



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:50 pm BST

PDB ID : 5K72
Title : IRAK4 in complex with Compound 21
Authors : Ferguson, A.D.
Deposited on : 2016-05-25
Resolution : 2.22 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 : 2.11
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) : 2.11

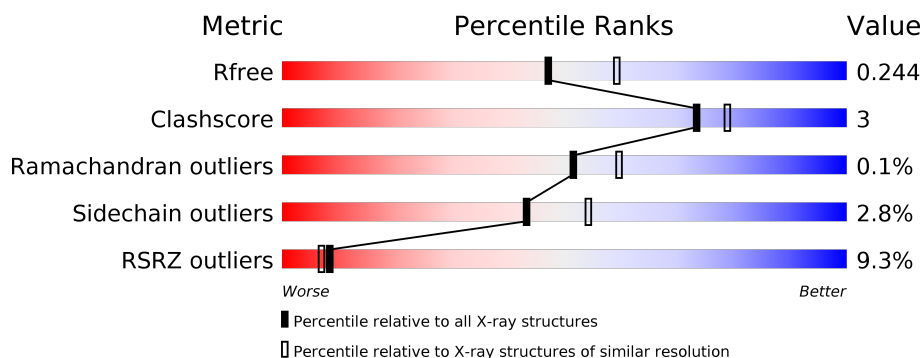
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	301	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	301	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>11%</div> </div> </div>
1	C	301	<div> <div>13%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	301	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9146 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	279	Total	C	N	O	P	S	0	0	0
			2205	1386	373	430	2	14			
1	B	267	Total	C	N	O	S		0	0	0
			2109	1333	355	408	13				
1	C	279	Total	C	N	O	P	S	0	0	0
			2212	1393	373	430	2	14			
1	D	278	Total	C	N	O	P	S	0	0	0
			2204	1387	372	429	2	14			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



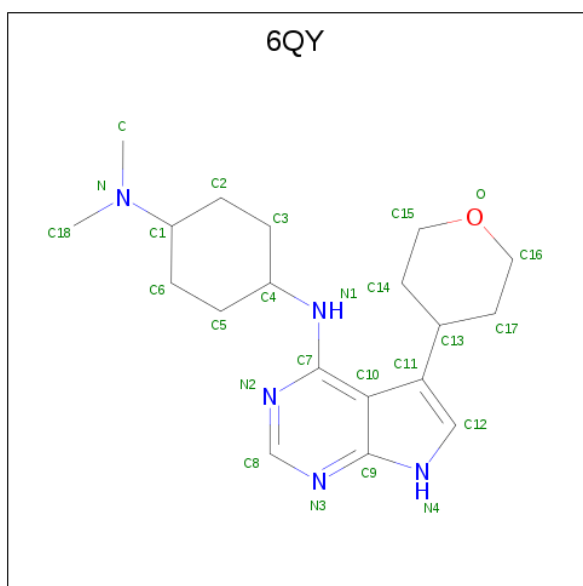
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is {N}4, {N}4-dimethyl- {N}1-[5-(oxan-4-yl)-7 {H}-pyrrolo[2,3-d]pyrimidin-4-yl]cyclohexane-1,4-diamine (three-letter code: 6QY) (formula: C₁₉H₂₉N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	19	5	1		
3	B	1	Total	C	N	O	0	0
			25	19	5	1		
3	C	1	Total	C	N	O	0	0
			25	19	5	1		
3	D	1	Total	C	N	O	0	0
			25	19	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	71	Total	O	0	0
			71	71		

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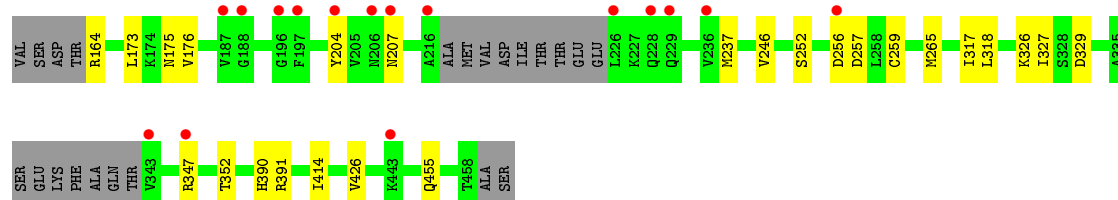
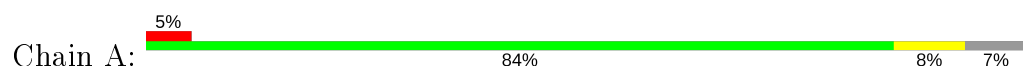
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	78	Total	O	0	0
			78	78		
4	D	70	Total	O	0	0
			70	70		

