



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 PM UTC

PDB ID : 8UCB / pdb_00008ucb
Title : IRAK4 in complex with compound 8
Authors : Metrick, C.M.; Chodaparambil, J.V.
Deposited on : 2023-09-26
Resolution : 1.85 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

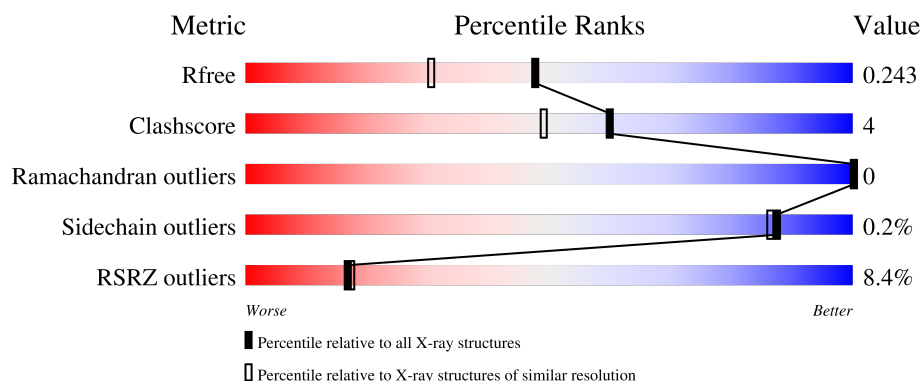
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	307	10% 82% 11% 6%
1	B	307	8% 84% 10% 6%
1	C	307	5% 84% 9% 7%
1	D	307	8% 84% 10% 5%

2 Entry composition [i](#)

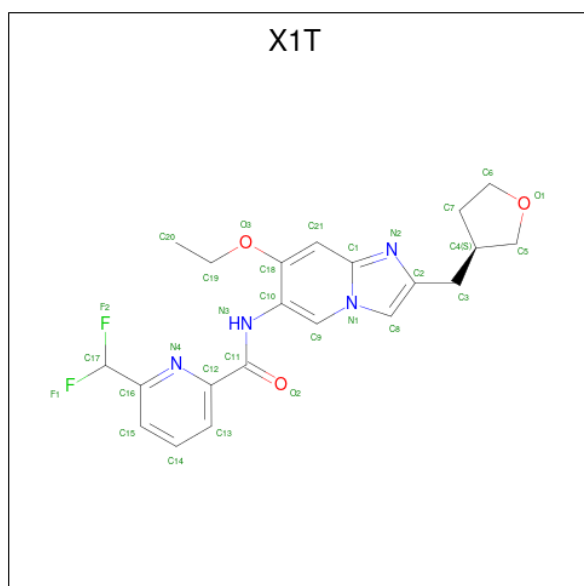
There are 3 unique types of molecules in this entry. The entry contains 9638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	P	S	0	0	0
			2272	1426	380	448	3	15			
1	B	288	Total	C	N	O	P	S	0	0	0
			2220	1397	370	436	3	14			
1	C	287	Total	C	N	O	P	S	0	0	0
			2209	1393	371	428	2	15			
1	D	291	Total	C	N	O	P	S	0	0	0
			2270	1424	379	449	3	15			

- Molecule 2 is 6-(difluoromethyl)-N-[(4R)-7-ethoxy-2-[(3R)-oxolan-3-yl]methyl]imidazo[1,2-a]pyridin-6-yl]pyridine-2-carboxamide (CCD ID: X1T) (formula: C₂₁H₂₂F₂N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	21	2	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			30	21	2	4	3		
2	C	1	Total	C	F	N	O	0	0
			30	21	2	4	3		
2	D	1	Total	C	F	N	O	0	0
			30	21	2	4	3		

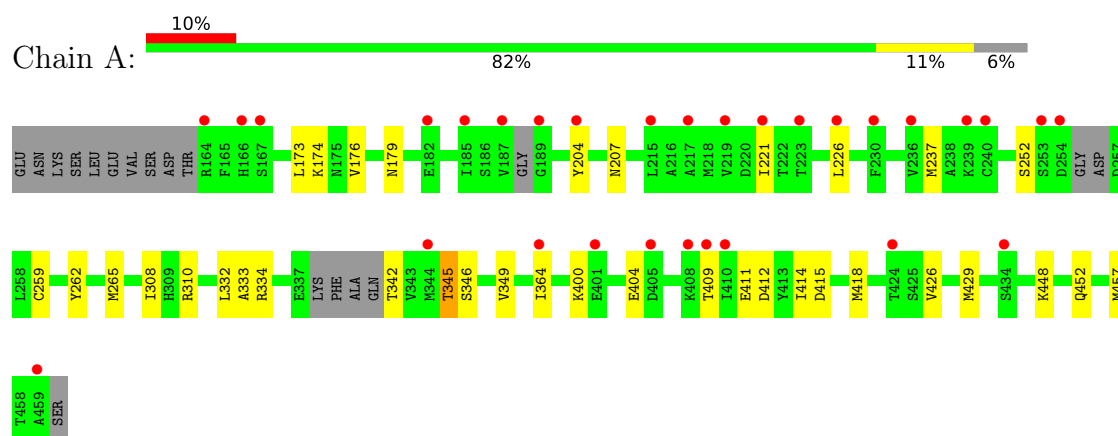
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	121	Total	O	0	0
			121	121		
3	C	165	Total	O	0	0
			165	165		
3	D	138	Total	O	0	0
			138	138		

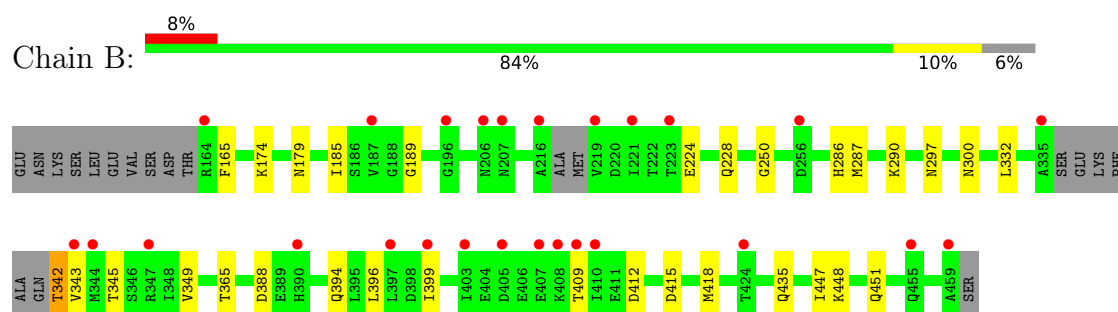
3 Residue-property plots [i](#)

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.

