



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:45 AM UTC

PDB ID : 8F9B / pdb_00008f9b
Title : Compound 19 bound to procaspase-6
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Deposited on : 2022-11-23
Resolution : 2.65 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

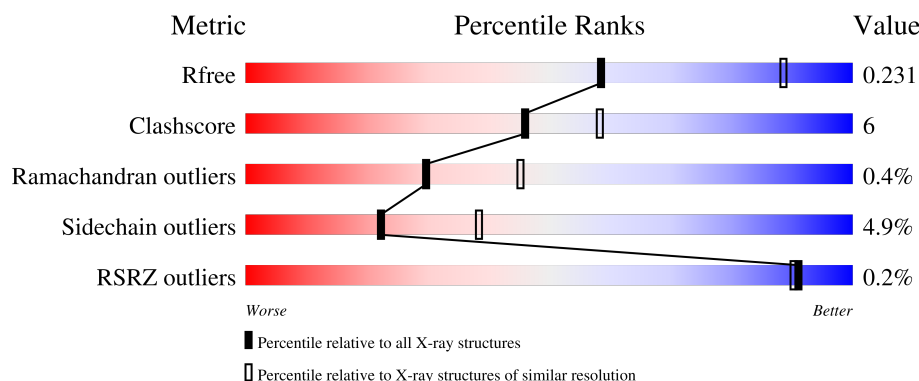
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	299	68% 13% 18%
1	B	299	68% 13% 18%
1	C	299	70% 13% 16%
1	D	299	70% 13% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8291 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 Procaspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	1	0
			1972	1258	342	357	15			
1	B	245	Total	C	N	O	S	0	0	0
			1967	1254	342	357	14			
1	C	251	Total	C	N	O	S	0	1	0
			2029	1296	350	368	15			
1	D	251	Total	C	N	O	S	0	1	0
			2029	1296	350	368	15			

There are 28 discrepancies between the modelled and reference sequences:

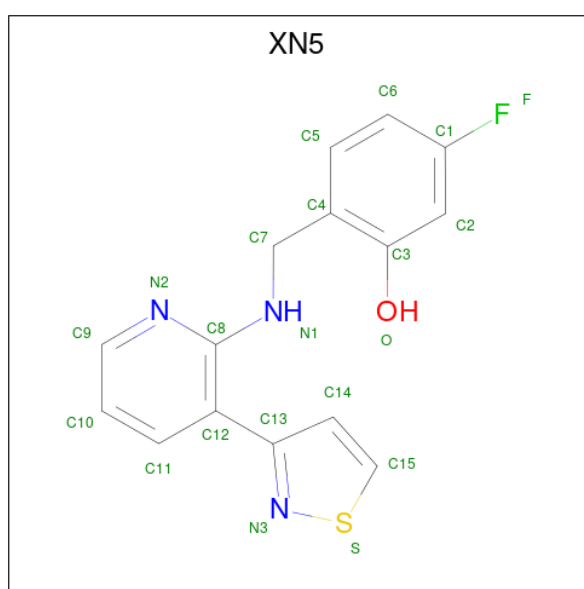
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ALA	CYS	conflict	UNP P55212
A	294	GLU	-	expression tag	UNP P55212
A	295	ASN	-	expression tag	UNP P55212
A	296	LEU	-	expression tag	UNP P55212
A	297	TYR	-	expression tag	UNP P55212
A	298	PHE	-	expression tag	UNP P55212
A	299	GLN	-	expression tag	UNP P55212
B	163	ALA	CYS	conflict	UNP P55212
B	294	GLU	-	expression tag	UNP P55212
B	295	ASN	-	expression tag	UNP P55212
B	296	LEU	-	expression tag	UNP P55212
B	297	TYR	-	expression tag	UNP P55212
B	298	PHE	-	expression tag	UNP P55212
B	299	GLN	-	expression tag	UNP P55212
C	163	ALA	CYS	conflict	UNP P55212
C	294	GLU	-	expression tag	UNP P55212
C	295	ASN	-	expression tag	UNP P55212
C	296	LEU	-	expression tag	UNP P55212
C	297	TYR	-	expression tag	UNP P55212
C	298	PHE	-	expression tag	UNP P55212
C	299	GLN	-	expression tag	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	163	ALA	CYS	conflict	UNP P55212
D	294	GLU	-	expression tag	UNP P55212
D	295	ASN	-	expression tag	UNP P55212
D	296	LEU	-	expression tag	UNP P55212
D	297	TYR	-	expression tag	UNP P55212
D	298	PHE	-	expression tag	UNP P55212
D	299	GLN	-	expression tag	UNP P55212

- Molecule 2 is 5-fluoro-2-({[(3M)-3-(1,2-thiazol-3-yl)pyridin-2-yl]amino}methyl)phenol (CCD ID: XN5) (formula: C₁₅H₁₂FN₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			42	30	2	6	2		
2	C	1	Total	C	F	N	O	0	1
			42	30	2	6	2		

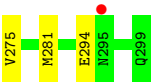
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	51	Total	O	0	0
			51	51		
3	C	52	Total	O	0	0
			52	52		

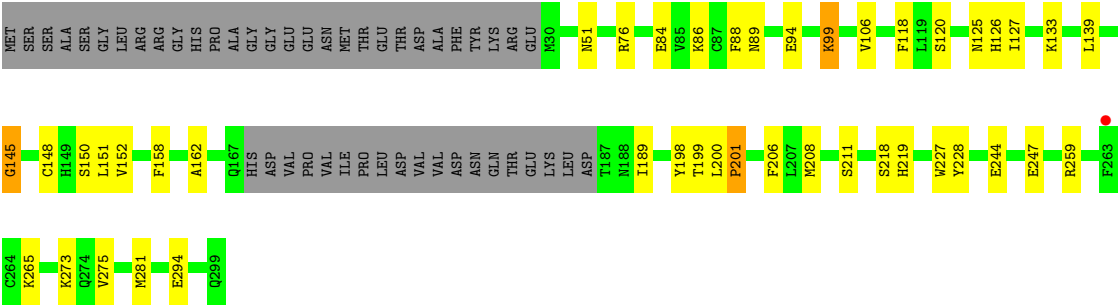
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	55	Total	O	0	0
			55	55		



