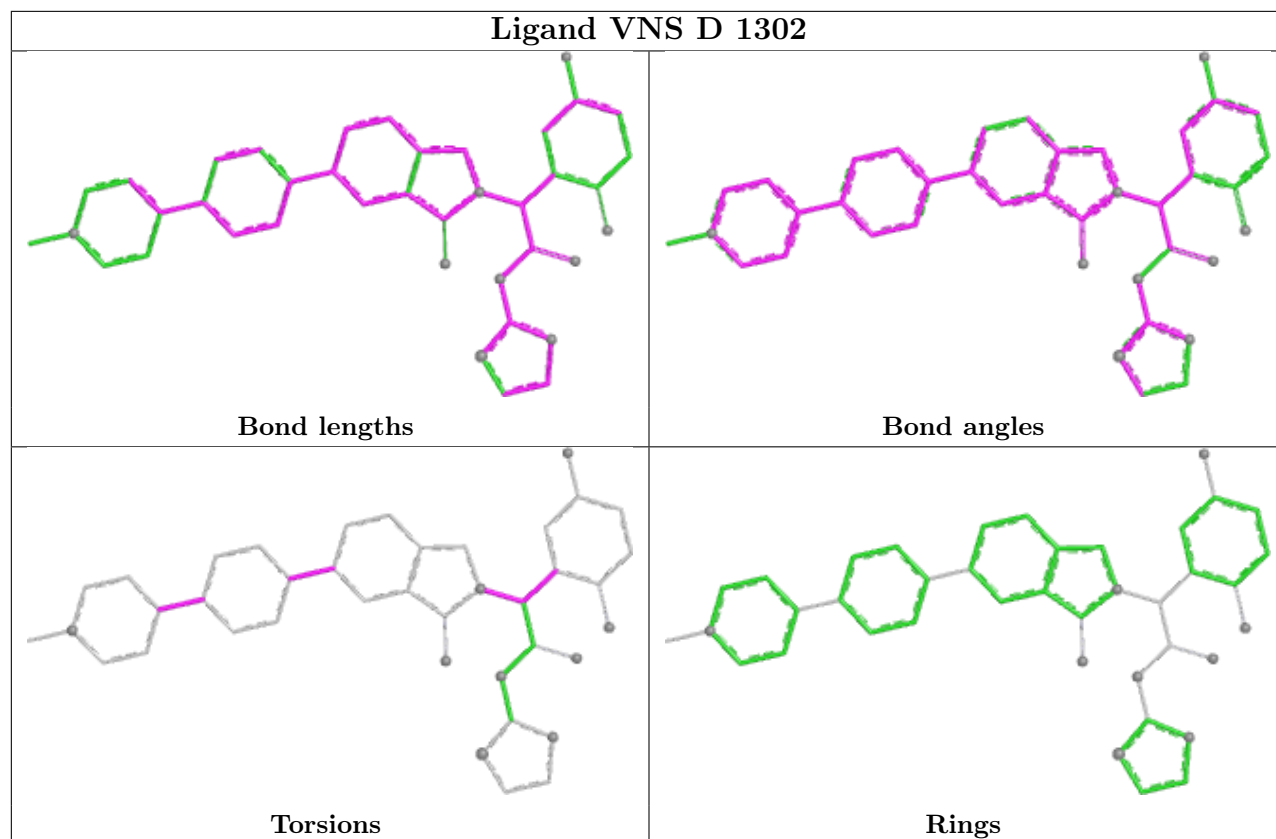
Mol	Chain	Res	Type	Atoms
2	C	1301	YY3	C6-C1-N-C7
3	C	1302	VNS	C02-C09-C33-C34
3	A	1302	VNS	C33-C09-N10-C31
3	C	1302	VNS	C33-C09-N10-C31
3	B	1302	VNS	C33-C09-N10-C31
3	D	1302	VNS	C13-C14-C15-C27
3	D	1302	VNS	C17-C18-C19-C20
2	C	1301	YY3	C2-C1-N-C7
3	D	1302	VNS	C26-C18-C19-C20
3	D	1302	VNS	C33-C09-N10-C31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

