



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:21 PM UTC

PDB ID : 2X1N / pdb_00002x1n
Title : Truncation and Optimisation of Peptide Inhibitors of CDK2, Cyclin A Through Structure Guided Design
Authors : Kontopidis, G.; Andrews, M.J.; McInnes, C.; Plater, A.; Innes, L.; Renachowski, S.; Cowan, A.; Fischer, P.M.; McIntyre, N.A.; Griffiths, G.; Barnett, A.L.; Slawin, A.M.Z.; Jackson, W.; Thomas, M.; Zheleva, D.I.; Wang, S.; Blake, D.G.; Westwood, N.J.
Deposited on : 2009-12-31
Resolution : 2.75 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)

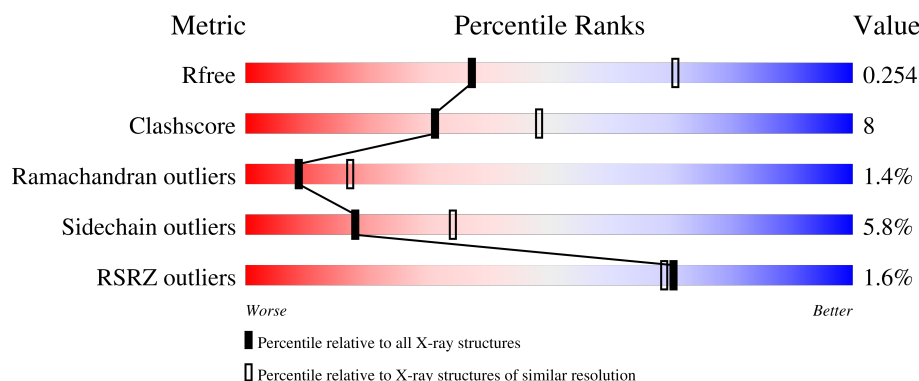
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

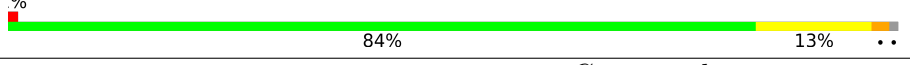
The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	298	
1	C	298	
2	B	261	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	261	% 88% 9% ..
3	H	5	60% 20% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9118 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2384	1551	403	422	8			
1	C	297	Total	C	N	O	S	0	2	1
			2393	1557	408	420	8			

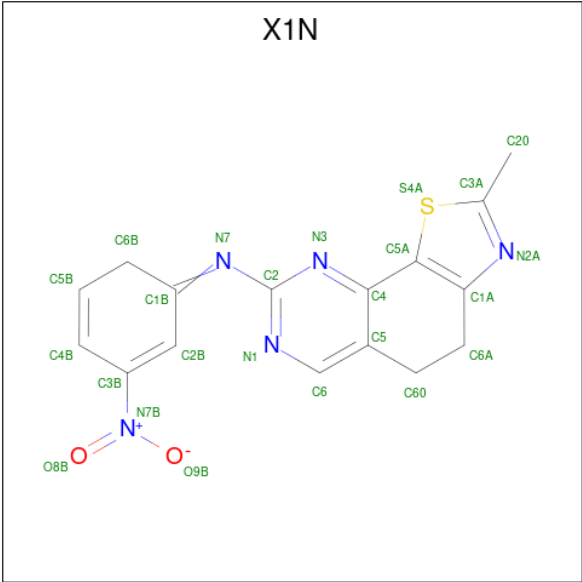
- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	1	0
			2091	1355	342	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is a protein called ACE-LEU-ASN-PFF-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	5	Total	C	F	N	O	0	0	1
			32	21	1	5	5			

- Molecule 4 is 2-METHYL-N-[(1Z)-3-NITROCYCLOHEXA-2,4-DIEN-1-YLIDENE]-4,5-DIHYDRO[1,3]THIAZOLO[4,5-H]QUINAZOLIN-8-AMINE (CCD ID: X1N) (formula: C₁₆H₁₃N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	16	5	2	1		
4	C	1	Total	C	N	O	S	0	0
			24	16	5	2	1		

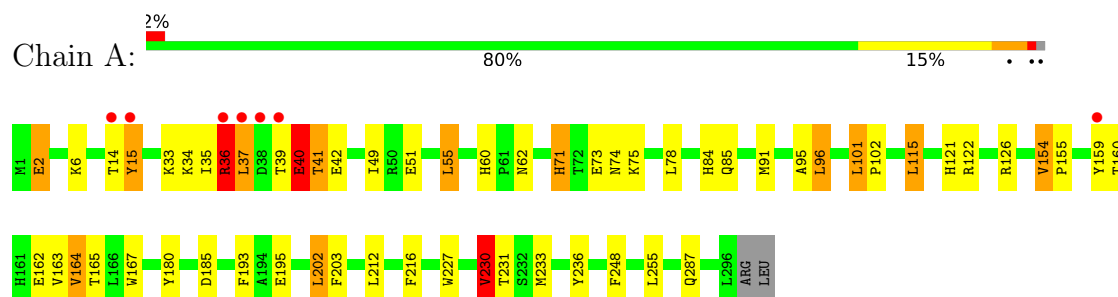
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	24	Total	O	0	0
			24	24		
5	C	17	Total	O	0	0
			17	17		
5	D	21	Total	O	0	0
			21	21		
5	H	2	Total	O	0	0
			2	2		