● Molecule 1: Procaspase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	101.94Å 101.94Å 321.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.08 – 2.65 52.08 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.08-2.65) 99.9 (52.08-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.193 , 0.230 0.198 , 0.231	Depositor DCC
R_{free} test set	2643 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8291	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XN5

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	1.02	0/2020	1.36	7/2719 (0.3%)
1	B	1.03	0/2012	1.37	6/2709 (0.2%)
1	C	1.02	0/2079	1.33	0/2799
1	D	1.02	0/2079	1.32	0/2799
All	All	1.02	0/8190	1.35	13/11026 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	CG-CD-NE	-6.92	96.79	112.00
1	A	131	ASP	N-CA-CB	-6.49	100.49	110.42
1	B	131	ASP	N-CA-CB	-6.46	100.54	110.42
1	A	102	GLU	CB-CA-C	5.82	120.12	110.81
1	B	30	MET	CA-C-N	5.77	129.04	120.90
1	B	30	MET	C-N-CA	5.77	129.04	120.90
1	B	130	TYR	CA-C-N	5.77	133.61	122.53
1	B	130	TYR	C-N-CA	5.77	133.61	122.53
1	A	30	MET	CA-C-N	5.54	128.71	120.90
1	A	30	MET	C-N-CA	5.54	128.71	120.90
1	A	130	TYR	CA-C-N	5.53	133.15	122.53
1	A	130	TYR	C-N-CA	5.53	133.15	122.53
1	B	201	PRO	N-CA-CB	-5.31	97.68	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1972	0	1945	21	0
1	B	1967	0	1936	19	0
1	C	2029	0	1994	30	0
1	D	2029	0	1994	32	0
2	A	42	0	0	2	0
2	C	42	0	0	3	0
3	A	52	0	0	3	0
3	B	51	0	0	2	0
3	C	52	0	0	1	0
3	D	55	0	0	3	0
All	All	8291	0	7869	93	0

