



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:31 PM BST

PDB ID : 6UYA
Title : Crystal structure of Compound 19 bound to IRAK4
Authors : Kiefer, J.R.; Bryan, M.C.; Lupardus, P.J.; Zarrin, A.A.; Rajapaksa, N.S.;
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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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

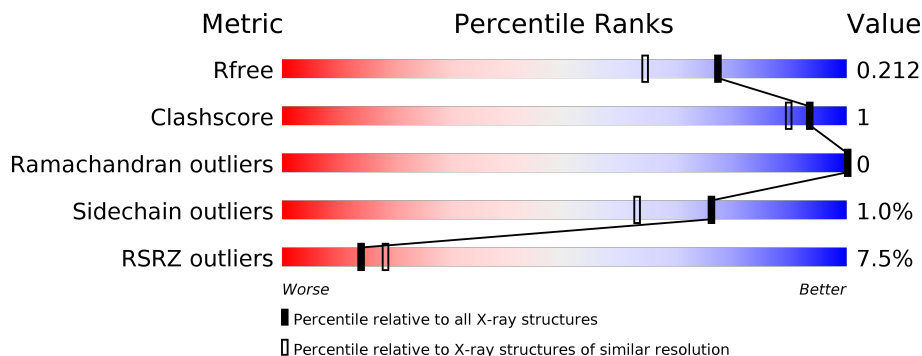
1 Overall quality at a glance i

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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 on 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	
1	B	320	
1	C	320	
1	D	320	

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
			Total	C	N	O	P	S			
1	A	288	2270	1423	380	450	3	14	0	1	0
1	B	290	2293	1439	384	452	3	15	0	2	0
1	C	278	2207	1384	371	434	3	15	0	1	0
1	D	291	2294	1439	386	451	3	15	0	1	0

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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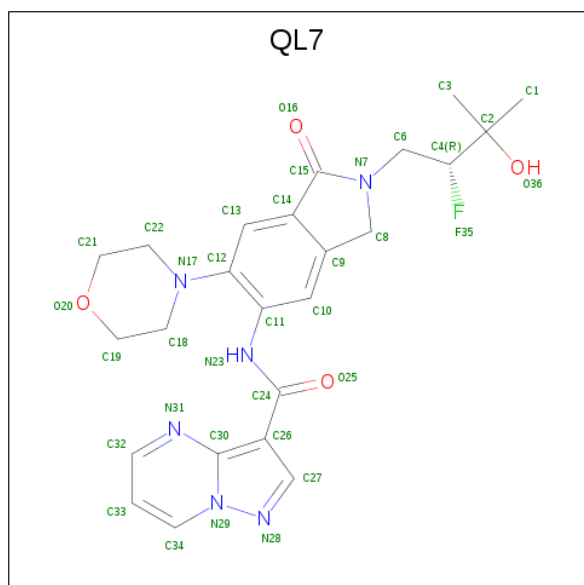
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	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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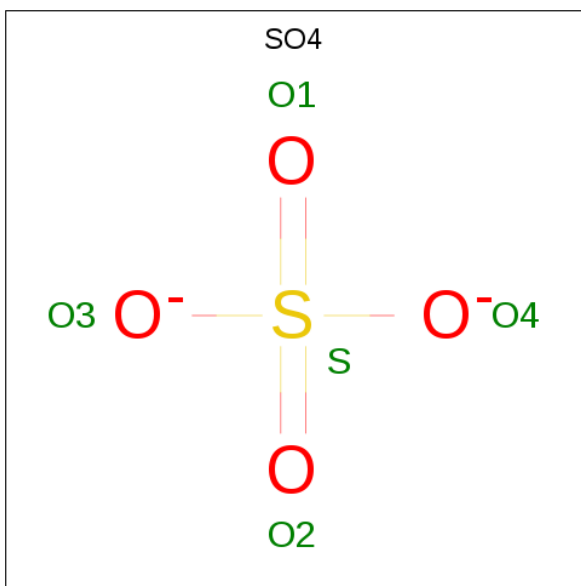
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	HIS	-	expression tag	UNP Q9NWZ3
D	151	GLY	-	expression tag	UNP Q9NWZ3
D	152	GLU	-	expression tag	UNP Q9NWZ3
D	153	ASN	-	expression tag	UNP Q9NWZ3
D	154	LEU	-	expression tag	UNP Q9NWZ3
D	155	TYR	-	expression tag	UNP Q9NWZ3
D	156	PHE	-	expression tag	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 (three-letter code: QL7) (formula: C₂₄H₂₇FN₆O₄) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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


- Molecule 4 is water.

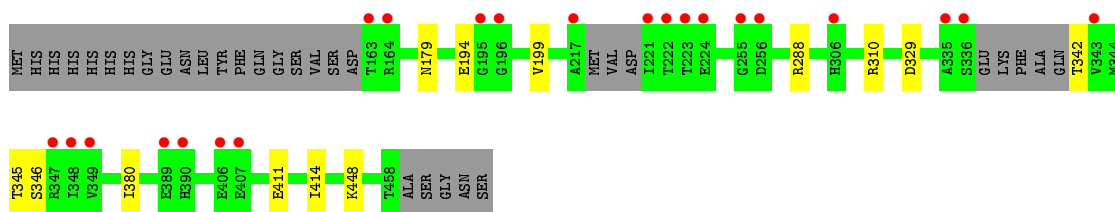
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	245	Total	O	0	0
			245	245		
4	B	253	Total	O	0	0
			253	253		
4	C	182	Total	O	0	0
			182	182		
4	D	207	Total	O	0	0
			207	207		

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.