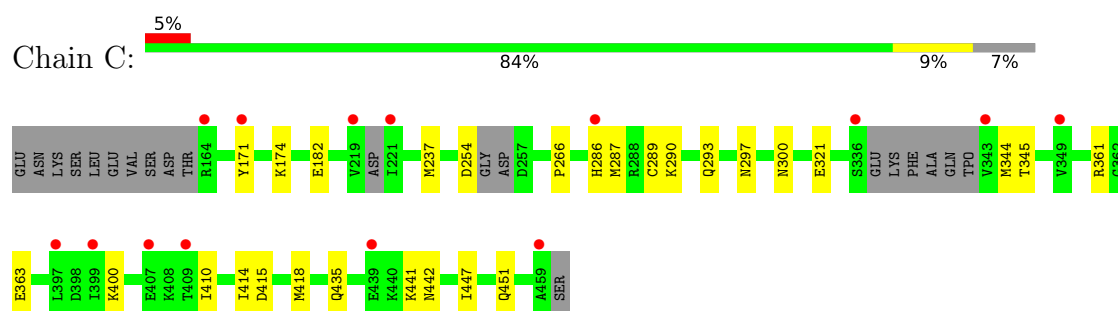
- Molecule 1: Interleukin-1 receptor-associated kinase 4



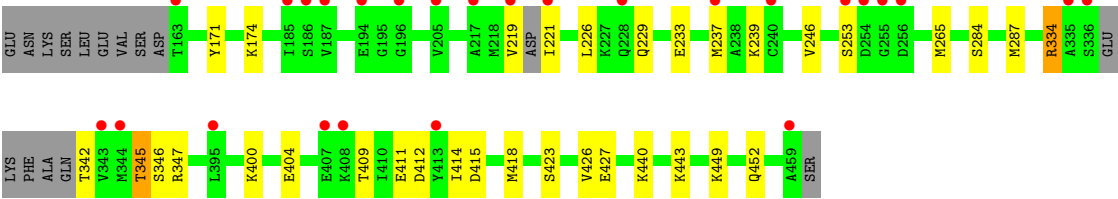
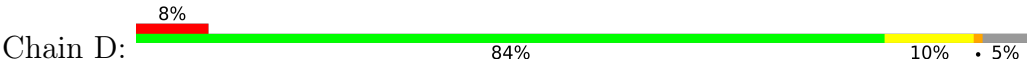
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.62Å 140.85Å 87.53Å 90.00° 125.70° 90.00°	Depositor
Resolution (Å)	48.31 – 1.85 48.31 – 1.85	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.31-1.85) 93.8 (48.31-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.207 , 0.243 0.207 , 0.243	Depositor DCC
R_{free} test set	5379 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9638	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 38.71 % 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 3.5396e-04. 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: TPO, X1T, SEP

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	0.14	0/2275	0.33	0/3065
1	B	0.19	0/2224	0.42	0/3005
1	C	0.18	0/2223	0.40	0/3002
1	D	0.34	1/2274 (0.0%)	0.36	0/3068
All	All	0.23	1/8996 (0.0%)	0.38	0/12140

