



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 02:18 PM EST

PDB ID : 7LG8
Title : EGFR (T79M/V948R) in complex with naquotinib and an allosteric inhibitor
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2021-01-19
Resolution : 2.93 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 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 : 2.26
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) : 2.26

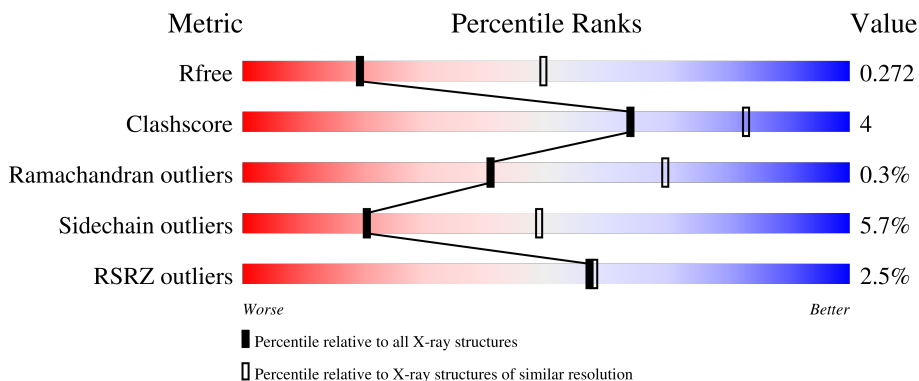
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	 72% 11% • 15%
1	B	331	 73% 10% • 17%
1	C	331	 69% 12% • 17%
1	D	331	 71% 10% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9222 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.

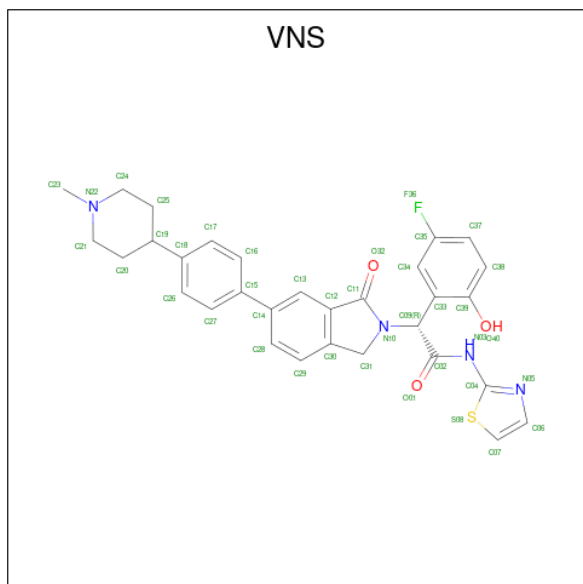
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2261	1457	383	404	17			
1	B	275	Total	C	N	O	S	0	0	0
			2218	1434	378	389	17			
1	C	274	Total	C	N	O	S	0	0	0
			2214	1432	376	389	17			
1	D	271	Total	C	N	O	S	0	0	0
			2192	1419	372	384	17			

There are 20 discrepancies between the modelled and reference sequences:

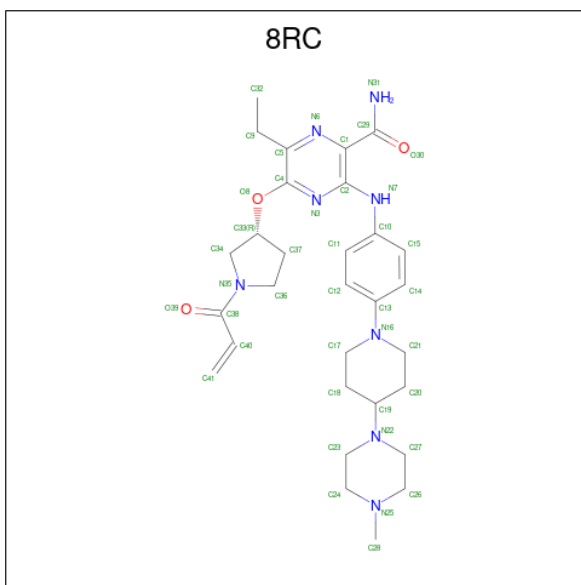
Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-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

- Molecule 2 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: $C_{31}H_{29}FN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 6-ethyl-3-[[4-[4-(4-methylpiperazin-1-yl)piperidin-1-yl]phenyl]amino]-5-[(3R)-1-prop-2-enoylpyrrolidin-3-yl]oxy-pyrazin e-2-carboxamide (three-letter code: 8RC) (formula: $C_{30}H_{42}N_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 41	C 30	N 8	O 3	0	0
3	B	1	Total 41	C 30	N 8	O 3	0	0
3	C	1	Total 41	C 30	N 8	O 3	0	0
3	D	1	Total 41	C 30	N 8	O 3	0	0

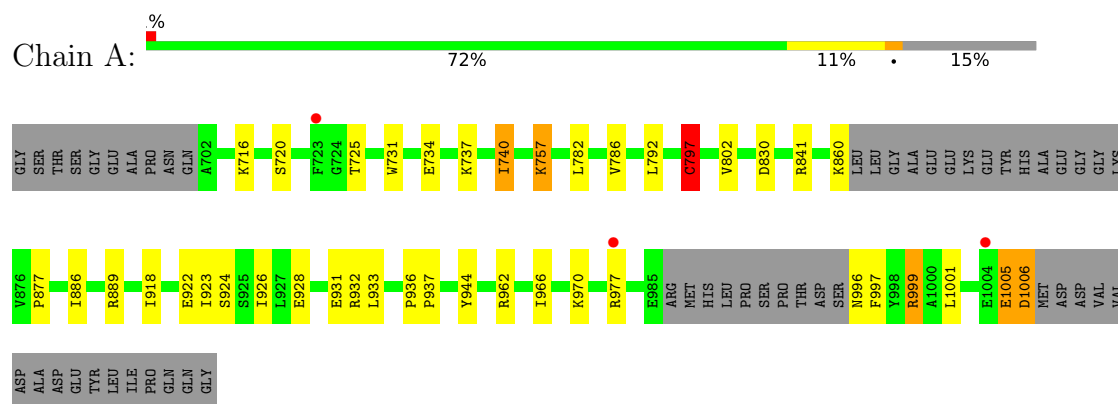
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	1	Total O 1 1	0	0
4	C	5	Total O 5 5	0	0
4	D	4	Total O 4 4	0	0

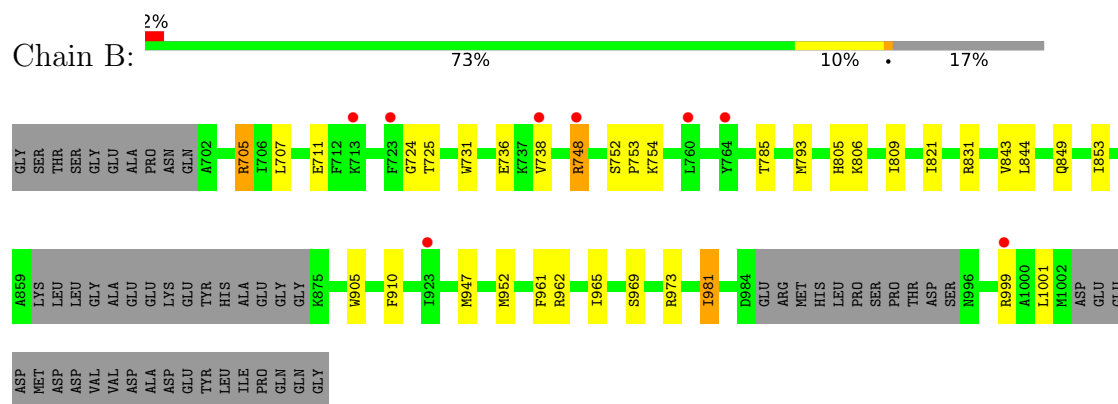
3 Residue-property plots

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.

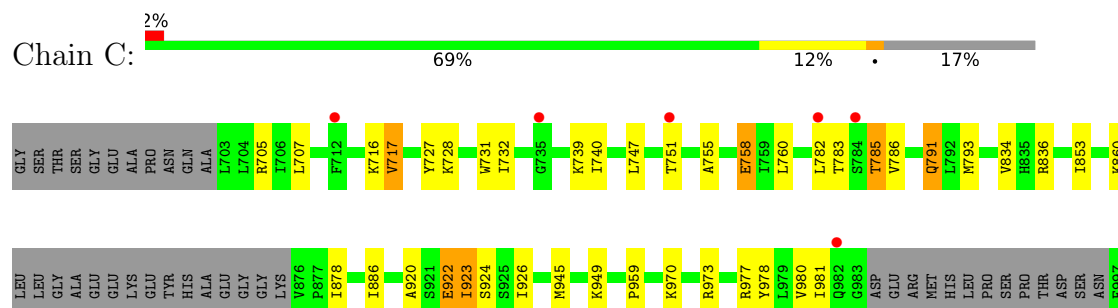
• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor



Y998	R999	A1000	L1001	M1002	D1003	E1004	GLU	ASP	ASP	MET	ASP	ASP	VAL	VAL	ASP	ALA	ASP	GLU	TYR	LEU	ILE	PRO	GLN	GLN	GLY
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● Molecule 1: Epidermal growth factor receptor



GLY	SER	THR	GLY	GLY	GLY	ALA	PRO	ASN	GLN	A702	T710	K713	V717	L718	K728	G729	E734	G735	E736	K737	V738	K739	E749	A750	T751	K754	I759	L760	Y764	V765	T783	S784	T785	Q791	D830	R836	V843	L858	ALA	LYS	LEU	GLY	ALA
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GLU	GLU	LYS	TYR	HIS	ALA	GLU	GLY	GLY	LYS	V876	K879	A882	L883	H893	V897	W898	Y905	Y915	I926	I946	M947	I953	D954	A955	F961	R962	I965	R977	Q982	GLY	ASP	GLU	ARG	MET	HIS	LEU	PRO	SER	PRO	THR	ASP	SER	ASN	F997	Y998
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R999	D1003	GLU	GLU	ASP	MET	ASP	ASP	VAL	VAL	ASP	ALA	ASP	GLU	TYR	LEU	ILE	PRO	GLN	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.65Å 75.95Å 150.98Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	50.81 – 2.93 50.81 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.81-2.93) 97.9 (50.81-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4080	Depositor
R, R_{free}	0.235 , 0.270 0.234 , 0.272	Depositor DCC
R_{free} test set	1345 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9222	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 20.71 % 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 8.1913e-03. 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: 8RC, 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	0.27	0/2309	0.55	1/3119 (0.0%)
1	B	0.26	0/2266	0.53	0/3061
1	C	0.26	0/2262	0.53	0/3055
1	D	0.26	0/2240	0.55	0/3027
All	All	0.26	0/9077	0.54	1/12262 (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	A	797	CYS	CB-CA-C	6.19	122.78	110.40

