



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:50 PM UTC

PDB ID : 8TGD / pdb_00008tgd
Title : STX-478, a Mutant-Selective, Allosteric Inhibitor bound to H1047R PI3Kalpha
Authors : Hilbert, B.; Brooijmans, N.; Buckbinder, L.; St.Jean Jr., D.J.
Deposited on : 2023-07-12
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 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

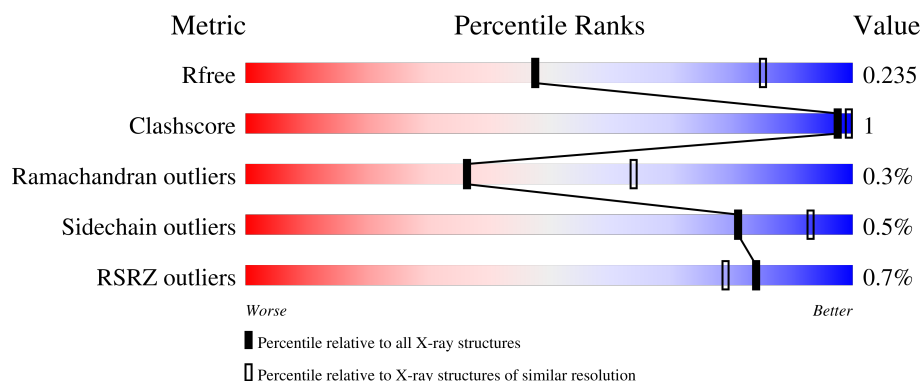
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	1068	 93%
1	C	1068	 91% 6%
2	B	293	 81% 16%
2	D	293	 80% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42029 atoms, of which 20849 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1027	Total	C	H	N	O	S	8467	4	0
			16899	5397	8467	1444	1522	69			
1	C	1008	Total	C	H	N	O	S	8270	0	0
			16530	5284	8270	1411	1497	68			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	ARG	HIS	variant	UNP P42336
C	1047	ARG	HIS	variant	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	245	Total	C	H	N	O	S	2059	2	0
			4155	1311	2059	373	406	6			
2	D	245	Total	C	H	N	O	S	2053	0	0
			4139	1306	2053	371	403	6			

There are 14 discrepancies between the modelled and reference sequences:

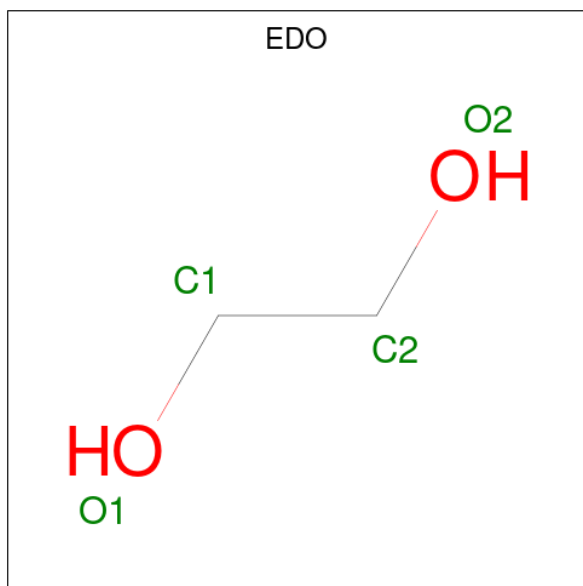
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P27986
B	302	HIS	-	expression tag	UNP P27986
B	303	HIS	-	expression tag	UNP P27986
B	304	HIS	-	expression tag	UNP P27986
B	305	HIS	-	expression tag	UNP P27986
B	306	HIS	-	expression tag	UNP P27986
B	307	HIS	-	expression tag	UNP P27986
D	301	MET	-	initiating methionine	UNP P27986
D	302	HIS	-	expression tag	UNP P27986

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Chain	Residue	Modelled	Actual	Comment	Reference
D	303	HIS	-	expression tag	UNP P27986
D	304	HIS	-	expression tag	UNP P27986
D	305	HIS	-	expression tag	UNP P27986
D	306	HIS	-	expression tag	UNP P27986
D	307	HIS	-	expression tag	UNP P27986

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



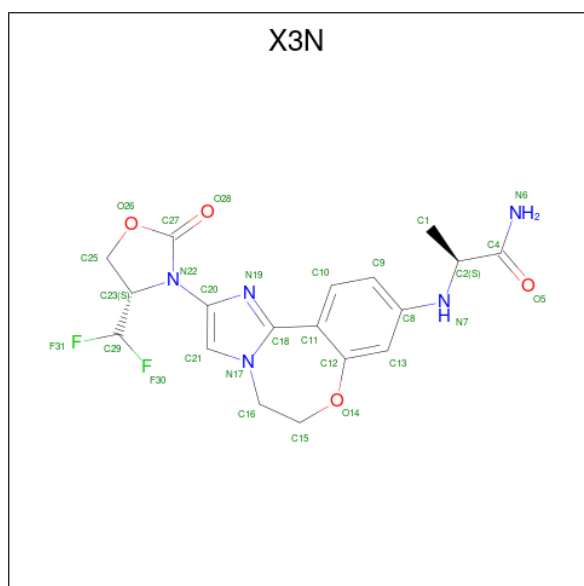
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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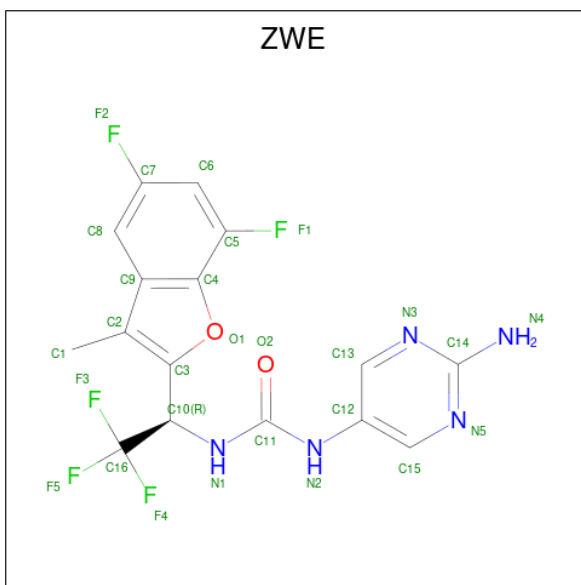
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is N 2 -{(4S,11aP)-2-[(4S)-4-(difluoromethyl)-2-oxo-1,3-oxazolidin-3-yl]-5,6-dihydroimidazo[1,2-d][1,4]benzoxazepin-9-yl}-L-alaninamide (CCD ID: X3N) (formula: C₁₈H₁₉F₂N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			29	18	2	5	4		
4	C	1	Total	C	F	N	O	0	0
			29	18	2	5	4		