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	334	ARG	C-N	14.41	1.52	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2272	0	2230	19	0
1	B	2220	0	2154	20	0
1	C	2209	0	2152	16	0
1	D	2270	0	2218	22	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	123	0	0	0	0
3	B	121	0	0	3	0
3	C	165	0	0	1	0
3	D	138	0	0	0	0
All	All	9638	0	8754	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:D:284:SER:H	1:D:287:MET:HE3	1.45	0.78
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.75	0.68
1:B:448:LYS:NZ	3:B:602:HOH:O	2.28	0.66
1:D:171:TYR:HA	1:D:174:LYS:HG3	1.77	0.66
1:C:361:ARG:HG2	1:C:361:ARG:HH11	1.60	0.66
1:D:423:SER:O	1:D:427:GLU:HG3	1.97	0.64
1:D:221:ILE:HD11	1:D:226:LEU:HD13	1.80	0.64
1:B:342:TPO:HG22	1:B:365:THR:HB	1.80	0.63
1:B:448:LYS:H	1:B:448:LYS:HE2	1.65	0.61
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.81	0.60
1:C:266:PRO:HG2	1:C:321:GLU:HG2	1.83	0.59
1:A:400:LYS:O	1:A:404:GLU:HG3	2.02	0.59
1:D:400:LYS:O	1:D:404:GLU:HG3	2.03	0.59
1:D:265:MET:HE2	1:D:265:MET:HA	1.84	0.58
1:B:435:GLN:NE2	3:B:603:HOH:O	2.32	0.56
1:C:435:GLN:NE2	3:C:601:HOH:O	2.34	0.56
1:A:414:ILE:HD11	1:A:426:VAL:HG11	1.88	0.56
1:D:229:GLN:HE22	1:D:347:ARG:HH22	1.53	0.56
1:D:229:GLN:HE21	1:D:347:ARG:HH12	1.55	0.55
1:D:237:MET:HE1	1:D:246:VAL:O	2.06	0.55
1:A:221:ILE:HG21	1:A:226:LEU:HD13	1.90	0.54
1:A:429:MET:HB2	1:A:457:MET:SD	2.47	0.54
1:C:289:CYS:O	1:C:293:GLN:HG3	2.09	0.52
1:A:448:LYS:O	1:A:452:GLN:HG3	2.10	0.52
1:A:310:ARG:HD3	1:A:364:ILE:HD12	1.92	0.51
1:A:411:GLU:HA	1:A:414:ILE:HD12	1.93	0.51
1:D:219:VAL:HG23	1:D:221:ILE:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.94	0.50
1:D:414:ILE:CD1	1:D:426:VAL:HG11	2.42	0.49
1:A:332:LEU:HD22	1:A:349:VAL:HG21	1.94	0.49
1:C:286:HIS:NE2	1:C:290:LYS:HE2	2.27	0.49
1:D:409:THR:HG22	1:D:412:ASP:OD1	2.12	0.49
1:A:334:ARG:NH2	1:A:345:TPO:O1P	2.42	0.49
1:C:254:ASP:OD1	1:C:254:ASP:N	2.40	0.49
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.94	0.48
1:C:344:MET:SD	1:C:363:GLU:HG2	2.54	0.48
1:C:287:MET:HA	1:C:287:MET:HE2	1.95	0.48
1:A:409:THR:HG22	1:A:412:ASP:OD2	2.14	0.48
1:B:297:ASN:OD1	1:B:451:GLN:NE2	2.25	0.47
1:B:185:ILE:HD13	1:B:189:GLY:O	2.13	0.47
1:D:409:THR:HG23	1:D:411:GLU:H	1.79	0.47
1:B:174:LYS:HE2	1:B:179:ASN:OD1	2.15	0.47
1:B:388:ASP:O	1:B:394:GLN:HG2	2.15	0.47
1:B:332:LEU:HD13	1:B:349:VAL:HG13	1.97	0.46
1:C:171:TYR:HA	1:C:174:LYS:HD3	1.96	0.46
1:B:224:GLU:O	1:B:228:GLN:HG3	2.15	0.46
1:D:449:LYS:NZ	1:D:452:GLN:HE22	2.14	0.45
1:B:409:THR:HG23	1:B:412:ASP:H	1.81	0.45
1:D:253:SER:O	1:D:253:SER:OG	2.28	0.45
1:C:410:ILE:O	1:C:414:ILE:HG13	2.16	0.45
1:D:239:LYS:HD3	1:D:239:LYS:HA	1.65	0.45
1:C:237:MET:HE2	1:C:237:MET:HA	2.00	0.44
1:D:233:GLU:O	1:D:237:MET:HG3	2.17	0.44
1:A:174:LYS:HE2	1:A:179:ASN:OD1	2.17	0.43
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.00	0.43
1:A:237:MET:HE1	1:A:262:TYR:CE2	2.54	0.43
1:A:448:LYS:HB2	1:A:448:LYS:HE2	1.73	0.43
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.01	0.43
1:A:204:TYR:CZ	1:A:207:ASN:HA	2.54	0.43
1:D:440:LYS:HD2	1:D:443:LYS:HD2	2.01	0.43
1:D:334:ARG:NH2	1:D:345:TPO:O3P	2.45	0.43
1:A:265:MET:HA	1:A:265:MET:HE2	2.00	0.43
1:C:441:LYS:HG3	1:C:442:ASN:N	2.33	0.43
1:D:229:GLN:NE2	1:D:347:ARG:HH12	2.17	0.42
1:C:297:ASN:OD1	1:C:451:GLN:NE2	2.51	0.42
1:B:287:MET:HE2	1:B:287:MET:HA	2.02	0.42
1:C:300:ASN:HA	1:C:447:ILE:HG21	2.02	0.42
1:B:287:MET:HG3	3:B:720:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:O	1:B:399:ILE:HB	2.19	0.41
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.02	0.41
1:A:308:ILE:O	1:A:333:ALA:HA	2.21	0.40
1:D:284:SER:H	1:D:287:MET:CE	2.24	0.40
1:B:286:HIS:CE1	1:B:290:LYS:HZ3	2.40	0.40
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.03	0.40
1:C:400:LYS:HD3	1:C:400:LYS:C	2.46	0.40
1:B:286:HIS:CE1	1:B:290:LYS:NZ	2.89	0.40
1:B:448:LYS:H	1:B:448:LYS:CE	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	279/307 (91%)	273 (98%)	6 (2%)	0	100	100
1	B	280/307 (91%)	275 (98%)	5 (2%)	0	100	100
1	C	277/307 (90%)	272 (98%)	5 (2%)	0	100	100
1	D	283/307 (92%)	276 (98%)	7 (2%)	0	100	100
All	All	1119/1228 (91%)	1096 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	246/265 (93%)	246 (100%)	0	100	100
1	B	235/265 (89%)	234 (100%)	1 (0%)	84	82
1	C	235/265 (89%)	234 (100%)	1 (0%)	84	82
1	D	244/265 (92%)	244 (100%)	0	100	100
All	All	960/1060 (91%)	958 (100%)	2 (0%)	87	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	343	VAL
1	C	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	232	GLN
1	A	293	GLN
1	A	394	GLN
1	A	452	GLN
1	B	286	HIS
1	B	394	GLN
1	B	435	GLN
1	B	442	ASN
1	C	229	GLN
1	C	305	ASN
1	D	229	GLN
1	D	451	GLN
1	D	452	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	B	345	1	8,10,11	0.73	0	10,14,16	0.97	1 (10%)
1	SEP	B	346	1	8,9,10	0.60	0	7,12,14	0.61	0
1	SEP	A	346	1	8,9,10	1.64	1 (12%)	7,12,14	1.38	1 (14%)
1	TPO	D	342	1	8,10,11	1.76	1 (12%)	10,14,16	1.67	1 (10%)
1	TPO	D	345	1	8,10,11	1.14	0	10,14,16	1.94	1 (10%)
1	SEP	D	346	1	8,9,10	1.62	1 (12%)	7,12,14	1.11	1 (14%)
1	TPO	B	342	1	8,10,11	0.77	0	10,14,16	1.13	1 (10%)
1	TPO	A	342	1	8,10,11	1.76	1 (12%)	10,14,16	1.70	1 (10%)
1	TPO	C	345	1	8,10,11	0.73	0	10,14,16	0.95	1 (10%)
1	SEP	C	346	1	8,9,10	0.66	0	7,12,14	0.63	0
1	TPO	A	345	1	8,10,11	1.66	1 (12%)	10,14,16	1.95	1 (10%)

