



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:18 AM UTC

PDB ID : 6UYA / pdb_00006uya
Title : Crystal structure of Compound 19 bound to IRAK4
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Deposited on : 2019-11-12
Resolution : 1.74 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

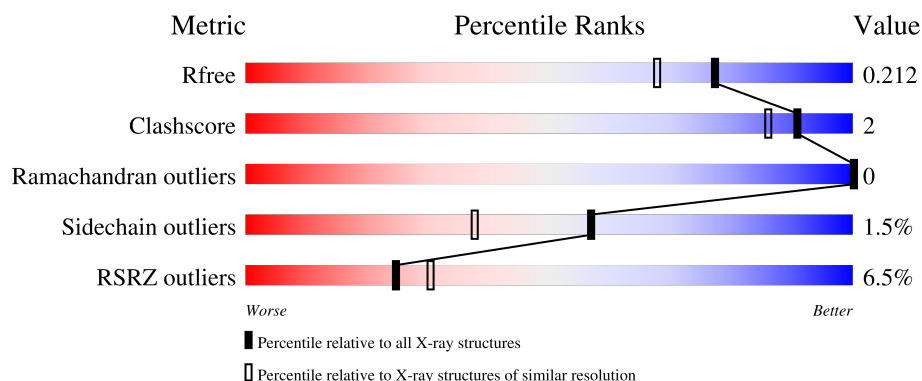
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	320	6% 84% 6% 10%
1	B	320	3% 85% 6% 9%
1	C	320	9% 79% 8% 13%
1	D	320	5% 86% 5% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10096 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	288	Total	C	N	O	P	S	0	1	0
			2270	1423	380	450	3	14			
1	B	290	Total	C	N	O	P	S	0	2	0
			2293	1439	384	452	3	15			
1	C	278	Total	C	N	O	P	S	0	1	0
			2207	1384	371	434	3	15			
1	D	291	Total	C	N	O	P	S	0	1	0
			2294	1439	386	451	3	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	-	initiating methionine	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	expression tag	UNP Q9NWZ3
A	147	HIS	-	expression tag	UNP Q9NWZ3
A	148	HIS	-	expression tag	UNP Q9NWZ3
A	149	HIS	-	expression tag	UNP Q9NWZ3
A	150	HIS	-	expression tag	UNP Q9NWZ3
A	151	GLY	-	expression tag	UNP Q9NWZ3
A	152	GLU	-	expression tag	UNP Q9NWZ3
A	153	ASN	-	expression tag	UNP Q9NWZ3
A	154	LEU	-	expression tag	UNP Q9NWZ3
A	155	TYR	-	expression tag	UNP Q9NWZ3
A	156	PHE	-	expression tag	UNP Q9NWZ3
A	157	GLN	-	expression tag	UNP Q9NWZ3
A	158	GLY	-	expression tag	UNP Q9NWZ3
A	159	SER	-	expression tag	UNP Q9NWZ3
A	461	GLY	-	expression tag	UNP Q9NWZ3
A	462	ASN	-	expression tag	UNP Q9NWZ3
A	463	SER	-	expression tag	UNP Q9NWZ3
B	144	MET	-	initiating methionine	UNP Q9NWZ3
B	145	HIS	-	expression tag	UNP Q9NWZ3

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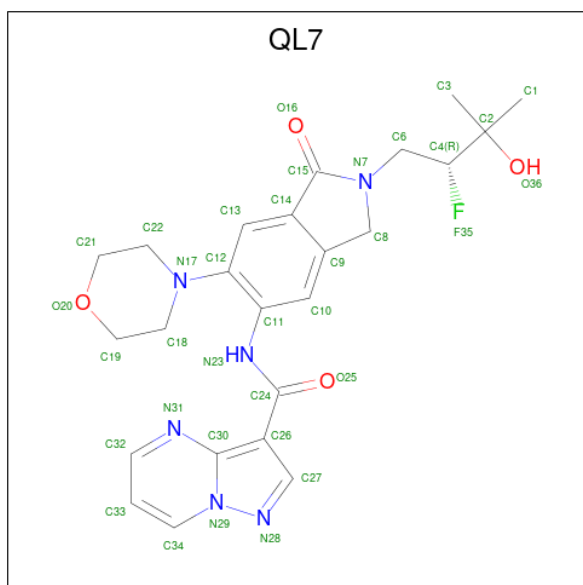
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	UNP Q9NWZ3
B	153	ASN	-	expression tag	UNP Q9NWZ3
B	154	LEU	-	expression tag	UNP Q9NWZ3
B	155	TYR	-	expression tag	UNP Q9NWZ3
B	156	PHE	-	expression tag	UNP Q9NWZ3
B	157	GLN	-	expression tag	UNP Q9NWZ3
B	158	GLY	-	expression tag	UNP Q9NWZ3
B	159	SER	-	expression tag	UNP Q9NWZ3
B	461	GLY	-	expression tag	UNP Q9NWZ3
B	462	ASN	-	expression tag	UNP Q9NWZ3
B	463	SER	-	expression tag	UNP Q9NWZ3
C	144	MET	-	initiating methionine	UNP Q9NWZ3
C	145	HIS	-	expression tag	UNP Q9NWZ3
C	146	HIS	-	expression tag	UNP Q9NWZ3
C	147	HIS	-	expression tag	UNP Q9NWZ3
C	148	HIS	-	expression tag	UNP Q9NWZ3
C	149	HIS	-	expression tag	UNP Q9NWZ3
C	150	HIS	-	expression tag	UNP Q9NWZ3
C	151	GLY	-	expression tag	UNP Q9NWZ3
C	152	GLU	-	expression tag	UNP Q9NWZ3
C	153	ASN	-	expression tag	UNP Q9NWZ3
C	154	LEU	-	expression tag	UNP Q9NWZ3
C	155	TYR	-	expression tag	UNP Q9NWZ3
C	156	PHE	-	expression tag	UNP Q9NWZ3
C	157	GLN	-	expression tag	UNP Q9NWZ3
C	158	GLY	-	expression tag	UNP Q9NWZ3
C	159	SER	-	expression tag	UNP Q9NWZ3
C	461	GLY	-	expression tag	UNP Q9NWZ3
C	462	ASN	-	expression tag	UNP Q9NWZ3
C	463	SER	-	expression tag	UNP Q9NWZ3
D	144	MET	-	initiating methionine	UNP Q9NWZ3
D	145	HIS	-	expression tag	UNP Q9NWZ3
D	146	HIS	-	expression tag	UNP Q9NWZ3
D	147	HIS	-	expression tag	UNP Q9NWZ3
D	148	HIS	-	expression tag	UNP Q9NWZ3
D	149	HIS	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	150	HIS	-	expression tag	UNP Q9NWZ3
D	151	GLY	-	expression tag	UNP Q9NWZ3
D	152	GLU	-	expression tag	UNP Q9NWZ3
D	153	ASN	-	expression tag	UNP Q9NWZ3
D	154	LEU	-	expression tag	UNP Q9NWZ3
D	155	TYR	-	expression tag	UNP Q9NWZ3
D	156	PHE	-	expression tag	UNP Q9NWZ3
D	157	GLN	-	expression tag	UNP Q9NWZ3
D	158	GLY	-	expression tag	UNP Q9NWZ3
D	159	SER	-	expression tag	UNP Q9NWZ3
D	461	GLY	-	expression tag	UNP Q9NWZ3
D	462	ASN	-	expression tag	UNP Q9NWZ3
D	463	SER	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-{2-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]-6-(morpholin-4-yl)-1-oxo-2,3-dihydro-1H-isoindol-5-yl}pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: QL7) (formula: C₂₄H₂₇FN₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 35	C 24	F 1	N 6	O 4	0	0
2	B	1	Total 35	C 24	F 1	N 6	O 4	0	0
2	C	1	Total 35	C 24	F 1	N 6	O 4	0	0
2	D	1	Total 35	C 24	F 1	N 6	O 4	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