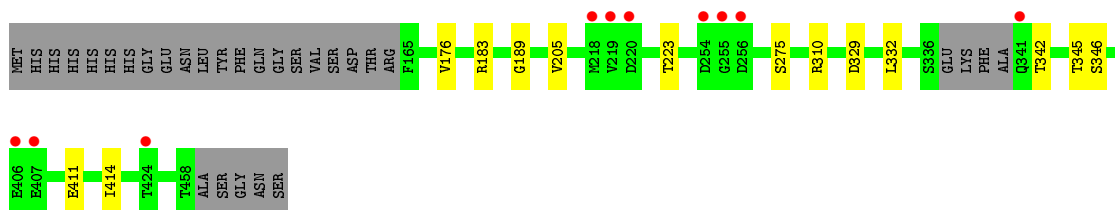
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A: 




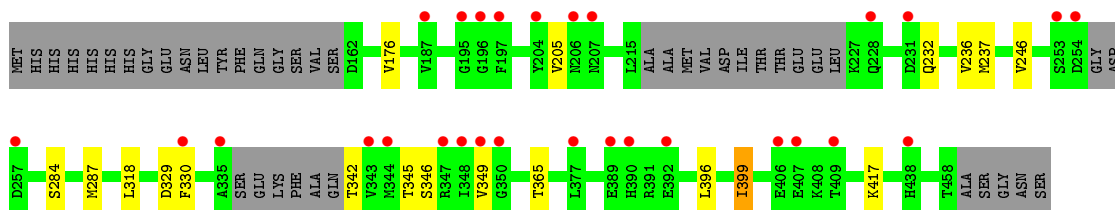
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B: 




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

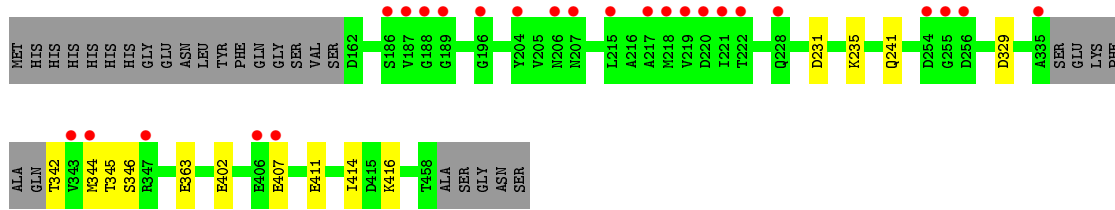
Chain C: 



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

Chain D: 





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 25.47 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.48-1.74) 99.7 (25.47-1.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.74Å)	Xtrriage
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	Xtrriage
Anisotropy	0.217	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: TPO, QL7, SO4, 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	0.51	0/2277	0.60	0/3069
1	B	0.51	0/2303	0.61	0/3104
1	C	0.50	0/2213	0.60	0/2979
1	D	0.50	0/2302	0.61	0/3103
All	All	0.50	0/9095	0.61	0/12255

There are no bond length outliers.

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	2270	0	2232	5	0
1	B	2293	0	2261	6	0
1	C	2207	0	2170	10	0
1	D	2294	0	2263	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	245	0	0	2	0
4	B	253	0	0	0	0
4	C	182	0	0	1	0
4	D	207	0	0	0	0
All	All	10096	0	8926	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (25) 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:231:ASP:O	1:D:235:LYS:HG2	2.00	0.61
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: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:C:284:SER:H	1:C:287[B]:MET:HE3	1.72	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:H	1:C:287[B]:MET:CE	2.23	0.51
1:D:344:MET:HG2	1:D:363:GLU:HA	1.96	0.48
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
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:A:310:ARG:HD2	4:A:796:HOH:O	2.19	0.42
1:C:237:MET:HE3	1:C:246:VAL:HG23	2.01	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: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 [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	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 [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	247/275 (90%)	245 (99%)	2 (1%)	81	72
1	B	250/275 (91%)	248 (99%)	2 (1%)	81	72
1	C	241/275 (88%)	237 (98%)	4 (2%)	60	41
1	D	249/275 (90%)	247 (99%)	2 (1%)	81	72
All	All	987/1100 (90%)	977 (99%)	10 (1%)	76	63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	448	LYS