- Molecule 5 is N-(2-aminopyrimidin-5-yl)-N'-[(1R)-1-(5,7-difluoro-3-methyl-1-benzofuran-2-yl)-2,2,2-trifluoroethyl]urea (CCD ID: ZWE) (formula: C₁₆H₁₂F₅N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			28	16	5	5	2		
5	C	1	Total	C	F	N	O	0	0
			28	16	5	5	2		

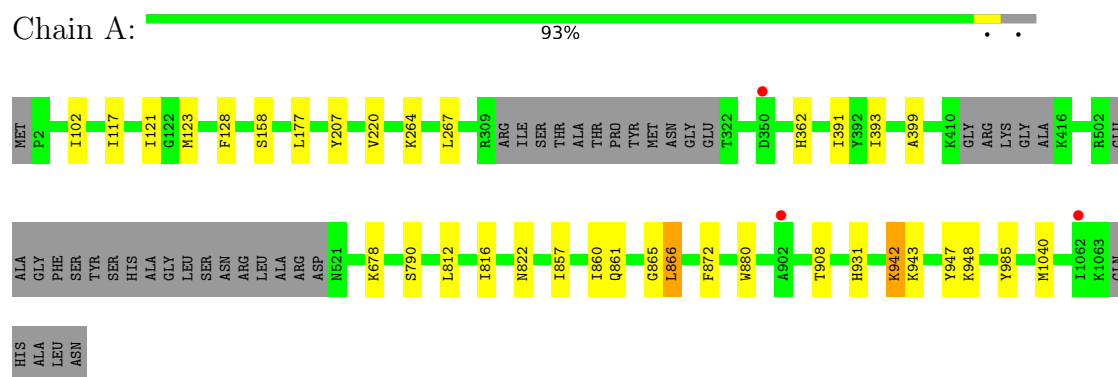
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	104	Total	O	0	0
			104	104		
6	B	5	Total	O	0	0
			5	5		
6	C	31	Total	O	0	0
			31	31		

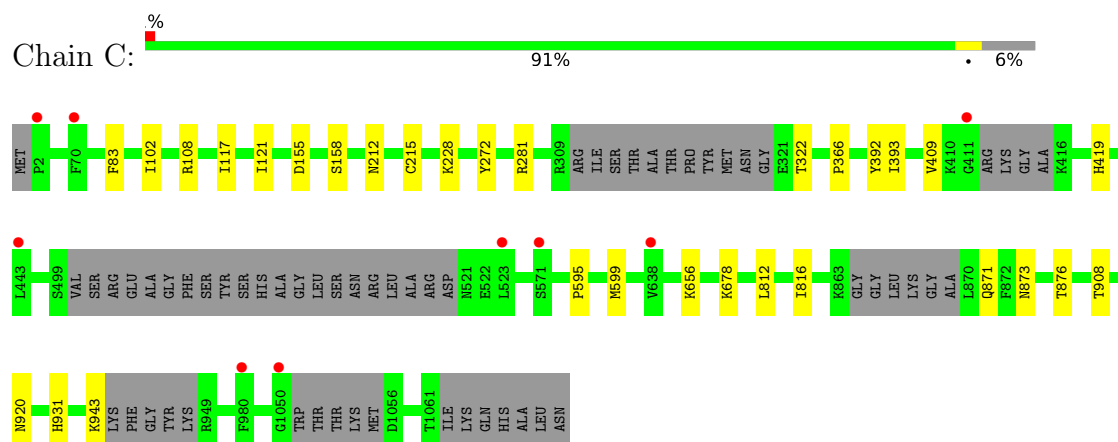
3 Residue-property plots [i](#)

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

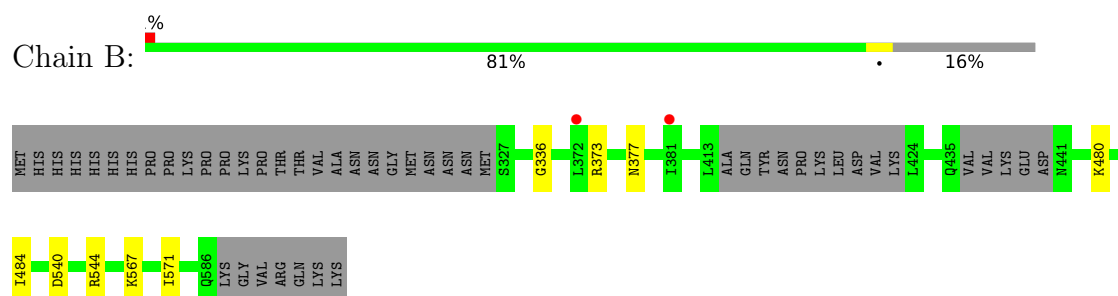
- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



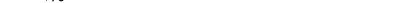
- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