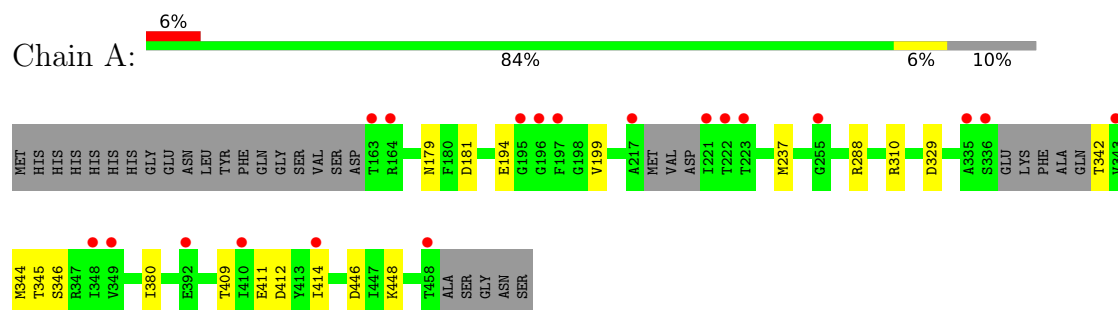
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	245	Total	O	0	0
			245	245		
4	B	253	Total	O	0	0
			253	253		
4	C	182	Total	O	0	0
			182	182		
4	D	207	Total	O	0	0
			207	207		

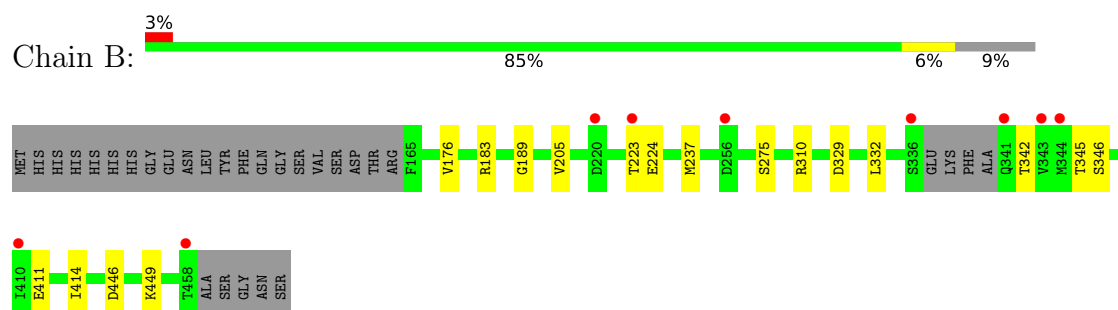
3 Residue-property plots [i](#)

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.

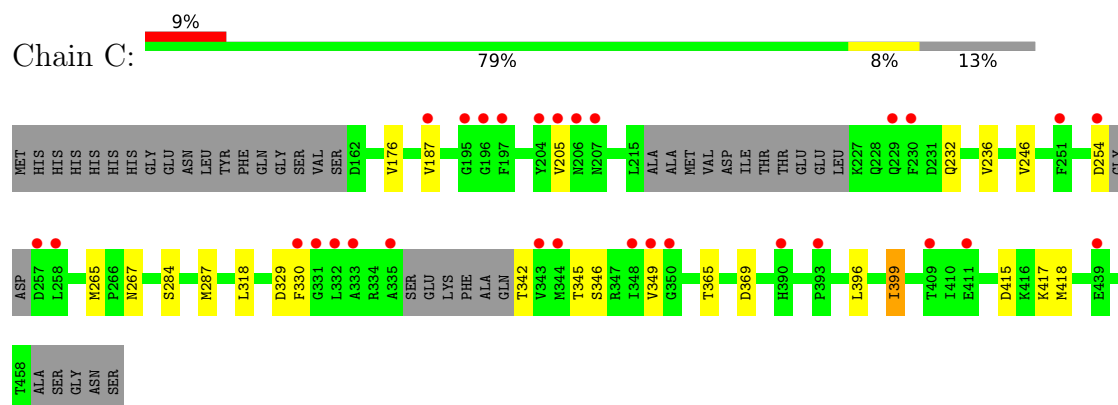
- Molecule 1: Interleukin-1 receptor-associated kinase 4



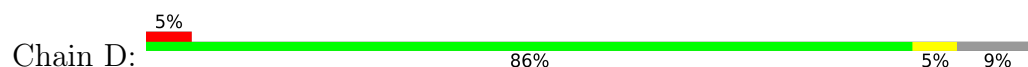
- Molecule 1: Interleukin-1 receptor-associated kinase 4