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	2261	0	2310	26	0
1	B	2218	0	2284	16	0
1	C	2214	0	2279	21	0
1	D	2192	0	2257	15	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	40	0	0	0	0
2	D	40	0	0	0	0
3	A	41	0	0	1	0
3	B	41	0	0	0	0
3	C	41	0	0	2	0
3	D	41	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	5	0	0	0	0
4	D	4	0	0	0	0
All	All	9222	0	9130	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:751:THR:HG21	1:C:786:VAL:HG23	1.62	0.82
1:C:834:VAL:HG12	1:C:836:ARG:HG3	1.72	0.70
1:A:928:GLU:OE1	1:D:754:LYS:NZ	2.28	0.66
1:B:910:PHE:HZ	1:B:981:ILE:HD11	1.60	0.66
1:C:791:GLN:O	3:C:1102:8RC:N31	2.30	0.65
1:C:970:LYS:HG2	1:C:973:ARG:NH2	2.13	0.64
1:C:731:TRP:CE3	1:C:740:ILE:HD11	2.35	0.62
1:A:797:CYS:SG	1:A:841:ARG:HA	2.41	0.61
1:A:923:ILE:HA	1:A:926:ILE:HG12	1.82	0.60
1:A:922:GLU:O	1:A:926:ILE:HG23	2.00	0.60
1:D:783:THR:OG1	1:D:785:THR:O	2.21	0.58
1:B:821:ILE:HG23	1:B:853:ILE:HD11	1.85	0.58
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.69	0.58
1:C:717:VAL:HA	1:C:727:TYR:HA	1.85	0.57
1:B:806:LYS:HG2	1:B:910:PHE:HB3	1.86	0.56
1:C:705:ARG:HD2	1:C:731:TRP:HH2	1.71	0.55
1:A:966:ILE:HG22	1:A:970:LYS:NZ	2.21	0.54
1:C:793:MET:N	3:C:1102:8RC:O30	2.27	0.53
1:A:923:ILE:HD13	1:A:926:ILE:HD11	1.91	0.52
1:A:926:ILE:HB	1:A:931:GLU:OE1	2.10	0.52
1:B:843:VAL:HG22	1:B:853:ILE:HD13	1.91	0.52
1:A:918:ILE:HG21	1:A:926:ILE:HD13	1.91	0.51
1:A:886:ILE:HG21	1:A:924:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:LYS:HE3	1:C:728:LYS:HE3	1.93	0.50
1:C:949:LYS:HB3	1:C:959:PRO:HD3	1.93	0.49
1:C:970:LYS:HG2	1:C:973:ARG:HH22	1.76	0.49
1:A:841:ARG:HH22	1:A:877:PRO:HB3	1.77	0.49
1:C:783:THR:OG1	1:C:785:THR:O	2.30	0.49
1:D:749:GLU:O	1:D:751:THR:HG23	2.13	0.49
1:C:732:ILE:HG12	1:C:739:LYS:HG2	1.95	0.48
1:A:830:ASP:OD1	1:A:962:ARG:NH2	2.46	0.48
1:B:753:PRO:HB2	1:B:754:LYS:HE2	1.96	0.48
1:A:931:GLU:O	1:A:932:ARG:NH1	2.42	0.48
1:D:710:THR:O	1:D:710:THR:OG1	2.32	0.47
1:D:879:LYS:HD3	1:D:915:TYR:HB2	1.97	0.47
1:C:707:LEU:HD21	1:C:731:TRP:CZ2	2.51	0.46
1:D:893:HIS:O	1:D:897:VAL:HG23	2.15	0.46
1:B:961:PHE:O	1:B:965:ILE:HG13	2.17	0.45
1:A:720:SER:HB2	1:A:725:THR:HG23	1.99	0.45
1:B:969:SER:O	1:B:973:ARG:HG3	2.17	0.45
1:C:760:LEU:HD11	1:C:782:LEU:HD11	1.97	0.45
1:A:792:LEU:HA	3:A:1102:8RC:N31	2.32	0.45
1:D:737:LYS:HA	1:D:737:LYS:HD3	1.77	0.44
1:A:977:ARG:C	1:A:977:ARG:HD3	2.37	0.44
1:B:725:THR:HB	1:B:748:ARG:HH21	1.83	0.44
1:C:886:ILE:HG21	1:C:924:SER:HB3	1.99	0.44
1:B:707:LEU:HA	1:B:711:GLU:OE2	2.18	0.44
1:C:922:GLU:O	1:C:926:ILE:HG23	2.19	0.43
1:D:883:LEU:HD13	1:D:953:ILE:HD12	2.00	0.43
1:B:724:GLY:HA2	1:B:748:ARG:HG2	1.99	0.43
1:A:734:GLU:HG2	1:A:734:GLU:O	2.18	0.43
1:D:751:THR:HG21	1:D:759:ILE:HD11	2.00	0.43
1:D:961:PHE:O	1:D:965:ILE:HG13	2.18	0.43
1:C:923:ILE:HA	1:C:926:ILE:HG12	2.01	0.42
1:A:926:ILE:HB	1:A:931:GLU:CD	2.38	0.42
1:C:977:ARG:HD2	1:C:978:TYR:CZ	2.54	0.42
1:D:926:ILE:HD12	1:D:926:ILE:HA	1.68	0.42
1:D:977:ARG:O	1:D:977:ARG:HD3	2.19	0.42
1:B:705:ARG:HG2	1:B:731:TRP:CZ2	2.55	0.42
1:C:878:ILE:HG21	1:C:920:ALA:HB1	2.01	0.42
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.85	0.42
1:B:831:ARG:HE	1:B:831:ARG:HB3	1.71	0.41
1:C:755:ALA:HA	1:C:758:GLU:OE2	2.20	0.41
1:D:718:LEU:HD11	1:D:728:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.55	0.41
1:A:716:LYS:HE3	1:A:716:LYS:HB3	1.84	0.41
1:A:933:LEU:O	1:A:944:TYR:OH	2.32	0.41
1:A:841:ARG:NH2	1:A:877:PRO:HB3	2.35	0.41
1:B:736:GLU:HB3	1:B:738:VAL:HG22	2.03	0.41
1:A:936:PRO:HA	1:A:937:PRO:HD3	1.98	0.41
1:A:1005:GLU:HB2	1:A:1006:ASP:H	1.62	0.41
1:A:966:ILE:HG22	1:A:970:LYS:HZ2	1.84	0.41
1:B:805:HIS:O	1:B:809:ILE:HG13	2.21	0.41
1:A:731:TRP:O	1:A:740:ILE:HG13	2.21	0.40
1:A:757:LYS:HB3	1:A:757:LYS:HE3	1.76	0.40
1:A:977:ARG:HD3	1:A:977:ARG:O	2.22	0.40
1:B:793:MET:HG3	1:B:844:LEU:HB3	2.02	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	274/331 (83%)	261 (95%)	12 (4%)	1 (0%)	34	64
1	B	269/331 (81%)	259 (96%)	10 (4%)	0	100	100
1	C	268/331 (81%)	257 (96%)	10 (4%)	1 (0%)	34	64
1	D	265/331 (80%)	255 (96%)	9 (3%)	1 (0%)	34	64
All	All	1076/1324 (81%)	1032 (96%)	41 (4%)	3 (0%)	41	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	734	GLU
1	A	999	ARG

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Mol	Chain	Res	Type
1	C	981	ILE

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	249/290 (86%)	234 (94%)	15 (6%)	19	46
1	B	244/290 (84%)	234 (96%)	10 (4%)	30	61
1	C	244/290 (84%)	228 (93%)	16 (7%)	16	42
1	D	242/290 (83%)	227 (94%)	15 (6%)	18	45
All	All	979/1160 (84%)	923 (94%)	56 (6%)	20	49

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	737	LYS
1	A	740	ILE
1	A	757	LYS
1	A	782	LEU
1	A	786	VAL
1	A	797	CYS
1	A	802	VAL
1	A	860	LYS
1	A	889	ARG
1	A	996	ASN
1	A	997	PHE
1	A	999	ARG
1	A	1001	LEU
1	A	1005	GLU
1	A	1006	ASP
1	B	705	ARG
1	B	748	ARG
1	B	752	SER
1	B	785	THR
1	B	849	GLN

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Mol	Chain	Res	Type
1	B	952	MET
1	B	962	ARG
1	B	981	ILE
1	B	999	ARG
1	B	1001	LEU
1	C	717	VAL
1	C	747	LEU
1	C	758	GLU
1	C	785	THR
1	C	791	GLN
1	C	853	ILE
1	C	860	LYS
1	C	922	GLU
1	C	923	ILE
1	C	945	MET
1	C	980	VAL
1	C	998	TYR
1	C	999	ARG
1	C	1001	LEU
1	C	1002	MET
1	C	1003	ASP
1	D	710	THR
1	D	717	VAL
1	D	734	GLU
1	D	736	GLU
1	D	739	LYS
1	D	765	VAL
1	D	791	GLN
1	D	830	ASP
1	D	836	ARG
1	D	843	VAL
1	D	962	ARG
1	D	977	ARG
1	D	997	PHE
1	D	998	TYR
1	D	999	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	VNS	D	1101	-	43,45,45	3.22	21 (48%)	54,65,65	4.67	28 (51%)
2	VNS	B	1101	-	43,45,45	3.15	20 (46%)	54,65,65	4.76	27 (50%)
2	VNS	A	1101	-	43,45,45	3.24	19 (44%)	54,65,65	4.68	26 (48%)
3	8RC	B	1102	1	44,45,45	2.77	23 (52%)	56,63,63	3.07	25 (44%)
3	8RC	D	1102	1	44,45,45	2.93	26 (59%)	56,63,63	2.83	27 (48%)
2	VNS	C	1101	-	43,45,45	3.31	19 (44%)	54,65,65	4.80	28 (51%)
3	8RC	A	1102	1	44,45,45	2.69	22 (50%)	56,63,63	2.61	24 (42%)
3	8RC	C	1102	1	44,45,45	2.95	25 (56%)	56,63,63	3.02	30 (53%)

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	VNS	D	1101	-	-	2/22/46/46	0/6/6/6
2	VNS	B	1101	-	-	2/22/46/46	0/6/6/6
2	VNS	A	1101	-	-	2/22/46/46	0/6/6/6
3	8RC	B	1102	1	-	10/28/57/57	0/5/5/5
3	8RC	D	1102	1	-	12/28/57/57	0/5/5/5
2	VNS	C	1101	-	-	1/22/46/46	0/6/6/6
3	8RC	A	1102	1	-	13/28/57/57	0/5/5/5
3	8RC	C	1102	1	-	10/28/57/57	0/5/5/5