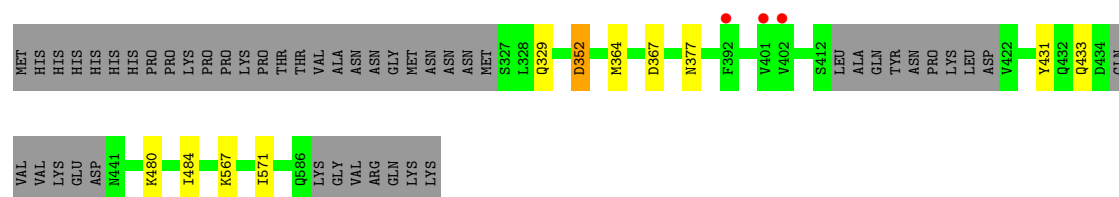


- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain D:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.15Å 124.50Å 165.42Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	34.42 – 2.93 34.42 – 2.93	Depositor EDS
% Data completeness (in resolution range)	74.5 (34.42-2.93) 74.3 (34.42-2.93)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.11.8, BUSTER 2.11.8	Depositor
R, R_{free}	0.217 , 0.252 (Not available) , 0.235	Depositor DCC
R_{free} test set	2840 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42029	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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: EDO, X3N, ZWE

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	0.76	1/8637 (0.0%)	0.97	2/11669 (0.0%)
1	C	0.74	2/8444 (0.0%)	0.95	3/11409 (0.0%)
2	B	0.75	0/2139	0.98	0/2862
2	D	0.75	0/2120	1.00	0/2836
All	All	0.75	3/21340 (0.0%)	0.97	5/28776 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ILE	CA-CB	6.83	1.57	1.54
1	C	393	ILE	CA-C	6.39	1.58	1.52
1	C	393	ILE	CA-CB	6.17	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	PHE	CA-CB-CG	6.45	120.25	113.80
1	C	920	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	822	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	392	TYR	CA-C-N	5.05	123.42	120.24
1	C	392	TYR	C-N-CA	5.05	123.42	120.24

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	8432	8467	8449	15	0
1	C	8260	8270	8270	12	0
2	B	2096	2059	2052	4	0
2	D	2086	2053	2053	5	0
3	A	40	0	60	1	0
3	C	12	0	18	1	0
4	A	29	0	0	0	0
4	C	29	0	0	0	0
5	A	28	0	0	0	0
5	C	28	0	0	0	0
6	A	104	0	0	0	0
6	B	5	0	0	0	0
6	C	31	0	0	0	0
All	All	21180	20849	20902	35	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 1.

All (35) 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:117:ILE:O	1:A:121:ILE:HG12	1.97	0.65
1:C:117:ILE:O	1:C:121:ILE:HG12	1.96	0.64
2:D:364:MET:HE3	2:D:367:ASP:OD2	1.98	0.63
1:A:207:TYR:HA	3:A:1505:EDO:H22	1.82	0.61
1:C:409:VAL:HG12	1:C:419:HIS:CE1	2.41	0.55
1:C:83:PHE:HD1	1:C:108:ARG:NH2	2.10	0.49
1:A:123:MET:SD	1:A:128:PHE:CZ	3.06	0.49
1:C:155:ASP:HA	1:C:158:SER:OG	2.14	0.47
1:A:362:HIS:CE1	1:A:399:ALA:HB3	2.49	0.47
1:A:865:GLY:O	1:A:866:LEU:HB2	2.14	0.46
1:C:595:PRO:O	1:C:599:MET:HG3	2.15	0.46
1:A:942:LYS:O	1:A:943:LYS:HG2	2.16	0.46
2:B:540:ASP:O	2:B:544:ARG:HB2	2.16	0.46
1:A:908:THR:HG21	1:A:931:HIS:CE1	2.52	0.44
2:B:567:LYS:O	2:B:571:ILE:HG12	2.17	0.44
1:C:212:ASN:HB2	1:C:215:CYS:SG	2.57	0.44
1:C:812:LEU:O	1:C:816:ILE:HG12	2.17	0.44
1:C:366:PRO:HD2	2:D:377:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:TYR:O	1:A:948:LYS:HG2	2.18	0.43
1:A:812:LEU:O	1:A:816:ILE:HG12	2.17	0.43
1:A:220:VAL:HG21	1:A:267:LEU:HD13	2.00	0.43
2:D:567:LYS:O	2:D:571:ILE:HG12	2.18	0.43
1:A:857:ILE:O	1:A:861:GLN:HG2	2.19	0.43
1:A:985:TYR:CE1	1:A:1040:MET:HG2	2.54	0.43
1:A:865:GLY:O	1:A:866:LEU:CB	2.66	0.42
1:C:873:ASN:OD1	1:C:876:THR:OG1	2.34	0.42
2:B:373:ARG:O	2:B:377:ASN:O	2.37	0.42
1:A:860:ILE:HD12	1:A:880:TRP:CE2	2.55	0.41
1:C:272:TYR:OH	1:C:281:ARG:NH2	2.50	0.41
2:D:329:GLN:O	2:D:431:TYR:OH	2.36	0.41
1:C:656:LYS:NZ	3:C:1503:EDO:H21	2.36	0.41
1:A:860:ILE:HD12	1:A:880:TRP:CD2	2.57	0.40
2:B:480:LYS:O	2:B:484:ILE:HG12	2.21	0.40
1:C:908:THR:HG21	1:C:931:HIS:CE1	2.56	0.40
2:D:480:LYS:O	2:D:484:ILE:HG12	2.21	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	1023/1068 (96%)	980 (96%)	40 (4%)	3 (0%)	36	64
1	C	994/1068 (93%)	950 (96%)	42 (4%)	2 (0%)	43	71
2	B	241/293 (82%)	224 (93%)	16 (7%)	1 (0%)	30	58
2	D	239/293 (82%)	224 (94%)	14 (6%)	1 (0%)	30	58
All	All	2497/2722 (92%)	2378 (95%)	112 (4%)	7 (0%)	36	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	866	LEU
2	B	336	GLY
1	A	942	LYS
2	D	352	ASP
1	C	871	GLN
1	A	264	LYS
1	C	322	THR