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

All (93) 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:281[B]:MET:HE2	1:B:275:VAL:CG1	2.18	0.73
1:C:51:ASN:HD22	1:C:89:ASN:HD22	1.36	0.73
1:D:51:ASN:HD22	1:D:89:ASN:HD22	1.36	0.73
1:A:281[B]:MET:HE2	1:B:275:VAL:HG11	1.73	0.71
1:B:51:ASN:HD22	1:B:89:ASN:HD22	1.40	0.70
1:A:51:ASN:HD22	1:A:89:ASN:HD22	1.40	0.69
1:C:201:PRO:HB2	1:C:281[A]:MET:SD	2.33	0.69
1:D:201:PRO:HB2	1:D:281[A]:MET:SD	2.34	0.67
1:A:149:HIS:HB2	3:A:448:HOH:O	1.95	0.66
1:A:203:GLY:N	1:A:281[B]:MET:SD	2.70	0.63
1:A:43:ARG:NH1	3:A:402:HOH:O	2.32	0.63
1:C:51:ASN:HD22	1:C:89:ASN:ND2	2.00	0.60
1:D:51:ASN:HD22	1:D:89:ASN:ND2	2.00	0.58
1:C:200:LEU:CD1	2:C:301[B]:XN5:C10	2.82	0.57
1:D:206:PHE:O	1:D:281[A]:MET:HE2	2.05	0.57
1:A:51:ASN:HD22	1:A:89:ASN:ND2	2.02	0.56
1:C:206:PHE:O	1:C:281[A]:MET:HE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281[B]:MET:HE2	1:D:275:VAL:HG11	1.88	0.55
1:B:51:ASN:HD22	1:B:89:ASN:ND2	2.02	0.55
1:B:76:ARG:HD3	1:B:80:ASP:OD2	2.07	0.55
1:D:118:PHE:CZ	1:D:139:LEU:HD13	2.42	0.55
1:D:76:ARG:NE	3:D:302:HOH:O	2.41	0.54
1:C:201:PRO:CB	1:C:281[A]:MET:SD	2.95	0.54
1:B:206:PHE:O	1:B:281:MET:HE2	2.08	0.54
1:C:221:GLU:OE2	1:C:224:ASN:HB2	2.09	0.53
1:C:281[B]:MET:HE2	1:D:275:VAL:CG1	2.38	0.53
1:D:198:TYR:HB3	1:D:200:LEU:CD1	2.39	0.52
1:D:201:PRO:CB	1:D:281[A]:MET:SD	2.96	0.52
1:C:200:LEU:HD12	2:C:301[A]:XN5:C9	2.40	0.52
1:C:118:PHE:CZ	1:C:139:LEU:HD13	2.45	0.52
1:C:200:LEU:HD12	2:C:301[B]:XN5:C10	2.40	0.51
1:C:275:VAL:HG11	1:D:281[B]:MET:HE2	1.93	0.50
1:A:206:PHE:O	1:A:281[A]:MET:HE2	2.10	0.50
1:D:198:TYR:HB2	1:D:200:LEU:HD13	1.93	0.49
1:C:201:PRO:HD3	1:D:199:THR:OG1	2.12	0.49
1:A:123:GLU:OE2	3:A:401:HOH:O	2.20	0.49
1:D:145:GLY:HA2	1:D:152:VAL:HG22	1.95	0.48
1:C:198:TYR:HB3	1:C:200:LEU:CD1	2.43	0.48
1:C:198:TYR:HB2	1:C:200:LEU:HD13	1.96	0.48
1:D:198:TYR:CB	1:D:200:LEU:HD13	2.44	0.47
1:A:211:SER:HA	1:A:228:TYR:CG	2.49	0.47
1:B:211:SER:HA	1:B:228:TYR:CG	2.49	0.47
1:C:275:VAL:CG1	1:D:281[B]:MET:HE2	2.44	0.47
1:A:118:PHE:CZ	1:A:139:LEU:HD13	2.50	0.47
1:B:118:PHE:CZ	1:B:139:LEU:HD13	2.50	0.46
1:D:211:SER:HA	1:D:228:TYR:CG	2.50	0.46
1:C:199:THR:OG1	1:D:201:PRO:HD3	2.14	0.46
1:C:211:SER:HA	1:C:228:TYR:CG	2.50	0.46
1:C:145:GLY:HA2	1:C:152:VAL:HG22	1.99	0.45
1:C:281[B]:MET:CE	1:D:275:VAL:CG1	2.95	0.45
1:D:273:LYS:HD2	3:D:353:HOH:O	2.16	0.44
1:D:198:TYR:CB	1:D:200:LEU:CD1	2.95	0.44
1:C:198:TYR:CB	1:C:200:LEU:CD1	2.94	0.44
1:B:123:GLU:OE2	3:B:301:HOH:O	2.20	0.44
1:C:126:HIS:HB3	1:C:133:LYS:HB2	2.00	0.43
1:D:158:PHE:HB2	1:D:208:MET:SD	2.59	0.43
1:B:88:PHE:CZ	1:B:99:LYS:HG2	2.53	0.43
1:D:88:PHE:CZ	1:D:99:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:HA2	1:B:152:VAL:HG22	2.00	0.43
1:B:71:ARG:HE	1:B:89:ASN:HD21	1.66	0.42
1:A:71:ARG:HE	1:A:89:ASN:HD21	1.66	0.42
1:B:43:ARG:NH2	3:B:306:HOH:O	2.49	0.42
1:A:126:HIS:HB3	1:A:133:LYS:HB2	2.01	0.42
1:D:84:GLU:HB2	3:D:317:HOH:O	2.19	0.42
1:D:227:TRP:CD2	1:D:259:ARG:HD3	2.55	0.42
1:A:227:TRP:CD2	1:A:259:ARG:HD3	2.55	0.42
1:C:164:ARG:HA	3:C:431:HOH:O	2.19	0.42
1:A:244:GLU:O	1:A:247:GLU:HB2	2.20	0.42
1:B:227:TRP:CD2	1:B:259:ARG:HD3	2.55	0.42
1:A:56:PHE:CE1	1:D:94:GLU:HG2	2.55	0.42
1:A:88:PHE:CZ	1:A:99:LYS:HG2	2.54	0.42
1:B:74:LEU:HD13	1:B:117:VAL:HG11	2.02	0.42
1:B:126:HIS:HB3	1:B:133:LYS:HB2	2.02	0.42
1:A:76:ARG:HD2	1:A:80:ASP:OD2	2.20	0.41
1:B:167:GLN:O	1:B:167:GLN:CG	2.67	0.41
1:C:227:TRP:CD2	1:C:259:ARG:HD3	2.54	0.41
2:A:301[B]:XN5:N1	2:A:301[B]:XN5:N3	2.68	0.41
1:B:244:GLU:O	1:B:247:GLU:HB2	2.20	0.41
1:D:126:HIS:HB3	1:D:133:LYS:HB2	2.01	0.41
2:A:301[A]:XN5:N1	2:A:301[A]:XN5:N3	2.68	0.41
1:C:158:PHE:HB2	1:C:208:MET:SD	2.61	0.41
1:C:219:HIS:HB2	1:C:227:TRP:CD2	2.56	0.41
1:D:120:SER:O	1:D:162:ALA:HA	2.20	0.41
1:D:148:CYS:SG	1:D:151:LEU:HD12	2.60	0.41
1:B:219:HIS:HB2	1:B:227:TRP:CD2	2.55	0.41
1:C:244:GLU:O	1:C:247:GLU:HB2	2.21	0.41
1:C:148:CYS:SG	1:C:151:LEU:HD12	2.61	0.40
1:D:244:GLU:O	1:D:247:GLU:HB2	2.21	0.40
1:A:120:SER:O	1:A:162:ALA:HA	2.21	0.40
1:A:131:ASP:OD1	1:D:94:GLU:HG3	2.22	0.40
1:C:120:SER:O	1:C:162:ALA:HA	2.21	0.40
1:A:158:PHE:HB2	1:A:208:MET:SD	2.62	0.40
1:D:219:HIS:HB2	1:D:227:TRP:CD2	2.56	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	242/299 (81%)	228 (94%)	14 (6%)	0	100	100
1	B	241/299 (81%)	228 (95%)	10 (4%)	3 (1%)	10	17
1	C	248/299 (83%)	232 (94%)	16 (6%)	0	100	100
1	D	248/299 (83%)	232 (94%)	15 (6%)	1 (0%)	30	45
All	All	979/1196 (82%)	920 (94%)	55 (6%)	4 (0%)	30	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ALA
1	B	201	PRO
1	B	145	GLY
1	D	145	GLY

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	214/260 (82%)	204 (95%)	10 (5%)	23	40
1	B	213/260 (82%)	203 (95%)	10 (5%)	23	40
1	C	220/260 (85%)	209 (95%)	11 (5%)	22	37
1	D	220/260 (85%)	209 (95%)	11 (5%)	22	37
All	All	867/1040 (83%)	825 (95%)	42 (5%)	22	39