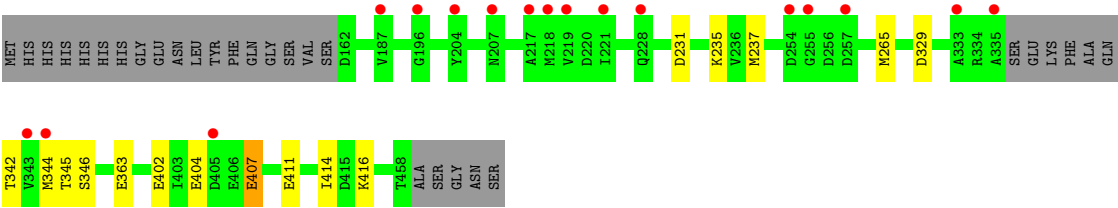


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	140.88Å 140.18Å 87.56Å 90.00° 123.20° 90.00°	Depositor
Resolution (Å)	25.48 – 1.74 25.48 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.48-1.74) 99.6 (25.48-1.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.181 , 0.207 0.186 , 0.212	Depositor DCC
R_{free} test set	7278 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	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	0.96	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 19.97 % 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 9.6386e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QL7, SEP, SO4, TPO

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	0.83	0/2277	1.13	2/3069 (0.1%)
1	B	0.82	0/2303	1.08	1/3104 (0.0%)
1	C	0.83	1/2213 (0.0%)	1.11	3/2979 (0.1%)
1	D	0.82	1/2302 (0.0%)	1.12	0/3103
All	All	0.82	2/9095 (0.0%)	1.11	6/12255 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	265	MET	SD-CE	-7.28	1.61	1.79
1	C	265	MET	SD-CE	-5.27	1.66	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	446	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	369	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	181	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	254	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	446	ASP	CA-CB-CG	5.11	117.71	112.60

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	2270	0	2232	7	0
1	B	2293	0	2261	7	0
1	C	2207	0	2170	12	0
1	D	2294	0	2263	6	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	B	5	0	0	0	0
4	A	245	0	0	2	0
4	B	253	0	0	0	0
4	C	182	0	0	3	0
4	D	207	0	0	0	0
All	All	10096	0	8926	31	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 2.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:SER:H	1:C:287[B]:MET:HE3	1.26	0.98
1:D:231:ASP:O	1:D:235:LYS:HG2	2.00	0.61
1:C:287[B]:MET:HE2	4:C:747:HOH:O	2.04	0.58
1:A:411:GLU:O	1:A:414:ILE:HG22	2.04	0.58
1:C:236:VAL:HG21	1:C:330:PHE:HB3	1.86	0.58
1:C:284:SER:OG	1:C:287[B]:MET:HG3	2.04	0.58
1:D:237:MET:HA	1:D:237:MET:HE2	1.87	0.57
1:C:287[B]:MET:HE1	4:C:653:HOH:O	2.06	0.55
1:B:176:VAL:HG21	1:B:205[A]:VAL:HG12	1.89	0.55
1:B:183[B]:ARG:HB2	1:B:189:GLY:HA3	1.89	0.54
1:A:237:MET:HA	1:A:237:MET:HE2	1.91	0.53
1:A:179:ASN:HB2	4:A:809:HOH:O	2.09	0.51
1:C:232:GLN:O	1:C:236:VAL:HG22	2.10	0.51
1:C:284:SER:N	1:C:287[B]:MET:HE3	2.10	0.50
1:D:344:MET:HG2	1:D:363:GLU:HA	1.96	0.48
1:A:409:THR:HG22	1:A:412:ASP:CG	2.42	0.44
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.99	0.44
1:C:417:LYS:HE2	4:C:613:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:HB2	1:D:416:LYS:HD2	2.00	0.44
1:D:411:GLU:O	1:D:414:ILE:HG22	2.17	0.44
1:C:176:VAL:HG11	1:C:205:VAL:HG22	2.01	0.43
1:B:176:VAL:CG2	1:B:205[A]:VAL:HG12	2.48	0.43
1:C:396:LEU:O	1:C:399:ILE:HB	2.19	0.43
1:B:237:MET:HA	1:B:237:MET:HE2	2.00	0.43
1:A:310:ARG:HD2	4:A:796:HOH:O	2.19	0.42
1:B:411:GLU:O	1:B:414:ILE:HG22	2.20	0.42
1:A:288:ARG:HB3	1:A:380:ILE:HG23	2.02	0.41
1:C:415:ASP:HB3	1:C:418:MET:HE2	2.02	0.41
1:B:310:ARG:HD3	1:B:332:LEU:O	2.21	0.41
1:D:402:GLU:O	1:D:407:GLU:HG2	2.21	0.40
1:A:194:GLU:HB3	1:A:199:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/320 (88%)	276 (98%)	5 (2%)	0	100	100
1	B	285/320 (89%)	279 (98%)	6 (2%)	0	100	100
1	C	269/320 (84%)	263 (98%)	6 (2%)	0	100	100
1	D	286/320 (89%)	276 (96%)	10 (4%)	0	100	100
All	All	1121/1280 (88%)	1094 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/275 (90%)	244 (99%)	3 (1%)	63	47
1	B	250/275 (91%)	246 (98%)	4 (2%)	55	35
1	C	241/275 (88%)	236 (98%)	5 (2%)	47	24
1	D	249/275 (90%)	246 (99%)	3 (1%)	63	47
All	All	987/1100 (90%)	972 (98%)	15 (2%)	57	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	344	MET
1	A	448	LYS
1	B	223	THR
1	B	224	GLU
1	B	329	ASP
1	B	449	LYS
1	C	187	VAL
1	C	329	ASP
1	C	349	VAL
1	C	365	THR
1	C	399	ILE
1	D	329	ASP
1	D	404	GLU
1	D	407	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	B	206	ASN
1	B	390	HIS
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	390	HIS
1	C	452	GLN
1	D	166	HIS
1	D	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	A	345	1	8,10,11	1.24	1 (12%)	10,14,16	1.20	1 (10%)
1	TPO	D	342	1	8,10,11	1.17	1 (12%)	10,14,16	1.49	2 (20%)
1	TPO	D	345	1	8,10,11	1.44	1 (12%)	10,14,16	1.31	1 (10%)
1	TPO	C	342	1	8,10,11	1.47	1 (12%)	10,14,16	1.23	1 (10%)
1	SEP	A	346	1	8,9,10	0.83	0	7,12,14	1.93	2 (28%)
1	TPO	B	342	1	8,10,11	1.42	1 (12%)	10,14,16	1.03	1 (10%)
1	SEP	D	346	1	8,9,10	0.82	0	7,12,14	2.81	2 (28%)
1	TPO	A	342	1	8,10,11	1.00	1 (12%)	10,14,16	1.35	2 (20%)
1	SEP	C	346	1	8,9,10	0.91	0	7,12,14	2.51	2 (28%)
1	TPO	B	345	1	8,10,11	1.09	1 (12%)	10,14,16	1.37	1 (10%)
1	SEP	B	346	1	8,9,10	1.12	0	7,12,14	1.29	1 (14%)
1	TPO	C	345	1	8,10,11	1.21	1 (12%)	10,14,16	1.35	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
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	D	342	1	-	0/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-
1	TPO	C	342	1	-	2/9/11/13	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	A	342	1	-	0/9/11/13	-
1	SEP	C	346	1	-	2/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-3.38	1.53	1.59
1	B	342	TPO	P-OG1	-3.36	1.53	1.59
1	A	345	TPO	CB-CA	2.72	1.59	1.53
1	D	342	TPO	P-OG1	-2.54	1.55	1.59
1	D	345	TPO	P-OG1	-2.42	1.55	1.59
1	C	345	TPO	P-OG1	-2.16	1.55	1.59
1	A	342	TPO	P-OG1	-2.15	1.55	1.59
1	B	345	TPO	CG2-CB	2.08	1.56	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	6.93	114.89	108.14
1	C	346	SEP	OG-CB-CA	5.96	113.95	108.14
1	A	346	SEP	OG-CB-CA	4.14	112.17	108.14
1	D	342	TPO	P-OG1-CB	-3.43	114.00	123.33
1	D	345	TPO	O3P-P-OG1	2.91	117.20	105.85
1	B	346	SEP	OG-P-O1P	2.91	114.31	106.44
1	B	345	TPO	O2P-P-OG1	2.82	116.83	105.85
1	C	345	TPO	O2P-P-OG1	2.66	116.21	105.85
1	A	342	TPO	P-OG1-CB	-2.44	116.70	123.33
1	C	346	SEP	OG-P-O1P	2.43	113.02	106.44
1	D	346	SEP	O3P-P-OG	2.39	112.90	106.67
1	A	346	SEP	O3P-P-OG	2.37	112.85	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	CG2-CB-CA	-2.25	108.88	113.26
1	C	345	TPO	P-OG1-CB	-2.19	117.38	123.33
1	A	345	TPO	OG1-P-O1P	2.18	117.12	109.33
1	D	342	TPO	O3P-P-OG1	2.14	114.18	105.85
1	B	342	TPO	O3P-P-OG1	2.09	114.00	105.85
1	C	342	TPO	O3P-P-OG1	2.03	113.76	105.85