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	948/974 (97%)	942 (99%)	6 (1%)	78	92
1	C	929/974 (95%)	925 (100%)	4 (0%)	84	94
2	B	230/272 (85%)	230 (100%)	0	100	100
2	D	228/272 (84%)	226 (99%)	2 (1%)	70	88
All	All	2335/2492 (94%)	2323 (100%)	12 (0%)	81	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ILE
1	A	158	SER
1	A	177	LEU
1	A	391	ILE
1	A	678	LYS
1	A	790	SER
1	C	102	ILE
1	C	228	LYS
1	C	678	LYS
1	C	943	LYS
2	D	352	ASP
2	D	433	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	160	HIS
1	A	205	GLN
1	A	219	GLN
1	A	362	HIS
1	A	756	ASN
1	A	785	ASN
2	B	435	GLN
2	B	457	GLN
2	B	552	GLN
1	C	107	ASN
1	C	160	HIS
1	C	219	GLN
1	C	467	ASN
1	C	756	ASN
1	C	785	ASN
1	C	879	GLN
2	D	457	GLN
2	D	552	GLN

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](#)

17 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	EDO	A	1502	-	3,3,3	0.23	0	2,2,2	0.33	0
3	EDO	C	1501	-	3,3,3	0.26	0	2,2,2	0.27	0
5	ZWE	A	1512	-	29,30,30	1.84	4 (13%)	36,45,45	1.21	4 (11%)
5	ZWE	C	1505	-	29,30,30	1.86	5 (17%)	36,45,45	1.19	3 (8%)
3	EDO	A	1509	-	3,3,3	0.39	0	2,2,2	0.05	0
3	EDO	C	1503	-	3,3,3	0.28	0	2,2,2	0.23	0
3	EDO	A	1508	-	3,3,3	0.31	0	2,2,2	0.14	0
3	EDO	A	1503	-	3,3,3	0.26	0	2,2,2	0.20	0
3	EDO	C	1502	-	3,3,3	0.28	0	2,2,2	0.28	0
3	EDO	A	1506	-	3,3,3	0.38	0	2,2,2	0.09	0
3	EDO	A	1510	-	3,3,3	0.36	0	2,2,2	0.09	0
4	X3N	A	1511	-	30,32,32	1.44	5 (16%)	36,47,47	1.38	4 (11%)
3	EDO	A	1507	-	3,3,3	0.34	0	2,2,2	0.12	0
3	EDO	A	1501	-	3,3,3	0.36	0	2,2,2	0.18	0
3	EDO	A	1504	-	3,3,3	0.34	0	2,2,2	0.19	0
3	EDO	A	1505	-	3,3,3	0.33	0	2,2,2	0.02	0
4	X3N	C	1504	-	30,32,32	1.41	3 (10%)	36,47,47	1.38	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1502	-	-	1/1/1/1	-
3	EDO	C	1501	-	-	0/1/1/1	-
5	ZWE	A	1512	-	-	2/15/18/18	0/3/3/3
5	ZWE	C	1505	-	-	2/15/18/18	0/3/3/3
3	EDO	A	1509	-	-	0/1/1/1	-
3	EDO	C	1503	-	-	1/1/1/1	-
3	EDO	A	1508	-	-	0/1/1/1	-
3	EDO	A	1503	-	-	1/1/1/1	-
3	EDO	C	1502	-	-	1/1/1/1	-
3	EDO	A	1506	-	-	0/1/1/1	-
3	EDO	A	1510	-	-	0/1/1/1	-
4	X3N	A	1511	-	-	4/13/39/39	0/4/4/4
3	EDO	A	1507	-	-	1/1/1/1	-
3	EDO	A	1501	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1504	-	-	0/1/1/1	-
3	EDO	A	1505	-	-	1/1/1/1	-
4	X3N	C	1504	-	-	4/13/39/39	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1505	ZWE	C16-C10	7.33	1.59	1.51
5	A	1512	ZWE	C16-C10	6.85	1.58	1.51
5	A	1512	ZWE	C14-N3	4.19	1.41	1.35
5	C	1505	ZWE	C14-N3	3.42	1.40	1.35
4	C	1504	X3N	C20-N19	2.77	1.39	1.35
4	A	1511	X3N	C18-N19	2.58	1.37	1.33
4	A	1511	X3N	C27-N22	2.57	1.43	1.39
4	A	1511	X3N	C20-N19	2.37	1.39	1.35
5	A	1512	ZWE	C14-N5	2.34	1.38	1.35
4	C	1504	X3N	C27-N22	2.31	1.43	1.39
5	C	1505	ZWE	C14-N5	2.30	1.38	1.35
4	C	1504	X3N	C18-N17	2.24	1.38	1.36
4	A	1511	X3N	O26-C27	2.21	1.37	1.35
5	C	1505	ZWE	C1-C2	-2.15	1.47	1.50
5	C	1505	ZWE	C11-N1	2.02	1.41	1.35
4	A	1511	X3N	C18-N17	2.00	1.38	1.36
5	A	1512	ZWE	C14-N4	2.00	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1511	X3N	C21-C20-N19	-3.75	110.31	112.77
4	C	1504	X3N	C21-C20-N19	-3.60	110.41	112.77
4	C	1504	X3N	F30-C29-C23	3.49	113.41	109.29
5	C	1505	ZWE	C6-C5-C4	-3.48	118.35	123.24
5	A	1512	ZWE	C6-C5-C4	-3.35	118.54	123.24
4	A	1511	X3N	F30-C29-C23	3.30	113.18	109.29
5	C	1505	ZWE	C12-N2-C11	-2.97	120.56	126.61
5	A	1512	ZWE	C12-N2-C11	-2.85	120.79	126.61
5	C	1505	ZWE	F1-C5-C4	2.67	121.17	117.62
5	A	1512	ZWE	F1-C5-C4	2.55	121.01	117.62
4	C	1504	X3N	O28-C27-N22	2.50	131.42	128.62
4	A	1511	X3N	O28-C27-N22	2.47	131.38	128.62
5	A	1512	ZWE	C12-C13-N3	-2.29	122.17	124.07
4	C	1504	X3N	O26-C27-O28	-2.10	120.03	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1511	X3N	O26-C27-O28	-2.05	120.08	122.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1511	X3N	N22-C23-C29-F30
4	A	1511	X3N	N22-C23-C29-F31
4	A	1511	X3N	C25-C23-C29-F31
4	C	1504	X3N	N22-C23-C29-F30
4	C	1504	X3N	N22-C23-C29-F31
4	C	1504	X3N	C25-C23-C29-F31
5	A	1512	ZWE	C13-C12-N2-C11
5	A	1512	ZWE	C15-C12-N2-C11
5	C	1505	ZWE	C13-C12-N2-C11
5	C	1505	ZWE	C15-C12-N2-C11
3	A	1507	EDO	O1-C1-C2-O2
3	C	1502	EDO	O1-C1-C2-O2
3	C	1503	EDO	O1-C1-C2-O2
3	A	1502	EDO	O1-C1-C2-O2
4	A	1511	X3N	N19-C20-N22-C23
4	C	1504	X3N	N19-C20-N22-C23
3	A	1505	EDO	O1-C1-C2-O2
3	A	1503	EDO	O1-C1-C2-O2