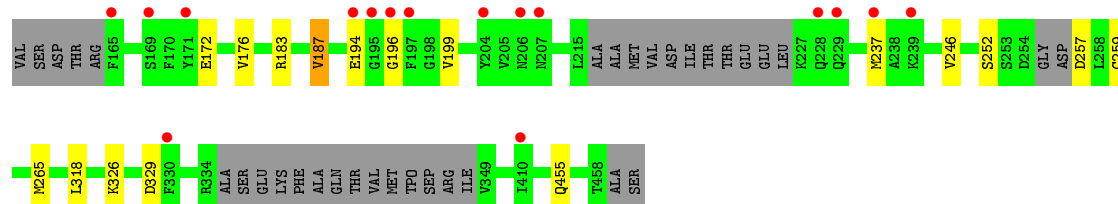
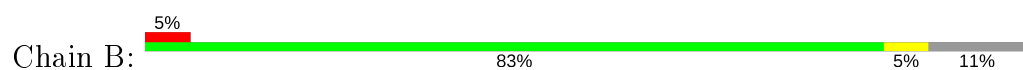
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

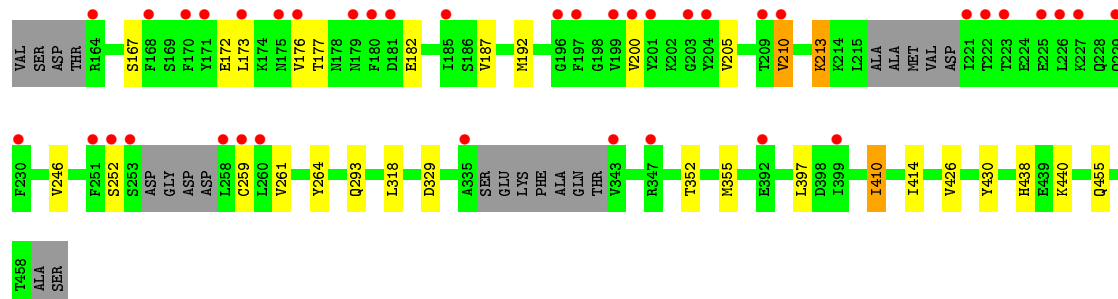
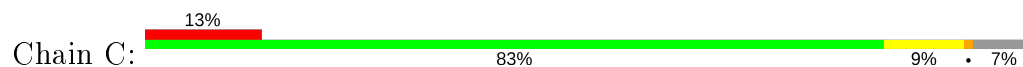
- Molecule 1: Interleukin-1 receptor-associated kinase 4



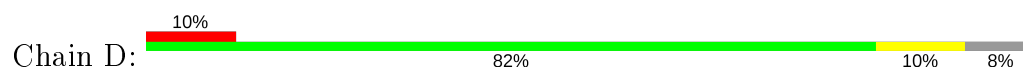
- Molecule 1: Interleukin-1 receptor-associated kinase 4

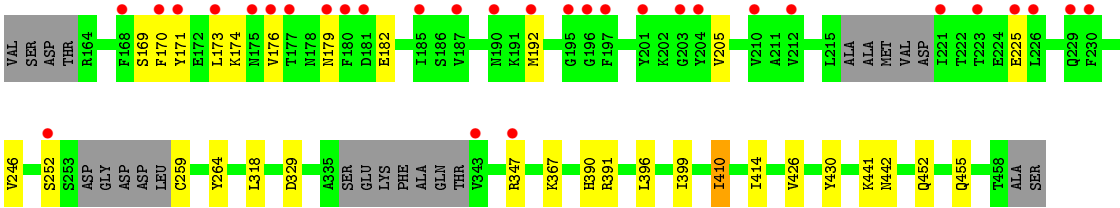


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	145.08Å 140.97Å 87.52Å 90.00° 125.77° 90.00°	Depositor
Resolution (Å)	58.86 – 2.22 58.86 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.0 (58.86-2.22) 93.1 (58.86-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.7	Depositor
R, R_{free}	0.215 , 0.225 0.227 , 0.244	Depositor DCC
R_{free} test set	3419 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.206 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9146	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 6QY, 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	0.48	0/2220	0.64	1/2989 (0.0%)
1	B	0.49	0/2145	0.64	0/2889
1	C	0.50	0/2226	0.66	0/2996
1	D	0.50	0/2218	0.66	0/2985
All	All	0.49	0/8809	0.65	1/11859 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	MET	CB-CG-SD	5.67	129.41	112.40

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	2205	0	2176	10	0
1	B	2109	0	2084	8	0
1	C	2212	0	2193	23	0
1	D	2204	0	2181	18	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	1	0
3	D	25	0	0	0	0
4	A	72	0	0	0	0
4	B	71	0	0	0	0
4	C	78	0	0	8	0
4	D	70	0	0	2	0
All	All	9146	0	8634	57	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 3.