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	N-CA-CB-OG
1	C	346	SEP	C-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	A	345	TPO	CB-OG1-P-O2P
1	C	342	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O1P
1	B	342	TPO	C-CA-CB-CG2
1	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	QL7	D	501	-	37,39,39	0.60	1 (2%)	48,58,58	0.86	3 (6%)
2	QL7	B	502	-	37,39,39	0.61	0	48,58,58	0.95	3 (6%)
2	QL7	A	501	-	37,39,39	0.61	0	48,58,58	0.89	3 (6%)
2	QL7	C	501	-	37,39,39	0.55	0	48,58,58	0.85	2 (4%)
3	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.07	0

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	QL7	C	501	-	-	4/19/42/42	0/5/5/5
2	QL7	D	501	-	-	4/19/42/42	0/5/5/5
2	QL7	B	502	-	-	4/19/42/42	0/5/5/5
2	QL7	A	501	-	-	4/19/42/42	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	QL7	C26-C30	-2.12	1.39	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	QL7	C32-N31-C30	2.86	117.77	115.55
2	B	502	QL7	C11-C10-C9	-2.68	117.77	121.81
2	C	501	QL7	C11-C10-C9	-2.51	118.02	121.81
2	A	501	QL7	C11-C10-C9	-2.46	118.09	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	QL7	C6-N7-C15	2.31	125.97	123.67
2	C	501	QL7	C32-N31-C30	2.10	117.18	115.55
2	D	501	QL7	C11-C10-C9	-2.07	118.68	121.81
2	A	501	QL7	C34-N29-C30	-2.05	118.71	122.70
2	D	501	QL7	C34-N29-C30	-2.04	118.73	122.70
2	B	502	QL7	C34-N29-C30	-2.01	118.79	122.70
2	A	501	QL7	C32-N31-C30	2.00	117.10	115.55

There are no chirality outliers.

All (16) torsion outliers are listed below:

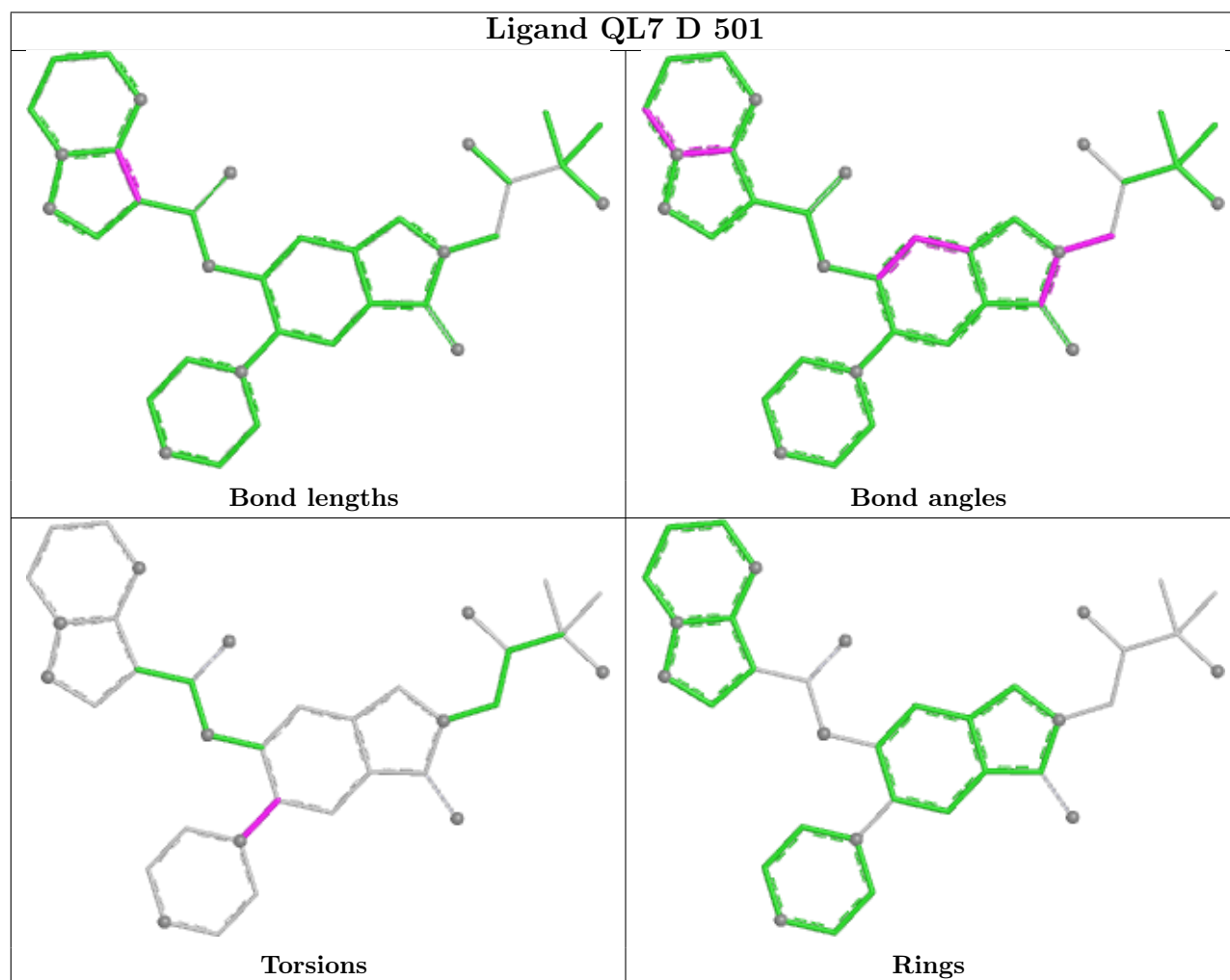
Mol	Chain	Res	Type	Atoms
2	B	502	QL7	C13-C12-N17-C22
2	A	501	QL7	C13-C12-N17-C22
2	C	501	QL7	C13-C12-N17-C18
2	C	501	QL7	C13-C12-N17-C22
2	A	501	QL7	C13-C12-N17-C18
2	D	501	QL7	C13-C12-N17-C22
2	B	502	QL7	C13-C12-N17-C18
2	D	501	QL7	C13-C12-N17-C18
2	A	501	QL7	C11-C12-N17-C18
2	C	501	QL7	C11-C12-N17-C18
2	C	501	QL7	C11-C12-N17-C22
2	D	501	QL7	C11-C12-N17-C18
2	A	501	QL7	C11-C12-N17-C22
2	B	502	QL7	C11-C12-N17-C18
2	B	502	QL7	C11-C12-N17-C22
2	D	501	QL7	C11-C12-N17-C22

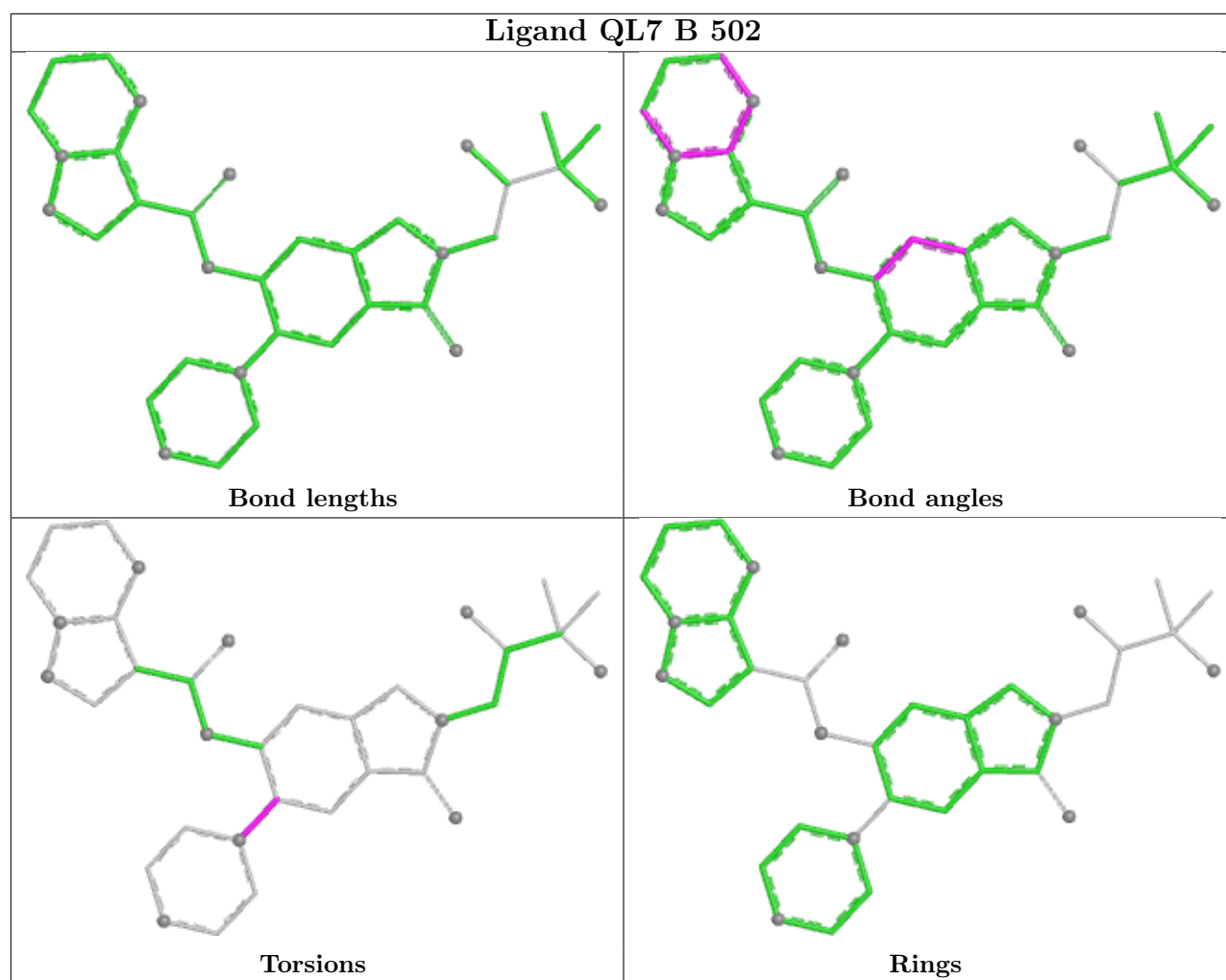
There are no ring outliers.