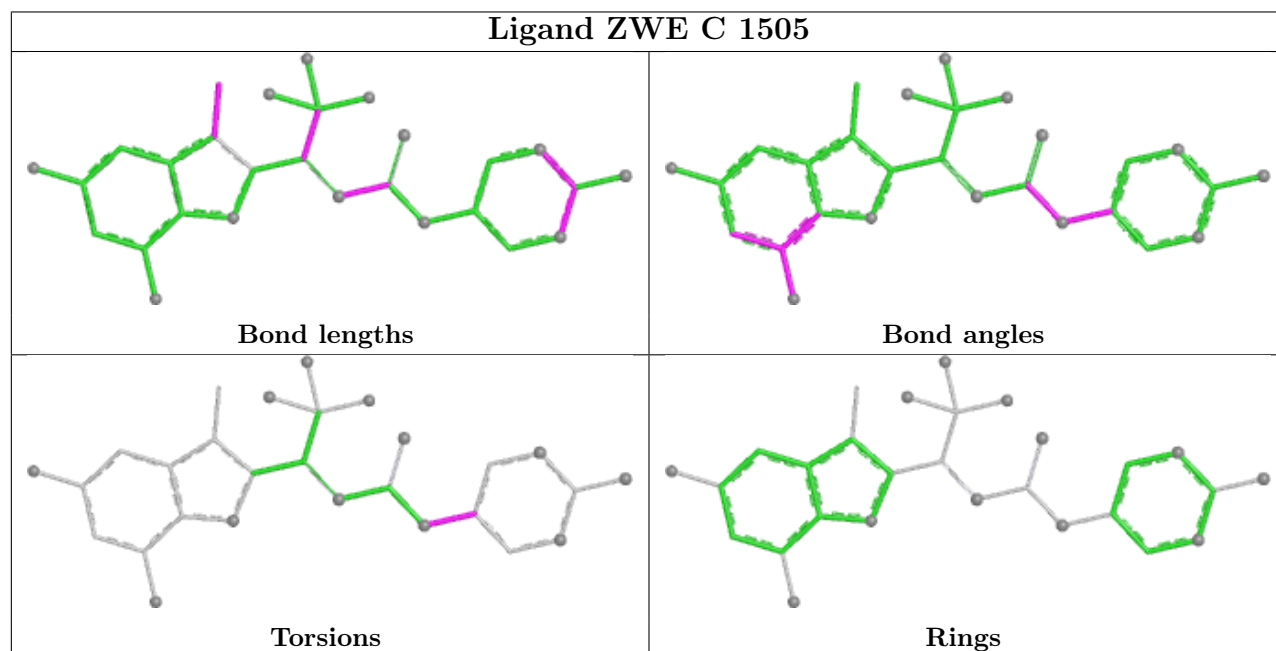
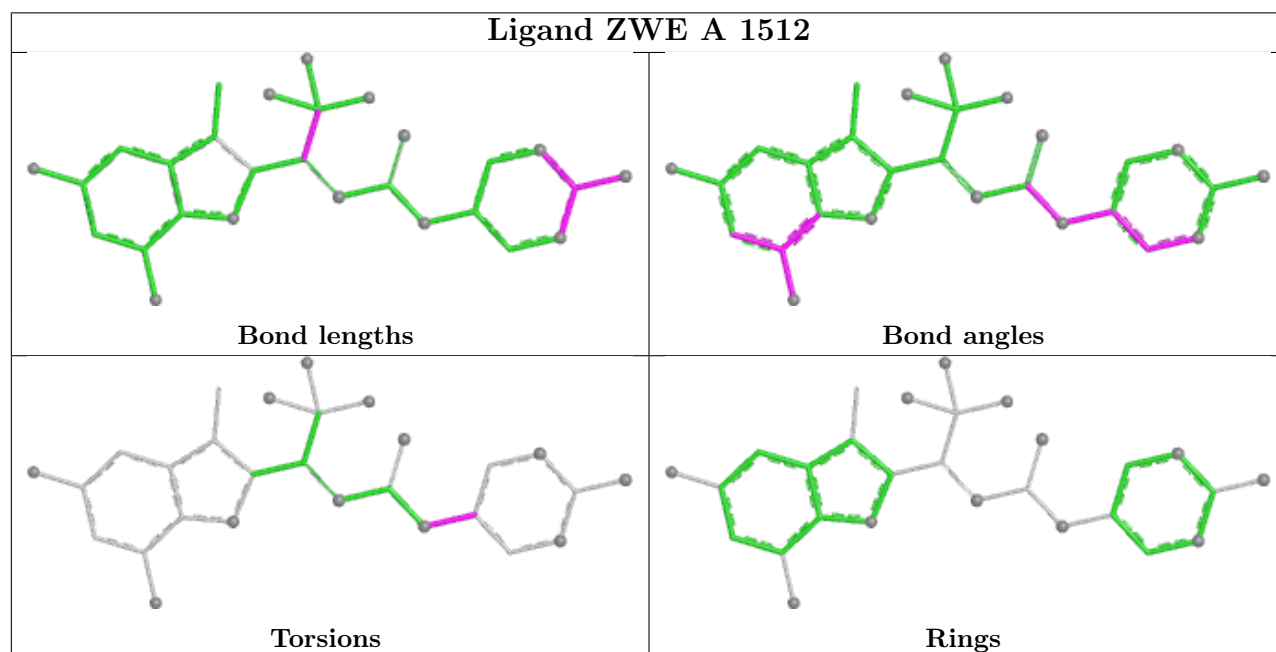
There are no ring outliers.