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	79	SER
1	A	86	LYS
1	A	106	VAL
1	A	125	ASN
1	A	127	ILE
1	A	147	LYS
1	A	150	SER
1	A	218	SER
1	A	265	LYS
1	B	76	ARG
1	B	79	SER
1	B	86	LYS
1	B	106	VAL
1	B	127	ILE
1	B	147	LYS
1	B	150	SER
1	B	189	ILE
1	B	218	SER
1	B	265	LYS
1	C	54	ARG
1	C	86	LYS
1	C	106	VAL
1	C	125	ASN
1	C	127	ILE
1	C	150	SER
1	C	189	ILE
1	C	201	PRO
1	C	218	SER
1	C	265	LYS
1	C	294	GLU
1	D	86	LYS
1	D	99	LYS
1	D	106	VAL
1	D	125	ASN
1	D	127	ILE
1	D	150	SER
1	D	189	ILE
1	D	201	PRO
1	D	218	SER
1	D	265	LYS
1	D	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	58	HIS
1	A	89	ASN
1	A	101	HIS
1	A	125	ASN
1	A	161	GLN
1	A	224	ASN
1	A	230	GLN
1	B	41	HIS
1	B	89	ASN
1	B	101	HIS
1	B	161	GLN
1	B	224	ASN
1	B	230	GLN
1	C	41	HIS
1	C	58	HIS
1	C	89	ASN
1	C	101	HIS
1	C	161	GLN
1	C	224	ASN
1	C	230	GLN
1	D	41	HIS
1	D	58	HIS
1	D	89	ASN
1	D	101	HIS
1	D	125	ASN
1	D	161	GLN
1	D	224	ASN
1	D	230	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	XN5	C	301[B]	-	22,23,23	2.19	2 (9%)	27,31,31	2.13	7 (25%)
2	XN5	C	301[A]	-	22,23,23	2.22	4 (18%)	27,31,31	2.33	7 (25%)
2	XN5	A	301[B]	-	22,23,23	2.02	3 (13%)	27,31,31	1.92	8 (29%)
2	XN5	A	301[A]	-	22,23,23	1.99	3 (13%)	27,31,31	2.00	7 (25%)

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	XN5	C	301[B]	-	-	0/9/9/9	0/3/3/3
2	XN5	C	301[A]	-	-	3/9/9/9	0/3/3/3
2	XN5	A	301[B]	-	-	0/9/9/9	0/3/3/3
2	XN5	A	301[A]	-	-	1/9/9/9	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	XN5	C8-N1	6.60	1.44	1.34
2	C	301[B]	XN5	C15-S	6.54	1.76	1.68
2	C	301[B]	XN5	C8-N1	6.38	1.44	1.34
2	A	301[B]	XN5	C8-N1	6.28	1.44	1.34
2	A	301[A]	XN5	C8-N1	6.02	1.43	1.34
2	C	301[A]	XN5	C15-S	5.81	1.76	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[A]	XN5	C15-S	5.25	1.75	1.68
2	A	301[B]	XN5	C15-S	5.07	1.75	1.68
2	A	301[A]	XN5	C13-N3	-2.38	1.32	1.35
2	A	301[B]	XN5	C6-C1	2.31	1.41	1.37
2	C	301[A]	XN5	C12-C8	2.21	1.45	1.42
2	C	301[A]	XN5	C7-N1	2.14	1.51	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	XN5	C12-C8-N1	6.11	125.46	121.81
2	A	301[A]	XN5	C14-C13-N3	5.16	116.59	110.92
2	C	301[B]	XN5	C12-C8-N2	-5.02	115.55	121.88
2	C	301[B]	XN5	C14-C13-N3	5.01	116.42	110.92
2	C	301[A]	XN5	C12-C8-N2	-4.89	115.72	121.88
2	C	301[A]	XN5	C14-C13-N3	4.73	116.12	110.92
2	A	301[B]	XN5	C12-C8-N2	-4.39	116.35	121.88
2	C	301[B]	XN5	C11-C12-C8	4.35	120.51	117.47
2	A	301[B]	XN5	C14-C13-N3	4.35	115.69	110.92
2	A	301[A]	XN5	C12-C8-N2	-4.29	116.48	121.88
2	C	301[A]	XN5	C9-N2-C8	4.06	124.64	116.74
2	C	301[B]	XN5	C9-N2-C8	3.75	124.03	116.74
2	A	301[B]	XN5	C9-N2-C8	3.74	124.01	116.74
2	A	301[A]	XN5	C9-N2-C8	3.47	123.48	116.74
2	A	301[A]	XN5	C11-C12-C8	3.11	119.64	117.47
2	C	301[A]	XN5	C11-C12-C8	3.02	119.58	117.47
2	A	301[B]	XN5	C11-C12-C8	2.99	119.56	117.47
2	A	301[A]	XN5	C5-C4-C3	2.99	121.41	118.16
2	C	301[B]	XN5	C12-C8-N1	2.92	123.55	121.81
2	C	301[B]	XN5	C11-C12-C13	-2.71	114.63	119.25
2	A	301[B]	XN5	C5-C4-C3	2.54	120.92	118.16
2	A	301[A]	XN5	C4-C7-N1	-2.49	105.35	113.35
2	C	301[A]	XN5	C7-C4-C3	2.38	123.17	119.86
2	C	301[A]	XN5	C7-N1-C8	2.35	126.12	123.08
2	A	301[A]	XN5	C7-N1-C8	2.34	126.11	123.08
2	A	301[B]	XN5	N1-C8-N2	2.30	122.17	118.47
2	A	301[B]	XN5	C7-N1-C8	2.15	125.86	123.08
2	A	301[B]	XN5	F-C1-C6	2.07	121.87	118.55
2	C	301[B]	XN5	C5-C4-C3	2.03	120.37	118.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301[A]	XN5	C12-C8-N1-C7
2	C	301[A]	XN5	N2-C8-N1-C7
2	A	301[A]	XN5	N2-C8-N1-C7
2	C	301[A]	XN5	C4-C7-N1-C8