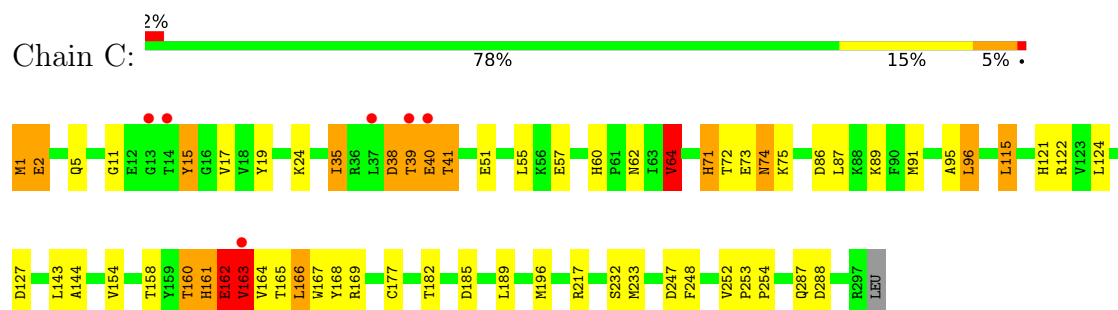
3 Residue-property plots

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.

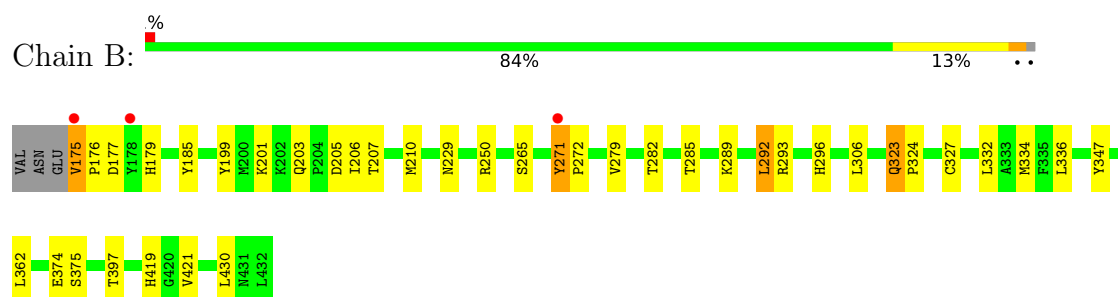
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



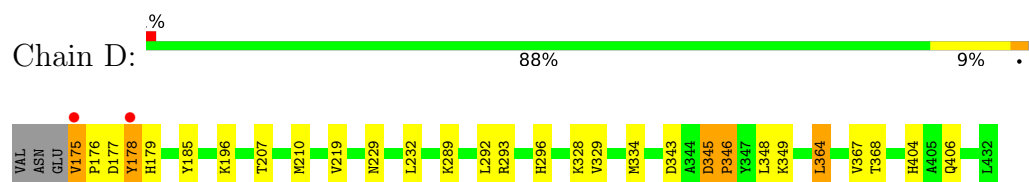
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN-A2



• Molecule 2: CYCLIN-A2



- Molecule 3: ACE-LEU-ASN-PFF-NH2

Chain H: 60% 20% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.56Å 114.26Å 157.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.75) 97.9 (30.00-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.255 0.204 , 0.254	Depositor DCC
R_{free} test set	1097 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9118	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: ACE, PFF, X1N, NH2

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	0.82	0/2449	1.06	5/3325 (0.2%)
1	C	0.78	0/2461	1.06	3/3340 (0.1%)
2	B	0.79	1/2144 (0.0%)	1.01	4/2910 (0.1%)
2	D	0.78	1/2134 (0.0%)	1.04	1/2897 (0.0%)
3	H	1.76	1/16 (6.2%)	2.12	1/21 (4.8%)
All	All	0.80	3/9204 (0.0%)	1.05	14/12493 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	175	VAL	N-CA	12.02	1.69	1.46
2	D	175	VAL	N-CA	6.91	1.59	1.46
3	H	3	ASN	CB-CG	-6.54	1.35	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	230	VAL	CB-CA-C	-6.83	103.14	111.88
1	C	161	HIS	N-CA-C	-6.79	105.40	113.21
1	C	64	VAL	CB-CA-C	-6.36	101.02	111.51
1	A	233	MET	CA-C-N	5.56	125.02	119.24
1	A	233	MET	C-N-CA	5.56	125.02	119.24
2	B	175	VAL	CA-C-N	5.52	126.74	119.84
2	B	175	VAL	C-N-CA	5.52	126.74	119.84
1	C	11	GLY	N-CA-C	5.38	117.85	110.69
2	B	177	ASP	N-CA-C	-5.28	107.01	113.50
2	B	203	GLN	CA-C-O	5.23	122.69	119.29
2	D	175	VAL	CB-CA-C	5.16	121.20	111.40
1	A	167	TRP	N-CA-C	5.14	117.55	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLU	N-CA-C	-5.06	100.02	110.80