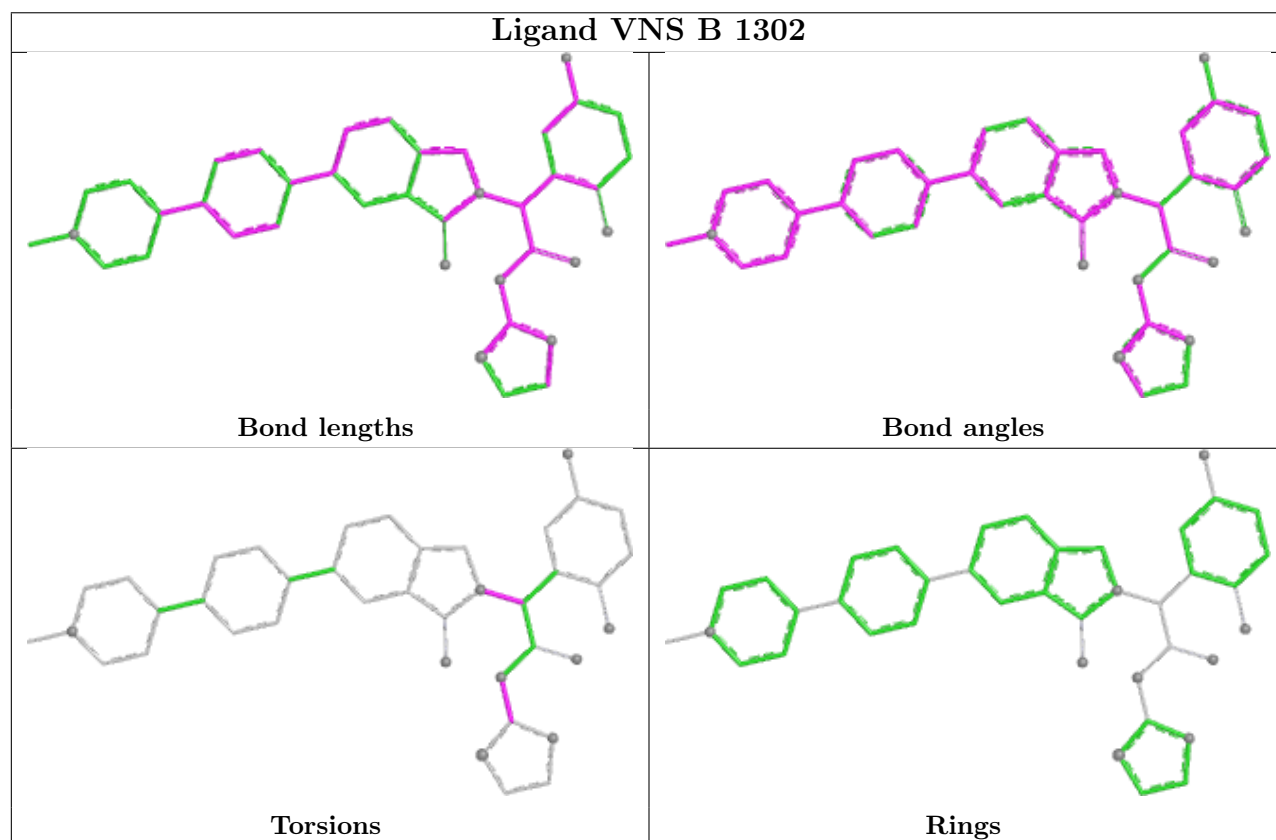
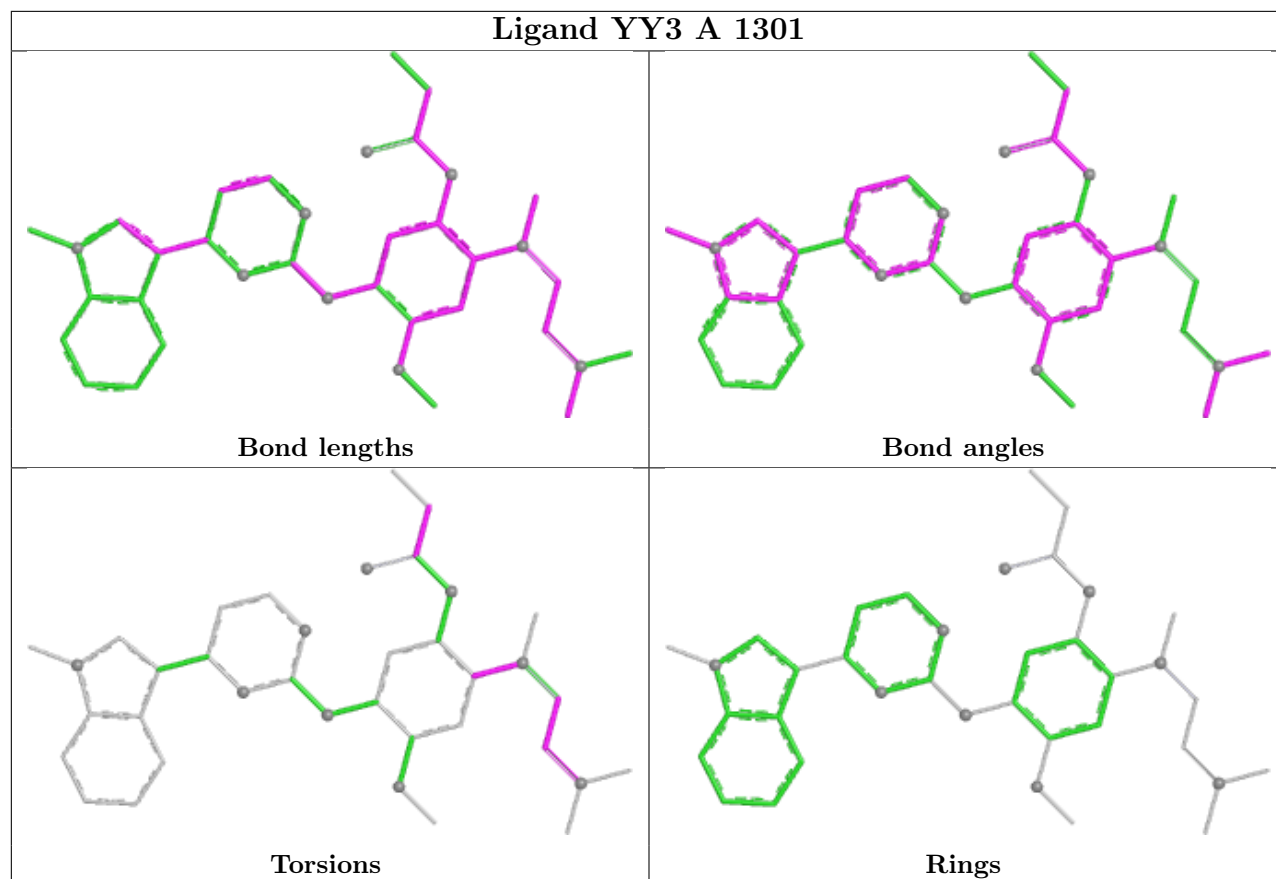
There are no ring outliers.