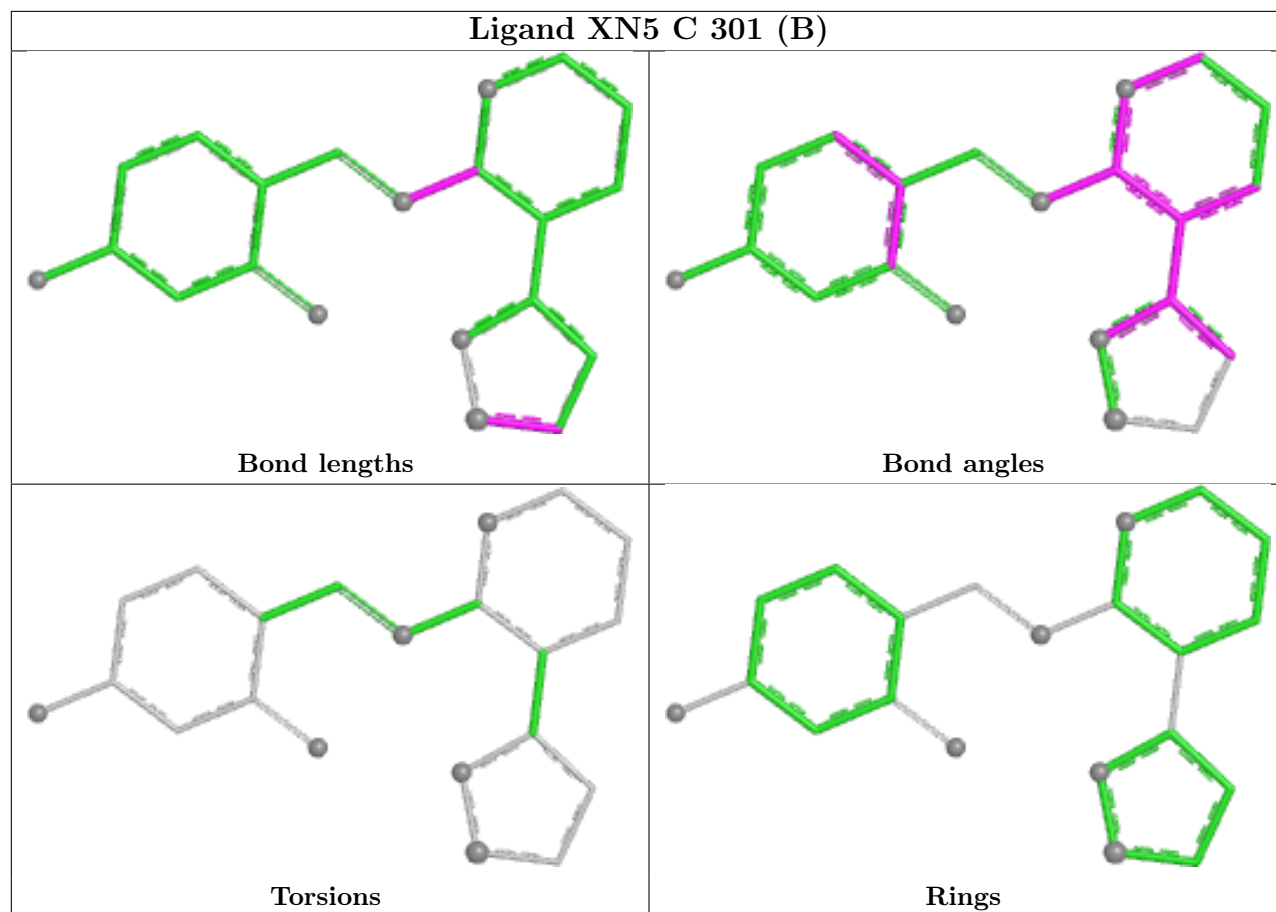
There are no ring outliers.

4 monomers are involved in 5 short contacts:

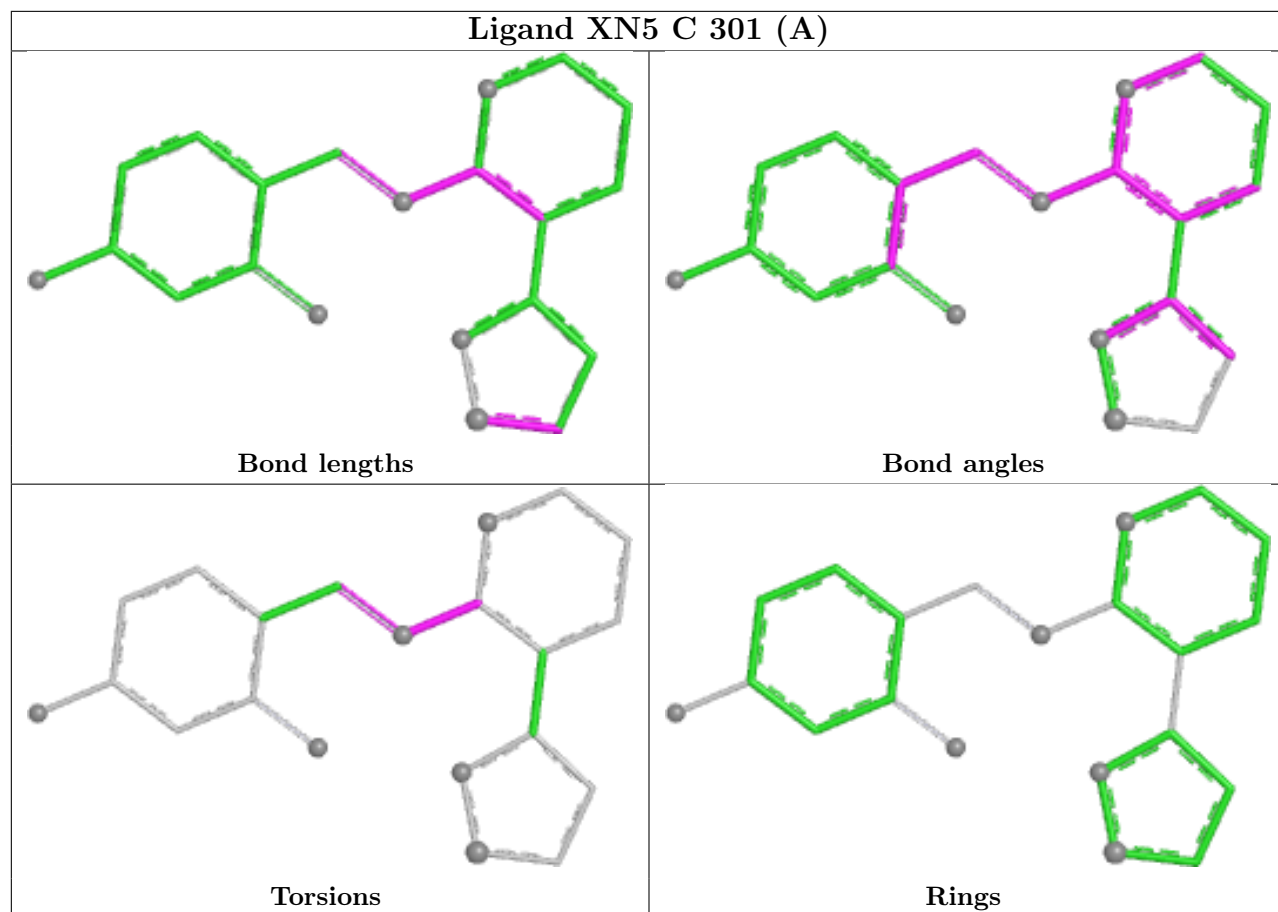
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[B]	XN5	2	0
2	C	301[A]	XN5	1	0
2	A	301[B]	XN5	1	0
2	A	301[A]	XN5	1	0