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Mol	Chain	Res	Type
1	B	223	THR
1	B	329	ASP
1	C	329	ASP
1	C	349	VAL
1	C	365	THR
1	C	399	ILE
1	D	241	GLN
1	D	329	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	B	342	1	8,10,11	1.30	1 (12%)	10,14,16	0.95	0
1	TPO	D	342	1	8,10,11	1.08	1 (12%)	10,14,16	1.35	1 (10%)
1	TPO	D	345	1	8,10,11	1.35	1 (12%)	10,14,16	1.18	1 (10%)
1	TPO	B	345	1	8,10,11	1.07	1 (12%)	10,14,16	1.25	1 (10%)
1	SEP	A	346	1	8,9,10	0.79	0	8,12,14	1.94	3 (37%)
1	SEP	B	346	1	8,9,10	1.07	0	8,12,14	1.20	1 (12%)
1	SEP	C	346	1	8,9,10	0.88	0	8,12,14	2.39	2 (25%)
1	TPO	A	342	1	8,10,11	0.91	0	10,14,16	1.25	2 (20%)
1	SEP	D	346	1	8,9,10	0.79	0	8,12,14	2.74	3 (37%)
1	TPO	C	345	1	8,10,11	1.12	0	10,14,16	1.23	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	342	1	8,10,11	1.35	1 (12%)	10,14,16	1.12	0
1	TPO	A	345	1	8,10,11	1.19	1 (12%)	10,14,16	1.11	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	B	342	1	-	0/9/11/13	-
1	TPO	D	342	1	-	0/9/11/13	-
1	TPO	D	345	1	-	2/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	SEP	A	346	1	-	1/5/8/10	-
1	SEP	B	346	1	-	0/5/8/10	-
1	SEP	C	346	1	-	1/5/8/10	-
1	TPO	A	342	1	-	0/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-3.02	1.53	1.59
1	B	342	TPO	P-OG1	-3.01	1.53	1.59
1	A	345	TPO	CB-CA	2.56	1.59	1.53
1	D	342	TPO	P-OG1	-2.24	1.55	1.59
1	D	345	TPO	P-OG1	-2.13	1.55	1.59
1	B	345	TPO	CG2-CB	2.08	1.56	1.51

All (16) 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	-3.05	114.00	123.21
1	B	346	SEP	OG-P-O1P	2.79	114.31	106.47
1	D	345	TPO	O3P-P-OG1	2.50	117.20	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	O2P-P-OG1	2.42	116.83	105.99
1	C	346	SEP	OG-P-O1P	2.33	113.02	106.47
1	D	346	SEP	O3P-P-OG	2.32	112.90	106.73
1	A	346	SEP	O3P-P-OG	2.30	112.85	106.73
1	D	346	SEP	P-OG-CB	-2.30	111.97	118.30
1	C	345	TPO	O2P-P-OG1	2.28	116.21	105.99
1	A	346	SEP	P-OG-CB	-2.19	112.26	118.30
1	A	342	TPO	CG2-CB-CA	-2.17	108.88	113.16
1	A	342	TPO	P-OG1-CB	-2.16	116.70	123.21
1	A	345	TPO	OG1-P-O1P	2.00	117.12	109.39

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	N-CA-CB-OG
1	C	346	SEP	N-CA-CB-OG
1	D	346	SEP	N-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	345	TPO	CB-OG1-P-O1P
1	C	342	TPO	CB-OG1-P-O2P
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	C	501	-	32,39,39	0.51	0	42,58,58	0.74	2 (4%)
3	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.05	0
2	QL7	B	502	-	32,39,39	0.56	0	42,58,58	0.80	1 (2%)
2	QL7	D	501	-	32,39,39	0.46	0	42,58,58	0.73	1 (2%)
2	QL7	A	501	-	32,39,39	0.54	0	42,58,58	0.77	2 (4%)

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	-	-	5/17/42/42	0/5/5/5
2	QL7	B	502	-	-	4/17/42/42	0/5/5/5
2	QL7	D	501	-	-	4/17/42/42	0/5/5/5
2	QL7	A	501	-	-	4/17/42/42	0/5/5/5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	QL7	C11-C10-C9	-2.49	117.77	121.92
2	C	501	QL7	C11-C10-C9	-2.34	118.02	121.92
2	A	501	QL7	C11-C10-C9	-2.30	118.09	121.92
2	C	501	QL7	C10-C11-C12	2.13	121.92	119.67
2	A	501	QL7	C8-N7-C6	-2.05	120.05	122.79
2	D	501	QL7	C8-N7-C6	-2.00	120.11	122.79

There are no chirality outliers.