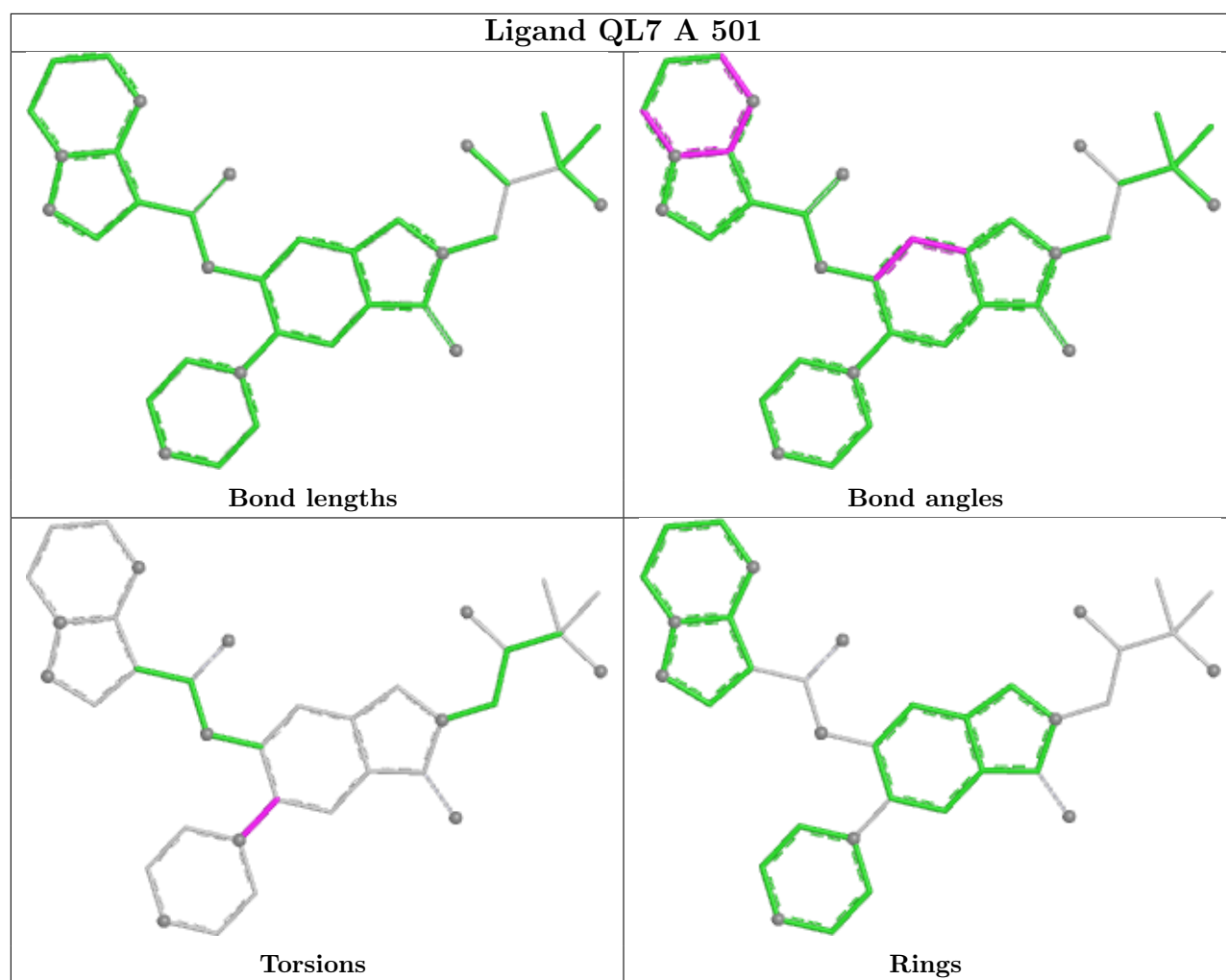
No monomer is involved in short contacts.