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

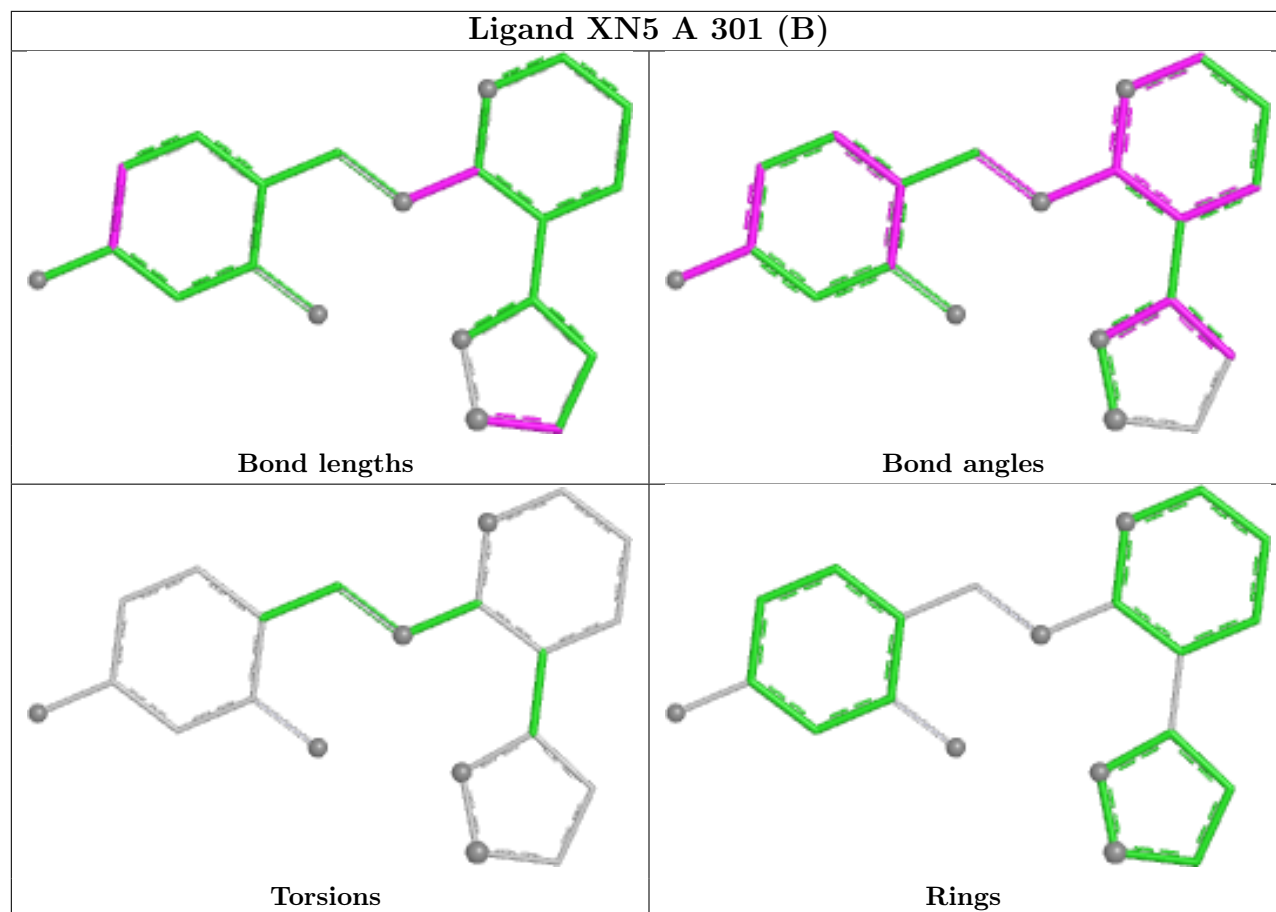
Ligand XN5 C 301 (B)