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	2384	0	2432	59	0
1	C	2393	0	2452	52	0
2	B	2091	0	2120	28	0
2	D	2084	0	2107	20	0
3	H	32	0	27	1	0
4	A	24	0	13	1	0
4	C	24	0	13	0	0
5	A	22	0	0	0	0
5	B	24	0	0	0	0
5	C	17	0	0	0	0
5	D	21	0	0	0	0
5	H	2	0	0	0	0
All	All	9118	0	9164	149	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 8.

All (149) 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)
2:B:175:VAL:N	2:B:175:VAL:CA	1.69	1.51
1:A:41:THR:HG22	1:A:42:GLU:H	1.08	1.11
1:C:164:VAL:HG12	1:C:165:THR:H	1.18	1.02
2:B:282:THR:O	2:B:285:THR:HG23	1.63	0.99
1:C:39:THR:O	1:C:40:GLU:HB2	1.63	0.96
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.24	0.96
1:A:39:THR:OG1	2:B:289:LYS:HD3	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:OE1	1:A:180:TYR:OH	1.89	0.91
2:D:176:PRO:HB3	2:D:179:HIS:ND1	1.88	0.89
1:A:41:THR:HG22	1:A:42:GLU:N	1.86	0.88
1:C:166:LEU:O	1:C:168:TYR:N	2.09	0.86
1:A:41:THR:CG2	1:A:42:GLU:H	1.91	0.83
1:A:36:ARG:HG2	1:A:36:ARG:NH1	1.83	0.82
1:A:36:ARG:O	1:A:37:LEU:HD13	1.81	0.81
1:A:36:ARG:HH11	1:A:36:ARG:CG	1.97	0.77
1:A:60:HIS:HD2	1:A:62:ASN:H	1.34	0.76
1:C:162:GLU:HG2	1:C:163:VAL:N	2.02	0.75
1:A:40:GLU:O	1:A:41:THR:HB	1.87	0.74
2:B:205:ASP:OD2	2:B:250:ARG:HD2	1.88	0.72
1:C:15:TYR:OH	1:C:51:GLU:OE1	2.04	0.71
1:C:51:GLU:O	1:C:55:LEU:HB2	1.91	0.71
2:B:175:VAL:N	2:B:175:VAL:C	2.48	0.71
1:C:91:MET:HE3	1:C:196:MET:HG2	1.73	0.70
1:A:164:VAL:CG1	1:A:164:VAL:O	2.40	0.69
1:A:164:VAL:O	1:A:164:VAL:HG13	1.92	0.69
2:B:282:THR:O	2:B:285:THR:CG2	2.40	0.69
1:A:39:THR:O	1:A:40:GLU:HB2	1.94	0.68
1:A:2:GLU:HG2	1:C:73:GLU:HG3	1.76	0.68
1:A:163:VAL:O	1:A:163:VAL:HG22	1.92	0.67
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.09	0.67
2:D:404:HIS:HD2	2:D:406:GLN:H	1.43	0.67
1:C:162:GLU:HG3	1:C:169:ARG:HH22	1.60	0.66
2:D:346:PRO:O	2:D:349:LYS:HG2	1.96	0.66
1:A:40:GLU:O	1:A:41:THR:CB	2.44	0.66
1:A:39:THR:O	1:A:40:GLU:CB	2.43	0.65
1:C:164:VAL:HG12	1:C:165:THR:N	1.97	0.65
1:A:162:GLU:HG3	1:A:164:VAL:HB	1.79	0.64
1:C:95:ALA:O	1:C:96:LEU:HD23	1.98	0.64
1:C:160:THR:C	1:C:162:GLU:H	2.06	0.63
2:D:343:ASP:HB3	2:D:345:ASP:OD2	1.97	0.63
1:A:60:HIS:CD2	1:A:62:ASN:H	2.18	0.62
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.35	0.62
2:D:207:THR:HG23	2:D:210:MET:H	1.65	0.62
1:C:164:VAL:CG1	1:C:165:THR:H	2.03	0.61
2:B:207:THR:HG23	2:B:210:MET:H	1.64	0.61
1:C:165:THR:O	1:C:166:LEU:HB2	2.00	0.60
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.84	0.60
1:C:60:HIS:HD2	1:C:62:ASN:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.83	0.59
1:C:60:HIS:CD2	1:C:62:ASN:H	2.20	0.59
1:A:14:THR:O	1:A:15:TYR:HB2	2.03	0.59
1:A:95:ALA:O	1:A:96:LEU:HD23	2.03	0.59
1:C:161:HIS:O	1:C:162:GLU:O	2.19	0.59
1:A:39:THR:OG1	2:B:289:LYS:CD	2.45	0.59
2:B:332:LEU:HD13	2:B:421:VAL:HB	1.86	0.58
1:A:39:THR:HG22	2:B:292:LEU:HB3	1.84	0.58
1:A:2:GLU:HG2	1:C:73:GLU:CG	2.33	0.58
1:A:91:MET:HE1	1:A:195:GLU:HG2	1.86	0.58
1:C:162:GLU:CG	1:C:163:VAL:N	2.66	0.58
4:A:1297:X1N:H2B	4:A:1297:X1N:N3	2.18	0.58
2:B:207:THR:HG22	2:B:210:MET:HE3	1.85	0.58
2:D:207:THR:HG22	2:D:210:MET:HG3	1.86	0.58
1:A:154:VAL:HG12	1:A:155:PRO:HD2	1.86	0.57
1:A:36:ARG:C	1:A:37:LEU:HD13	2.30	0.56
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.86	0.56
1:C:165:THR:O	1:C:166:LEU:CB	2.52	0.56
1:C:162:GLU:HG2	1:C:163:VAL:H	1.71	0.56
1:C:72:THR:HG22	1:C:73:GLU:N	2.22	0.54
2:B:176:PRO:HB3	2:B:179:HIS:ND1	2.22	0.54
1:A:41:THR:CG2	1:A:42:GLU:N	2.58	0.54
2:D:178:TYR:HD2	2:D:178:TYR:C	2.16	0.54
1:A:51:GLU:O	1:A:55:LEU:HB2	2.08	0.54
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.91	0.53
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.33	0.53
1:C:5:GLN:HB2	1:C:24:LYS:HE2	1.91	0.53
1:C:64:VAL:CG2	1:C:143:LEU:O	2.57	0.53
2:D:176:PRO:CB	2:D:179:HIS:ND1	2.69	0.52
1:A:6:LYS:NZ	1:A:34:LYS:NZ	2.57	0.52