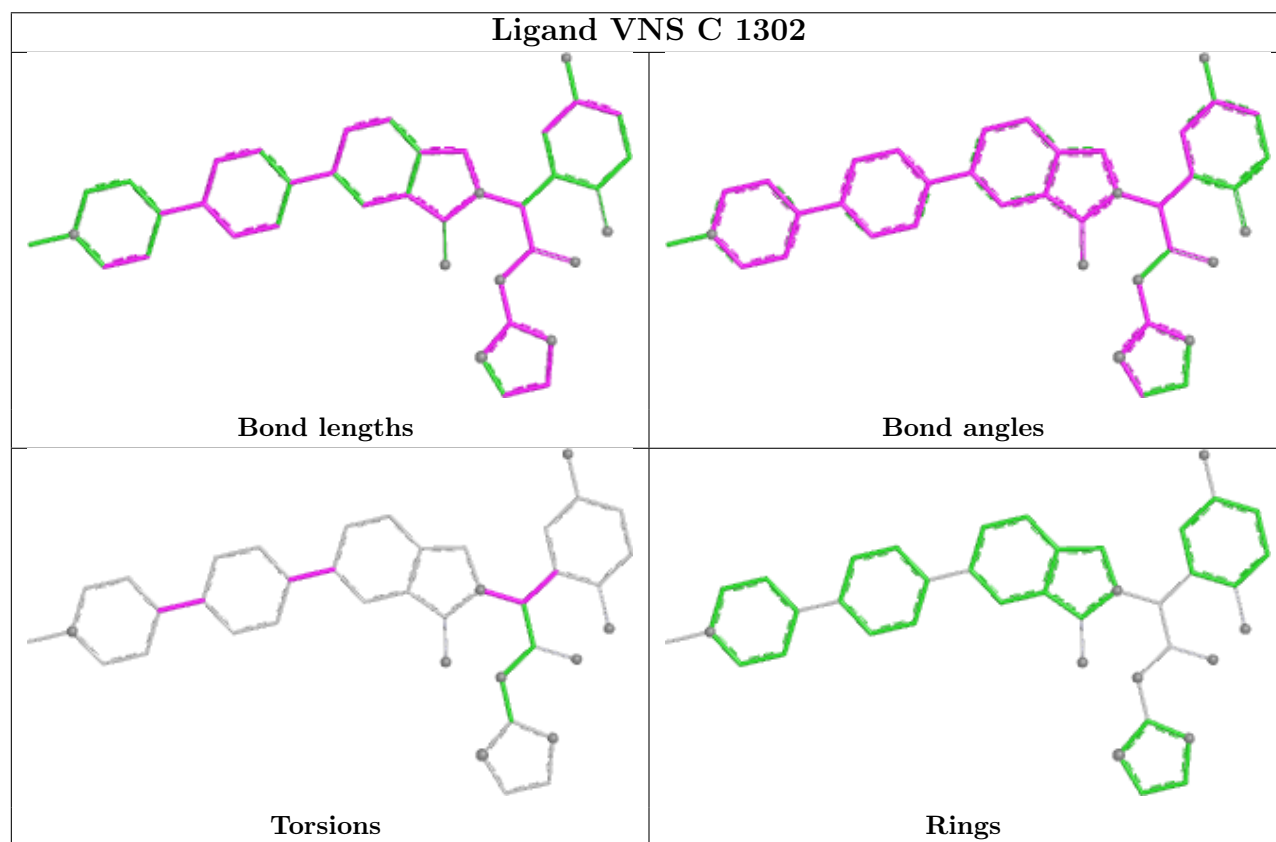
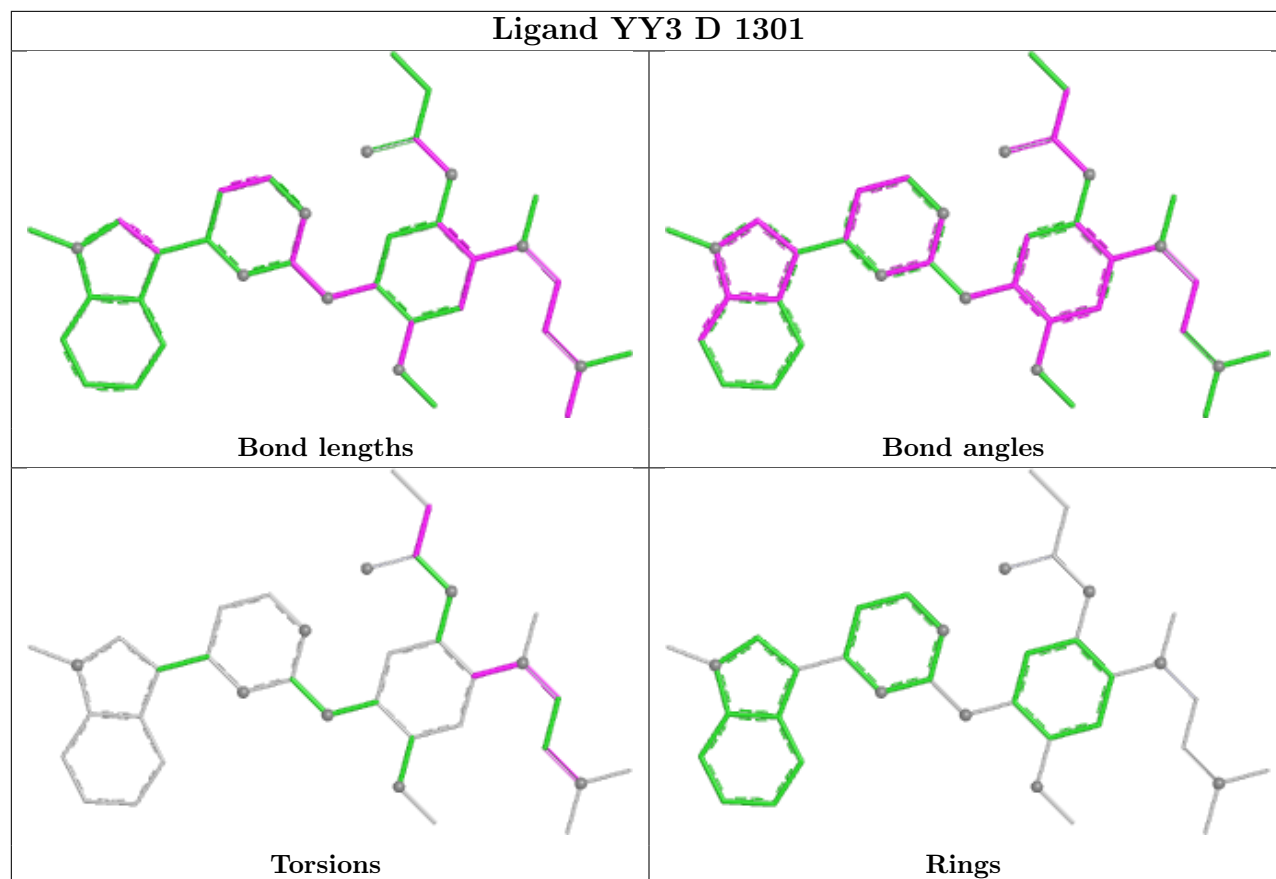
7 monomers are involved in 20 short contacts:

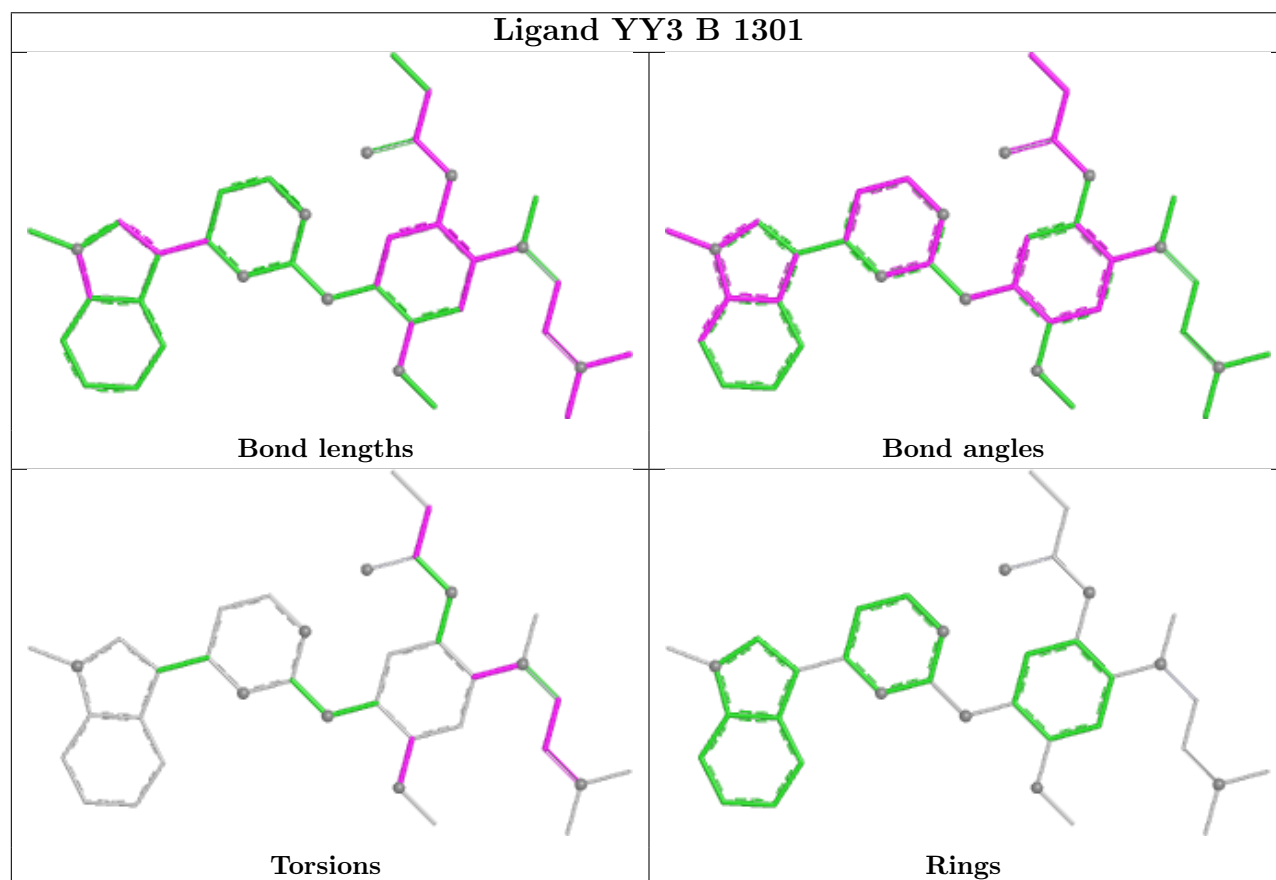
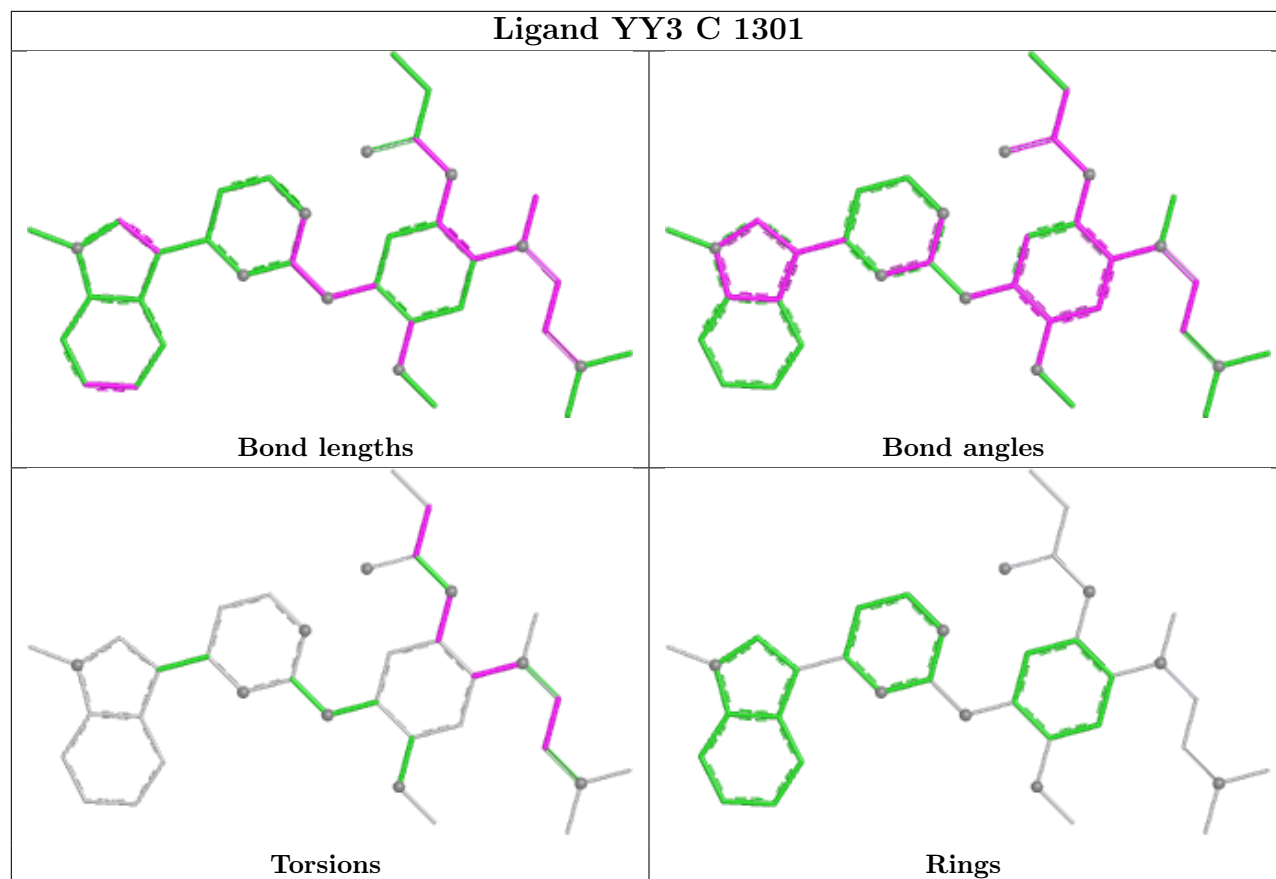
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1302	VNS	3	0
3	A	1302	VNS	1	0
2	A	1301	YY3	3	0
2	D	1301	YY3	4	0
3	C	1302	VNS	2	0
2	C	1301	YY3	4	0
2	B	1301	YY3	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/331 (87%)	1.18	52 (18%) 3 3	37, 65, 99, 117	0
1	B	291/331 (87%)	0.57	28 (9%) 13 11	22, 53, 98, 114	1 (0%)
1	C	293/331 (88%)	1.21	54 (18%) 3 2	35, 69, 113, 141	1 (0%)
1	D	287/331 (86%)	1.88	116 (40%) 0 0	44, 86, 129, 144	1 (0%)
All	All	1159/1324 (87%)	1.21	250 (21%) 2 2	22, 69, 114, 144	3 (0%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	782	LEU	5.3
1	D	882	ALA	5.0
1	C	979	LEU	4.9
1	D	883	LEU	4.8
1	C	946	ILE	4.8
1	A	717	VAL	4.8
1	D	886	ILE	4.7
1	C	938	ILE	4.7
1	D	923	ILE	4.6
1	D	789	ILE	4.5
1	D	878	ILE	4.4
1	D	876	VAL	4.3
1	D	885	SER	4.2
1	D	727	TYR	4.1
1	A	807	ASP	4.1
1	D	877	PRO	4.1
1	C	975	PRO	4.0
1	D	918	ILE	3.9
1	A	918	ILE	3.9
1	D	915	TYR	3.8
1	A	716	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	915	TYR	3.8
1	D	858	LEU	3.7
1	C	723	PHE	3.7
1	D	707	LEU	3.7
1	A	715	ILE	3.7
1	D	927	LEU	3.6
1	D	919	PRO	3.6
1	D	755	ALA	3.6
1	D	726	VAL	3.6
1	D	759	ILE	3.6
1	A	783	THR	3.5
1	D	920	ALA	3.5
1	D	837	ASP	3.5
1	B	807	ASP	3.5
1	D	717	VAL	3.5
1	A	876	VAL	3.5
1	D	731	TRP	3.5
1	D	946	ILE	3.5
1	D	931	GLU	3.5
1	C	983	GLY	3.4
1	D	913	LYS	3.4
1	D	881	MET	3.4
1	C	941	ILE	3.4
1	D	922	GLU	3.4
1	A	712	PHE	3.4
1	D	895	SER	3.4
1	D	924	SER	3.4
1	B	988	HIS	3.4
1	B	915	TYR	3.3
1	D	785	THR	3.3
1	D	723	PHE	3.3
1	D	788	LEU	3.3
1	D	917	GLY	3.3
1	D	780	ILE	3.3
1	C	759	ILE	3.3
1	D	926	ILE	3.3
1	D	1007	MET	3.3
1	D	747	LEU	3.3
1	C	937	PRO	3.2
1	D	786	VAL	3.2
1	D	834	VAL	3.2
1	D	903	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	833	LEU	3.2
1	A	781	CYS	3.2
1	B	918	ILE	3.2
1	D	856	PHE	3.2
1	A	753	PRO	3.2
1	C	982	GLN	3.1
1	C	877	PRO	3.1
1	B	982	GLN	3.1
1	C	907	LEU	3.1
1	C	813	TYR	3.1
1	C	903	THR	3.1
1	B	707	LEU	3.1
1	C	977	ARG	3.1
1	D	890	ILE	3.1
1	D	897	VAL	3.1
1	D	721	GLY	3.0
1	D	930	GLY	3.0
1	B	735	GLY	3.0
1	B	737	LYS	3.0
1	D	774	VAL	3.0
1	A	707	LEU	3.0
1	A	752	SER	3.0
1	D	703	LEU	3.0
1	A	730	LEU	2.9
1	A	786	VAL	2.9
1	D	898	TRP	2.9
1	A	720	SER	2.9
1	D	704	LEU	2.9
1	C	989	LEU	2.9
1	D	951	TRP	2.9
1	C	976	GLN	2.9
1	D	925	SER	2.9
1	A	722	ALA	2.9
1	D	760	LEU	2.9
1	A	718	LEU	2.9
1	A	747	LEU	2.9
1	D	956	ASP	2.9
1	A	988	HIS	2.8
1	D	781	CYS	2.8
1	A	782	LEU	2.8
1	C	988	HIS	2.8
1	B	700	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	891	TYR	2.8
1	C	987	MET	2.8
1	D	900	TYR	2.8
1	A	785	THR	2.8
1	B	703	LEU	2.8
1	D	937	PRO	2.7
1	D	715	ILE	2.7
1	C	786	VAL	2.7
1	C	915	TYR	2.7
1	D	722	ALA	2.7
1	D	884	GLU	2.7
1	D	712	PHE	2.7
1	C	923	ILE	2.7
1	B	712	PHE	2.7
1	D	742	VAL	2.7
1	D	807	ASP	2.6
1	C	910	PHE	2.6
1	D	894	GLN	2.6
1	B	750	ALA	2.6
1	D	994	ASP	2.6
1	D	732	ILE	2.6
1	A	1007	MET	2.6
1	D	714	LYS	2.6
1	D	887	LEU	2.6
1	D	928	GLU	2.6
1	A	738	VAL	2.6
1	B	715	ILE	2.6
1	B	717	VAL	2.6
1	A	888	HIS	2.6
1	D	806	LYS	2.6
1	D	766	MET	2.5
1	D	880	TRP	2.5
1	B	994	ASP	2.5
1	D	784	SER	2.5
1	D	929	LYS	2.5
1	D	705	ARG	2.5
1	D	744	ILE	2.5
1	D	809	ILE	2.5
1	D	988	HIS	2.5
1	B	751	THR	2.5
1	D	977	ARG	2.5
1	D	914	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	704	LEU	2.5
1	D	713	LYS	2.5
1	D	888	HIS	2.5
1	C	980	VAL	2.5
1	B	928	GLU	2.5
1	A	923	ILE	2.5
1	D	763	ALA	2.5
1	D	854	THR	2.5
1	D	746	GLU	2.4
1	A	928	GLU	2.4
1	A	878	ILE	2.4
1	C	994	ASP	2.4
1	D	982	GLN	2.4
1	D	892	THR	2.4
1	C	990	PRO	2.4
1	D	797	CYS	2.4
1	C	939	CYS	2.4
1	B	781	CYS	2.4
1	A	789	ILE	2.4
1	C	918	ILE	2.4
1	C	945	MET	2.4
1	A	732	ILE	2.4
1	C	897	VAL	2.4
1	B	931	GLU	2.4
1	C	900	TYR	2.4
1	C	936	PRO	2.3
1	B	783	THR	2.3
1	B	784	SER	2.3
1	A	917	GLY	2.3
1	A	713	LYS	2.3
1	C	943	VAL	2.3
1	C	722	ALA	2.3
1	A	924	SER	2.3
1	A	989	LEU	2.3
1	C	984	ASP	2.3
1	C	860	LYS	2.3
1	A	1000	ALA	2.3
1	C	972	ALA	2.3
1	C	973	ARG	2.3
1	D	905	TRP	2.3
1	D	798	LEU	2.3
1	D	828	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	838	LEU	2.3
1	C	981	ILE	2.3
1	A	723	PHE	2.3
1	B	738	VAL	2.3
1	A	977	ARG	2.3
1	C	783	THR	2.3
1	D	921	SER	2.3
1	C	1007	MET	2.3
1	B	723	PHE	2.3
1	D	738	VAL	2.3
1	D	719	GLY	2.2
1	D	778	LEU	2.2
1	D	953	ILE	2.2
1	A	858	LEU	2.2
1	A	987	MET	2.2
1	C	953	ILE	2.2
1	D	948	ARG	2.2
1	A	834	VAL	2.2
1	A	990	PRO	2.2
1	A	788	LEU	2.2
1	C	815	LEU	2.2
1	C	715	ILE	2.2
1	C	966	ILE	2.2
1	B	916	ASP	2.2
1	D	765	VAL	2.2
1	A	919	PRO	2.2
1	D	822	ALA	2.2
1	D	777	LEU	2.2
1	C	754	LYS	2.2
1	C	751	THR	2.1
1	B	782	LEU	2.1
1	B	788	LEU	2.1
1	C	749	GLU	2.1
1	D	855	ASP	2.1
1	D	912	SER	2.1
1	A	994	ASP	2.1
1	D	745	LYS	2.1
1	C	913	LYS	2.1
1	A	980	VAL	2.1
1	A	755	ALA	2.1
1	D	803	ARG	2.1
1	B	1007	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	902	VAL	2.1
1	D	839	ALA	2.1
1	D	779	GLY	2.1
1	A	927	LEU	2.1
1	C	785	THR	2.1
1	C	944	TYR	2.1
1	A	991	SER	2.1
1	D	979	LEU	2.1
1	C	700	ASN	2.1
1	C	951	TRP	2.1
1	B	760	LEU	2.1
1	D	725	THR	2.1
1	D	706	ILE	2.1
1	D	959	PRO	2.1
1	A	733	PRO	2.0
1	D	700	ASN	2.0
1	A	926	ILE	2.0
1	A	1006	ASP	2.0
1	C	752	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