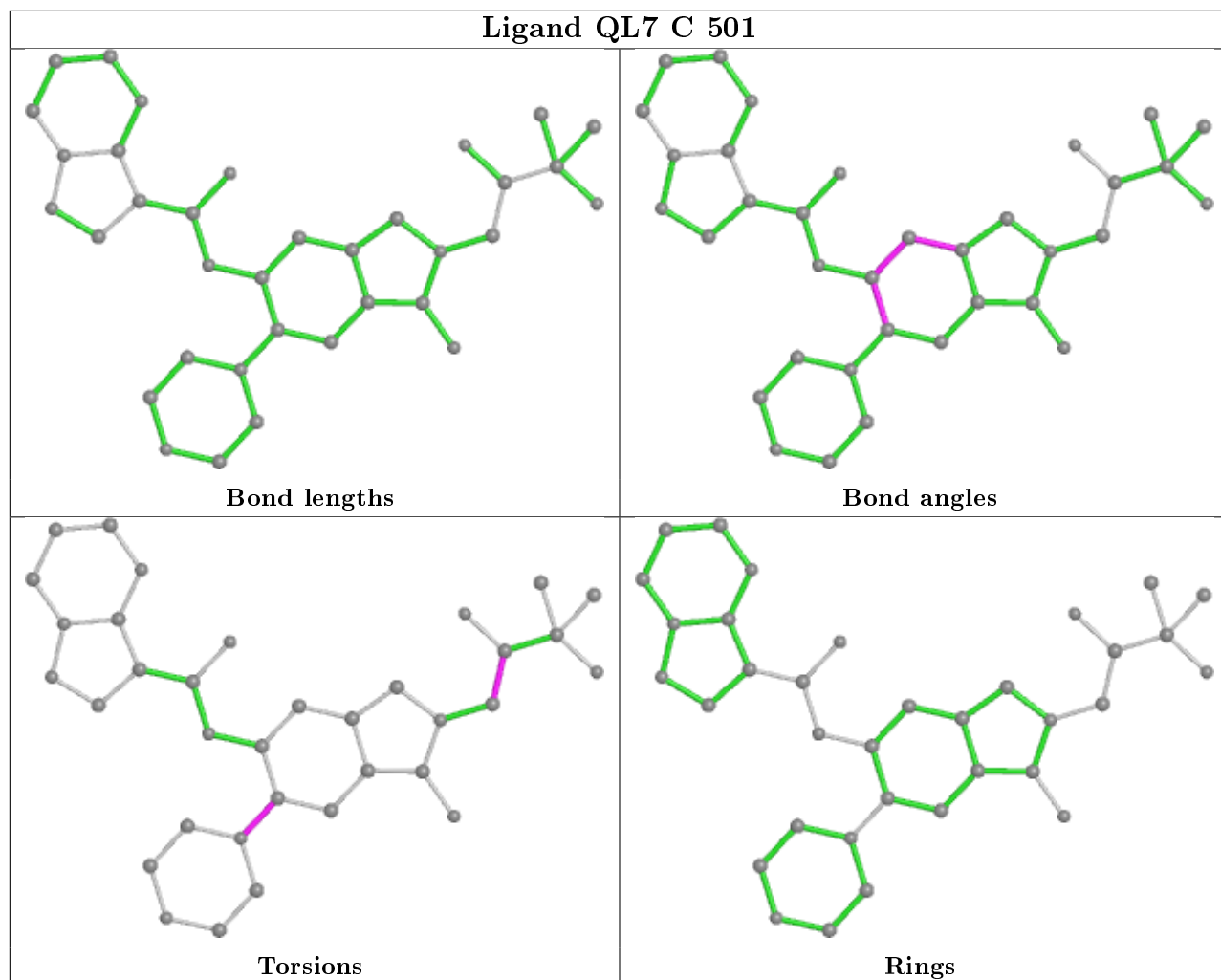
All (17) torsion outliers are listed below:

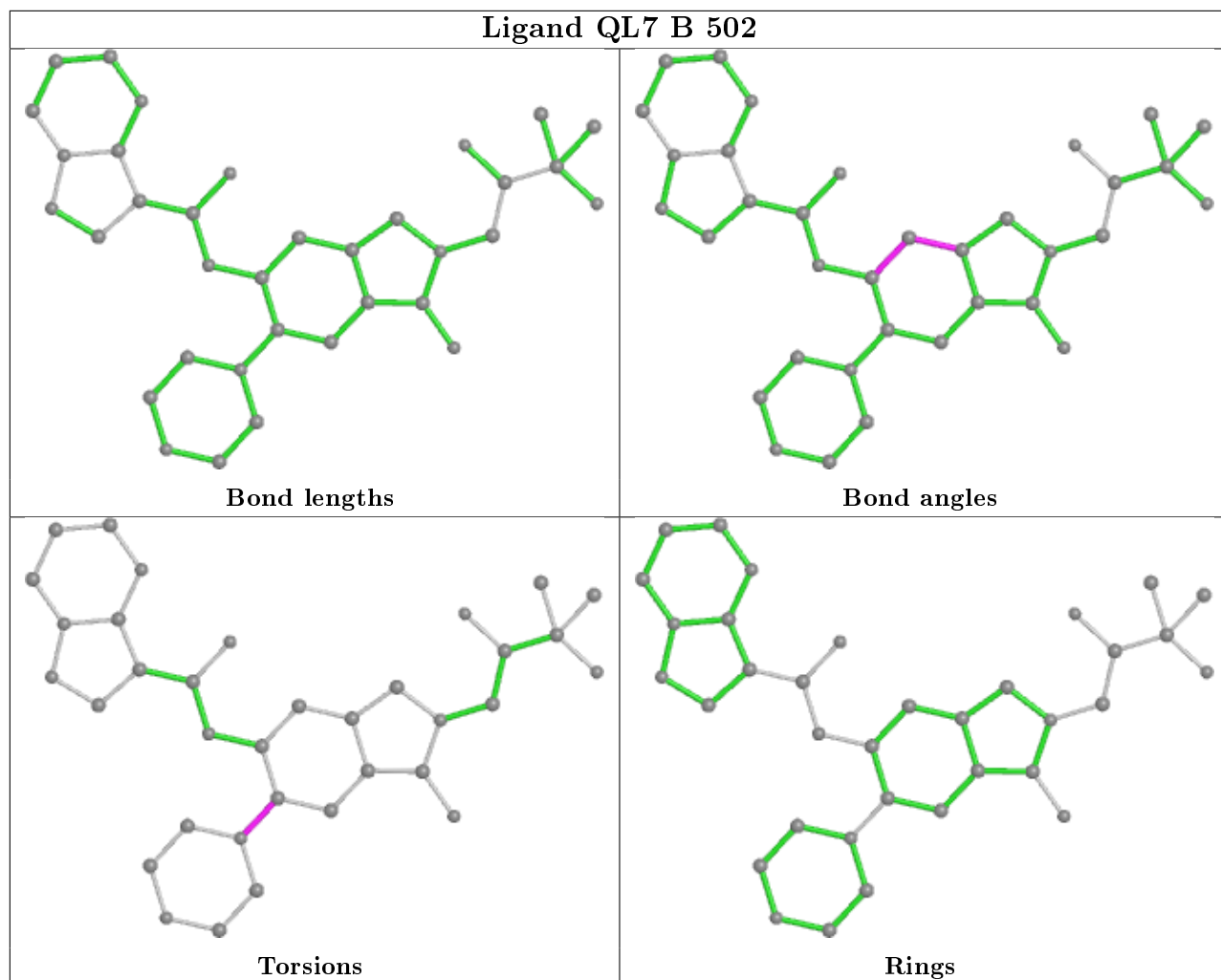
Mol	Chain	Res	Type	Atoms
2	B	502	QL7	C13-C12-N17-C22
2	A	501	QL7	C13-C12-N17-C22
2	C	501	QL7	C13-C12-N17-C18
2	C	501	QL7	C13-C12-N17-C22
2	D	501	QL7	C13-C12-N17-C22
2	A	501	QL7	C13-C12-N17-C18
2	D	501	QL7	C13-C12-N17-C18
2	B	502	QL7	C13-C12-N17-C18
2	C	501	QL7	C11-C12-N17-C18
2	C	501	QL7	C11-C12-N17-C22
2	D	501	QL7	C11-C12-N17-C18
2	A	501	QL7	C11-C12-N17-C18
2	C	501	QL7	F35-C4-C6-N7
2	B	502	QL7	C11-C12-N17-C18
2	B	502	QL7	C11-C12-N17-C22
2	A	501	QL7	C11-C12-N17-C22
2	D	501	QL7	C11-C12-N17-C22