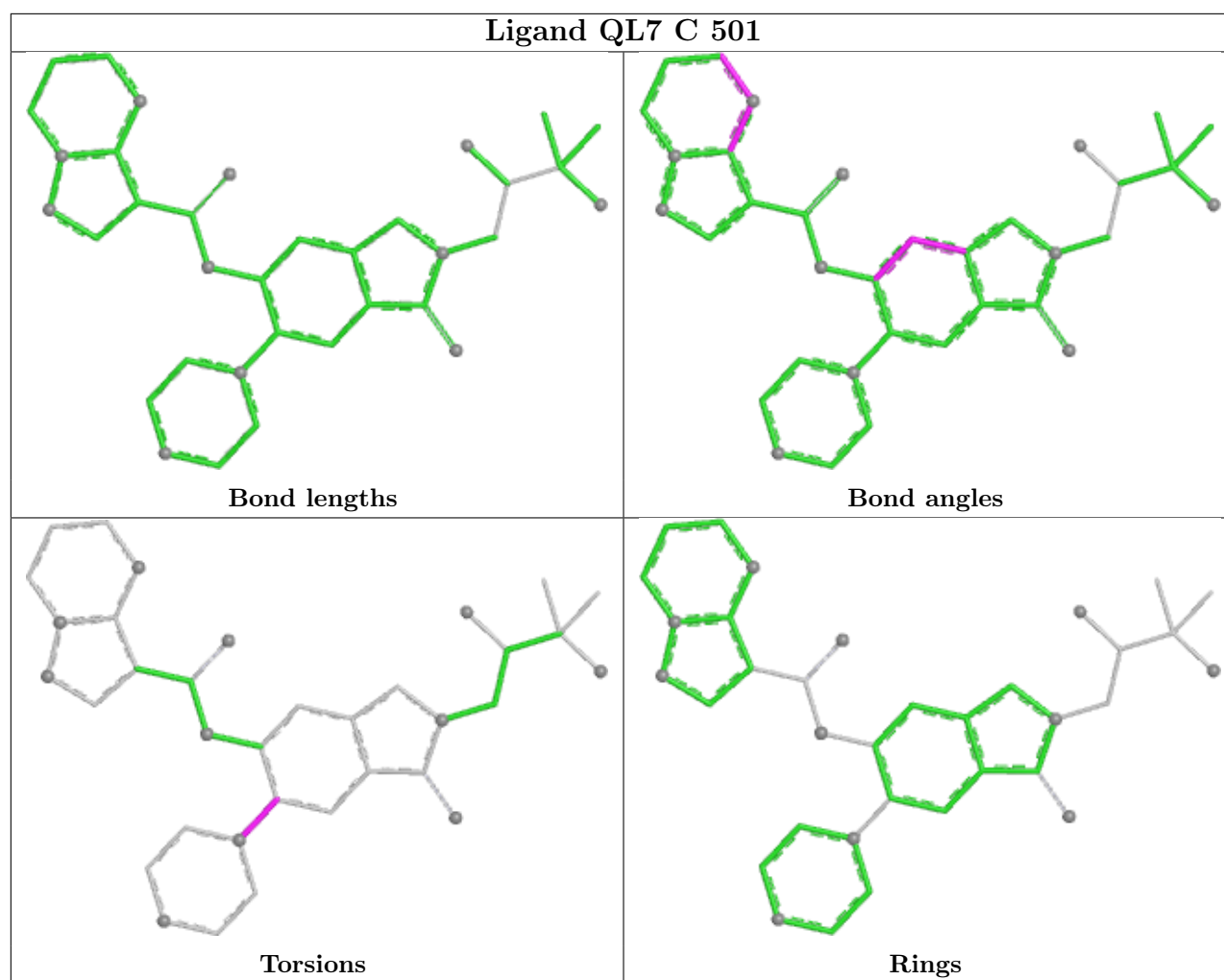
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	285/320 (89%)	0.24	19 (6%)	24 29	13, 27, 55, 79	1 (0%)
1	B	287/320 (89%)	0.02	9 (3%)	51 60	15, 25, 47, 67	2 (0%)
1	C	275/320 (85%)	0.51	29 (10%)	11 15	13, 30, 60, 87	1 (0%)
1	D	288/320 (90%)	0.27	17 (5%)	28 34	14, 29, 56, 71	1 (0%)
All	All	1135/1280 (88%)	0.26	74 (6%)	25 30	13, 27, 56, 87	5 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	VAL	7.0
1	A	343	VAL	6.3
1	C	335	ALA	6.0
1	C	349	VAL	5.5
1	A	163	THR	5.5
1	D	335	ALA	5.5
1	A	217	ALA	4.8
1	C	254	ASP	4.0
1	C	330	PHE	4.0
1	C	348	ILE	3.9
1	C	344	MET	3.8
1	B	256	ASP	3.6
1	A	223	THR	3.5
1	A	222	THR	3.5
1	C	197	PHE	3.5
1	A	196	GLY	3.4
1	C	204	TYR	3.3
1	D	219	VAL	3.3
1	A	195	GLY	3.2
1	C	333	ALA	3.2
1	C	196	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	3.0
1	D	204	TYR	3.0
1	D	221	ILE	3.0
1	D	187	VAL	3.0
1	D	217	ALA	2.9
1	C	409	THR	2.8
1	D	405	ASP	2.8
1	B	343	VAL	2.8
1	D	207	ASN	2.8
1	A	336	SER	2.8
1	C	207	ASN	2.7
1	A	349	VAL	2.7
1	A	458	THR	2.7
1	C	331	GLY	2.7
1	A	164	ARG	2.7
1	C	195	GLY	2.7
1	D	196	GLY	2.7
1	C	393	PRO	2.6
1	A	221	ILE	2.6
1	B	336	SER	2.6
1	B	341	GLN	2.6
1	D	344	MET	2.6
1	B	220	ASP	2.6
1	D	343	VAL	2.6
1	D	228	GLN	2.5
1	C	332	LEU	2.4
1	B	458	THR	2.4
1	C	205	VAL	2.4
1	A	335	ALA	2.4
1	C	187	VAL	2.4
1	D	218	MET	2.3
1	A	414	ILE	2.3
1	A	197	PHE	2.3
1	C	251	PHE	2.3
1	D	255	GLY	2.2
1	C	390	HIS	2.2
1	C	350	GLY	2.2
1	C	257	ASP	2.2
1	D	257	ASP	2.2
1	B	344	MET	2.2
1	D	333	ALA	2.2
1	C	258	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	230	PHE	2.1
1	C	206	ASN	2.1
1	C	229	GLN	2.1
1	D	254	ASP	2.1
1	A	410	ILE	2.1
1	B	410	ILE	2.1
1	A	392	GLU	2.1
1	A	348	ILE	2.1
1	C	411	GLU	2.0
1	B	223	THR	2.0
1	C	439	GLU	2.0

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(Å ²)	Q<0.9
1	TPO	C	342	11/12	0.44	0.25	78,79,82,83	3
1	TPO	A	342	11/12	0.64	0.17	64,64,66,66	4
1	SEP	C	346	10/11	0.66	0.12	66,68,68,69	3
1	TPO	D	342	11/12	0.66	0.15	63,63,66,67	3
1	TPO	B	342	11/12	0.70	0.18	54,56,56,57	3
1	SEP	A	346	10/11	0.71	0.13	56,60,61,62	4
1	SEP	D	346	10/11	0.81	0.13	54,57,61,62	2
1	SEP	B	346	10/11	0.86	0.11	38,42,48,48	4
1	TPO	C	345	11/12	0.88	0.14	70,71,71,72	0
1	TPO	A	345	11/12	0.91	0.11	51,53,56,57	0
1	TPO	B	345	11/12	0.91	0.12	35,40,45,45	0
1	TPO	D	345	11/12	0.92	0.12	53,54,58,58	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,