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	VNS	C09-C02	11.77	1.66	1.54
2	A	1101	VNS	C09-C02	11.52	1.66	1.54
2	D	1101	VNS	C09-C02	10.85	1.65	1.54
2	B	1101	VNS	C09-C02	10.11	1.65	1.54
2	C	1101	VNS	C11-N10	9.25	1.45	1.36
2	B	1101	VNS	C11-N10	9.23	1.45	1.36
2	A	1101	VNS	C11-N10	9.19	1.45	1.36
2	D	1101	VNS	C11-N10	9.16	1.45	1.36
3	C	1102	8RC	C2-N7	7.23	1.49	1.36
3	D	1102	8RC	C2-N7	7.21	1.49	1.36
3	B	1102	8RC	C2-N7	6.93	1.48	1.36
3	A	1102	8RC	C2-N7	6.93	1.48	1.36
3	C	1102	8RC	C13-N16	6.80	1.57	1.38
3	A	1102	8RC	C13-N16	6.78	1.57	1.38
3	D	1102	8RC	C13-N16	6.69	1.57	1.38
3	D	1102	8RC	C38-N35	6.60	1.48	1.35
3	B	1102	8RC	C13-N16	6.60	1.56	1.38
3	C	1102	8RC	C38-N35	6.53	1.47	1.35
3	B	1102	8RC	C38-N35	6.41	1.47	1.35
3	A	1102	8RC	C38-N35	6.13	1.47	1.35
2	C	1101	VNS	C02-N03	5.46	1.47	1.35
2	A	1101	VNS	O01-C02	-5.41	1.12	1.23
2	B	1101	VNS	C02-N03	5.30	1.47	1.35
2	D	1101	VNS	C02-N03	5.17	1.47	1.35
2	A	1101	VNS	C02-N03	5.15	1.47	1.35
2	D	1101	VNS	O01-C02	-5.07	1.13	1.23
2	B	1101	VNS	O01-C02	-4.92	1.13	1.23
2	C	1101	VNS	O01-C02	-4.74	1.14	1.23
2	A	1101	VNS	C31-N10	4.72	1.50	1.46
2	C	1101	VNS	C09-N10	4.67	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	VNS	C09-N10	4.67	1.51	1.46
2	C	1101	VNS	C31-N10	4.59	1.50	1.46
2	C	1101	VNS	C04-N03	4.55	1.44	1.36
2	B	1101	VNS	C15-C14	4.54	1.60	1.49
2	B	1101	VNS	C04-N03	4.42	1.44	1.36
2	D	1101	VNS	C04-N03	4.40	1.44	1.36
2	C	1101	VNS	C15-C14	4.37	1.59	1.49
2	D	1101	VNS	C15-C14	4.34	1.59	1.49
2	D	1101	VNS	C31-N10	4.30	1.50	1.46
2	D	1101	VNS	C33-C09	4.29	1.57	1.52
3	D	1102	8RC	C21-N16	4.27	1.53	1.46
3	B	1102	8RC	C34-C33	4.27	1.59	1.52
2	A	1101	VNS	C04-N03	4.23	1.44	1.36
3	C	1102	8RC	C17-N16	4.18	1.53	1.46
3	D	1102	8RC	C36-N35	4.18	1.56	1.47
3	C	1102	8RC	C36-N35	4.18	1.56	1.47
2	B	1101	VNS	C31-N10	4.14	1.50	1.46
3	C	1102	8RC	C9-C5	4.09	1.58	1.51
3	D	1102	8RC	C9-C5	4.07	1.58	1.51
3	C	1102	8RC	C21-N16	4.05	1.53	1.46
3	B	1102	8RC	C9-C5	4.02	1.58	1.51
3	C	1102	8RC	C10-N7	3.95	1.49	1.40
2	A	1101	VNS	C15-C14	3.92	1.58	1.49
3	D	1102	8RC	C17-N16	3.92	1.52	1.46
3	D	1102	8RC	C10-N7	3.82	1.49	1.40
3	C	1102	8RC	C34-C33	3.79	1.59	1.52
3	B	1102	8RC	C10-N7	3.77	1.49	1.40
3	B	1102	8RC	C36-N35	3.76	1.55	1.47
2	B	1101	VNS	C09-N10	3.74	1.50	1.46
2	D	1101	VNS	C09-N10	3.71	1.50	1.46
3	D	1102	8RC	C40-C38	3.69	1.59	1.49
3	A	1102	8RC	C10-N7	3.68	1.48	1.40
3	D	1102	8RC	C34-C33	3.68	1.59	1.52
3	C	1102	8RC	C40-C38	3.67	1.59	1.49
3	B	1102	8RC	C40-C38	3.67	1.59	1.49
3	A	1102	8RC	C36-N35	3.65	1.55	1.47
3	A	1102	8RC	C9-C5	3.64	1.57	1.51
2	C	1101	VNS	C33-C09	3.62	1.57	1.52
2	A	1101	VNS	C33-C09	3.62	1.57	1.52
2	B	1101	VNS	C33-C09	3.56	1.56	1.52
3	A	1102	8RC	C17-N16	3.53	1.52	1.46
3	B	1102	8RC	C21-N16	3.44	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	VNS	C18-C19	3.38	1.59	1.52
3	A	1102	8RC	C21-N16	3.33	1.51	1.46
3	D	1102	8RC	C1-C29	3.31	1.61	1.51
3	A	1102	8RC	C40-C38	3.30	1.58	1.49
3	B	1102	8RC	C17-N16	3.26	1.51	1.46
2	B	1101	VNS	C31-C30	3.24	1.54	1.50
3	A	1102	8RC	C34-C33	3.23	1.58	1.52
3	C	1102	8RC	C1-C29	3.21	1.61	1.51
3	C	1102	8RC	C4-N3	3.09	1.36	1.32
3	C	1102	8RC	C29-N31	3.08	1.38	1.33
2	D	1101	VNS	C31-C30	3.07	1.54	1.50
2	C	1101	VNS	C17-C16	3.06	1.44	1.38
2	C	1101	VNS	C18-C19	3.03	1.58	1.52
3	D	1102	8RC	C2-N3	3.03	1.40	1.34
3	C	1102	8RC	C26-N25	3.01	1.52	1.46
2	D	1101	VNS	C17-C16	3.00	1.44	1.38
3	C	1102	8RC	C2-N3	3.00	1.40	1.34
3	D	1102	8RC	C4-N3	2.98	1.36	1.32
2	B	1101	VNS	C17-C16	2.98	1.44	1.38
2	D	1101	VNS	C39-C33	2.96	1.43	1.40
3	C	1102	8RC	C15-C14	2.95	1.44	1.38
3	D	1102	8RC	C29-N31	2.95	1.38	1.33
3	A	1102	8RC	C15-C14	2.92	1.44	1.38
2	C	1101	VNS	C31-C30	2.89	1.54	1.50
2	A	1101	VNS	C17-C16	2.88	1.44	1.38
2	D	1101	VNS	C18-C19	2.82	1.57	1.52
3	A	1102	8RC	C4-N3	2.82	1.36	1.32
3	B	1102	8RC	C4-N3	2.82	1.36	1.32
3	B	1102	8RC	C15-C14	2.81	1.43	1.38
3	B	1102	8RC	C1-C29	2.80	1.60	1.51
3	D	1102	8RC	C15-C14	2.76	1.43	1.38
3	B	1102	8RC	C2-N3	2.75	1.39	1.34
2	C	1101	VNS	C34-C35	2.75	1.42	1.37
3	A	1102	8RC	C1-C29	2.73	1.60	1.51
2	A	1101	VNS	C18-C19	2.71	1.57	1.52
2	C	1101	VNS	C13-C12	2.69	1.44	1.39
2	B	1101	VNS	C34-C35	2.67	1.42	1.37
2	D	1101	VNS	C34-C35	2.65	1.42	1.37
3	D	1102	8RC	C37-C36	2.64	1.57	1.52
3	A	1102	8RC	C2-N3	2.63	1.39	1.34
3	C	1102	8RC	C15-C10	2.61	1.43	1.39
2	D	1101	VNS	C13-C12	2.60	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	VNS	C34-C35	2.59	1.42	1.37
2	B	1101	VNS	C27-C26	2.58	1.43	1.38
2	A	1101	VNS	C31-C30	2.58	1.53	1.50
3	C	1102	8RC	C37-C36	2.57	1.57	1.52
2	A	1101	VNS	C39-C33	2.57	1.43	1.40
3	B	1102	8RC	C23-N22	2.56	1.52	1.47
2	B	1101	VNS	C39-C33	2.56	1.43	1.40
3	D	1102	8RC	C11-C12	2.55	1.43	1.38
2	B	1101	VNS	C13-C12	2.54	1.43	1.39
3	D	1102	8RC	C26-N25	2.53	1.51	1.46
2	D	1101	VNS	C27-C26	2.49	1.43	1.38
3	D	1102	8RC	C12-C13	2.47	1.44	1.39
3	B	1102	8RC	C11-C12	2.46	1.43	1.38
3	D	1102	8RC	C15-C10	2.45	1.43	1.39
2	C	1101	VNS	C39-C33	2.44	1.43	1.40
2	A	1101	VNS	F36-C35	-2.43	1.30	1.36
3	D	1102	8RC	C23-N22	2.42	1.51	1.47
3	C	1102	8RC	C11-C12	2.41	1.43	1.38
3	C	1102	8RC	C18-C17	2.40	1.59	1.52
3	B	1102	8RC	C29-N31	2.39	1.37	1.33
2	C	1101	VNS	C27-C26	2.38	1.43	1.38
2	D	1101	VNS	C29-C28	2.36	1.43	1.38
3	A	1102	8RC	C15-C10	2.36	1.43	1.39
3	C	1102	8RC	C12-C13	2.35	1.43	1.39
3	C	1102	8RC	C19-N22	-2.34	1.42	1.48
2	D	1101	VNS	F36-C35	-2.34	1.30	1.36
2	B	1101	VNS	C29-C28	2.33	1.43	1.38
2	C	1101	VNS	C29-C28	2.31	1.43	1.38
2	A	1101	VNS	C13-C12	2.26	1.43	1.39
3	A	1102	8RC	C18-C17	2.26	1.58	1.52
2	C	1101	VNS	F36-C35	-2.24	1.30	1.36
3	B	1102	8RC	C18-C17	2.23	1.58	1.52
3	B	1102	8RC	C12-C13	2.23	1.43	1.39
3	C	1102	8RC	C24-N25	2.23	1.51	1.46
3	A	1102	8RC	C11-C12	2.21	1.42	1.38
3	B	1102	8RC	C15-C10	2.21	1.43	1.39
2	A	1101	VNS	C29-C28	2.21	1.42	1.38
2	B	1101	VNS	F36-C35	-2.20	1.31	1.36
2	B	1101	VNS	C26-C18	2.19	1.42	1.39
3	A	1102	8RC	C12-C13	2.19	1.43	1.39
2	D	1101	VNS	C37-C35	2.18	1.41	1.37
3	D	1102	8RC	C18-C17	2.18	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	8RC	C37-C36	2.18	1.56	1.52
3	B	1102	8RC	C19-N22	-2.18	1.42	1.48
3	D	1102	8RC	C19-N22	-2.16	1.42	1.48
3	C	1102	8RC	C11-C10	2.14	1.42	1.39
2	D	1101	VNS	C12-C11	2.14	1.52	1.48
3	A	1102	8RC	C23-N22	2.14	1.51	1.47
2	C	1101	VNS	C37-C35	2.13	1.41	1.37
3	D	1102	8RC	C11-C10	2.12	1.42	1.39
3	A	1102	8RC	C26-N25	2.12	1.50	1.46
3	B	1102	8RC	C26-N25	2.10	1.50	1.46
2	A	1101	VNS	C27-C26	2.09	1.42	1.38
2	B	1101	VNS	C37-C35	2.08	1.41	1.37
2	A	1101	VNS	C37-C35	2.07	1.41	1.37
2	D	1101	VNS	C26-C18	2.05	1.42	1.39
3	C	1102	8RC	C23-N22	2.05	1.51	1.47
3	D	1102	8RC	C5-N6	2.04	1.37	1.34
3	B	1102	8RC	C24-N25	2.02	1.50	1.46
3	A	1102	8RC	C29-N31	2.00	1.36	1.33
3	D	1102	8RC	C24-N25	2.00	1.50	1.46