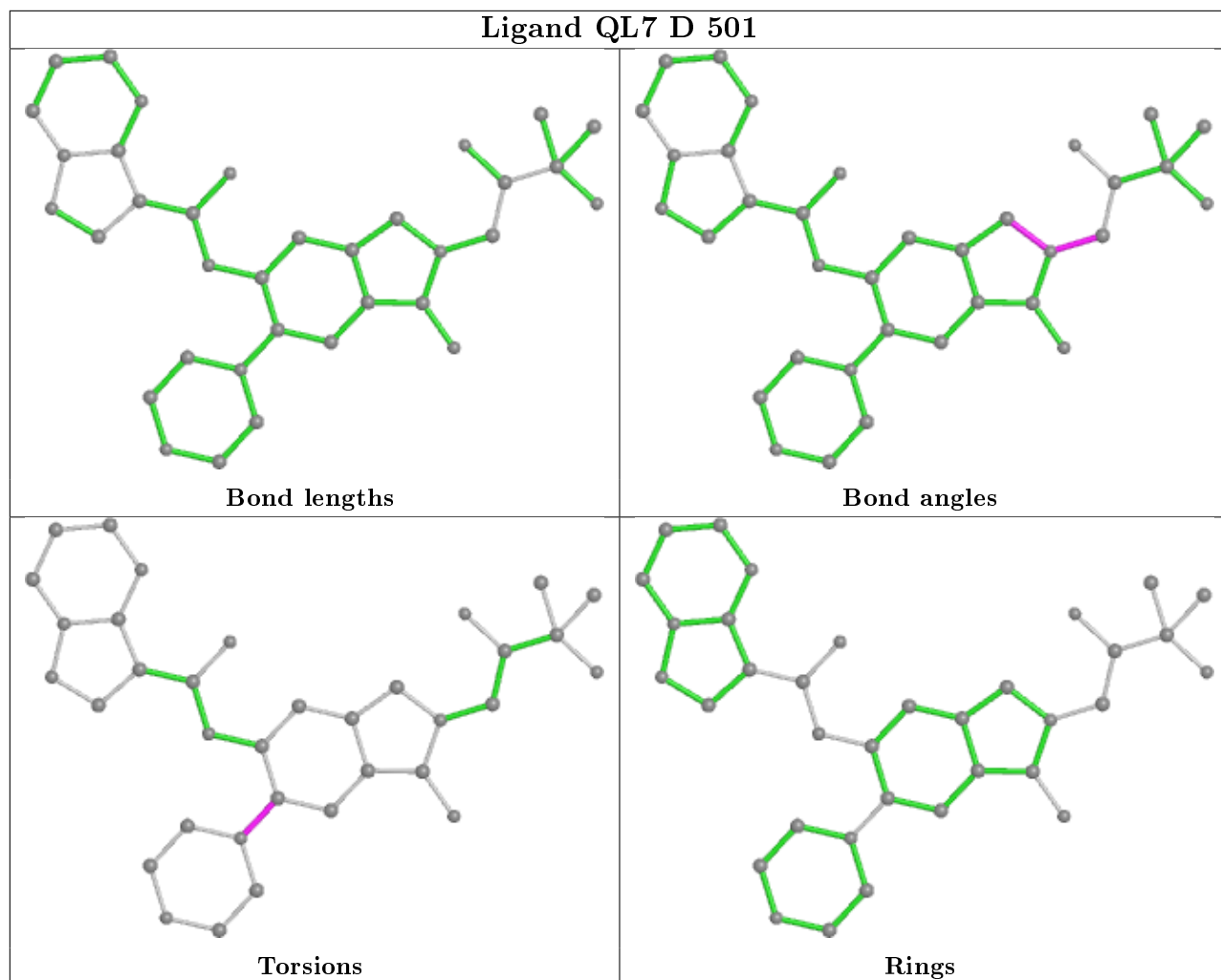
There are no ring outliers.