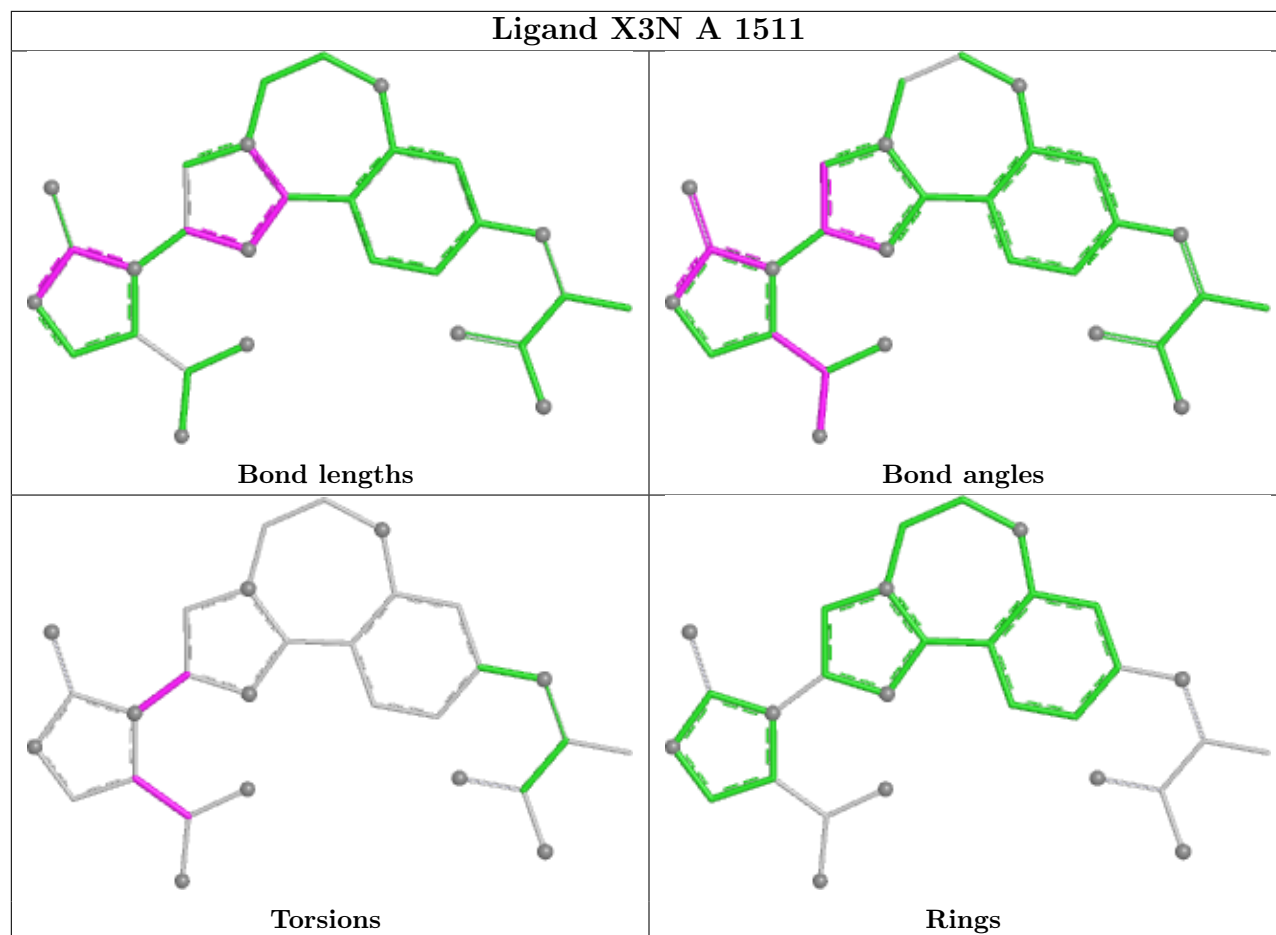
2 monomers are involved in 2 short contacts:

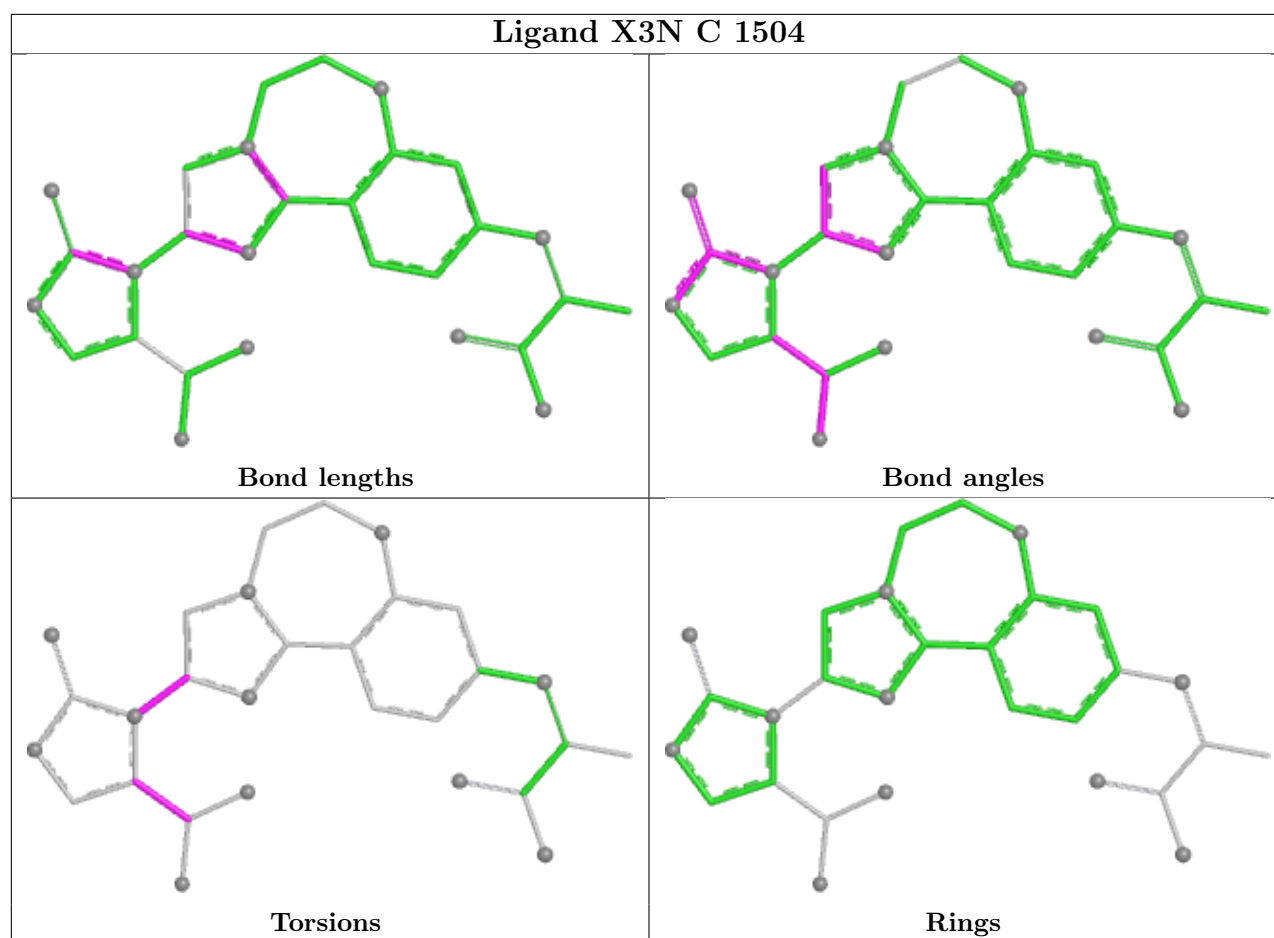
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1503	EDO	1	0
3	A	1505	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1027/1068 (96%)	-0.20	3 (0%) 90 87	14, 46, 73, 109	2 (0%)
1	C	1008/1068 (94%)	0.00	9 (0%) 81 74	36, 67, 108, 159	0
2	B	245/293 (83%)	0.01	2 (0%) 82 76	29, 75, 119, 143	1 (0%)
2	D	245/293 (83%)	0.14	3 (1%) 76 69	59, 108, 152, 168	0
All	All	2525/2722 (92%)	-0.07	17 (0%) 84 79	14, 60, 118, 168	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	381	ILE	4.1
1	C	980	PHE	3.3
1	C	411	GLY	3.1
2	D	392	PHE	2.7
1	C	571	SER	2.7
1	C	1050	GLY	2.7
1	A	350	ASP	2.5
1	C	2	PRO	2.5
2	D	402	VAL	2.5
2	B	372	LEU	2.4
1	C	523	LEU	2.3
1	C	443	LEU	2.3
1	A	902	ALA	2.2
1	C	70	PHE	2.2
2	D	401	VAL	2.1
1	A	1062	ILE	2.1
1	C	638	VAL	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

There are no oligosaccharides in this entry.

6.4 Ligands

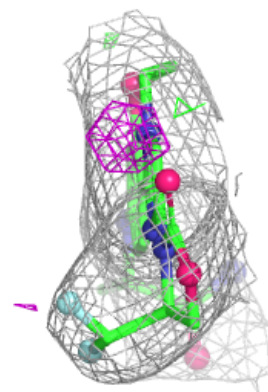
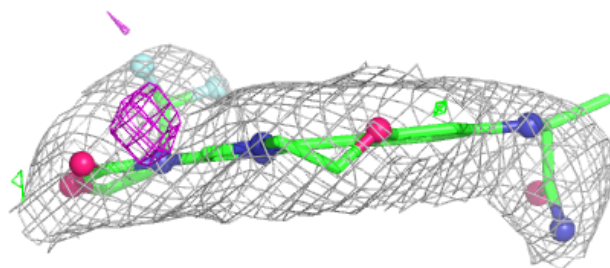
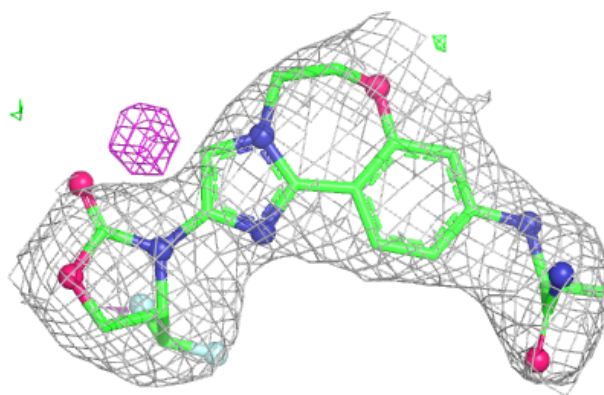
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	1503	4/4	0.39	0.24	133,133,133,133	0
3	EDO	A	1505	4/4	0.66	0.15	107,107,107,107	0
3	EDO	C	1501	4/4	0.77	0.07	120,120,120,120	0
3	EDO	A	1508	4/4	0.77	0.13	100,100,101,101	0
3	EDO	C	1502	4/4	0.79	0.09	98,98,98,98	0
3	EDO	A	1502	4/4	0.80	0.13	94,94,94,94	0
3	EDO	A	1509	4/4	0.84	0.15	101,101,101,101	0
3	EDO	A	1501	4/4	0.84	0.09	97,98,98,98	0
3	EDO	A	1507	4/4	0.87	0.22	94,94,95,95	0
3	EDO	A	1504	4/4	0.87	0.10	99,99,100,100	0
3	EDO	A	1510	4/4	0.89	0.09	104,104,104,104	0
3	EDO	A	1506	4/4	0.92	0.19	97,97,97,97	0
4	X3N	C	1504	29/29	0.92	0.10	109,110,111,111	0
3	EDO	A	1503	4/4	0.93	0.13	93,93,93,93	0
5	ZWE	C	1505	28/28	0.94	0.07	108,111,113,114	0
5	ZWE	A	1512	28/28	0.96	0.07	69,73,77,77	0
4	X3N	A	1511	29/29	0.96	0.07	60,61,66,66	0