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	VNS	C31-N10-C11	-21.80	104.15	113.12
2	B	1101	VNS	C31-N10-C11	-21.63	104.22	113.12
2	A	1101	VNS	C31-N10-C11	-21.51	104.27	113.12
2	D	1101	VNS	C31-N10-C11	-21.06	104.45	113.12
2	A	1101	VNS	C30-C31-N10	15.88	107.47	102.18
2	D	1101	VNS	C30-C31-N10	15.69	107.41	102.18
2	C	1101	VNS	C30-C31-N10	15.44	107.32	102.18
2	B	1101	VNS	C30-C31-N10	15.28	107.27	102.18
3	B	1102	8RC	C40-C38-N35	12.11	131.71	117.66
2	B	1101	VNS	C12-C11-N10	11.59	113.28	106.44
2	C	1101	VNS	C12-C11-N10	11.51	113.24	106.44
2	D	1101	VNS	C12-C11-N10	10.87	112.86	106.44
2	A	1101	VNS	C12-C11-N10	10.80	112.82	106.44
3	D	1102	8RC	C20-C19-N22	-8.14	91.37	112.52
3	C	1102	8RC	C20-C19-N22	-7.99	91.78	112.52
2	C	1101	VNS	O32-C11-N10	-7.61	119.53	125.24
2	C	1101	VNS	C30-C12-C11	-7.52	104.91	108.94
2	D	1101	VNS	O32-C11-N10	-7.49	119.62	125.24
3	C	1102	8RC	C40-C38-N35	7.44	126.30	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	VNS	O32-C11-N10	-7.43	119.67	125.24
2	B	1101	VNS	C30-C12-C11	-7.36	105.00	108.94
3	D	1102	8RC	C40-C38-N35	7.30	126.14	117.66
3	C	1102	8RC	C26-N25-C24	7.12	119.47	109.52
3	C	1102	8RC	C1-C29-N31	7.06	126.89	115.75
3	D	1102	8RC	C1-C29-N31	7.05	126.88	115.75
3	B	1102	8RC	C1-C29-N31	7.03	126.85	115.75
2	D	1101	VNS	C30-C12-C11	-7.03	105.17	108.94
2	A	1101	VNS	O32-C11-N10	-7.01	119.99	125.24
3	A	1102	8RC	C40-C38-N35	6.87	125.63	117.66
3	A	1102	8RC	C1-C29-N31	6.82	126.52	115.75
3	B	1102	8RC	C20-C19-N22	-6.79	94.89	112.52
3	A	1102	8RC	C1-C2-N3	-6.78	115.03	121.63
2	A	1101	VNS	C30-C12-C11	-6.64	105.38	108.94
3	B	1102	8RC	C1-C2-N3	-6.64	115.16	121.63
3	C	1102	8RC	C1-C2-N3	-6.57	115.23	121.63
3	D	1102	8RC	C1-C2-N3	-6.47	115.33	121.63
3	A	1102	8RC	C20-C19-N22	-6.41	95.88	112.52
3	C	1102	8RC	C27-C26-N25	5.24	116.72	110.80
2	C	1101	VNS	C21-C20-C19	5.12	117.09	111.04
2	D	1101	VNS	C20-C19-C18	-4.81	101.51	112.79
2	A	1101	VNS	C24-N22-C21	4.80	116.23	109.52
2	B	1101	VNS	C21-C20-C19	4.65	116.54	111.04
3	B	1102	8RC	O39-C38-N35	-4.64	114.44	121.13
2	A	1101	VNS	C21-C20-C19	4.59	116.47	111.04
3	D	1102	8RC	C27-N22-C23	4.57	117.43	109.08
2	C	1101	VNS	C24-N22-C21	4.53	115.86	109.52
2	A	1101	VNS	C20-C21-N22	4.47	117.22	111.22
2	B	1101	VNS	C24-C25-C19	4.45	116.30	111.04
2	B	1101	VNS	C24-N22-C21	4.43	115.72	109.52
2	B	1101	VNS	C26-C18-C17	-4.43	112.76	118.29
2	C	1101	VNS	C26-C18-C17	-4.43	112.77	118.29
3	D	1102	8RC	C26-N25-C24	4.38	115.65	109.52
2	C	1101	VNS	C20-C21-N22	4.38	117.09	111.22
2	C	1101	VNS	C23-N22-C24	-4.37	104.12	110.66
2	A	1101	VNS	C23-N22-C24	-4.35	104.15	110.66
2	D	1101	VNS	C21-C20-C19	4.26	116.08	111.04
3	D	1102	8RC	C1-C2-N7	4.22	125.67	119.06
2	A	1101	VNS	C23-N22-C21	-4.15	104.45	110.66
3	C	1102	8RC	C20-C21-N16	4.10	119.55	111.10
2	D	1101	VNS	C26-C18-C17	-4.09	113.19	118.29
2	D	1101	VNS	C24-N22-C21	4.09	115.24	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	VNS	C23-N22-C21	-4.09	104.55	110.66
2	A	1101	VNS	C26-C18-C17	-4.07	113.22	118.29
3	B	1102	8RC	C33-C34-N35	4.07	107.80	102.75
3	C	1102	8RC	C1-N6-C5	4.04	125.64	116.84
2	D	1101	VNS	C23-N22-C21	-4.00	104.67	110.66
2	B	1101	VNS	C23-N22-C24	-3.97	104.72	110.66
3	D	1102	8RC	C1-N6-C5	3.96	125.47	116.84
2	D	1101	VNS	C24-C25-C19	3.93	115.68	111.04
2	B	1101	VNS	C20-C19-C18	-3.91	103.64	112.79
3	C	1102	8RC	C1-C2-N7	3.89	125.14	119.06
3	A	1102	8RC	C1-N6-C5	3.87	125.28	116.84
3	B	1102	8RC	C1-N6-C5	3.87	125.28	116.84
2	D	1101	VNS	C23-N22-C24	-3.86	104.89	110.66
3	A	1102	8RC	C28-N25-C26	-3.80	104.97	110.66
3	C	1102	8RC	O8-C33-C34	3.77	117.35	108.19
3	A	1102	8RC	C23-C24-N25	-3.76	106.56	110.80
2	B	1101	VNS	C20-C21-N22	3.75	116.26	111.22
2	B	1101	VNS	C23-N22-C21	-3.73	105.08	110.66
3	B	1102	8RC	C28-N25-C26	-3.73	105.08	110.66
3	B	1102	8RC	C18-C19-N22	3.71	122.16	112.52
3	D	1102	8RC	C28-N25-C26	-3.63	105.23	110.66
3	B	1102	8RC	C41-C40-C38	3.61	128.72	121.33
2	A	1101	VNS	C24-C25-C19	3.57	115.26	111.04
2	C	1101	VNS	C24-C25-C19	3.56	115.25	111.04
2	C	1101	VNS	C20-C19-C18	-3.52	104.53	112.79
3	B	1102	8RC	O8-C33-C34	3.50	116.69	108.19
2	A	1101	VNS	C20-C19-C18	-3.45	104.70	112.79
3	A	1102	8RC	C1-C2-N7	3.43	124.43	119.06
3	C	1102	8RC	C18-C17-N16	3.42	118.16	111.10
2	C	1101	VNS	C16-C15-C14	3.42	127.29	121.36
2	A	1101	VNS	C16-C15-C14	3.41	127.27	121.36
3	A	1102	8RC	C28-N25-C24	-3.41	105.56	110.66
3	D	1102	8RC	O8-C33-C34	3.39	116.42	108.19
2	B	1101	VNS	C31-N10-C09	3.38	127.02	123.86
3	D	1102	8RC	C36-N35-C34	-3.33	102.94	111.55
3	C	1102	8RC	C36-N35-C34	-3.32	102.97	111.55
3	A	1102	8RC	C36-N35-C34	-3.27	103.09	111.55
3	D	1102	8RC	C20-C21-N16	3.27	117.84	111.10
2	D	1101	VNS	C33-C34-C35	3.25	122.81	118.59
3	C	1102	8RC	C18-C19-N22	3.22	120.88	112.52
2	D	1101	VNS	C31-N10-C09	3.16	126.82	123.86
2	B	1101	VNS	C33-C34-C35	3.16	122.69	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	8RC	C1-C2-N7	3.15	123.99	119.06
3	C	1102	8RC	C23-N22-C19	-3.13	103.82	112.64
3	B	1102	8RC	C36-N35-C34	-3.12	103.49	111.55
2	B	1101	VNS	C28-C14-C13	-3.11	113.76	118.16
2	C	1101	VNS	C31-N10-C09	3.10	126.76	123.86
2	B	1101	VNS	C29-C30-C12	-3.07	117.52	120.31
3	B	1102	8RC	C28-N25-C24	-3.07	106.07	110.66
2	D	1101	VNS	C20-C21-N22	3.05	115.32	111.22
3	A	1102	8RC	C18-C19-N22	3.05	120.44	112.52
2	C	1101	VNS	C28-C14-C13	-3.05	113.86	118.16
3	A	1102	8RC	O30-C29-N31	-3.04	118.26	122.58
2	D	1101	VNS	C28-C14-C13	-3.03	113.88	118.16
2	C	1101	VNS	C27-C15-C16	-3.03	111.56	117.59
2	B	1101	VNS	C27-C15-C16	-3.00	111.61	117.59
3	D	1102	8RC	C28-N25-C24	-2.99	106.18	110.66
3	D	1102	8RC	O30-C29-N31	-2.98	118.34	122.58
2	A	1101	VNS	C33-C34-C35	2.97	122.44	118.59
3	B	1102	8RC	O30-C29-N31	-2.93	118.41	122.58
2	B	1101	VNS	C16-C15-C14	2.93	126.42	121.36
2	D	1101	VNS	C27-C15-C16	-2.92	111.77	117.59
2	D	1101	VNS	C16-C15-C14	2.92	126.41	121.36
2	A	1101	VNS	C27-C15-C16	-2.86	111.89	117.59
2	C	1101	VNS	C33-C34-C35	2.86	122.30	118.59
2	C	1101	VNS	C29-C30-C12	-2.83	117.75	120.31
2	C	1101	VNS	C25-C19-C18	2.83	119.42	112.79
3	C	1102	8RC	O30-C29-N31	-2.82	118.56	122.58
2	D	1101	VNS	C29-C30-C12	-2.82	117.75	120.31
3	B	1102	8RC	C26-C27-N22	-2.82	105.21	110.59
3	B	1102	8RC	C37-C33-C34	-2.81	97.64	104.39
3	A	1102	8RC	O8-C33-C34	2.80	114.98	108.19
2	A	1101	VNS	C28-C14-C13	-2.78	114.23	118.16
3	B	1102	8RC	C27-C26-N25	-2.78	107.67	110.80
2	D	1101	VNS	C25-C19-C18	2.75	119.25	112.79
3	A	1102	8RC	C37-C33-C34	-2.73	97.83	104.39
2	C	1101	VNS	C13-C12-C11	2.70	133.87	129.36
2	B	1101	VNS	C25-C19-C18	2.68	119.08	112.79
2	D	1101	VNS	O01-C02-C09	-2.68	117.38	120.97
2	B	1101	VNS	O01-C02-C09	-2.66	117.40	120.97
2	D	1101	VNS	C13-C12-C11	2.65	133.80	129.36
3	A	1102	8RC	C14-C13-N16	2.64	125.02	121.38
2	B	1101	VNS	C37-C35-C34	-2.61	119.90	123.29
2	A	1101	VNS	C29-C30-C12	-2.61	117.94	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	VNS	C13-C12-C11	2.59	133.70	129.36
3	C	1102	8RC	C15-C14-C13	2.58	123.72	120.32
2	A	1101	VNS	C13-C12-C11	2.56	133.64	129.36
3	D	1102	8RC	C21-C20-C19	2.55	115.67	110.81
3	C	1102	8RC	C37-C36-N35	2.55	106.29	103.28
3	C	1102	8RC	C33-C34-N35	2.54	105.90	102.75
3	C	1102	8RC	C28-N25-C24	-2.52	106.89	110.66
2	C	1101	VNS	C37-C35-C34	-2.51	120.02	123.29
3	D	1102	8RC	C15-C14-C13	2.51	123.63	120.32
3	B	1102	8RC	C15-C14-C13	2.50	123.61	120.32
3	C	1102	8RC	O39-C38-N35	-2.47	117.58	121.13
3	D	1102	8RC	C33-C34-N35	2.46	105.80	102.75
3	D	1102	8RC	C37-C36-N35	2.45	106.17	103.28
3	C	1102	8RC	C28-N25-C26	-2.45	107.00	110.66
2	A	1101	VNS	C37-C35-C34	-2.43	120.13	123.29
2	C	1101	VNS	C04-N03-C02	-2.41	123.65	129.02
3	D	1102	8RC	C36-N35-C38	2.41	133.10	123.89
2	B	1101	VNS	C17-C16-C15	2.39	124.58	121.13
2	A	1101	VNS	C04-N03-C02	-2.38	123.73	129.02
3	D	1102	8RC	O39-C38-N35	-2.37	117.71	121.13
3	D	1102	8RC	C9-C5-N6	2.37	121.86	116.66
2	C	1101	VNS	C27-C26-C18	2.37	123.58	121.20
3	A	1102	8RC	C36-N35-C38	2.37	132.94	123.89
3	C	1102	8RC	C36-N35-C38	2.36	132.92	123.89
3	A	1102	8RC	C15-C14-C13	2.36	123.43	120.32
2	D	1101	VNS	C04-N03-C02	-2.36	123.77	129.02
2	A	1101	VNS	C26-C27-C15	2.36	124.53	121.13
2	A	1101	VNS	C31-N10-C09	2.36	126.06	123.86
2	C	1101	VNS	C26-C27-C15	2.36	124.53	121.13
3	C	1102	8RC	C21-C20-C19	2.34	115.25	110.81
2	D	1101	VNS	C17-C16-C15	2.33	124.49	121.13
3	D	1102	8RC	C37-C33-C34	-2.33	98.78	104.39
3	B	1102	8RC	C23-C24-N25	-2.33	108.17	110.80
3	D	1102	8RC	C18-C17-N16	2.31	115.87	111.10
3	C	1102	8RC	C37-C33-C34	-2.30	98.85	104.39
2	C	1101	VNS	C17-C16-C15	2.30	124.44	121.13
2	B	1101	VNS	C26-C27-C15	2.29	124.43	121.13
2	D	1101	VNS	C37-C35-C34	-2.28	120.33	123.29
3	B	1102	8RC	O39-C38-C40	-2.28	113.83	120.34
3	A	1102	8RC	C14-C13-C12	-2.26	114.56	119.16
2	B	1101	VNS	C04-N03-C02	-2.25	124.00	129.02
2	D	1101	VNS	C26-C27-C15	2.25	124.37	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	8RC	O30-C29-C1	-2.23	114.54	119.89
3	C	1102	8RC	C17-N16-C13	2.23	124.11	118.09
3	B	1102	8RC	C14-C13-C12	-2.23	114.63	119.16
3	A	1102	8RC	C33-C34-N35	2.22	105.50	102.75
2	B	1101	VNS	C27-C26-C18	2.22	123.43	121.20
2	A	1101	VNS	C17-C16-C15	2.19	124.29	121.13
3	C	1102	8RC	C14-C13-C12	-2.16	114.77	119.16
3	D	1102	8RC	C27-C26-N25	2.16	113.24	110.80
3	B	1102	8RC	O30-C29-C1	-2.15	114.74	119.89
3	D	1102	8RC	O30-C29-C1	-2.13	114.78	119.89
3	A	1102	8RC	O39-C38-N35	-2.13	118.07	121.13
3	B	1102	8RC	C21-N16-C17	-2.13	106.82	111.52
2	A	1101	VNS	C25-C19-C18	2.10	117.73	112.79
2	C	1101	VNS	O01-C02-C09	-2.09	118.17	120.97
2	D	1101	VNS	C38-C39-C33	2.07	122.29	120.41
2	D	1101	VNS	C27-C26-C18	2.06	123.27	121.20
3	C	1102	8RC	C21-N16-C17	2.06	116.06	111.52
3	D	1102	8RC	C4-O8-C33	2.06	121.52	118.56
3	B	1102	8RC	C15-C10-C11	-2.06	116.22	119.03
3	C	1102	8RC	C12-C11-C10	2.05	122.66	120.30
3	D	1102	8RC	C14-C13-C12	-2.05	115.00	119.16
2	A	1101	VNS	C27-C26-C18	2.04	123.25	121.20
3	C	1102	8RC	C15-C10-C11	-2.03	116.25	119.03
2	C	1101	VNS	C38-C39-C33	2.03	122.26	120.41
3	A	1102	8RC	C18-C17-N16	2.02	115.27	111.10
3	A	1102	8RC	C15-C10-C11	-2.02	116.27	119.03
3	A	1102	8RC	C37-C36-N35	2.01	105.65	103.28
3	A	1102	8RC	C41-C40-C38	2.00	125.43	121.33