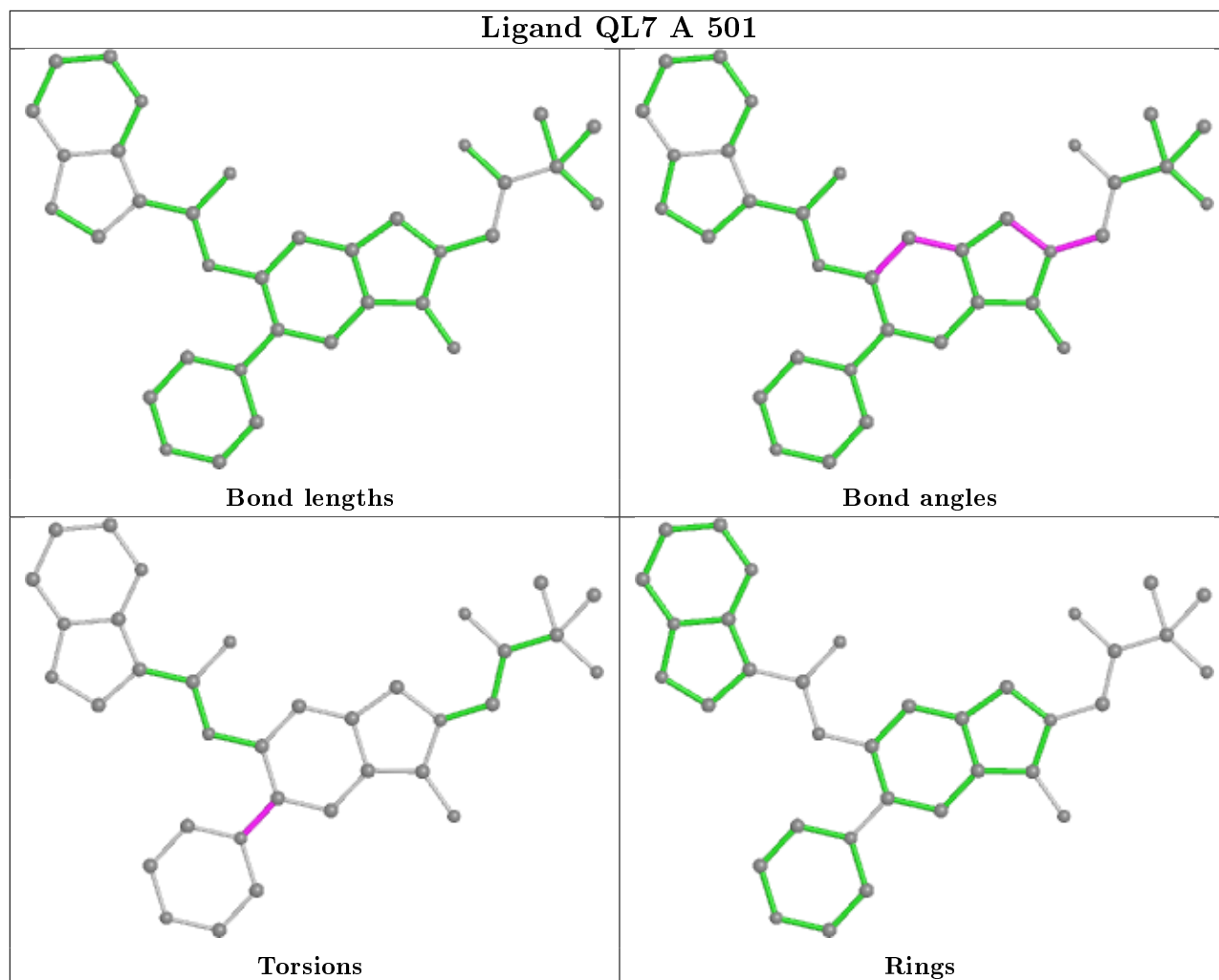
No monomer is involved in short contacts.