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
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	D	342	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	1/6/8/10	-
1	TPO	B	342	1	-	6/9/11/13	-
1	TPO	A	342	1	-	3/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	SEP	P-O1P	3.58	1.61	1.50
1	A	342	TPO	P-O1P	3.57	1.61	1.50
1	D	342	TPO	P-O1P	3.54	1.61	1.50
1	A	345	TPO	P-O1P	3.53	1.61	1.50
1	D	346	SEP	P-O1P	3.53	1.61	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	TPO	P-OG1-CB	-5.51	108.35	123.33
1	A	345	TPO	P-OG1-CB	-5.51	108.36	123.33
1	A	342	TPO	P-OG1-CB	-4.56	110.95	123.33
1	D	342	TPO	P-OG1-CB	-4.55	110.96	123.33
1	A	346	SEP	OG-CB-CA	3.02	111.09	108.14
1	B	342	TPO	O-C-CA	-2.54	118.23	124.77
1	B	345	TPO	O-C-CA	-2.39	118.63	124.77
1	C	345	TPO	O-C-CA	-2.28	118.91	124.77
1	D	346	SEP	OG-CB-CA	2.26	110.35	108.14

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	342	TPO	N-CA-CB-OG1
1	A	342	TPO	C-CA-CB-CG2
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	C-CA-CB-OG
1	B	342	TPO	N-CA-CB-CG2
1	B	342	TPO	N-CA-CB-OG1
1	B	342	TPO	C-CA-CB-CG2
1	B	342	TPO	O-C-CA-CB
1	B	342	TPO	CG2-CB-OG1-P
1	B	345	TPO	N-CA-CB-OG1
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	D	342	TPO	N-CA-CB-OG1
1	D	342	TPO	C-CA-CB-CG2
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	A	342	TPO	N-CA-CB-CG2
1	D	342	TPO	N-CA-CB-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	346	SEP	CA-CB-OG-P
1	C	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O1P
1	D	346	SEP	CB-OG-P-O1P
1	B	342	TPO	CB-OG1-P-O3P
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	345	TPO	1	0
1	B	342	TPO	1	0
1	A	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	X1T	D	501	-	32,33,33	0.57	0	34,46,46	0.85	2 (5%)
2	X1T	C	501	-	32,33,33	0.58	0	34,46,46	0.83	1 (2%)
2	X1T	A	501	-	32,33,33	0.57	0	34,46,46	0.85	2 (5%)
2	X1T	B	501	-	32,33,33	0.57	0	34,46,46	0.86	2 (5%)

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	X1T	D	501	-	-	2/19/26/26	0/4/4/4
2	X1T	C	501	-	-	1/19/26/26	0/4/4/4
2	X1T	A	501	-	-	2/19/26/26	0/4/4/4
2	X1T	B	501	-	-	2/19/26/26	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	X1T	O2-C11-N3	2.44	125.84	122.27
2	B	501	X1T	O2-C11-N3	2.41	125.80	122.27
2	A	501	X1T	O2-C11-N3	2.40	125.77	122.27
2	C	501	X1T	O2-C11-N3	2.40	125.77	122.27
2	B	501	X1T	C10-N3-C11	2.14	129.82	123.04
2	A	501	X1T	C10-N3-C11	2.13	129.81	123.04
2	D	501	X1T	C10-N3-C11	2.12	129.76	123.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

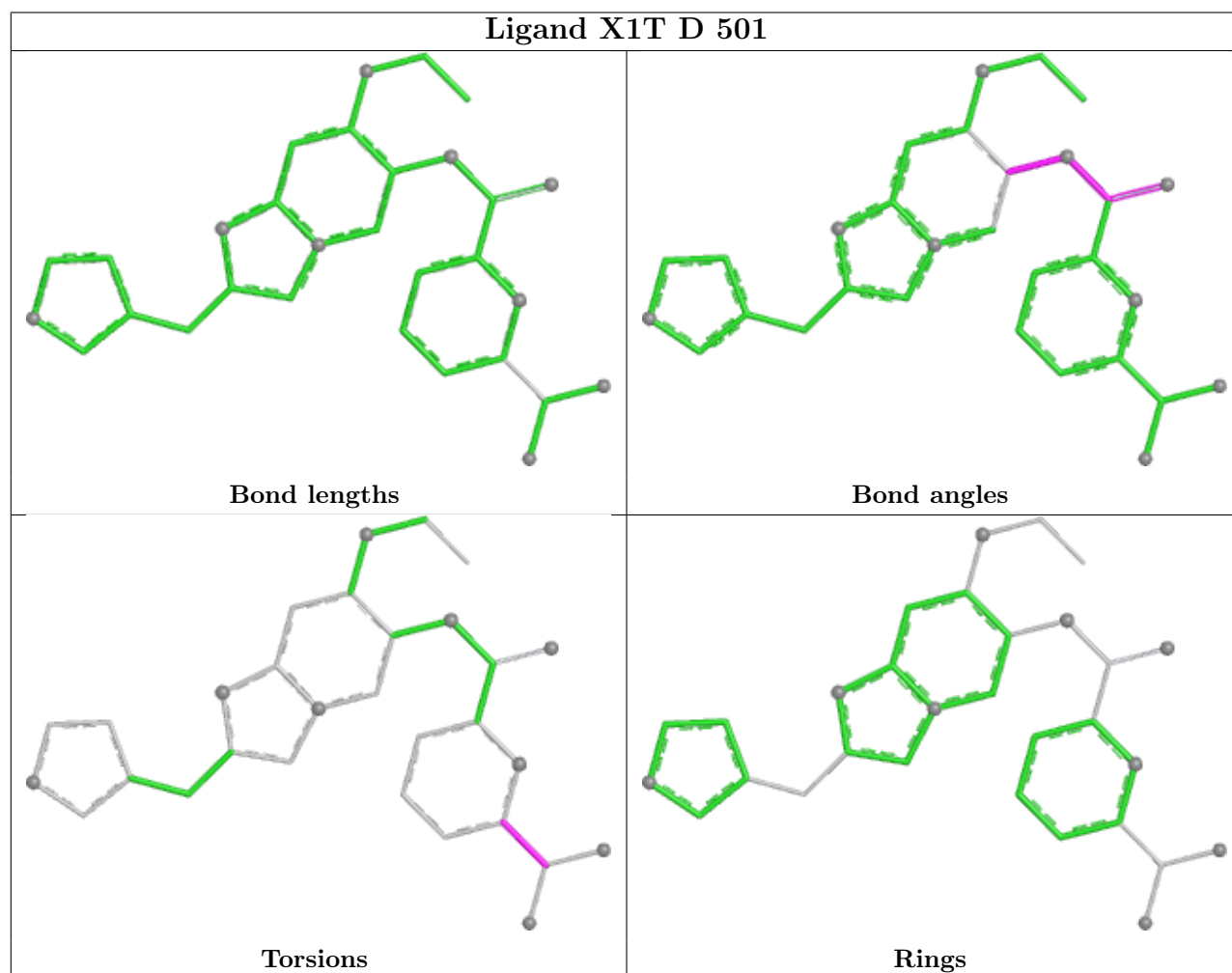
Mol	Chain	Res	Type	Atoms
2	A	501	X1T	N4-C16-C17-F1
2	B	501	X1T	N4-C16-C17-F1
2	D	501	X1T	N4-C16-C17-F1
2	A	501	X1T	N4-C16-C17-F2
2	B	501	X1T	N4-C16-C17-F2
2	C	501	X1T	N4-C16-C17-F2
2	D	501	X1T	N4-C16-C17-F2