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	8RC	C2-C1-C29-N31
3	A	1102	8RC	C2-C1-C29-O30
3	A	1102	8RC	N6-C1-C29-N31
3	A	1102	8RC	N6-C1-C29-O30
3	A	1102	8RC	C1-C2-N7-C10
3	A	1102	8RC	C37-C33-O8-C4
3	B	1102	8RC	C1-C2-N7-C10
3	B	1102	8RC	N35-C38-C40-C41
3	B	1102	8RC	O39-C38-C40-C41

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Mol	Chain	Res	Type	Atoms
3	C	1102	8RC	C1-C2-N7-C10
3	C	1102	8RC	C37-C33-O8-C4
3	D	1102	8RC	C1-C2-N7-C10
3	D	1102	8RC	C37-C33-O8-C4
3	D	1102	8RC	C12-C13-N16-C17
3	D	1102	8RC	C14-C13-N16-C17
3	B	1102	8RC	N3-C2-N7-C10
3	B	1102	8RC	C18-C19-N22-C27
3	D	1102	8RC	C18-C19-N22-C27
3	A	1102	8RC	C34-C33-O8-C4
3	C	1102	8RC	C34-C33-O8-C4
3	D	1102	8RC	C34-C33-O8-C4
3	A	1102	8RC	N3-C2-N7-C10
3	C	1102	8RC	N3-C2-N7-C10
3	D	1102	8RC	N3-C2-N7-C10
3	C	1102	8RC	O39-C38-C40-C41
3	C	1102	8RC	N35-C38-C40-C41
3	C	1102	8RC	C18-C19-N22-C27
3	D	1102	8RC	N35-C38-C40-C41
3	B	1102	8RC	C34-C33-O8-C4
3	B	1102	8RC	C37-C33-O8-C4
3	D	1102	8RC	C4-C5-C9-C32
3	C	1102	8RC	C12-C13-N16-C21
3	D	1102	8RC	O39-C38-C40-C41
3	A	1102	8RC	N35-C38-C40-C41
3	B	1102	8RC	C18-C19-N22-C23
3	D	1102	8RC	C20-C19-N22-C27
2	D	1101	VNS	C02-C09-N10-C31
3	A	1102	8RC	C4-C5-C9-C32
3	A	1102	8RC	C18-C19-N22-C23
3	B	1102	8RC	C20-C19-N22-C23
3	B	1102	8RC	C20-C19-N22-C27
2	A	1101	VNS	C33-C09-N10-C31
2	B	1101	VNS	C33-C09-N10-C31
2	C	1101	VNS	C33-C09-N10-C31
2	D	1101	VNS	C33-C09-N10-C31
3	A	1102	8RC	O39-C38-C40-C41
3	C	1102	8RC	C20-C19-N22-C23
3	C	1102	8RC	C14-C13-N16-C21
2	B	1101	VNS	C02-C09-C33-C34
2	A	1101	VNS	C02-C09-N10-C31
3	A	1102	8RC	N6-C5-C9-C32

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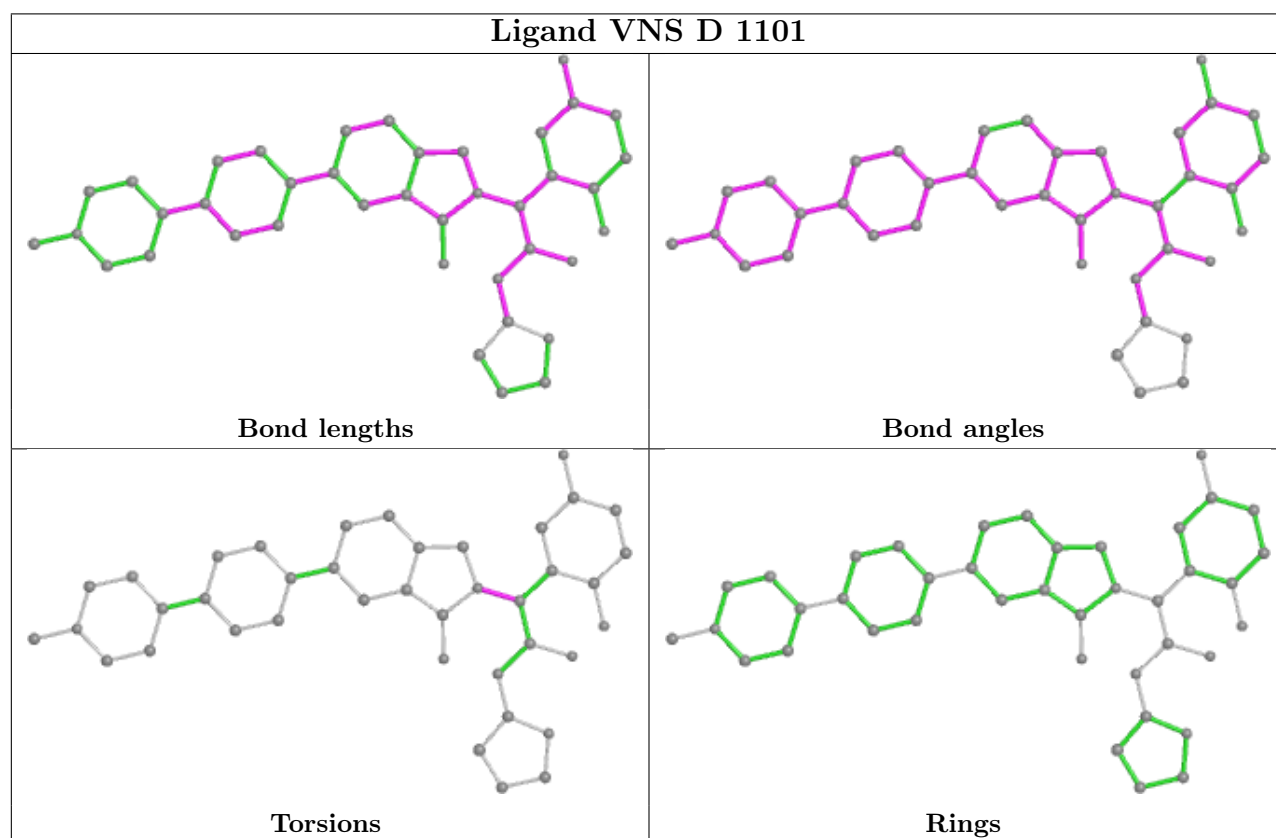
Mol	Chain	Res	Type	Atoms
3	D	1102	8RC	N6-C5-C9-C32