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

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	285/320 (89%)	0.24	22 (7%) 13 17	15, 27, 55, 79	0
1	B	287/320 (89%)	0.07	10 (3%) 44 49	15, 25, 47, 67	0
1	C	275/320 (85%)	0.52	28 (10%) 6 8	16, 30, 60, 87	0
1	D	288/320 (90%)	0.33	25 (8%) 10 12	16, 29, 56, 71	0
All	All	1135/1280 (88%)	0.29	85 (7%) 14 18	15, 27, 56, 87	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	VAL	10.5
1	C	349	VAL	7.2
1	D	219	VAL	7.1
1	A	164	ARG	6.3
1	B	256	ASP	5.8
1	C	196	GLY	5.5
1	A	163	THR	5.4
1	A	196	GLY	5.3
1	C	228	GLN	5.2
1	B	341	GLN	5.1
1	C	195	GLY	5.0
1	A	195	GLY	5.0
1	C	335	ALA	4.9
1	A	255	GLY	4.9
1	D	217	ALA	4.7
1	A	336	SER	4.6
1	C	207	ASN	4.6
1	C	187	VAL	4.4
1	A	222	THR	4.4
1	D	254	ASP	4.2
1	A	223	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	344	MET	4.2
1	D	220	ASP	4.1
1	D	222	THR	4.0
1	A	343	VAL	4.0
1	D	187	VAL	4.0
1	D	207	ASN	3.8
1	D	406	GLU	3.8
1	C	389	GLU	3.8
1	D	343	VAL	3.8
1	C	407	GLU	3.8
1	A	224	GLU	3.7
1	C	206	ASN	3.6
1	A	335	ALA	3.6
1	D	221	ILE	3.6
1	A	217	ALA	3.5
1	B	407	GLU	3.5
1	A	347	ARG	3.5
1	A	256	ASP	3.5
1	C	409	THR	3.3
1	C	257	ASP	3.2
1	A	221	ILE	3.1
1	C	253	SER	3.1
1	D	218	MET	3.1
1	D	186	SER	3.1
1	D	204	TYR	3.0
1	B	220	ASP	3.0
1	D	335	ALA	3.0
1	C	347	ARG	2.9
1	D	347	ARG	2.9
1	D	256	ASP	2.9
1	B	255	GLY	2.8
1	D	407	GLU	2.8
1	C	390	HIS	2.8
1	D	206	ASN	2.8
1	C	197	PHE	2.8
1	C	204	TYR	2.7
1	C	348	ILE	2.7
1	A	389	GLU	2.7
1	A	407	GLU	2.7
1	D	228	GLN	2.7
1	D	255	GLY	2.6
1	C	330	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	218	MET	2.5
1	D	344	MET	2.5
1	D	196	GLY	2.5
1	B	254	ASP	2.4
1	A	348	ILE	2.4
1	D	188	GLY	2.4
1	C	231	ASP	2.3
1	C	406	GLU	2.3
1	B	219	VAL	2.3
1	C	254	ASP	2.3
1	A	349	VAL	2.3
1	B	406	GLU	2.3
1	C	350	GLY	2.3
1	B	424	THR	2.2
1	A	306	HIS	2.2
1	D	189	GLY	2.2
1	C	377	LEU	2.1
1	C	392	GLU	2.1
1	A	390	HIS	2.1
1	A	406	GLU	2.1
1	D	215	LEU	2.1
1	C	438	HIS	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	0.12	0.39	78,79,82,83	3
1	TPO	A	342	11/12	0.64	0.25	64,64,66,66	4
1	TPO	B	342	11/12	0.66	0.21	54,56,56,57	3
1	TPO	D	342	11/12	0.68	0.36	63,63,66,67	3
1	SEP	A	346	10/11	0.70	0.36	56,60,61,62	4
1	SEP	C	346	10/11	0.73	0.34	66,68,68,69	3
1	SEP	D	346	10/11	0.86	0.28	54,57,61,62	2
1	TPO	C	345	11/12	0.87	0.27	70,71,71,72	0
1	SEP	B	346	10/11	0.89	0.28	38,42,48,48	4
1	TPO	B	345	11/12	0.92	0.15	35,40,45,45	0
1	TPO	D	345	11/12	0.92	0.21	53,54,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	A	345	11/12	0.93	0.15	51,53,56,57	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

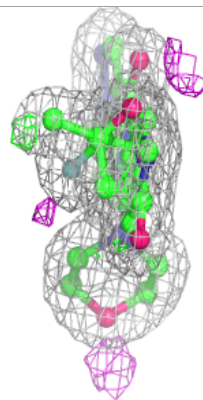
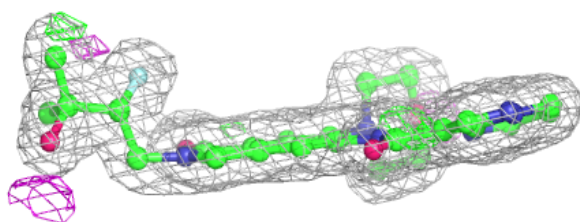
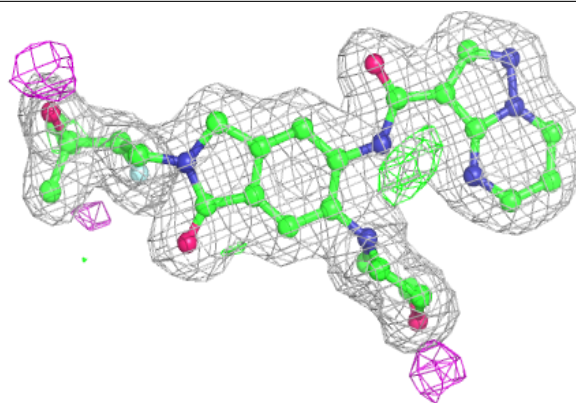
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	QL7	C	501	35/35	0.95	0.09	15,20,25,29	0
2	QL7	D	501	35/35	0.95	0.08	18,22,26,30	0
2	QL7	A	501	35/35	0.97	0.08	15,18,24,24	0
2	QL7	B	502	35/35	0.98	0.08	13,17,21,24	0
3	SO4	B	501	5/5	0.98	0.15	44,46,49,50	0