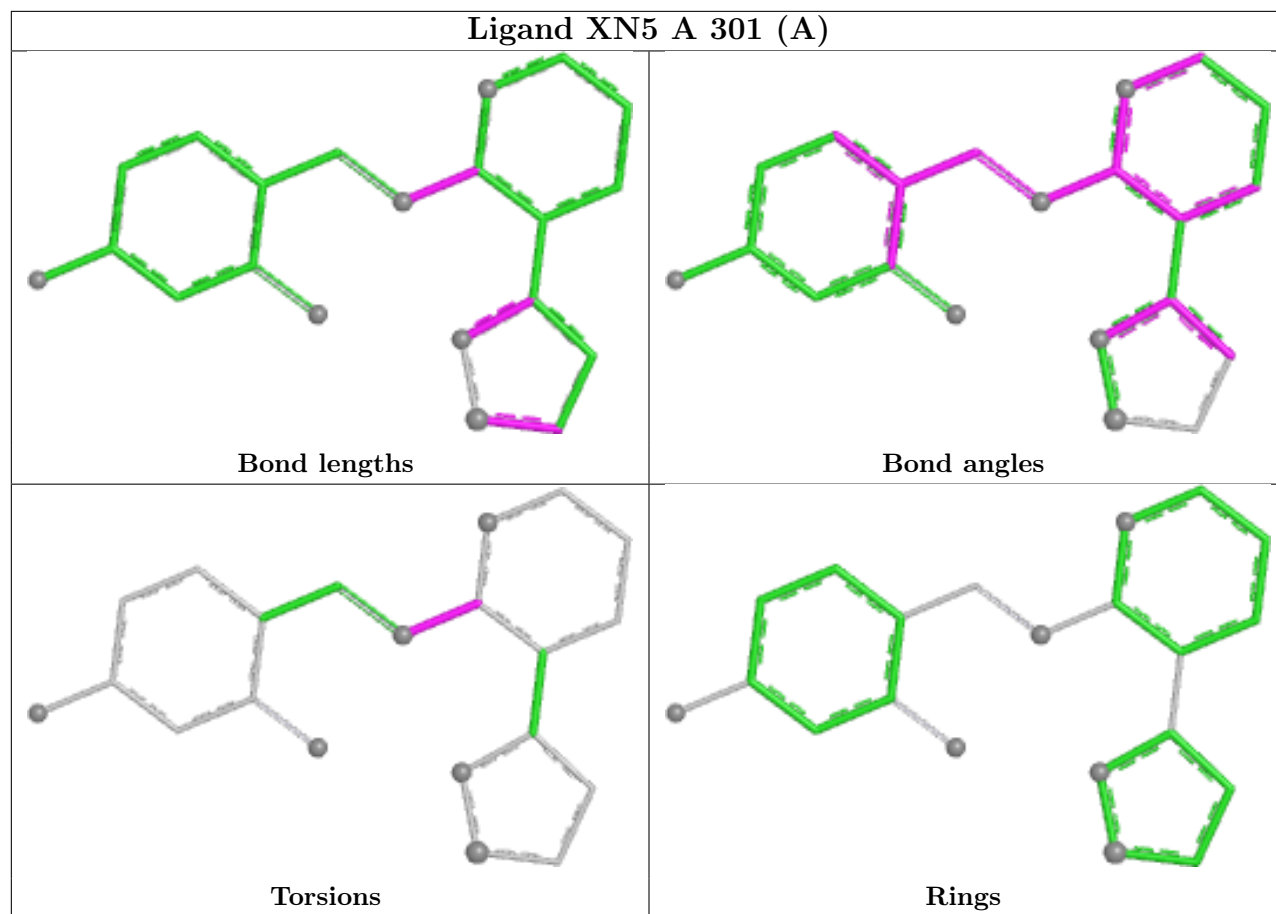


Ligand XN5 C 301 (A)



Ligand XN5 A 301 (B)





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	245/299 (81%)	-1.12	0 100 100	33, 67, 109, 150	1 (0%)
1	B	245/299 (81%)	-1.08	0 100 100	51, 67, 107, 142	0
1	C	251/299 (83%)	-1.17	1 (0%) 88 87	36, 68, 118, 155	1 (0%)
1	D	251/299 (83%)	-1.16	1 (0%) 88 87	34, 68, 115, 153	1 (0%)
All	All	992/1196 (82%)	-1.13	2 (0%) 91 90	33, 68, 113, 155	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	ASN	2.5
1	D	263	PHE	2.2

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](#)

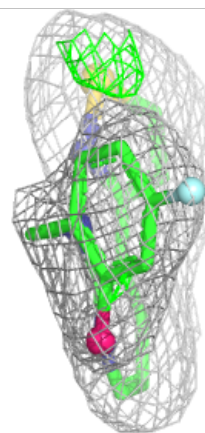
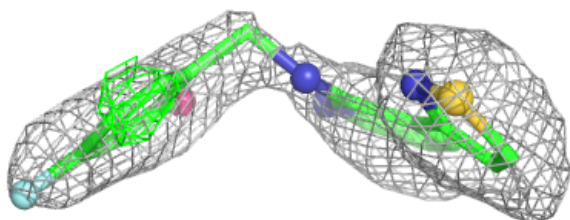
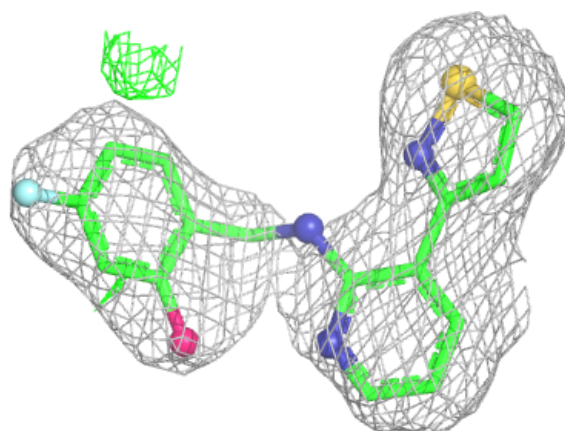
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XN5	A	301[A]	21/21	0.97	0.09	37,52,68,71	21
2	XN5	A	301[B]	21/21	0.97	0.09	40,58,73,74	21
2	XN5	C	301[A]	21/21	0.98	0.09	47,81,115,121	21
2	XN5	C	301[B]	21/21	0.98	0.09	47,79,98,100	21

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.