There are no ring outliers.

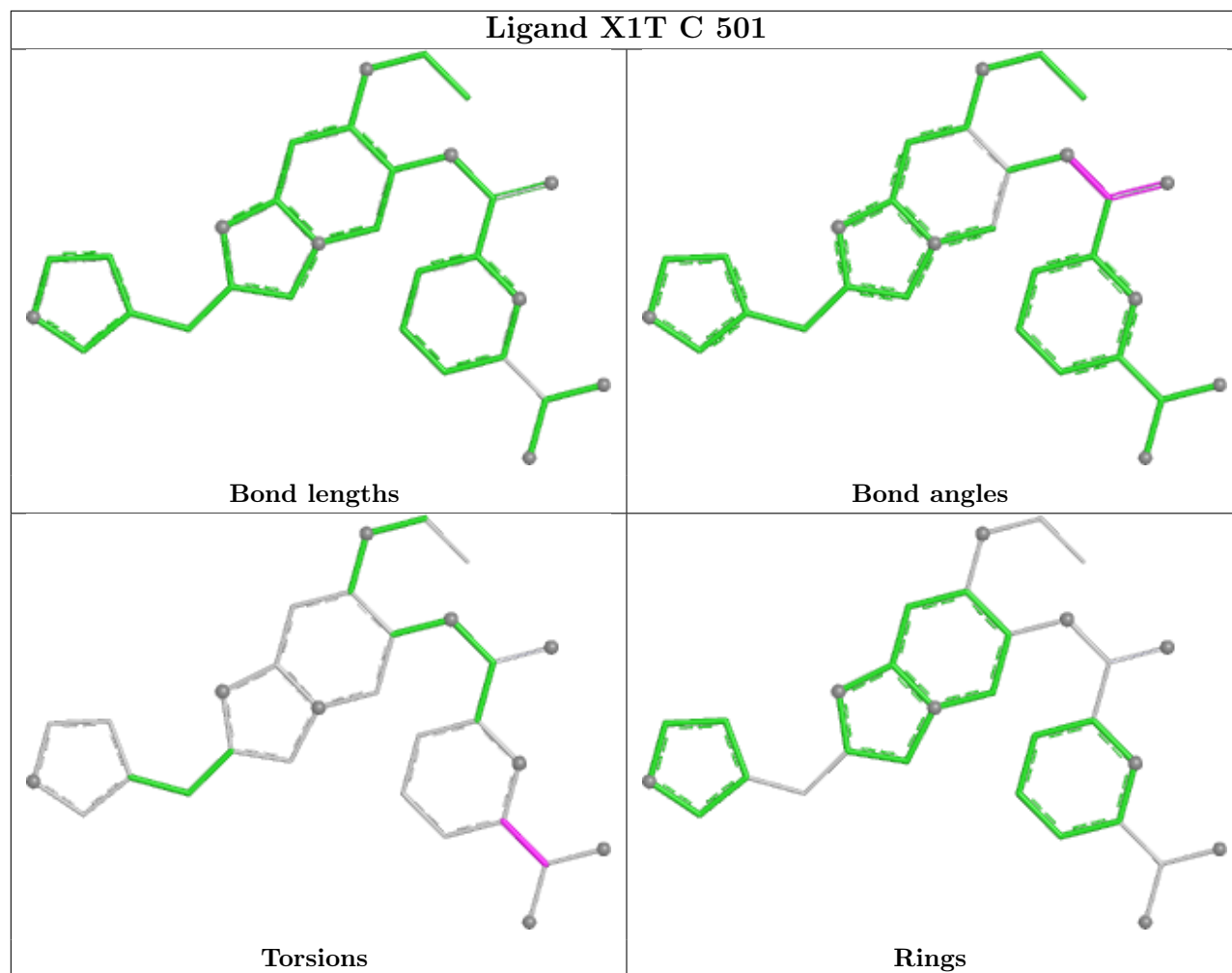
No monomer is involved in short contacts.