All (57) 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:177:THR:HG22	4:C:640:HOH:O	1.30	1.23
1:C:200:VAL:HG12	4:C:605:HOH:O	1.41	1.16
1:C:192:MET:HE2	4:C:605:HOH:O	1.62	1.00
1:C:192:MET:CE	4:C:605:HOH:O	2.13	0.96
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.58	0.86
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.58	0.86
1:B:265:MET:CE	1:B:326:LYS:HG3	2.11	0.81
1:A:390:HIS:O	1:D:391:ARG:HA	1.84	0.78
1:C:352:THR:HA	1:C:355:MET:HE3	1.67	0.77
1:A:391:ARG:HA	1:D:390:HIS:O	1.85	0.76
1:C:172:GLU:O	1:C:176:VAL:HG13	1.92	0.70
1:A:265:MET:CE	1:A:326:LYS:HG3	2.26	0.65
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.78	0.65
1:D:192:MET:SD	1:D:264:TYR:HE1	2.18	0.65
1:B:194:GLU:HG3	1:B:199:VAL:HG22	1.80	0.64
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.81	0.62
1:D:452:GLN:O	1:D:455:GLN:HG3	1.99	0.62
1:C:167:SER:HB2	4:C:669:HOH:O	2.00	0.61
1:C:213:LYS:HE3	3:C:501:6QY:O	2.01	0.60
1:C:192:MET:SD	1:C:264:TYR:HE1	2.25	0.60
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.82	0.60
1:C:246:VAL:HG21	1:C:318:LEU:HD12	1.83	0.59
1:A:204:TYR:CE2	1:A:207:ASN:HA	2.38	0.59
1:B:172:GLU:O	1:B:176:VAL:HG13	2.05	0.56
1:C:210:VAL:HG21	1:C:261:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.91	0.53
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.91	0.52
1:C:177:THR:CG2	4:C:640:HOH:O	2.14	0.52
1:D:442:ASN:C	4:D:601:HOH:O	2.48	0.51
1:C:438:HIS:HD2	1:C:440:LYS:H	1.61	0.48
1:D:367:LYS:NZ	4:D:601:HOH:O	2.47	0.47
1:B:265:MET:HE2	1:B:326:LYS:HG3	1.92	0.47
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.96	0.47
1:C:210:VAL:CG2	1:C:261:VAL:HG12	2.45	0.46
1:D:170:PHE:HD2	1:D:171:TYR:CE1	2.34	0.46
1:C:200:VAL:CG1	4:C:605:HOH:O	2.23	0.46
1:D:396:LEU:O	1:D:399:ILE:HG12	2.15	0.45
1:D:410:ILE:HG12	1:D:430:TYR:CD2	2.51	0.45
1:C:210:VAL:CG2	1:C:261:VAL:CG1	2.94	0.45
1:C:293:GLN:HG2	4:C:611:HOH:O	2.18	0.44
1:C:210:VAL:HG21	1:C:261:VAL:HG12	1.99	0.44
1:A:317:ILE:HG12	1:A:327:ILE:HD13	2.00	0.43
1:C:414:ILE:HG12	1:C:426:VAL:HG11	2.01	0.43
1:D:174:LYS:HE3	1:D:179:ASN:OD1	2.19	0.43
1:C:176:VAL:HG11	1:C:205:VAL:HG22	2.01	0.42
1:D:171:TYR:HD1	1:D:174:LYS:HD3	1.85	0.42
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.01	0.42
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.02	0.41
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.01	0.41
1:C:410:ILE:HG12	1:C:430:TYR:CD2	2.56	0.41
1:B:183:ARG:HB3	1:B:187:VAL:CG1	2.51	0.41
1:D:367:LYS:HD2	1:D:441:LYS:O	2.19	0.41
1:C:173:LEU:HA	1:C:176:VAL:HG22	2.02	0.41
1:D:176:VAL:HG11	1:D:205:VAL:HG22	2.02	0.41
1:D:410:ILE:HG12	1:D:430:TYR:CG	2.55	0.41
1:D:414:ILE:HG12	1:D:426:VAL:HG11	2.03	0.40
1:A:173:LEU:HA	1:A:176: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	271/301 (90%)	263 (97%)	8 (3%)	0	100	100
1	B	259/301 (86%)	251 (97%)	7 (3%)	1 (0%)	34	37
1	C	269/301 (89%)	264 (98%)	5 (2%)	0	100	100
1	D	268/301 (89%)	262 (98%)	6 (2%)	0	100	100
All	All	1067/1204 (89%)	1040 (98%)	26 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/260 (93%)	233 (97%)	8 (3%)	38	47
1	B	234/260 (90%)	229 (98%)	5 (2%)	53	65
1	C	243/260 (94%)	235 (97%)	8 (3%)	38	47
1	D	242/260 (93%)	236 (98%)	6 (2%)	47	58
All	All	960/1040 (92%)	933 (97%)	27 (3%)	43	54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	175	ASN
1	A	256	ASP
1	A	257	ASP
1	A	329	ASP