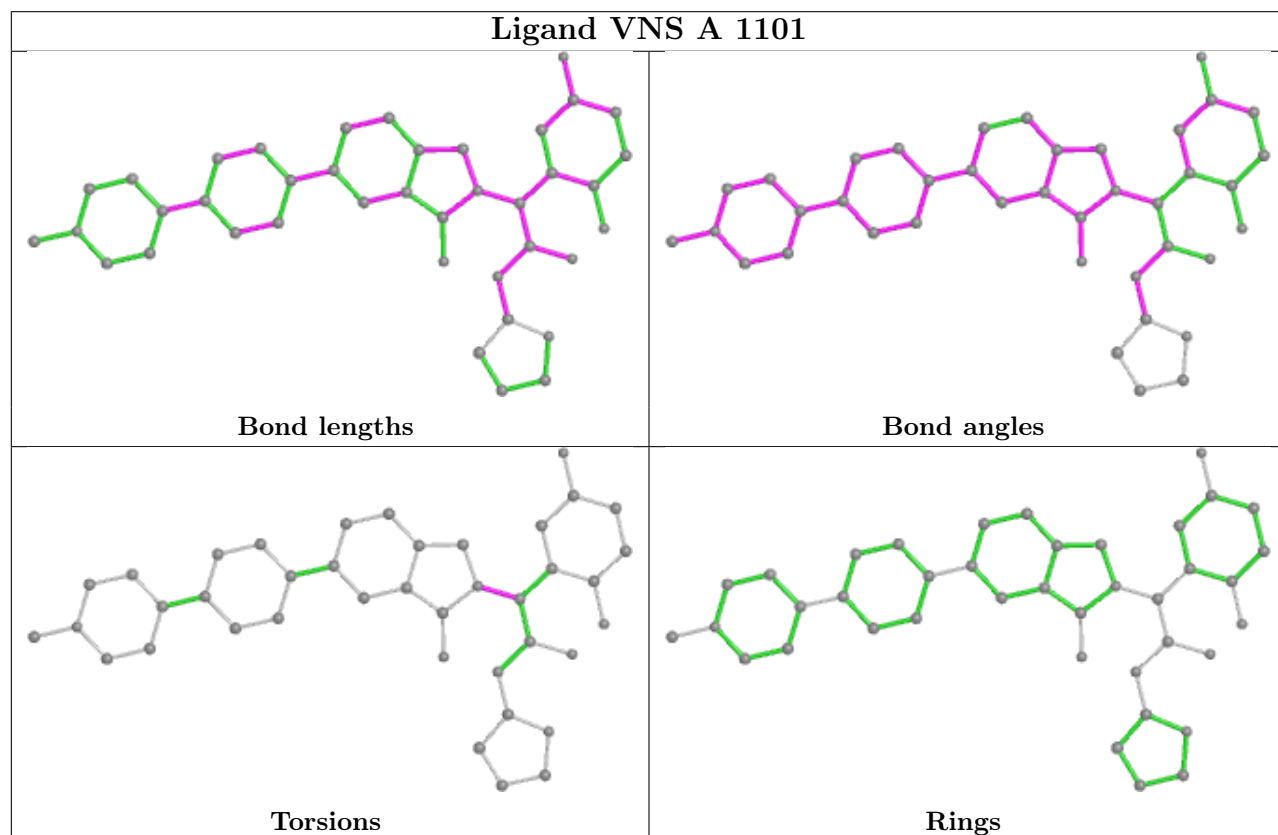
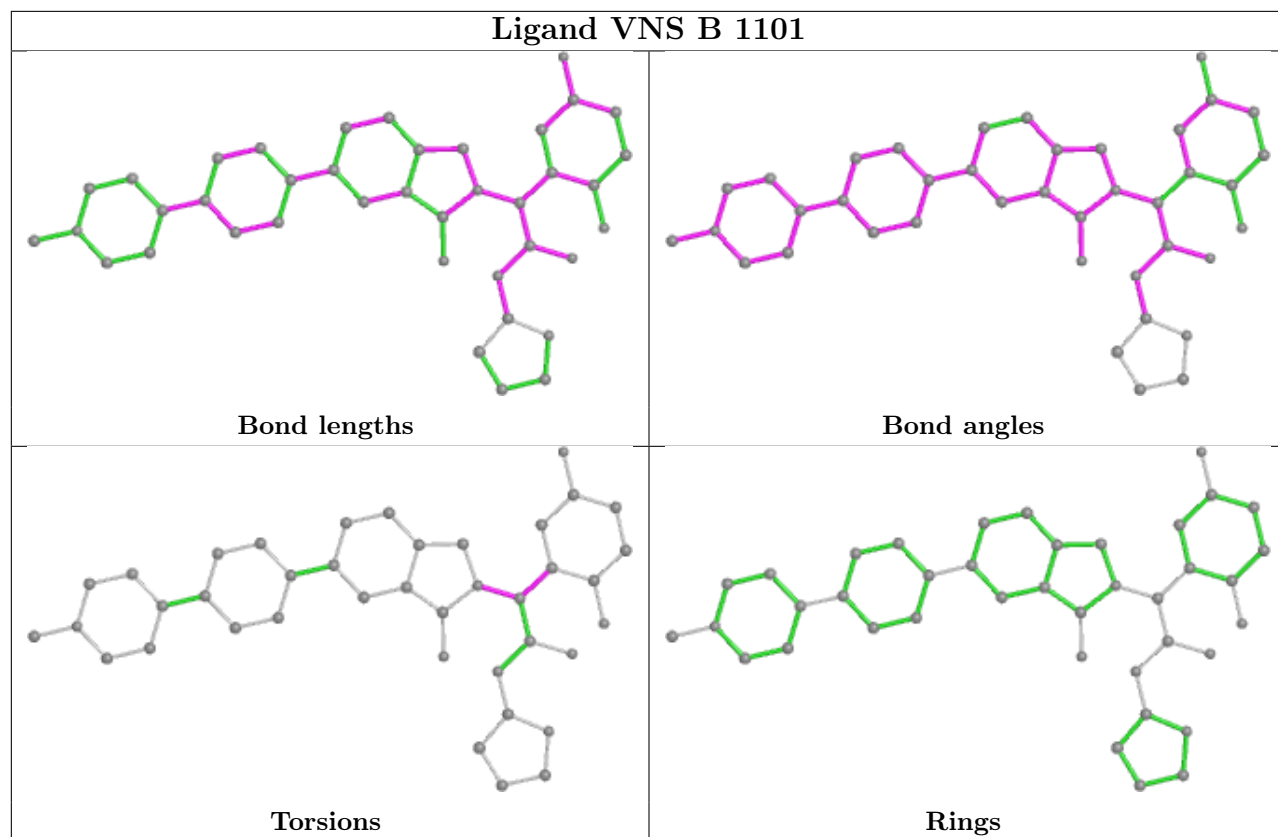
There are no ring outliers.

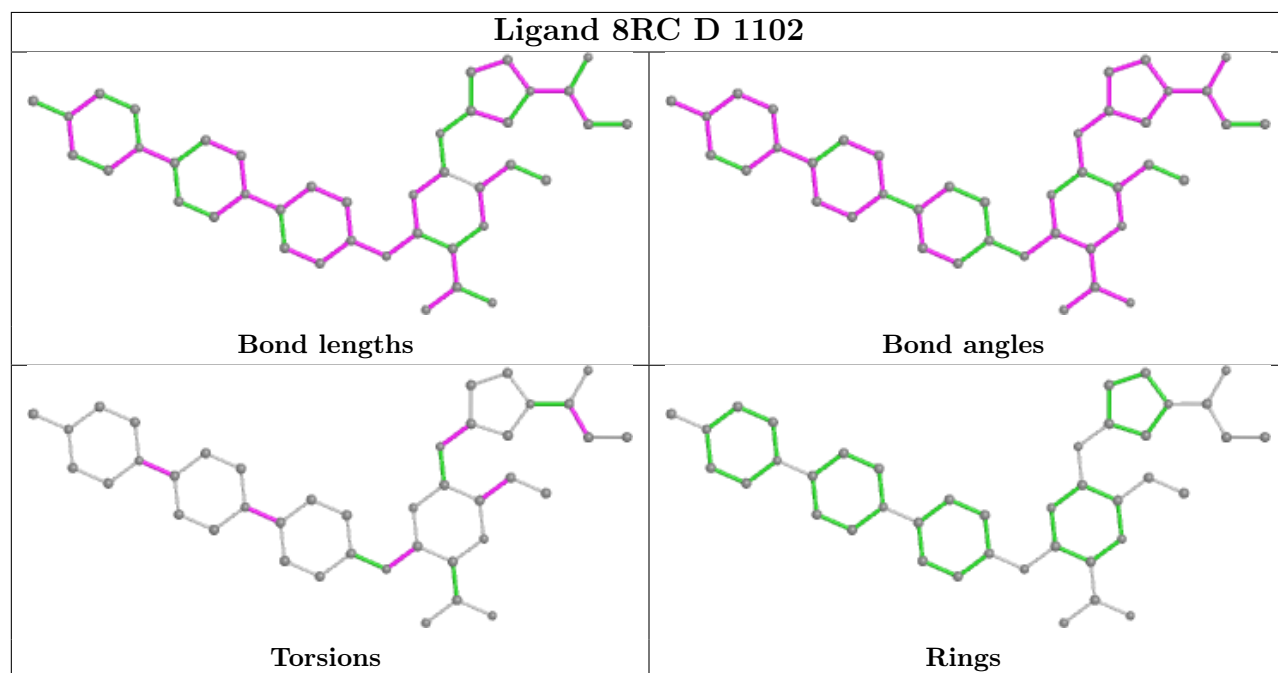
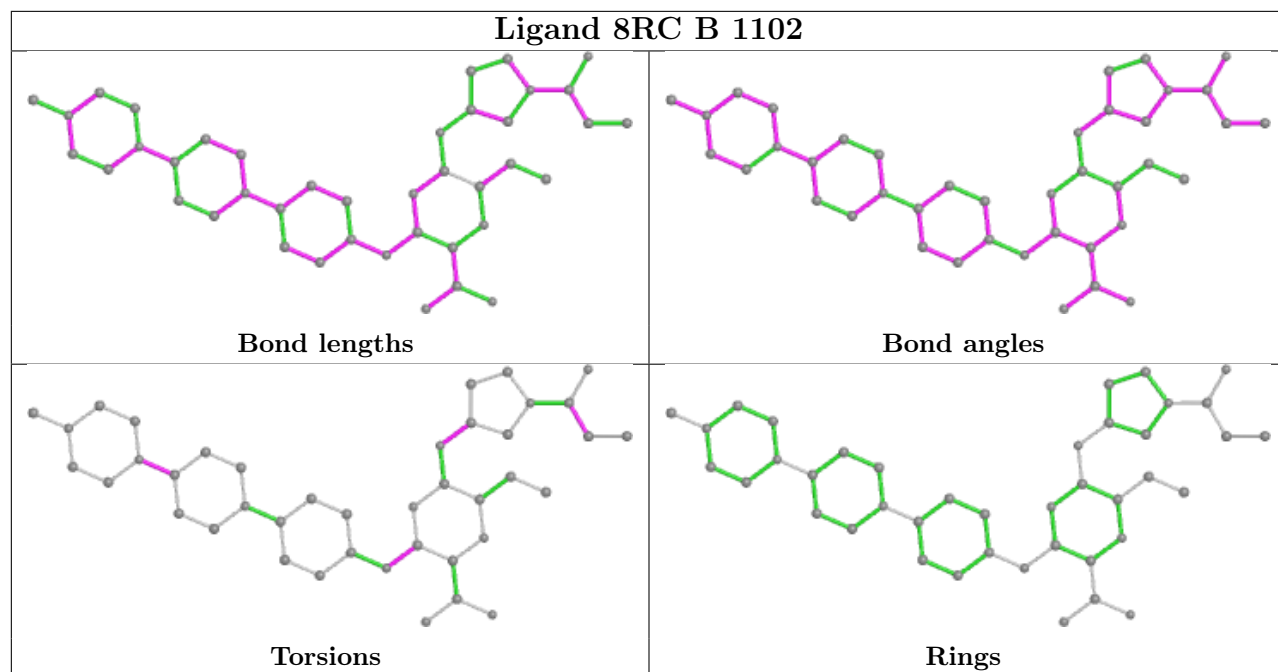
2 monomers are involved in 3 short contacts:

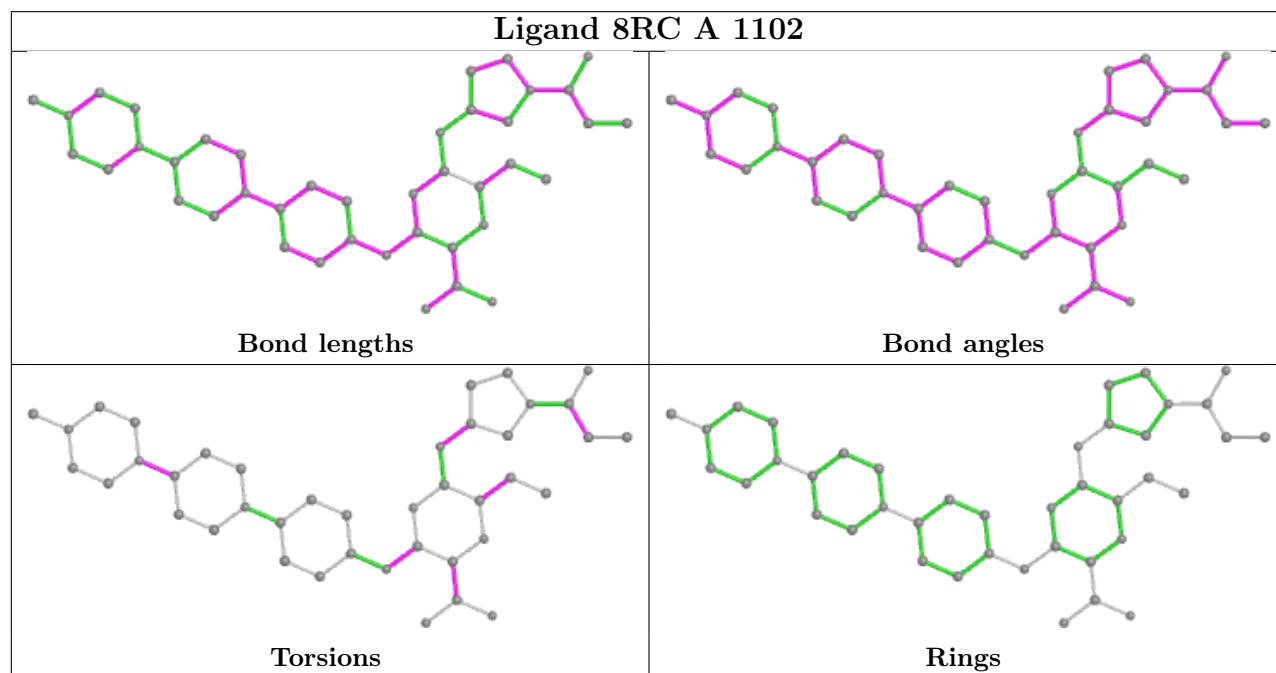
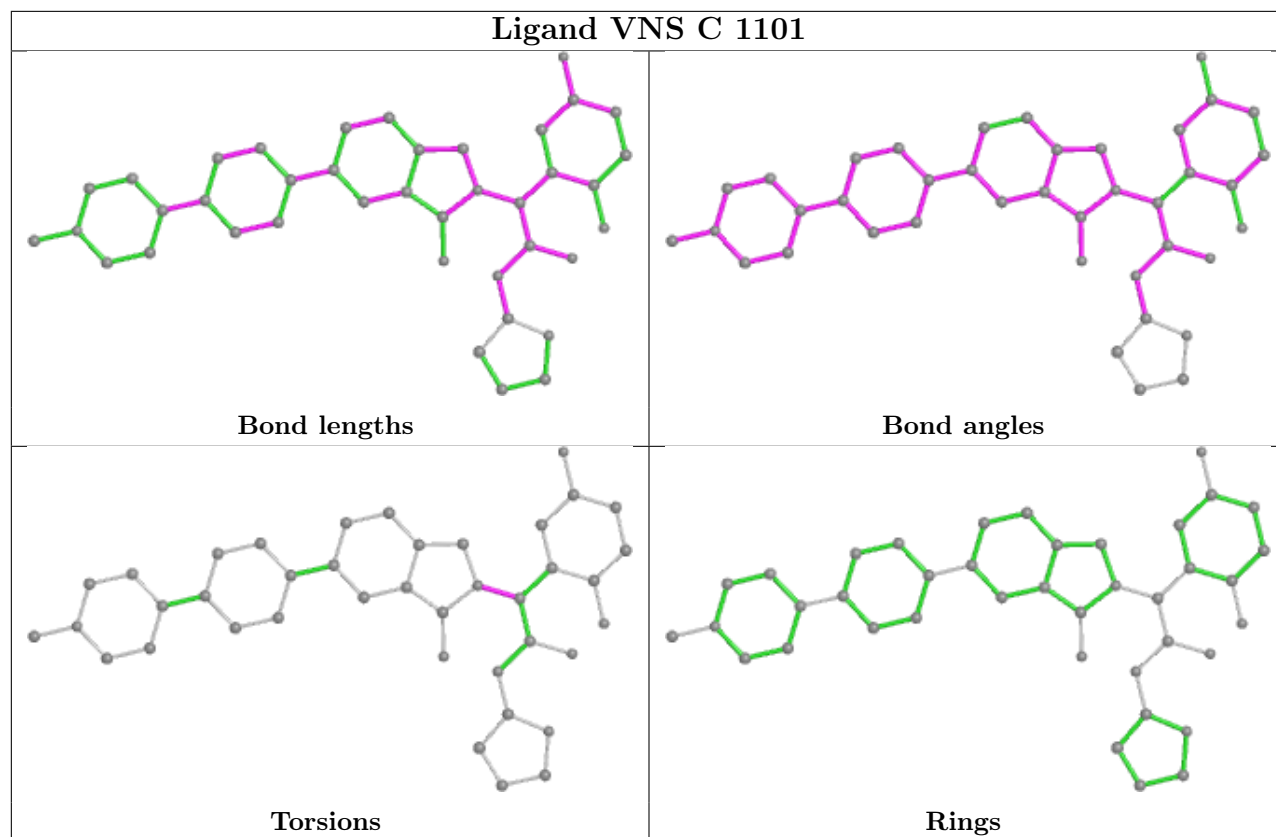
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	8RC	1	0
3	C	1102	8RC	2	0

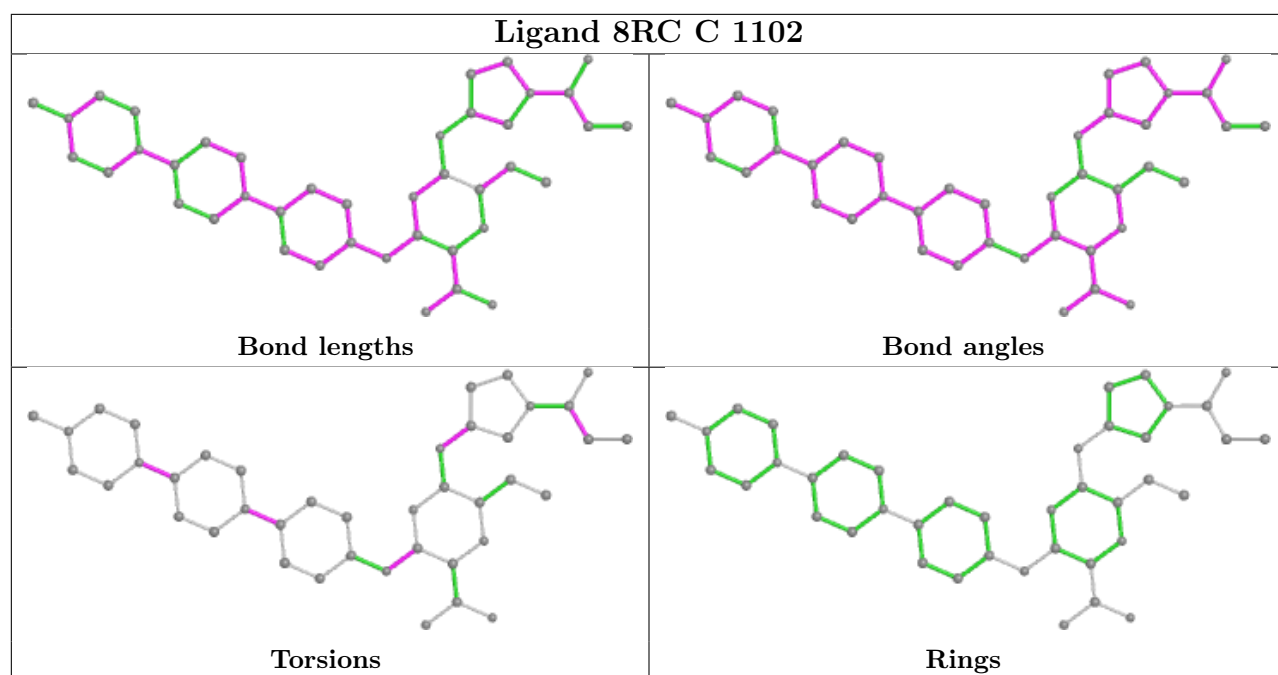
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	280/331 (84%)	0.09	3 (1%) 80 82	35, 53, 76, 93	0
1	B	275/331 (83%)	0.19	8 (2%) 51 51	39, 61, 95, 114	0
1	C	274/331 (82%)	0.10	6 (2%) 62 63	36, 54, 83, 98	0
1	D	271/331 (81%)	0.31	11 (4%) 37 36	44, 67, 93, 106	0
All	All	1100/1324 (83%)	0.17	28 (2%) 57 58	35, 59, 88, 114	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	723	PHE	3.9
1	D	784	SER	3.9
1	B	923	ILE	3.4
1	B	764	TYR	3.3
1	D	893	HIS	3.0
1	C	735	GLY	2.9
1	C	712	PHE	2.7
1	B	999	ARG	2.6
1	A	977	ARG	2.6
1	C	982	GLN	2.5
1	A	1004	GLU	2.5
1	D	713	LYS	2.5
1	D	955	ALA	2.5
1	D	760	LEU	2.5
1	D	946	ILE	2.5
1	D	729	GLY	2.4
1	B	748	ARG	2.3
1	C	751	THR	2.3
1	C	782	LEU	2.3
1	B	738	VAL	2.3
1	B	760	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	764	TYR	2.3
1	C	784	SER	2.1
1	D	751	THR	2.1
1	D	735	GLY	2.1
1	A	723	PHE	2.1
1	B	713	LYS	2.0
1	D	858	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

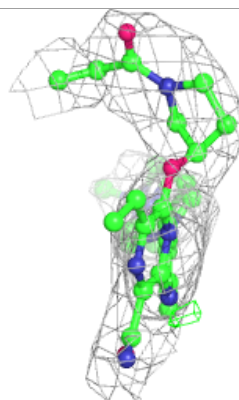
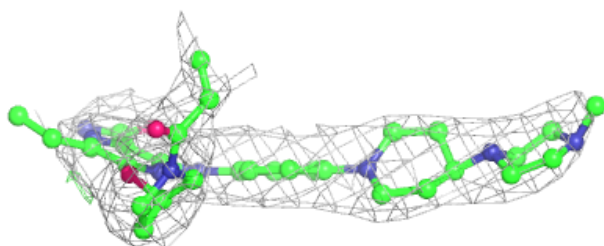
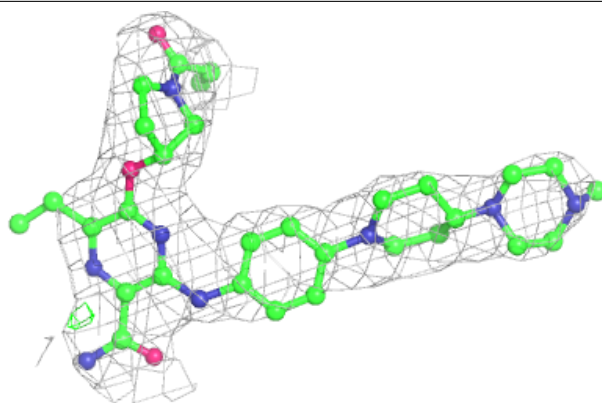
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8RC	C	1102	41/41	0.91	0.23	44,54,85,91	0
2	VNS	D	1101	40/40	0.92	0.24	52,61,98,102	0
3	8RC	A	1102	41/41	0.92	0.23	37,50,67,69	0
3	8RC	B	1102	41/41	0.92	0.20	46,56,76,81	0
2	VNS	B	1101	40/40	0.92	0.23	50,60,89,92	0
2	VNS	A	1101	40/40	0.93	0.23	37,47,77,81	0
2	VNS	C	1101	40/40	0.93	0.21	44,56,75,81	0
3	8RC	D	1102	41/41	0.93	0.19	47,55,76,80	0