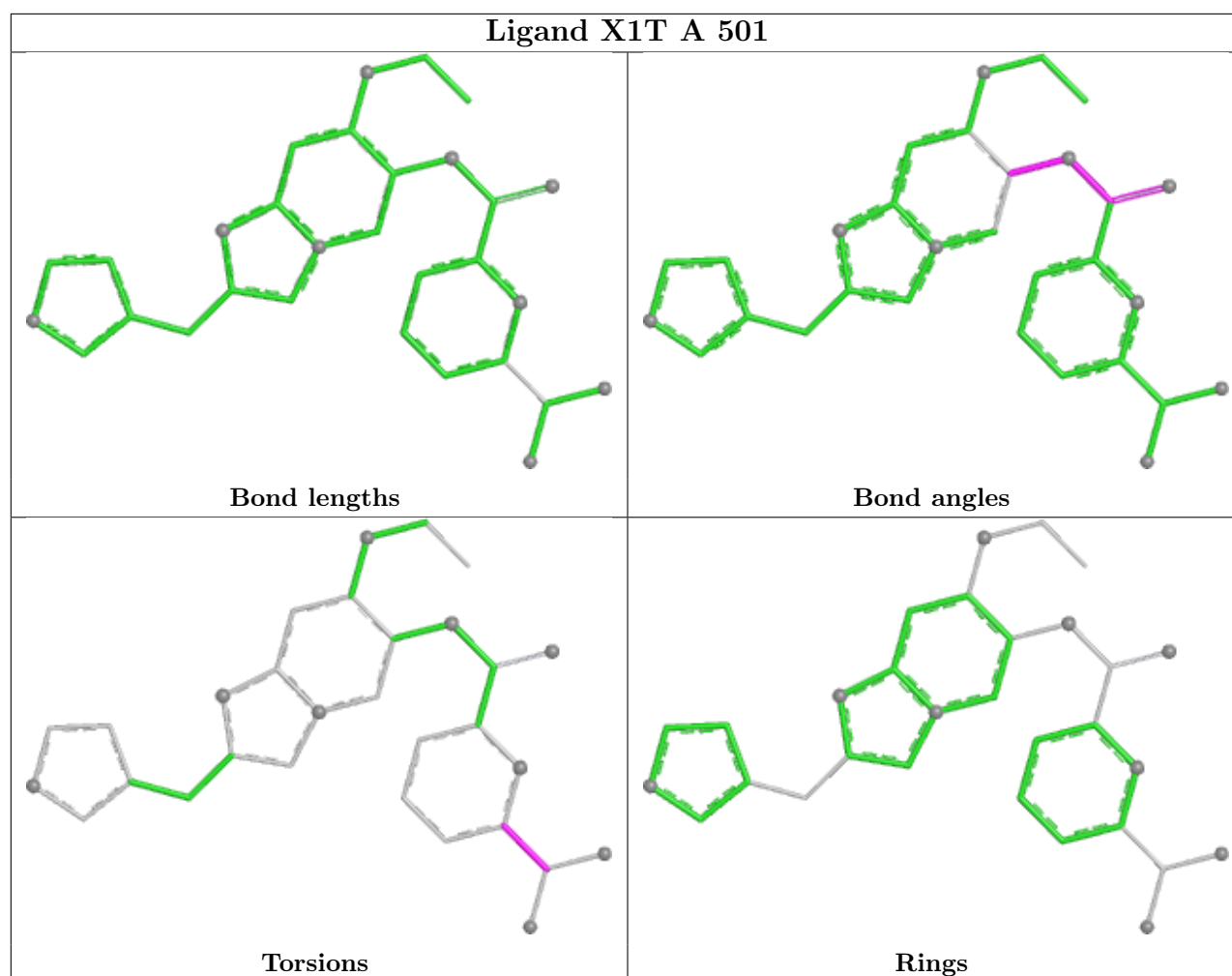
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

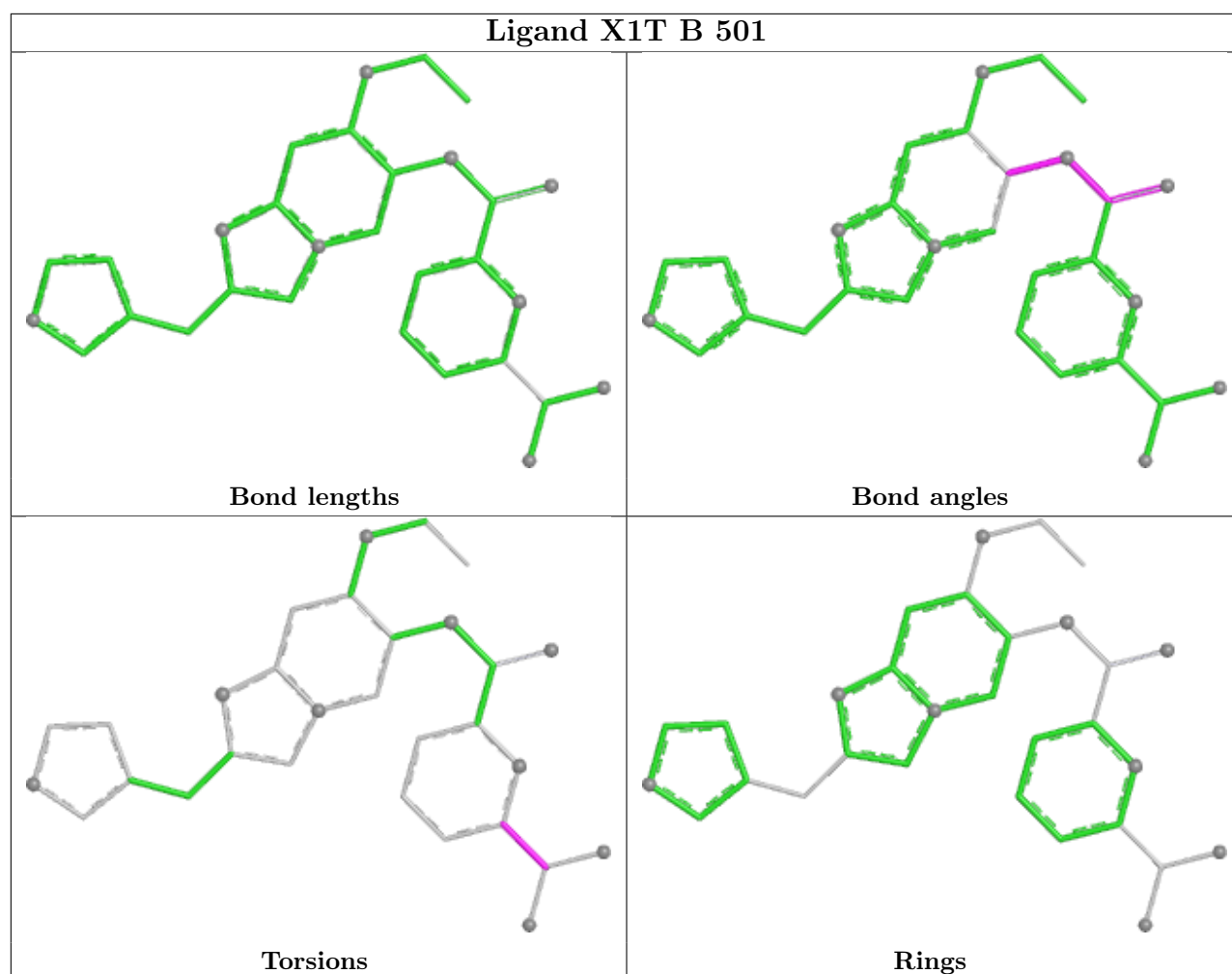
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 X1T C 501