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Mol	Chain	Res	Type
1	A	347	ARG
1	A	352	THR
1	A	455	GLN
1	B	187	VAL
1	B	237	MET
1	B	257	ASP
1	B	329	ASP
1	B	455	GLN
1	C	182	GLU
1	C	187	VAL
1	C	210	VAL
1	C	213	LYS
1	C	329	ASP
1	C	397	LEU
1	C	410	ILE
1	C	455	GLN
1	D	169	SER
1	D	182	GLU
1	D	225	GLU
1	D	329	ASP
1	D	347	ARG
1	D	410	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	394	GLN
1	B	394	GLN
1	C	207	ASN
1	C	394	GLN
1	C	438	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	D	345	1	8,10,11	1.28	1 (12%)	10,14,16	1.07	0
1	SEP	D	346	1	8,9,10	0.76	0	8,12,14	1.92	4 (50%)
1	SEP	C	346	1	8,9,10	0.85	0	8,12,14	2.85	2 (25%)
1	SEP	A	346	1	8,9,10	0.72	0	8,12,14	2.12	4 (50%)
1	TPO	C	345	1	8,10,11	0.92	0	10,14,16	2.02	2 (20%)
1	TPO	A	345	1	8,10,11	1.04	0	10,14,16	1.22	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	D	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	C	345	1	-	5/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	CG2-CB	2.10	1.56	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	7.09	115.05	108.14
1	C	345	TPO	CG2-CB-CA	4.97	122.97	113.16
1	D	346	SEP	OG-CB-CA	3.30	111.36	108.14
1	A	346	SEP	P-OG-CB	-3.20	109.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	OG-P-O1P	3.04	114.99	106.47
1	A	346	SEP	OG-CB-CA	3.02	111.08	108.14
1	C	345	TPO	O2P-P-OG1	2.79	118.50	105.99
1	C	346	SEP	P-OG-CB	-2.66	110.96	118.30
1	D	346	SEP	O3P-P-OG	2.57	113.57	106.73
1	A	345	TPO	O3P-P-OG1	2.44	116.93	105.99
1	D	346	SEP	P-OG-CB	-2.44	111.58	118.30
1	A	346	SEP	O3P-P-OG	2.37	113.05	106.73
1	D	346	SEP	OG-P-O1P	2.15	112.50	106.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	SO4	B	501	-	4,4,4	0.31	0	6,6,6	0.25	0
2	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.32	0
2	SO4	A	502	-	4,4,4	0.17	0	6,6,6	0.15	0
3	6QY	C	501	-	26,28,28	0.85	1 (3%)	29,39,39	0.94	2 (6%)
3	6QY	D	501	-	26,28,28	0.77	1 (3%)	29,39,39	0.92	2 (6%)
3	6QY	B	504	-	26,28,28	0.82	1 (3%)	29,39,39	0.82	1 (3%)
2	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.10	0
3	6QY	A	503	-	26,28,28	1.03	1 (3%)	29,39,39	1.59	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6QY	D	501	-	-	2/10/30/30	0/4/4/4
3	6QY	C	501	-	-	0/10/30/30	0/4/4/4
3	6QY	B	504	-	-	2/10/30/30	0/4/4/4
3	6QY	A	503	-	-	6/10/30/30	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	6QY	C11-C10	4.12	1.45	1.40
3	B	504	6QY	C11-C10	3.01	1.44	1.40
3	C	501	6QY	C11-C10	2.95	1.44	1.40
3	D	501	6QY	C11-C10	2.36	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	6QY	C7-N1-C4	6.36	136.25	124.16
3	A	503	6QY	C-N-C1	3.74	118.82	112.39
3	C	501	6QY	C-N-C1	3.35	118.15	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	6QY	C18-N-C1	3.06	117.65	112.39
3	B	504	6QY	C18-N-C1	2.39	116.50	112.39
3	A	503	6QY	C3-C4-N1	2.21	114.05	110.60
3	A	503	6QY	C18-N-C1	-2.16	108.67	112.39
3	D	501	6QY	C-N-C1	2.03	115.89	112.39
3	C	501	6QY	C18-N-C1	2.01	115.84	112.39
3	A	503	6QY	C5-C4-N1	2.00	113.72	110.60

There are no chirality outliers.