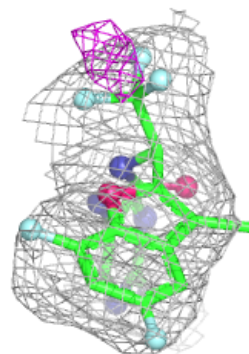
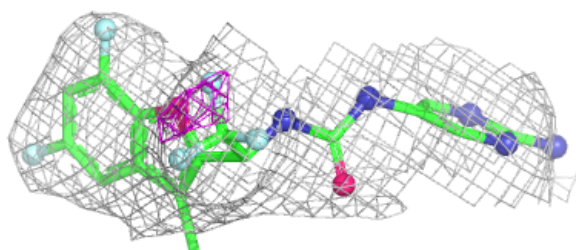
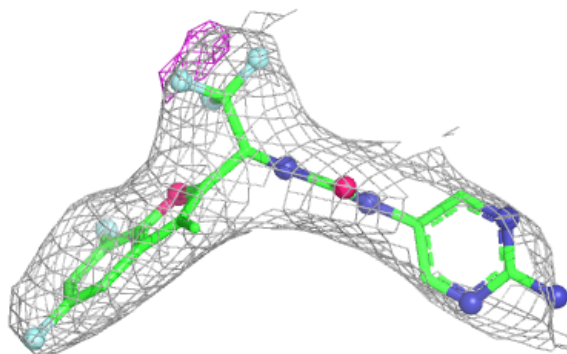
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X3N C 1504:

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

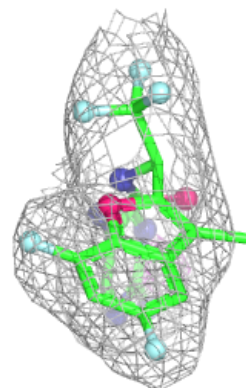
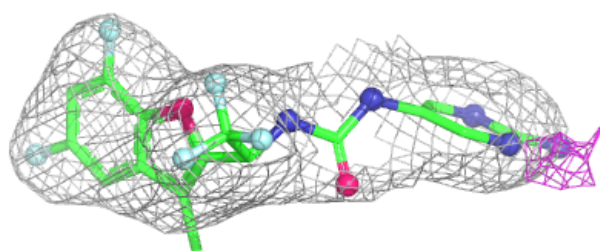
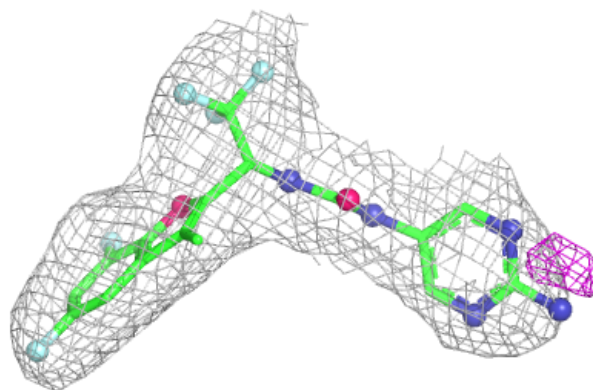
**Electron density around ZWE C 1505:**

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

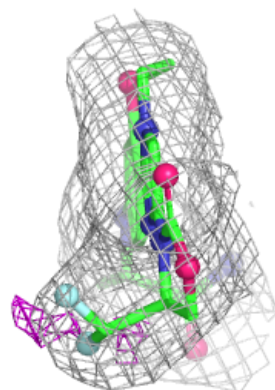
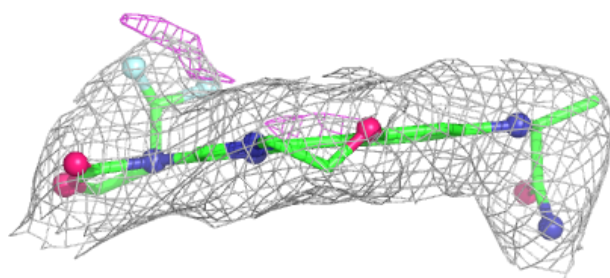
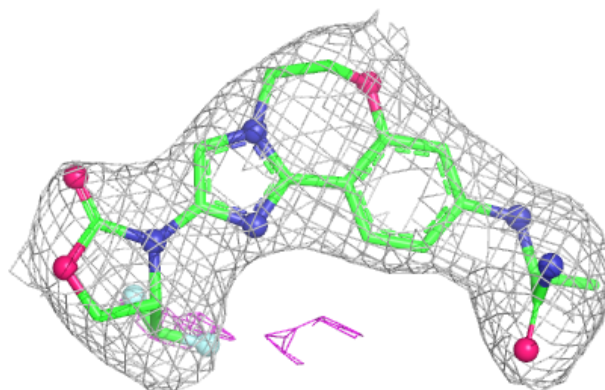


Electron density around ZWE A 1512:

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

**Electron density around X3N A 1511:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.