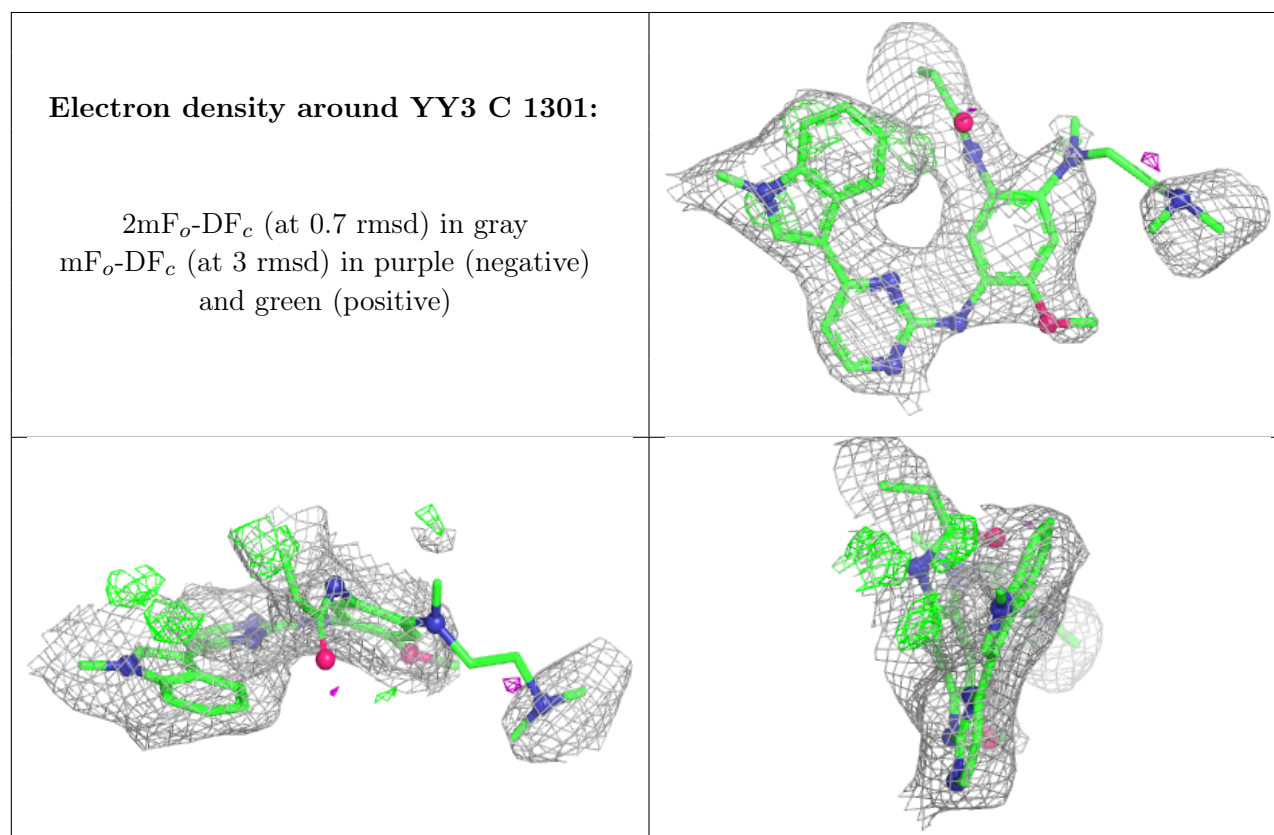
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YY3	C	1301	37/37	0.76	0.16	38,62,89,91	0
2	YY3	D	1301	37/37	0.80	0.17	46,69,88,90	0
2	YY3	A	1301	37/37	0.84	0.15	34,53,77,81	0
3	VNS	A	1302	40/40	0.84	0.16	29,49,80,109	0