All (10) torsion outliers are listed below:

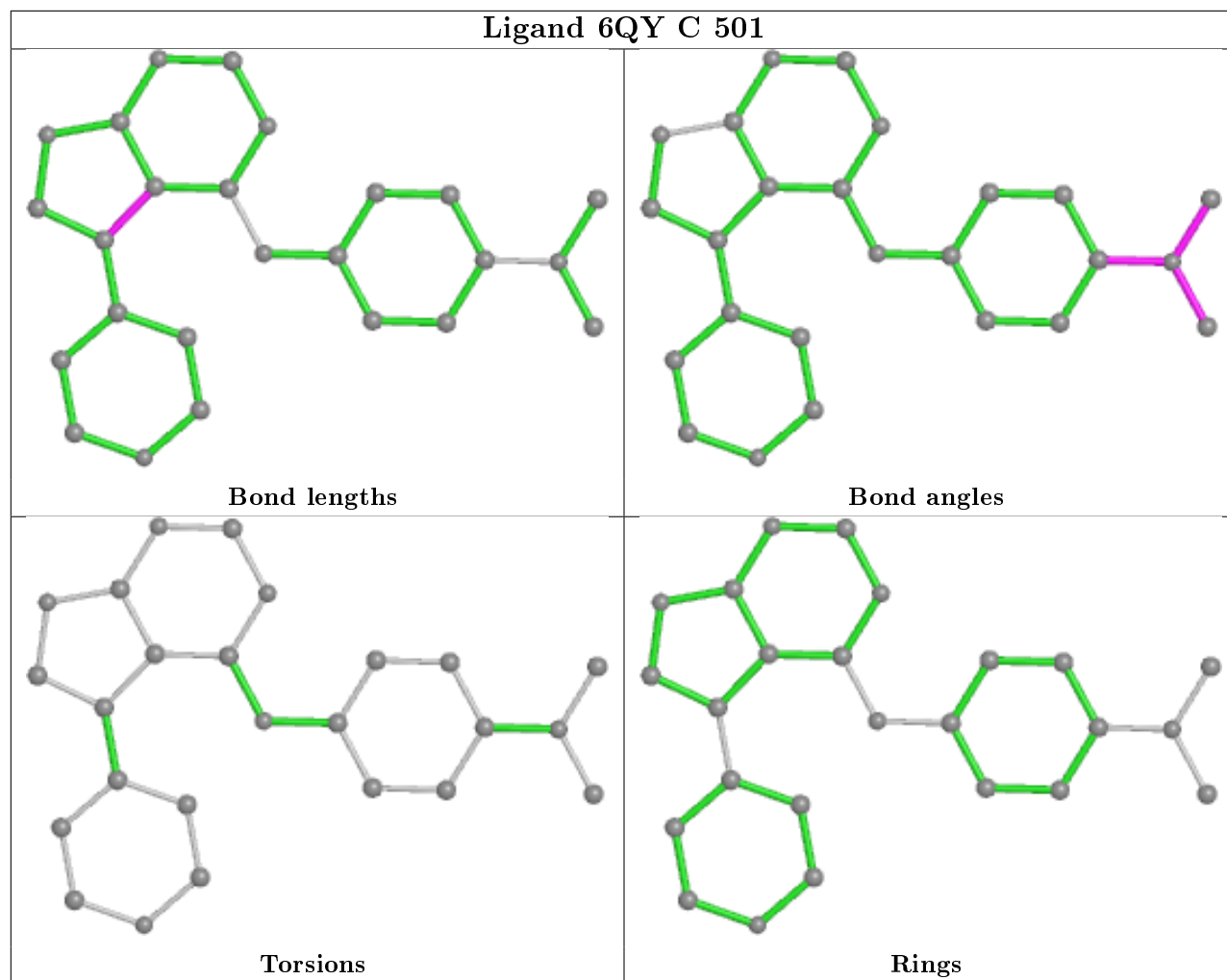
Mol	Chain	Res	Type	Atoms
3	A	503	6QY	C2-C1-N-C
3	A	503	6QY	N2-C7-N1-C4
3	A	503	6QY	C5-C4-N1-C7
3	A	503	6QY	C2-C1-N-C18
3	A	503	6QY	C6-C1-N-C18
3	A	503	6QY	C6-C1-N-C
3	D	501	6QY	C12-C11-C13-C14
3	D	501	6QY	C12-C11-C13-C17
3	B	504	6QY	C12-C11-C13-C14
3	B	504	6QY	C12-C11-C13-C17