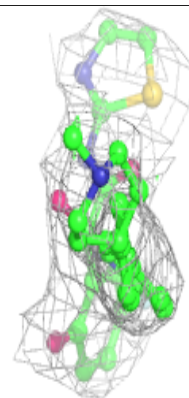
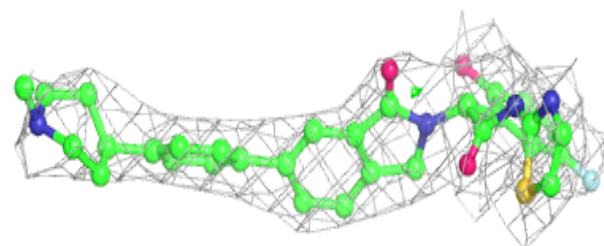
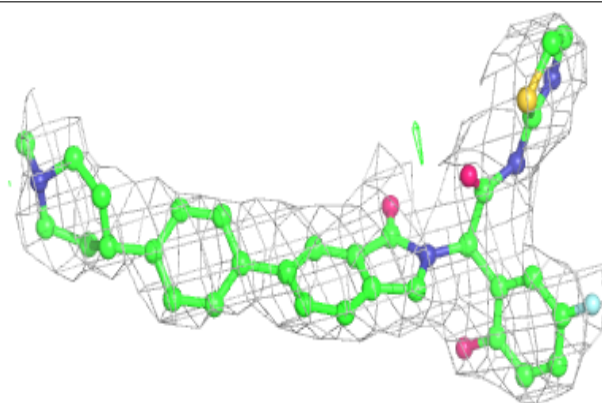
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8RC C 1102:

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

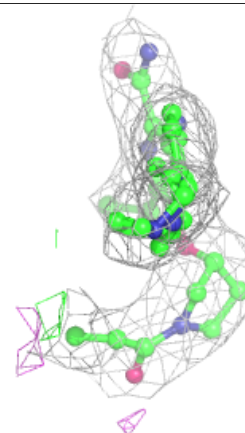
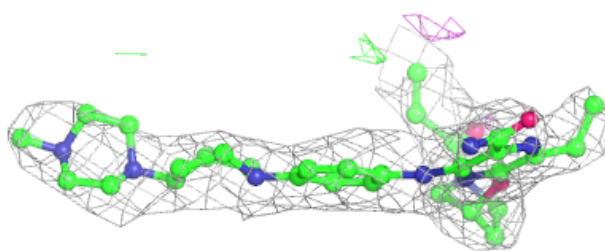
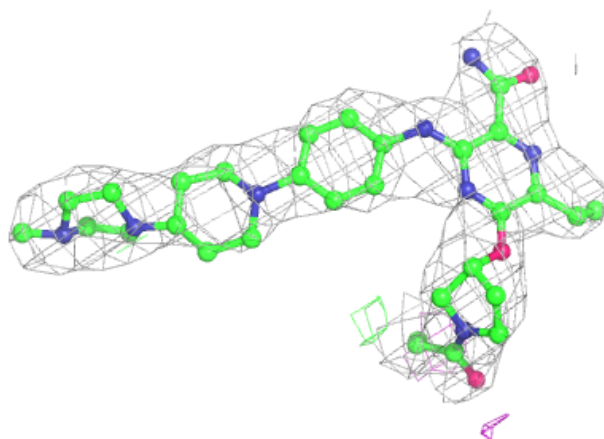
**Electron density around VNS D 1101:**

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

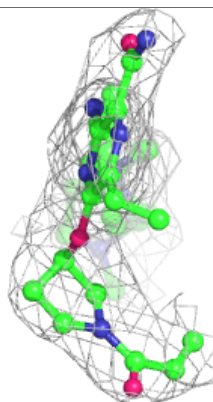
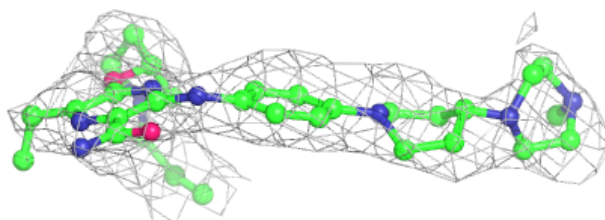
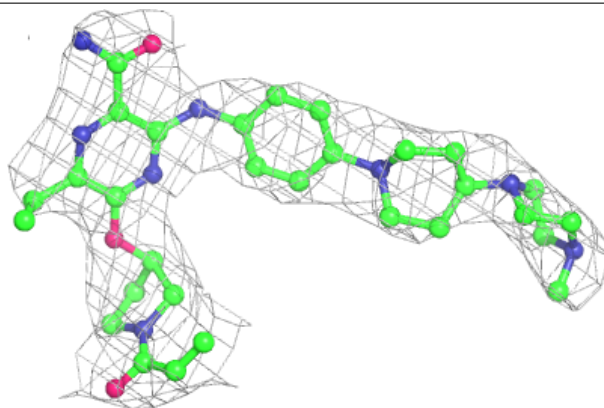


Electron density around 8RC A 1102:

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

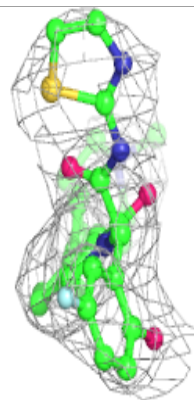
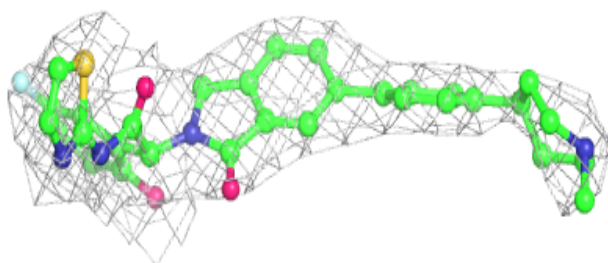
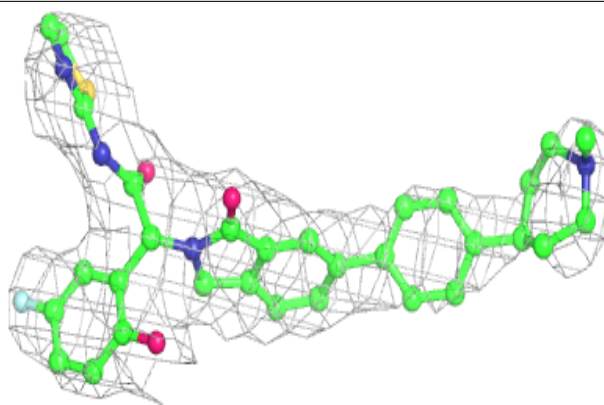
**Electron density around 8RC B 1102:**

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

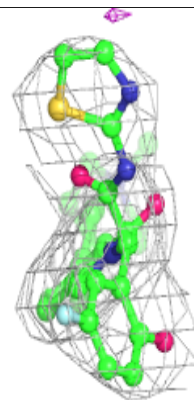
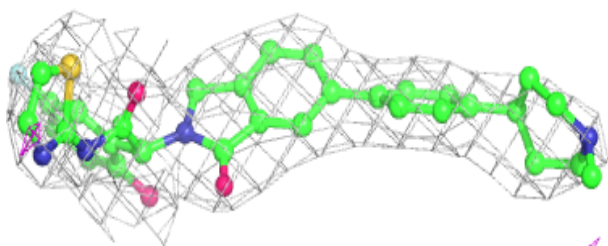
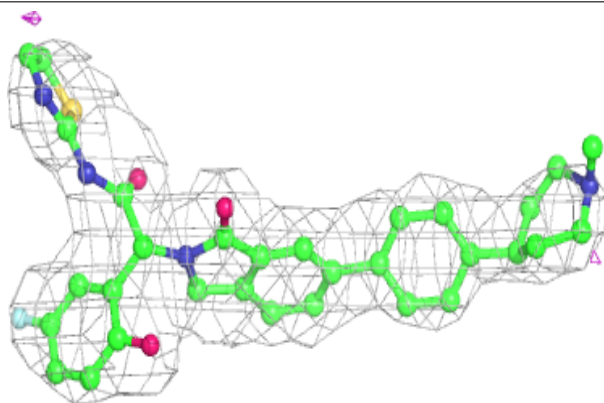


Electron density around VNS B 1101:

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

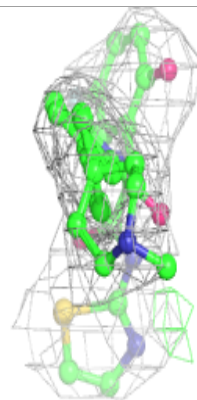
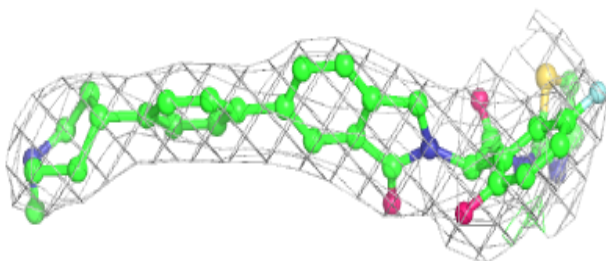
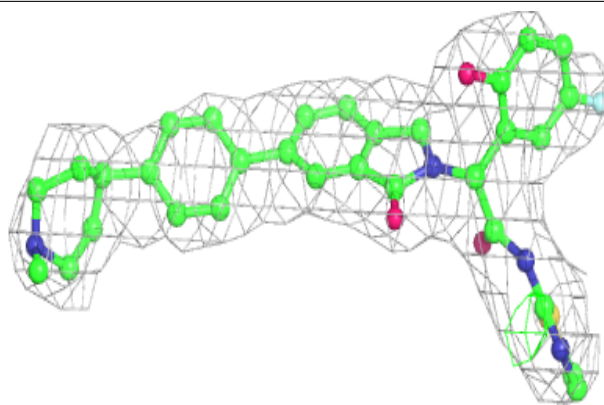
**Electron density around VNS A 1101:**

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

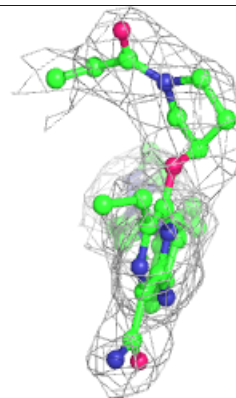
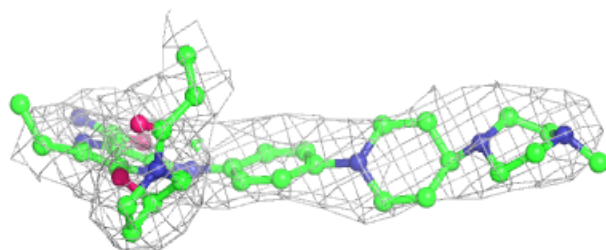
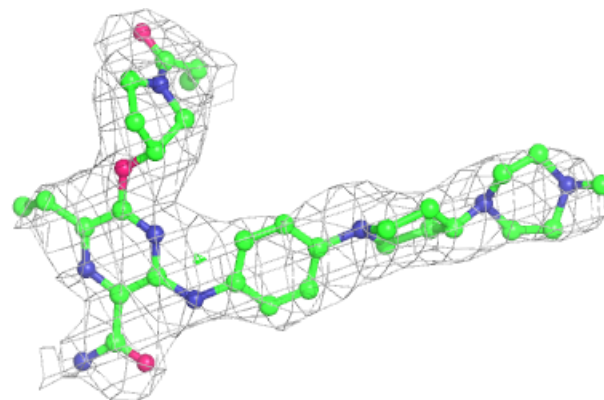


Electron density around VNS C 1101:

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

**Electron density around 8RC D 1102:**

$2mF_o-DF_c$ (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.