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.90	0.52
1:C:91:MET:HE3	1:C:196:MET:CG	2.40	0.52
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.92	0.51
2:B:265:SER:HB3	2:B:272:PRO:HB3	1.90	0.51
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.91	0.51
1:A:84:HIS:O	1:A:85:GLN:HB3	2.10	0.51
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.46	0.51
2:D:229:ASN:HD22	2:D:334:MET:CE	2.24	0.51
2:D:178:TYR:C	2:D:178:TYR:CD2	2.88	0.51
2:D:404:HIS:CD2	2:D:406:GLN:H	2.26	0.50
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:TRP:O	1:A:230:VAL:HG22	2.11	0.49
1:C:64:VAL:HG22	1:C:143:LEU:O	2.13	0.49
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.00	0.49
2:B:229:ASN:HD22	2:B:334:MET:HE3	1.78	0.49
1:A:91:MET:CE	1:A:195:GLU:HG2	2.43	0.48
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.48	0.48
1:A:36:ARG:O	1:A:36:ARG:HD3	2.13	0.48
1:C:127:ASP:OD1	1:C:165:THR:HG23	2.13	0.48
1:C:57:GLU:OE1	2:D:185:TYR:OH	2.31	0.48
1:C:161:HIS:O	1:C:162:GLU:C	2.57	0.48
2:B:327:CYS:HB3	2:B:419:HIS:NE2	2.29	0.48
2:D:289:LYS:HZ3	2:D:293:ARG:HD2	1.79	0.47
2:B:176:PRO:CA	2:B:179:HIS:ND1	2.77	0.47
1:C:160:THR:C	1:C:162:GLU:N	2.71	0.47
1:C:177:CYS:HB3	1:C:233:MET:HE1	1.95	0.47
1:C:1:MET:HA	1:C:1:MET:HE3	1.97	0.47
1:C:164:VAL:CG1	1:C:165:THR:N	2.70	0.46
1:A:121:HIS:C	1:A:122:ARG:HG3	2.40	0.46
1:C:162:GLU:HG2	1:C:164:VAL:H	1.80	0.46
1:A:121:HIS:O	1:A:122:ARG:HG3	2.15	0.46
2:B:279:VAL:O	2:B:282:THR:OG1	2.33	0.46
1:A:35:ILE:C	1:A:36:ARG:HG3	2.41	0.46
2:D:345:ASP:OD2	2:D:346:PRO:HD3	2.15	0.46
1:A:6:LYS:HZ1	1:A:34:LYS:NZ	2.14	0.46
1:C:86:ASP:OD2	1:C:89:LYS:HD3	2.15	0.46
1:C:15:TYR:HD2	1:C:35:ILE:HG12	1.82	0.45
2:B:289:LYS:O	2:B:293:ARG:HG2	2.16	0.45
1:C:74:ASN:OD1	1:C:74:ASN:N	2.50	0.45
1:C:39:THR:O	1:C:40:GLU:CB	2.45	0.45
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.72	0.45
1:A:101:LEU:N	1:A:102:PRO:CD	2.79	0.44
1:A:230:VAL:HG23	1:A:231:THR:HG23	1.99	0.44
1:A:39:THR:O	1:A:40:GLU:CG	2.66	0.44
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.82	0.44
2:D:207:THR:CG2	2:D:210:MET:HG3	2.47	0.44
2:B:199:TYR:CD1	2:B:199:TYR:C	2.96	0.44
1:A:159:TYR:N	1:A:159:TYR:CD1	2.86	0.43
1:C:64:VAL:CG2	1:C:144:ALA:HA	2.48	0.43
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.99	0.43
1:A:163:VAL:O	1:A:163:VAL:CG2	2.63	0.43
2:B:430:LEU:HD23	2:B:430:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLN:HA	2:B:324:PRO:HA	1.85	0.42
1:C:72:THR:HG22	1:C:73:GLU:H	1.83	0.42
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.49	0.42
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.62	0.42
1:C:124:LEU:HD21	1:C:182:THR:HA	2.02	0.42
1:C:64:VAL:HG23	1:C:143:LEU:O	2.20	0.41
1:A:159:TYR:N	1:A:159:TYR:HD1	2.17	0.41
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.89	0.41
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.56	0.41
2:B:347:TYR:OH	2:B:397:THR:OG1	2.32	0.41
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.39	0.41
1:A:227:TRP:CE3	1:A:230:VAL:CG1	3.04	0.41
1:C:288:ASP:OD1	1:C:288:ASP:N	2.53	0.41
2:B:271:TYR:O	2:B:271:TYR:HD1	2.03	0.41
2:D:210:MET:HG2	3:H:4:PFF:HB2	2.03	0.41
1:A:193:PHE:CZ	1:A:255:LEU:HD21	2.56	0.40
1:C:17:VAL:HG13	1:C:19:TYR:CE1	2.57	0.40
1:A:227:TRP:CG	1:A:230:VAL:HG13	2.57	0.40
1:C:121:HIS:C	1:C:122:ARG:HG3	2.47	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	295/298 (99%)	283 (96%)	8 (3%)	4 (1%)	9	17
1	C	297/298 (100%)	280 (94%)	8 (3%)	9 (3%)	3	6
2	B	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
2	D	256/261 (98%)	252 (98%)	2 (1%)	2 (1%)	16	30
3	H	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1107/1123 (99%)	1067 (96%)	25 (2%)	15 (1%)	9 17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	36	ARG
1	A	41	THR
1	C	162	GLU
1	C	163	VAL
1	C	167	TRP
1	C	40	GLU
1	C	41	THR
1	C	166	LEU
2	D	177	ASP
2	D	346	PRO
1	C	15	TYR
1	C	160	THR
1	A	40	GLU
1	C	38	ASP