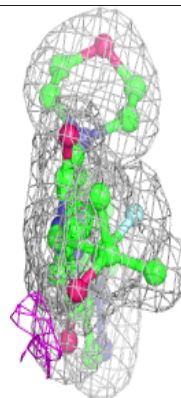
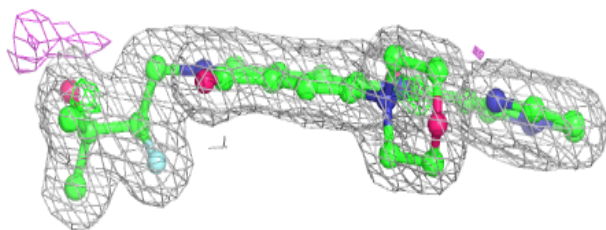
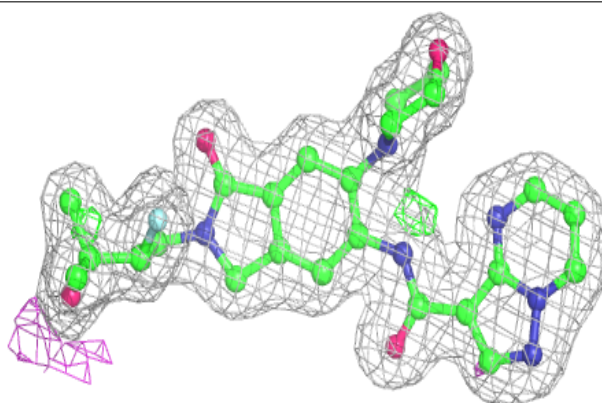
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

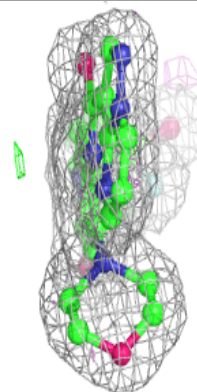
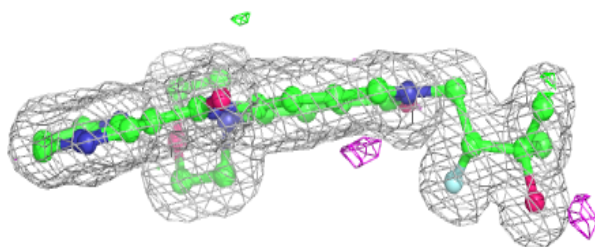
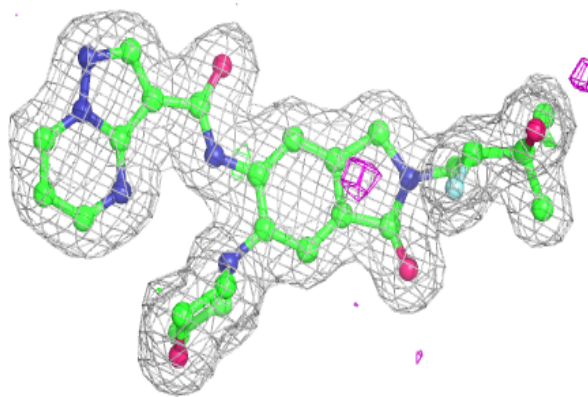
**Electron density around QL7 D 501:**

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

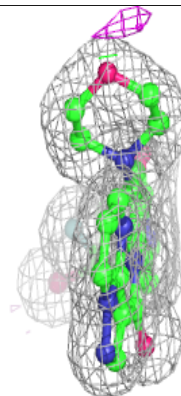
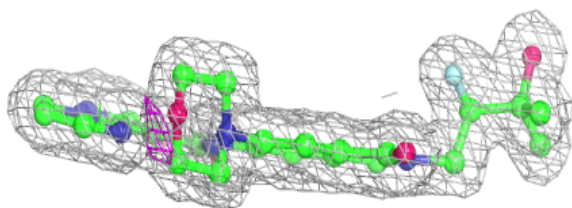
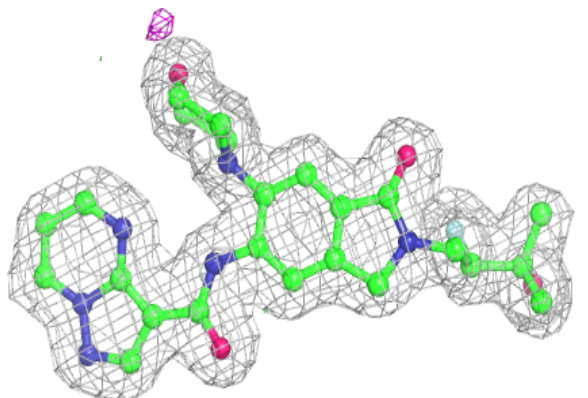


Electron density around QL7 A 501:

$2mF_o-DF_c$ (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

There are no such residues in this entry.