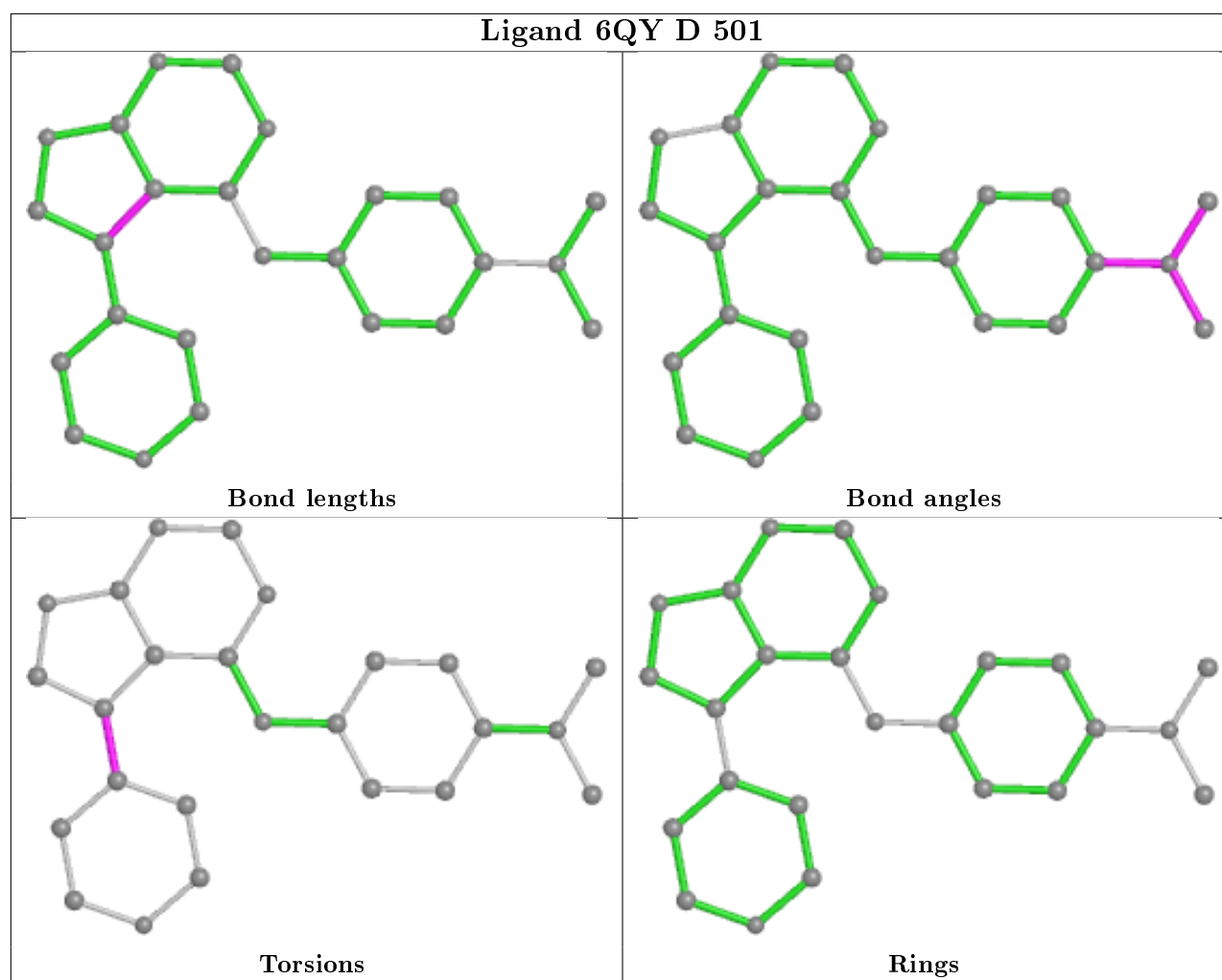
There are no ring outliers.