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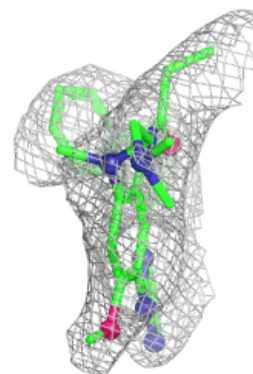
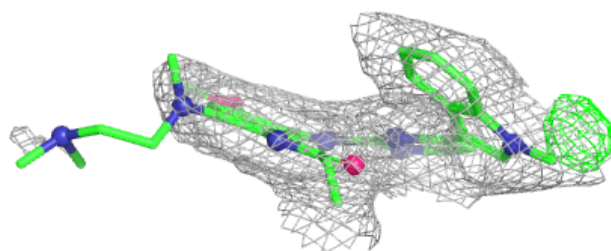
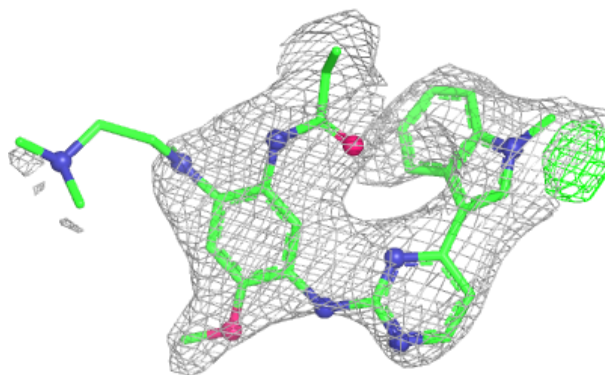
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VNS	D	1302	40/40	0.87	0.15	32,65,86,115	0
3	VNS	C	1302	40/40	0.87	0.14	24,42,80,84	0
2	YY3	B	1301	37/37	0.88	0.11	27,43,66,71	0
3	VNS	B	1302	40/40	0.88	0.13	18,45,76,92	0