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	262/263 (100%)	243 (93%)	19 (7%)	13 24
1	C	263/263 (100%)	240 (91%)	23 (9%)	9 18
2	B	233/235 (99%)	226 (97%)	7 (3%)	36 60
2	D	232/235 (99%)	224 (97%)	8 (3%)	32 57
3	H	2/2 (100%)	2 (100%)	0	100 100
All	All	992/998 (99%)	935 (94%)	57 (6%)	18 35

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	36	ARG
1	A	37	LEU
1	A	55	LEU
1	A	71	HIS
1	A	74	ASN
1	A	75	LYS
1	A	96	LEU
1	A	101	LEU
1	A	115	LEU
1	A	126	ARG
1	A	154	VAL
1	A	160	THR
1	A	164	VAL
1	A	165	THR
1	A	202	LEU
1	A	230	VAL
1	A	248	PHE
1	A	287	GLN
2	B	201	LYS
2	B	206	ILE
2	B	271	TYR
2	B	292	LEU
2	B	323	GLN
2	B	374	GLU
2	B	375	SER
1	C	1	MET
1	C	2	GLU
1	C	35	ILE
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	64	VAL
1	C	71	HIS
1	C	74	ASN
1	C	75	LYS
1	C	87	LEU
1	C	96	LEU
1	C	115	LEU
1	C	154	VAL
1	C	158	THR
1	C	162	GLU
1	C	163	VAL