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	286/307 (93%)	0.77	30 (10%)	11 11	25, 40, 69, 94	0
1	B	285/307 (92%)	0.70	26 (9%)	15 15	24, 37, 63, 84	0
1	C	285/307 (92%)	0.48	14 (4%)	35 38	22, 35, 60, 73	0
1	D	288/307 (93%)	0.69	26 (9%)	15 15	25, 40, 65, 85	0
All	All	1144/1228 (93%)	0.66	96 (8%)	17 17	22, 38, 65, 94	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	VAL	5.7
1	C	459	ALA	4.9
1	B	219	VAL	4.6
1	A	187	VAL	4.5
1	B	187	VAL	4.5
1	C	221	ILE	4.5
1	B	459	ALA	4.4
1	B	344	MET	4.1
1	D	336	SER	4.0
1	C	219	VAL	4.0
1	D	221	ILE	3.8
1	A	223	THR	3.8
1	C	343	VAL	3.7
1	B	335	ALA	3.7
1	A	221	ILE	3.6
1	A	219	VAL	3.6
1	D	335	ALA	3.5
1	D	163	THR	3.5
1	D	255	GLY	3.5
1	D	187	VAL	3.4
1	C	164	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	254	ASP	3.3
1	B	347	ARG	3.3
1	B	343	VAL	3.2
1	D	343	VAL	3.2
1	C	409	THR	3.0
1	B	399	ILE	3.0
1	C	407	GLU	2.9
1	D	253	SER	2.9
1	A	164	ARG	2.9
1	B	164	ARG	2.8
1	B	397	LEU	2.8
1	A	239	LYS	2.8
1	D	344	MET	2.8
1	A	166	HIS	2.8
1	A	236	VAL	2.8
1	A	408	LYS	2.7
1	C	399	ILE	2.7
1	B	409	THR	2.6
1	B	424	THR	2.6
1	A	185	ILE	2.6
1	D	256	ASP	2.6
1	D	254	ASP	2.5
1	A	189	GLY	2.5
1	C	439	GLU	2.5
1	A	409	THR	2.5
1	D	407	GLU	2.4
1	D	196	GLY	2.4
1	A	226	LEU	2.4
1	A	410	ILE	2.4
1	D	194	GLU	2.4
1	A	240	CYS	2.4
1	C	397	LEU	2.3
1	B	216	ALA	2.3
1	D	459	ALA	2.3
1	B	206	ASN	2.3
1	A	167	SER	2.3
1	D	186	SER	2.3
1	B	223	THR	2.3
1	A	217	ALA	2.3
1	C	171	TYR	2.3
1	B	256	ASP	2.3
1	D	205	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	207	ASN	2.3
1	A	204	TYR	2.2
1	C	336	SER	2.2
1	B	403	ILE	2.2
1	D	185	ILE	2.2
1	A	364	ILE	2.2
1	A	434	SER	2.2
1	D	240	CYS	2.2
1	B	408	LYS	2.2
1	A	344	MET	2.1
1	A	401	GLU	2.1
1	B	407	GLU	2.1
1	B	410	ILE	2.1
1	C	349	VAL	2.1
1	A	215	LEU	2.1
1	B	221	ILE	2.1
1	D	413	TYR	2.1
1	A	253	SER	2.1
1	A	182	GLU	2.1
1	B	390	HIS	2.1
1	B	455	GLN	2.1
1	C	286	HIS	2.1
1	D	228	GLN	2.1
1	D	395	LEU	2.1
1	D	217	ALA	2.1
1	B	405	ASP	2.1
1	A	230	PHE	2.0
1	D	408	LYS	2.0
1	A	459	ALA	2.0
1	A	405	ASP	2.0
1	D	237	MET	2.0
1	A	424	THR	2.0
1	B	196	GLY	2.0

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

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
1	TPO	D	342	11/12	0.60	0.21	70,76,88,91	0
1	TPO	A	342	11/12	0.62	0.22	70,76,88,91	0
1	TPO	B	342	11/12	0.70	0.20	70,76,88,91	0
1	SEP	C	346	10/11	0.71	0.17	53,68,91,92	0
1	SEP	D	346	10/11	0.77	0.14	56,74,105,109	0
1	SEP	B	346	10/11	0.82	0.12	53,68,91,92	0
1	SEP	A	346	10/11	0.82	0.11	53,68,91,92	0
1	TPO	B	345	11/12	0.84	0.14	41,50,56,72	0
1	TPO	A	345	11/12	0.88	0.11	41,50,56,72	0
1	TPO	D	345	11/12	0.91	0.10	41,50,56,72	0
1	TPO	C	345	11/12	0.91	0.11	43,45,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