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.



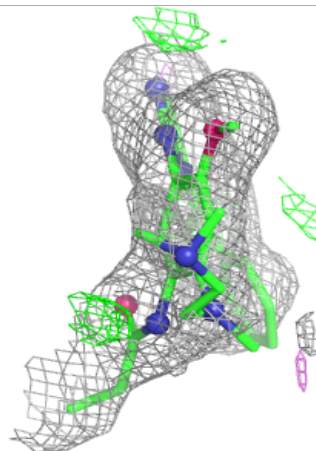
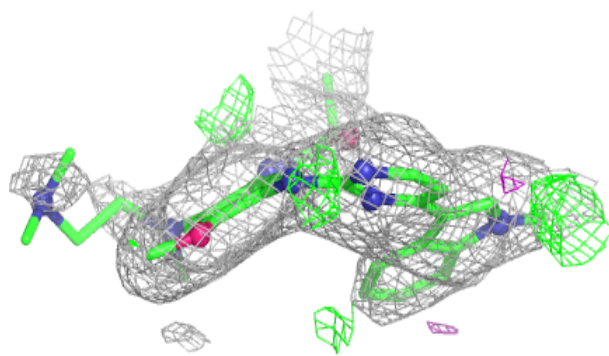
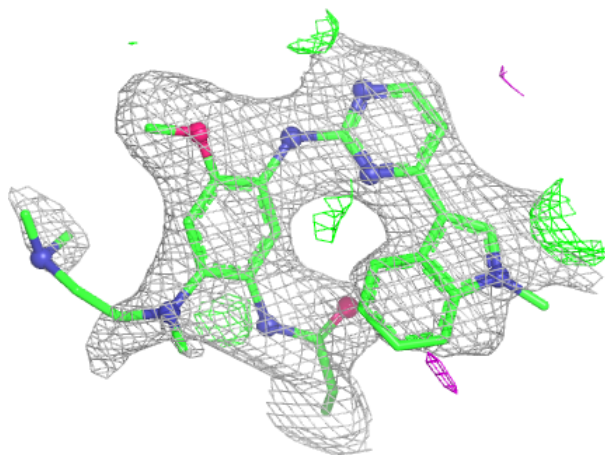
Electron density around YY3 D 1301:

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



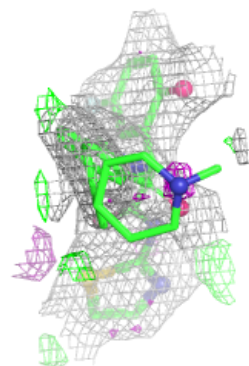
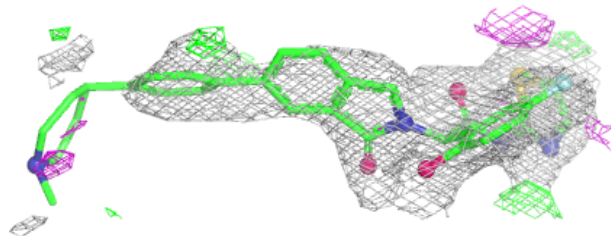
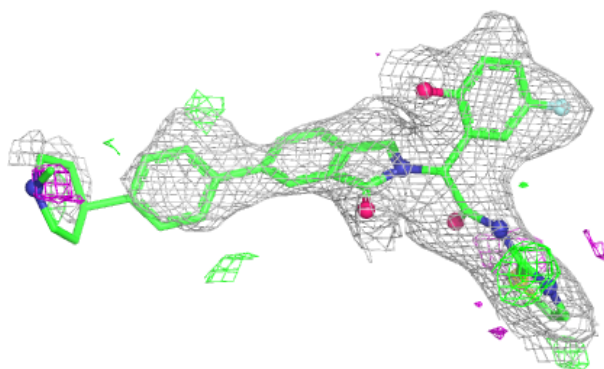
Electron density around YY3 A 1301:

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

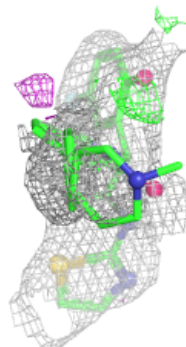
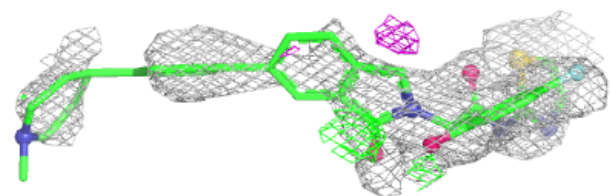
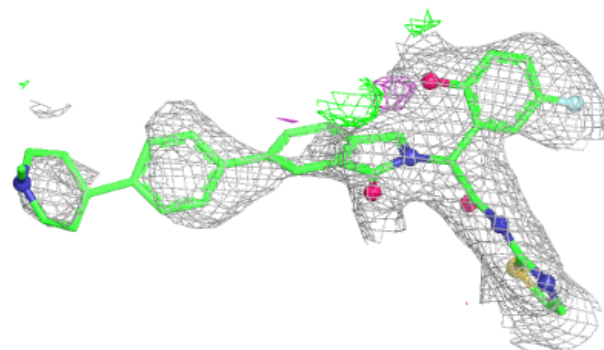


Electron density around VNS A 1302:

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

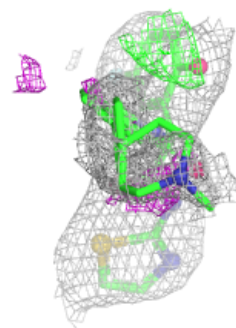
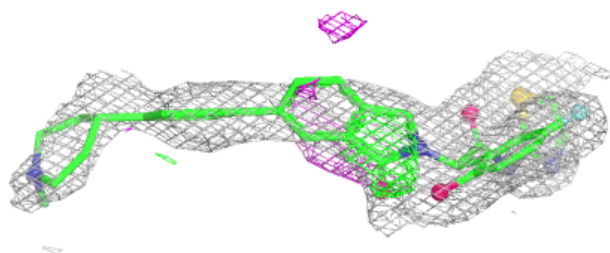
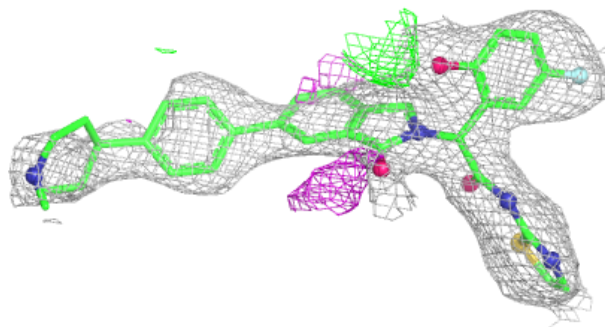
**Electron density around VNS D 1302:**

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

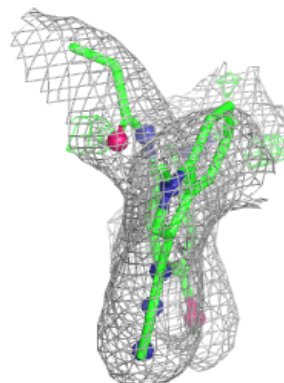
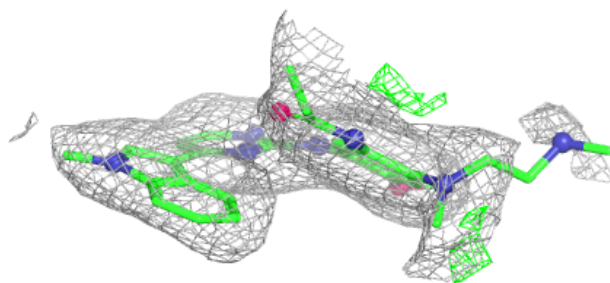
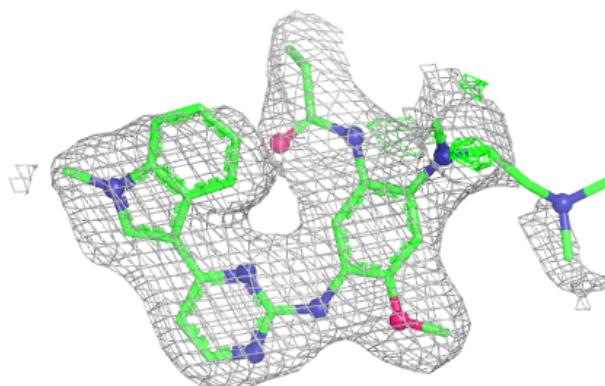


Electron density around VNS C 1302:

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

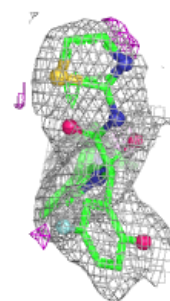
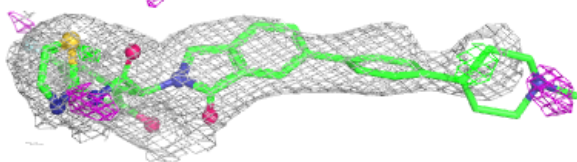
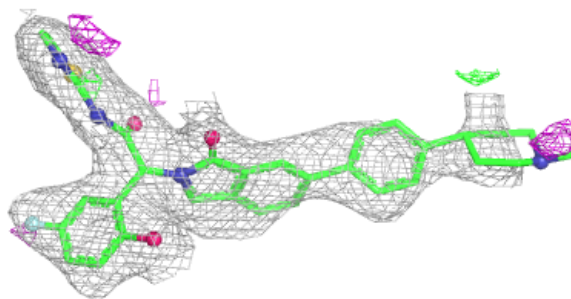
**Electron density around YY3 B 1301:**

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



Electron density around VNS 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 ⓘ

There are no such residues in this entry.