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Mol	Chain	Res	Type
1	C	217	ARG
1	C	232	SER
1	C	247	ASP
1	C	248	PHE
1	C	252	VAL
1	C	287	GLN
2	D	175	VAL
2	D	178	TYR
2	D	196	LYS
2	D	292	LEU
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	364	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	62	ASN
1	A	71	HIS
1	A	85	GLN
2	B	208	ASN
2	B	296	HIS
2	B	323	GLN
2	B	404	HIS
2	B	406	GLN
1	C	60	HIS
1	C	71	HIS
1	C	85	GLN
1	C	246	GLN
2	D	208	ASN
2	D	228	GLN
2	D	312	ASN
2	D	404	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PFF	H	4	3	11,12,13	0.74	0	10,15,17	1.72	2 (20%)

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	PFF	H	4	3	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4	PFF	F-CZ-CE2	4.10	125.11	118.55
3	H	4	PFF	F-CZ-CE1	-2.69	114.24	118.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	PFF	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	4	PFF	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
4	X1N	A	1297	-	23,27,27	3.28	7 (30%)	23,39,39	5.83	11 (47%)
4	X1N	C	1298	-	23,27,27	3.40	7 (30%)	23,39,39	5.32	10 (43%)

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
4	X1N	A	1297	-	-	0/3/27/27	0/4/4/4
4	X1N	C	1298	-	-	3/3/27/27	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1298	X1N	O8B-N7B	13.80	1.46	1.22
4	A	1297	X1N	O8B-N7B	13.40	1.46	1.22
4	C	1298	X1N	C20-C3A	-3.80	1.39	1.49
4	A	1297	X1N	C6B-C5B	-3.73	1.39	1.49
4	C	1298	X1N	C6B-C5B	-3.56	1.39	1.49
4	A	1297	X1N	C20-C3A	-3.50	1.40	1.49
4	C	1298	X1N	C4-C5	-3.05	1.37	1.40
4	C	1298	X1N	C2B-C1B	-2.65	1.38	1.44
4	C	1298	X1N	C5A-S4A	-2.47	1.68	1.74
4	A	1297	X1N	C4B-C5B	2.35	1.39	1.33
4	C	1298	X1N	C4B-C5B	2.31	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1297	X1N	C5A-S4A	-2.29	1.68	1.74
4	A	1297	X1N	C4-C5	-2.20	1.38	1.40
4	A	1297	X1N	C2B-C1B	-2.00	1.39	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1297	X1N	C3A-S4A-C5A	14.46	98.22	89.64
4	A	1297	X1N	S4A-C3A-N2A	-14.13	104.90	114.64
4	C	1298	X1N	C3A-S4A-C5A	13.55	97.68	89.64
4	A	1297	X1N	C6-N1-C2	12.49	124.57	115.52
4	C	1298	X1N	S4A-C3A-N2A	-11.74	106.55	114.64
4	C	1298	X1N	C6-N1-C2	11.61	123.92	115.52
4	A	1297	X1N	C1A-C5A-S4A	-10.50	103.85	109.59
4	C	1298	X1N	C1A-C5A-S4A	-9.25	104.53	109.59
4	C	1298	X1N	C20-C3A-N2A	5.29	134.93	123.74
4	A	1297	X1N	N1-C2-N3	-4.52	119.33	126.45
4	C	1298	X1N	N1-C2-N3	-4.52	119.33	126.45
4	A	1297	X1N	C5-C6-N1	-4.35	116.75	123.83
4	A	1297	X1N	C5B-C6B-C1B	4.22	123.03	112.64
4	C	1298	X1N	C5-C6-N1	-3.97	117.38	123.83
4	C	1298	X1N	C5B-C6B-C1B	3.93	122.31	112.64
4	A	1297	X1N	C20-C3A-N2A	3.92	132.03	123.74
4	A	1297	X1N	C60-C5-C6	-3.21	116.82	121.97
4	C	1298	X1N	C60-C5-C6	-2.70	117.63	121.97
4	A	1297	X1N	C60-C5-C4	2.64	124.60	120.09
4	A	1297	X1N	N3-C2-N7	2.31	124.72	116.92
4	C	1298	X1N	C60-C5-C4	2.17	123.80	120.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