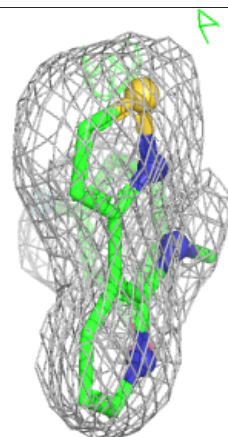
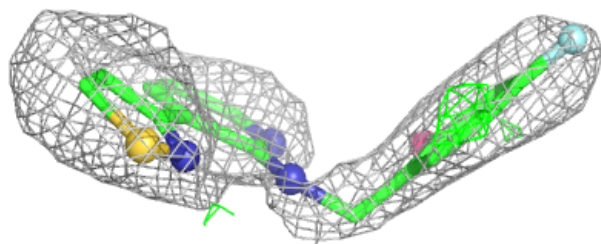
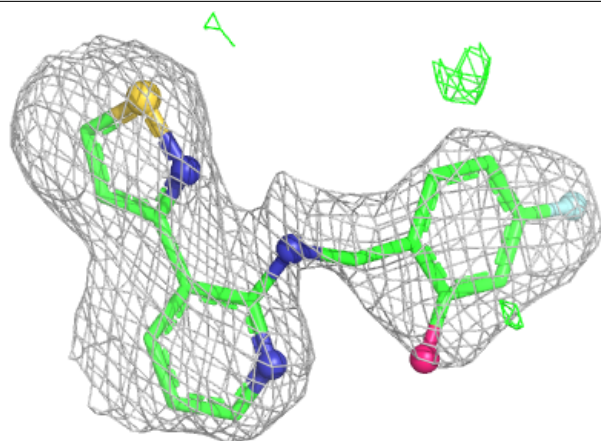
Electron density around XN5 A 301 (A):

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



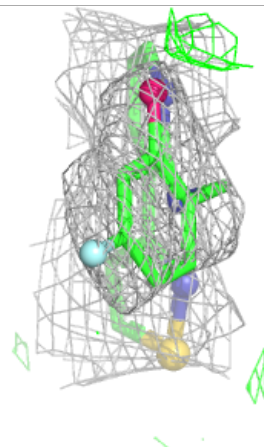
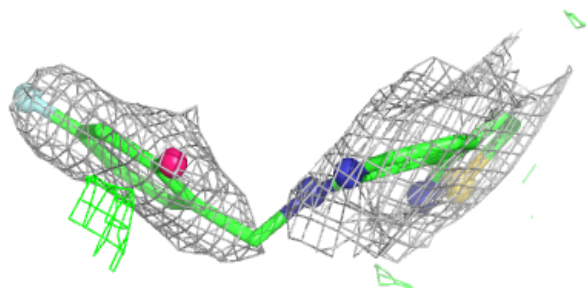
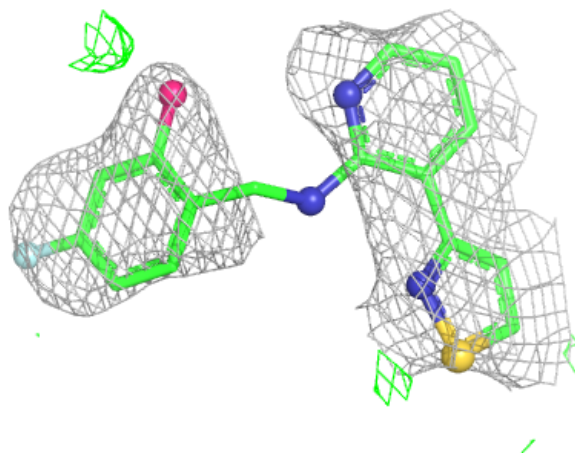
Electron density around XN5 A 301 (B):

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



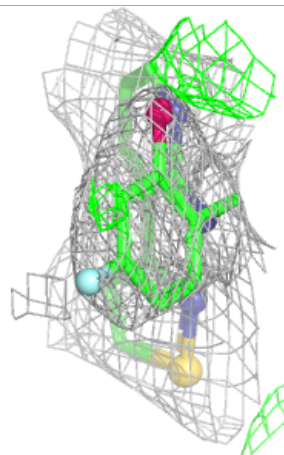
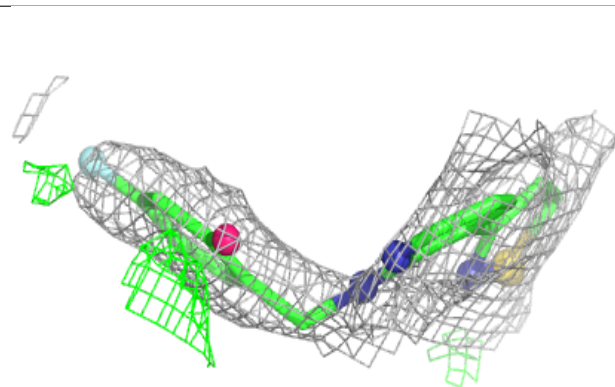
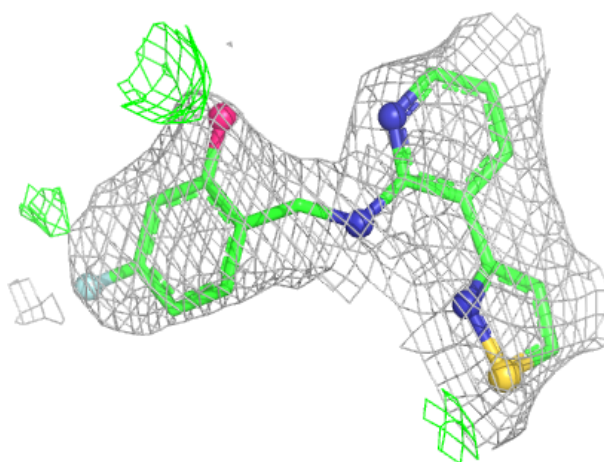
Electron density around XN5 C 301 (A):

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



Electron density around XN5 C 301 (B):

$2mF_o-DF_c$ (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.