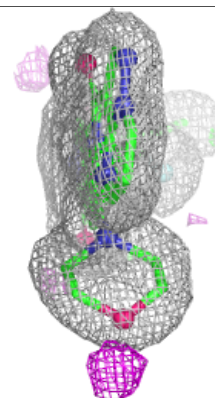
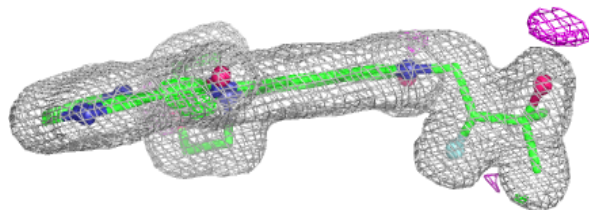
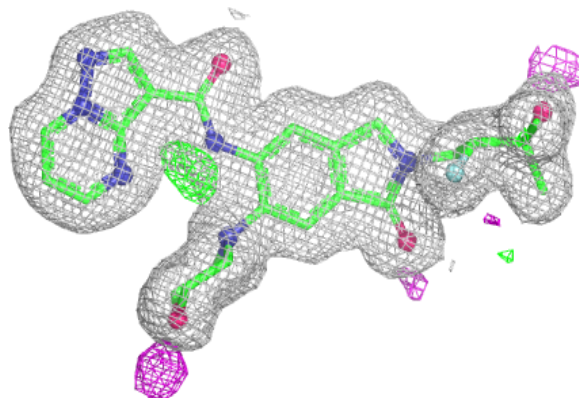
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	QL7	C	501	35/35	0.96	0.06	15,20,25,29	0
2	QL7	D	501	35/35	0.96	0.06	18,22,26,30	0
3	SO4	B	501	5/5	0.96	0.06	44,46,49,50	0
2	QL7	A	501	35/35	0.97	0.05	15,18,24,24	0
2	QL7	B	502	35/35	0.98	0.04	13,17,21,24	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.

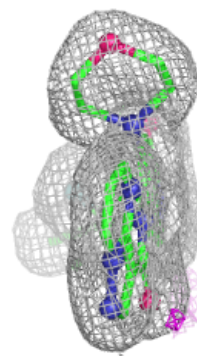
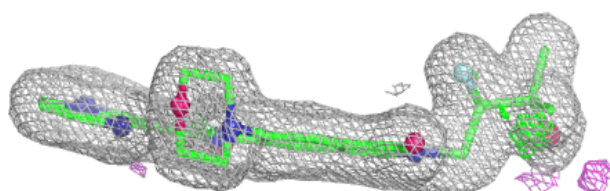
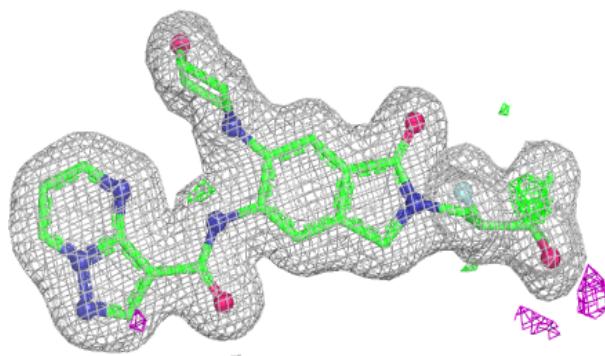
Electron density around QL7 C 501:

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

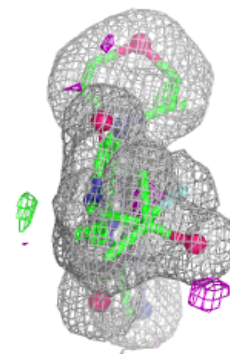
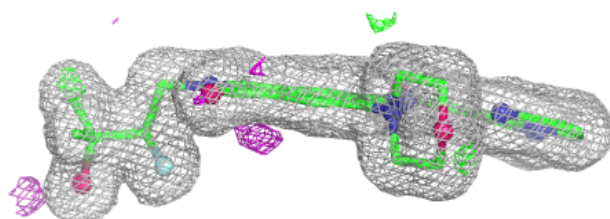
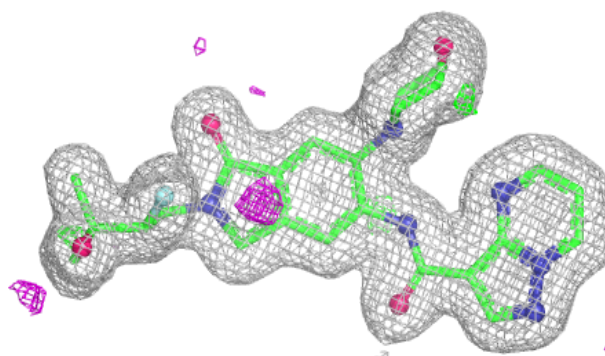


Electron density around QL7 D 501:

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

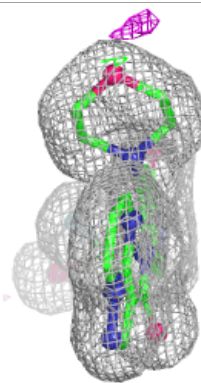
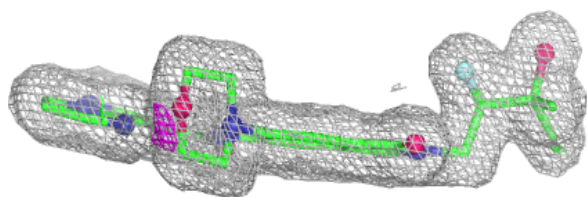
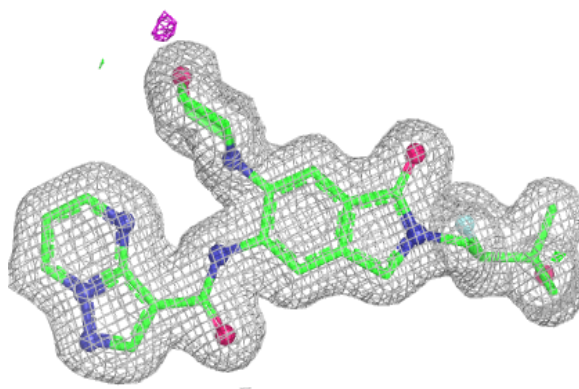
**Electron density around QL7 A 501:**

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



Electron density around QL7 B 502:

$2mF_o - DF_c$ (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.