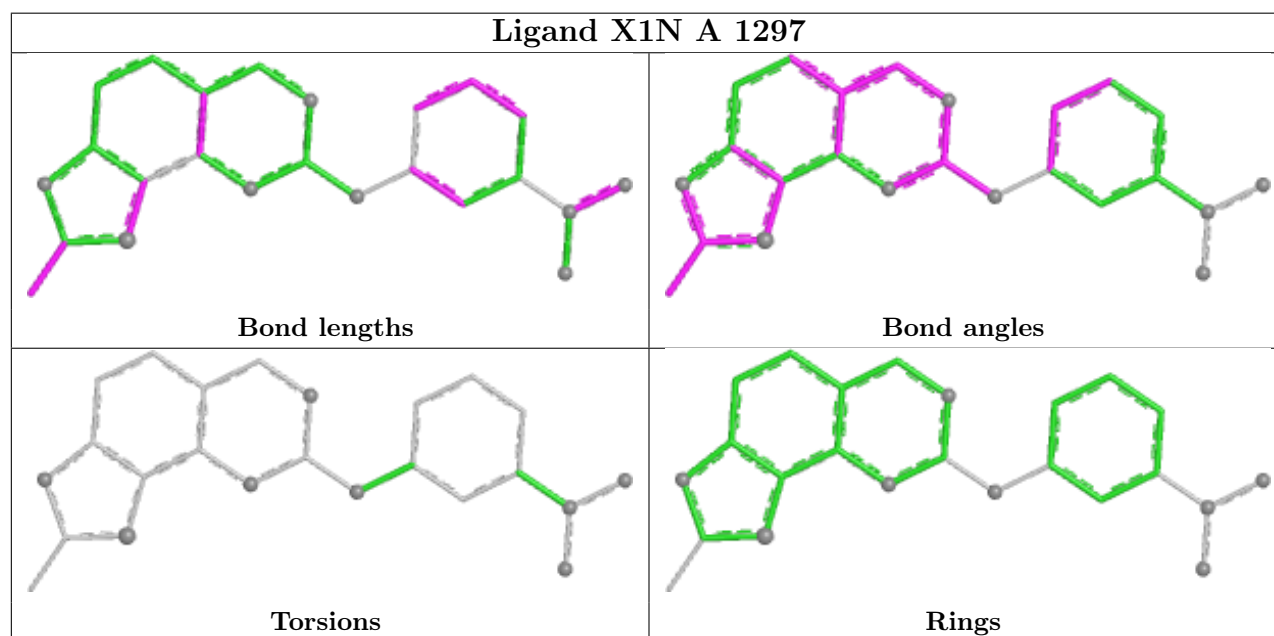
Mol	Chain	Res	Type	Atoms
4	C	1298	X1N	C2B-C3B-N7B-O8B
4	C	1298	X1N	C2B-C1B-N7-C2
4	C	1298	X1N	C4B-C3B-N7B-O8B

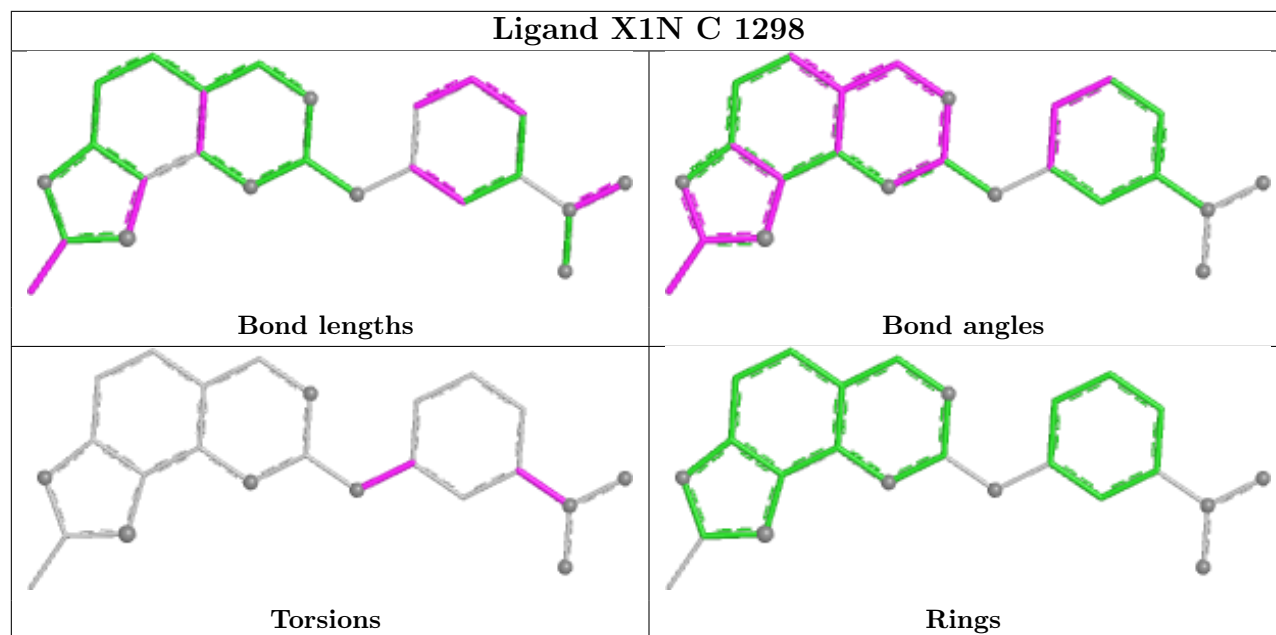
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1297	X1N	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