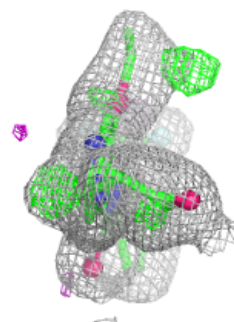
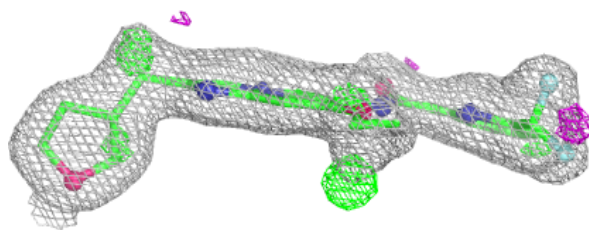
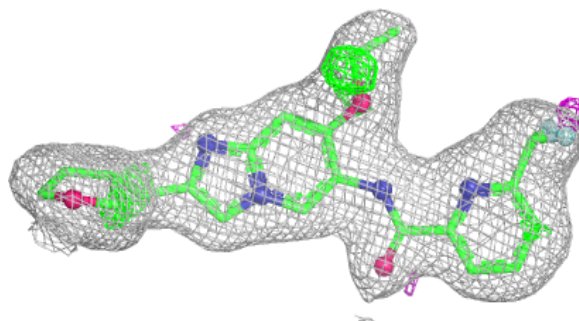
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	X1T	A	501	30/30	0.91	0.11	29,34,48,50	0
2	X1T	B	501	30/30	0.93	0.11	29,34,48,50	0
2	X1T	C	501	30/30	0.94	0.11	29,34,48,50	0
2	X1T	D	501	30/30	0.94	0.09	29,34,48,50	0

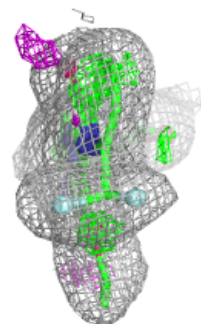
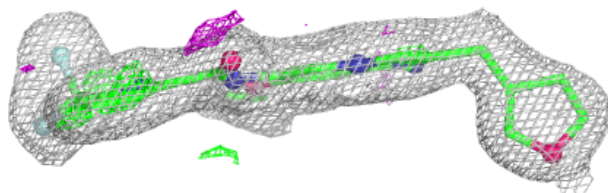
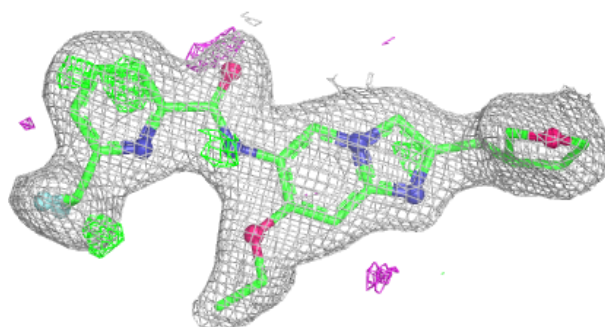
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X1T A 501:

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

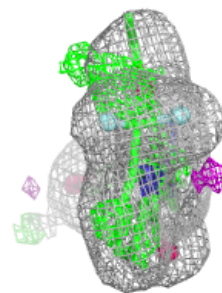
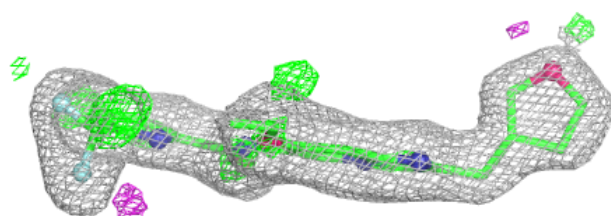
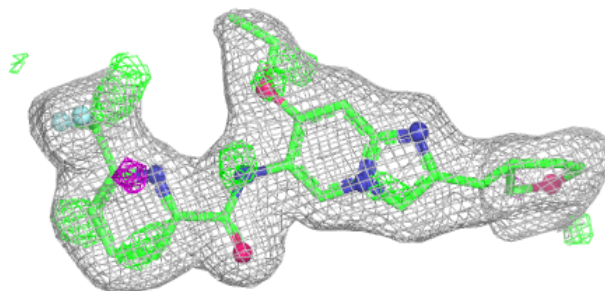
**Electron density around X1T B 501:**

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

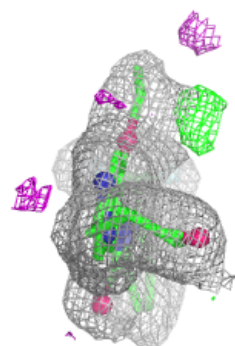
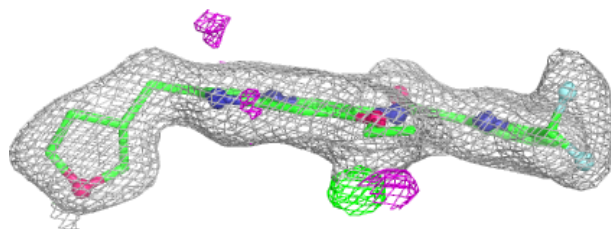
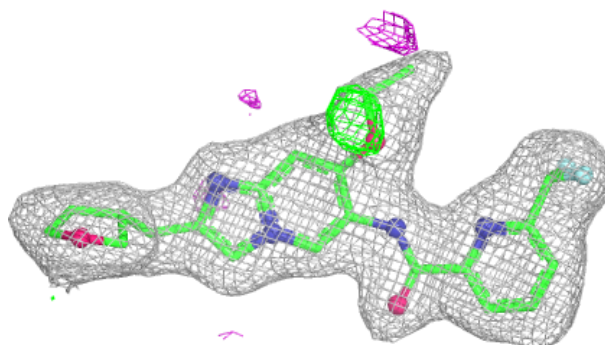


Electron density around X1T C 501:

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

**Electron density around X1T D 501:**

$2mF_o-DF_c$ (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.