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	296/298 (99%)	-0.25	7 (2%) 59 57	16, 36, 73, 98	2 (0%)
1	C	297/298 (99%)	-0.29	6 (2%) 65 63	19, 36, 74, 99	2 (0%)
2	B	258/261 (98%)	-0.34	3 (1%) 76 76	21, 40, 61, 99	1 (0%)
2	D	258/261 (98%)	-0.35	2 (0%) 82 82	21, 40, 60, 99	0
3	H	2/5 (40%)	0.23	0 100 100	52, 52, 52, 77	0
All	All	1111/1123 (98%)	-0.30	18 (1%) 70 69	16, 38, 70, 99	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	5.1
1	C	13	GLY	4.4
2	B	175	VAL	4.3
2	D	175	VAL	3.8
1	A	37	LEU	3.6
1	A	15	TYR	3.5
1	C	14	THR	2.7
1	A	159	TYR	2.6
1	C	37	LEU	2.6
1	A	36	ARG	2.6
1	A	14	THR	2.5
1	C	163	VAL	2.5
2	B	271	TYR	2.4
2	B	178	TYR	2.4
1	A	39	THR	2.3
1	C	40	GLU	2.3
1	A	38	ASP	2.2
2	D	178	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	PFF	H	4	12/13	0.86	0.10	40,49,68,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

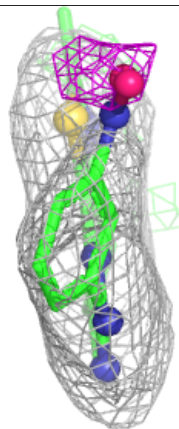
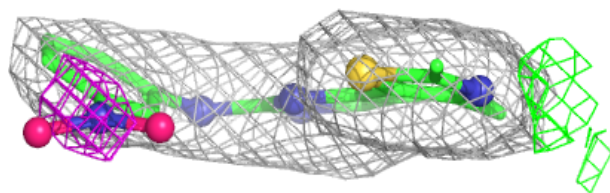
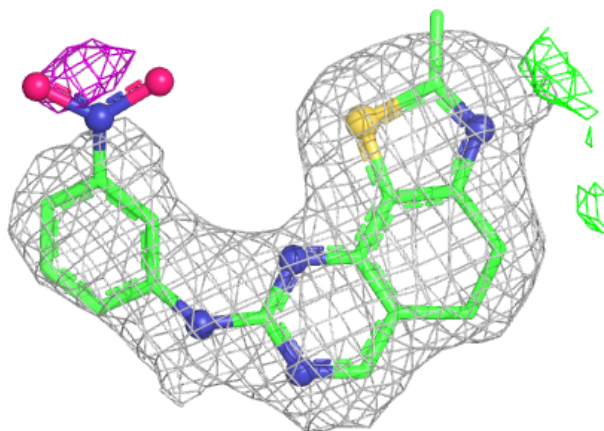
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	X1N	C	1298	24/24	0.91	0.11	41,52,86,95	0
4	X1N	A	1297	24/24	0.93	0.08	32,47,72,80	0

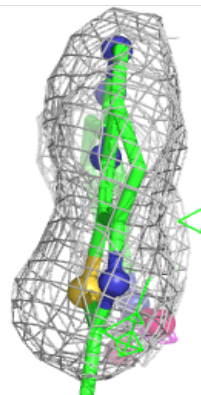
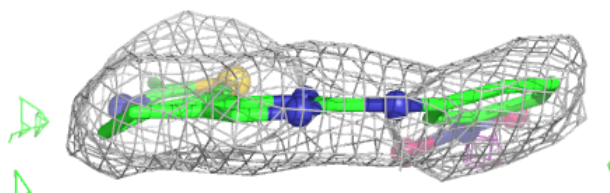
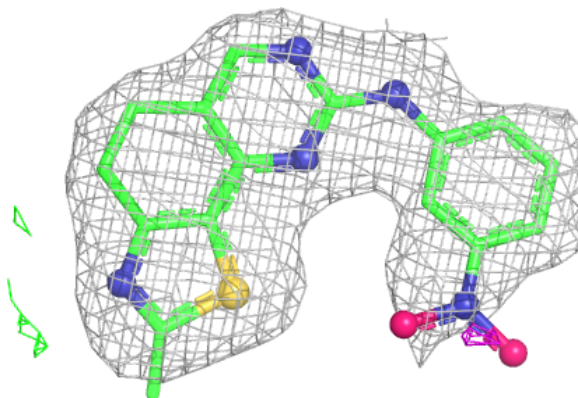
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X1N C 1298:

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

**Electron density around X1N A 1297:**

$2mF_o - DF_c$ (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.