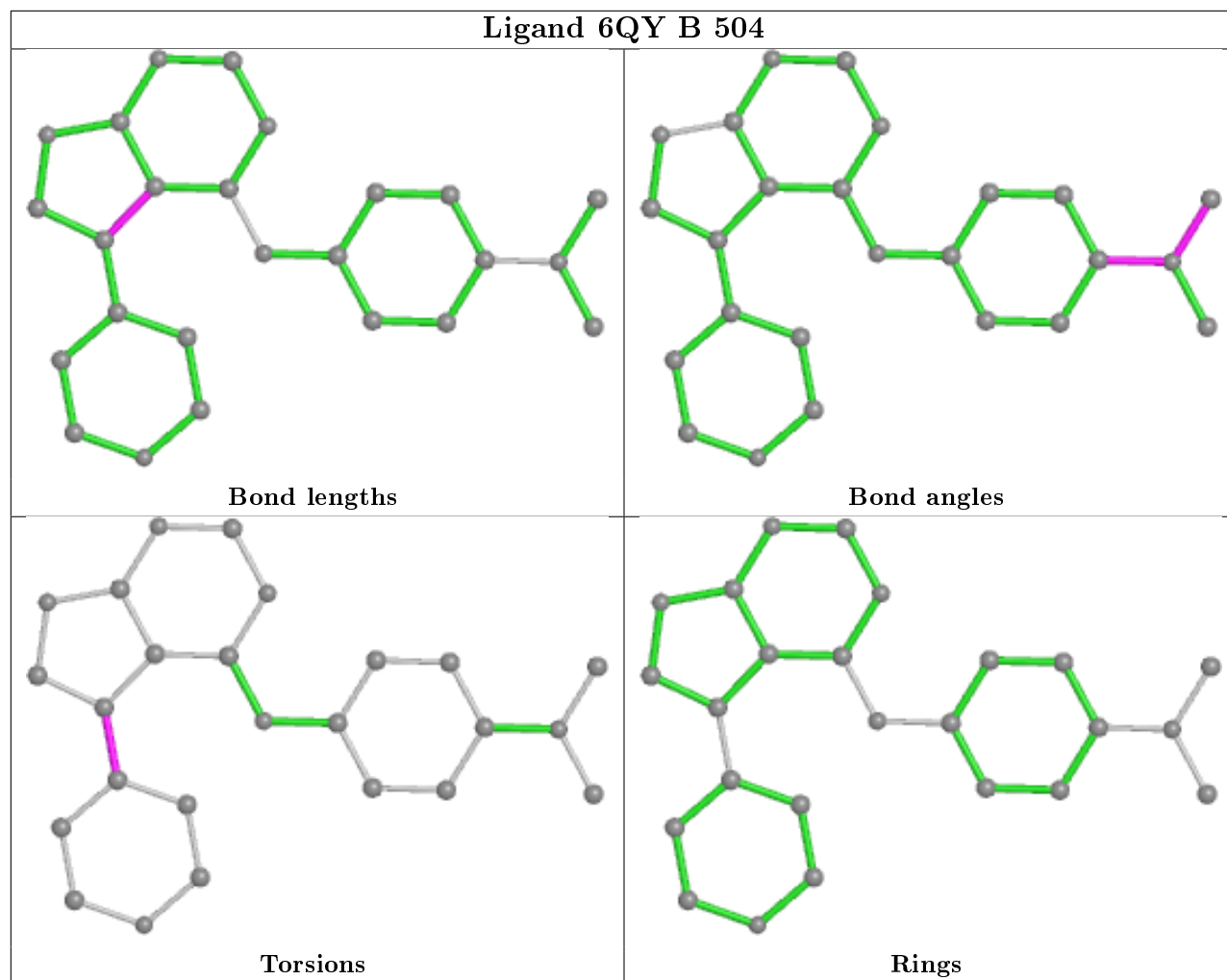
1 monomer is involved in 1 short contact:

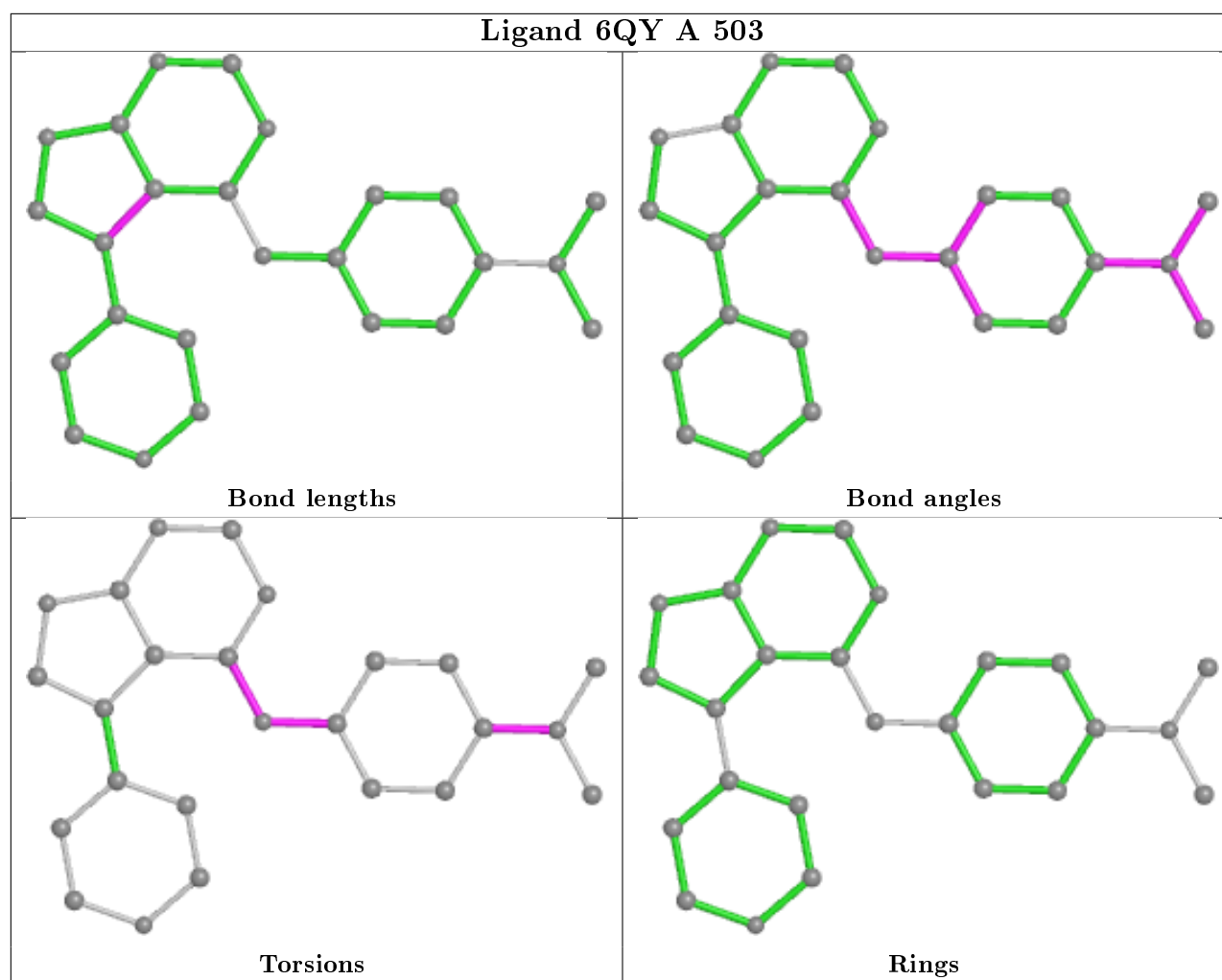
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	6QY	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	277/301 (92%)	0.37	16 (5%)	23 21	31, 55, 98, 133	0
1	B	267/301 (88%)	0.35	16 (5%)	21 20	33, 57, 98, 130	0
1	C	277/301 (92%)	0.72	39 (14%)	2 2	31, 60, 103, 136	0
1	D	276/301 (91%)	0.66	31 (11%)	5 4	32, 61, 111, 158	0
All	All	1097/1204 (91%)	0.53	102 (9%)	8 7	31, 59, 103, 158	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	TYR	12.1
1	C	225	GLU	10.7
1	C	203	GLY	7.8
1	B	196	GLY	6.2
1	A	196	GLY	5.9
1	D	343	VAL	5.7
1	C	168	PHE	5.5
1	D	201	TYR	5.2
1	A	256	ASP	5.0
1	D	221	ILE	5.0
1	D	196	GLY	5.0
1	C	176	VAL	4.8
1	D	180	PHE	4.7
1	A	226	LEU	4.5
1	C	221	ILE	4.3
1	C	251	PHE	4.2
1	B	207	ASN	4.2
1	D	197	PHE	4.2
1	C	201	TYR	4.2
1	C	197	PHE	4.1
1	C	399	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	170	PHE	4.0
1	A	216	ALA	4.0
1	A	197	PHE	3.9
1	B	197	PHE	3.9
1	D	226	LEU	3.7
1	D	168	PHE	3.7
1	C	343	VAL	3.7
1	C	170	PHE	3.6
1	D	252	SER	3.6
1	D	179	ASN	3.6
1	A	347	ARG	3.5
1	D	190	ASN	3.5
1	C	226	LEU	3.5
1	C	223	THR	3.5
1	D	173	LEU	3.4
1	D	225	GLU	3.4
1	C	173	LEU	3.4
1	D	187	VAL	3.3
1	C	171	TYR	3.3
1	D	177	THR	3.3
1	C	259	CYS	3.2
1	B	204	TYR	3.2
1	A	187	VAL	3.2
1	C	230	PHE	3.1
1	D	204	TYR	3.0
1	B	330	PHE	3.0
1	D	229	GLN	3.0
1	A	229	GLN	2.9
1	C	335	ALA	2.9
1	D	181	ASP	2.9
1	A	207	ASN	2.9
1	A	228	GLN	2.9
1	C	229	GLN	2.9
1	A	343	VAL	2.8
1	D	192	MET	2.8
1	C	196	GLY	2.8
1	C	258	LEU	2.8
1	B	206	ASN	2.8
1	B	410	ILE	2.8
1	C	180	PHE	2.7
1	D	230	PHE	2.7
1	D	212	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	176	VAL	2.6
1	A	206	ASN	2.5
1	B	237	MET	2.5
1	C	210	VAL	2.5
1	B	239	LYS	2.5
1	A	188	GLY	2.5
1	A	443	LYS	2.5
1	A	236	VAL	2.5
1	D	185	ILE	2.5
1	C	179	ASN	2.4
1	B	171	TYR	2.4
1	C	199	VAL	2.4
1	B	229	GLN	2.4
1	A	204	TYR	2.4
1	C	347	ARG	2.4
1	C	181	ASP	2.3
1	C	204	TYR	2.3
1	C	222	THR	2.3
1	D	175	ASN	2.3
1	C	227	LYS	2.3
1	C	185	ILE	2.2
1	B	195	GLY	2.2
1	C	260	LEU	2.2
1	C	200	VAL	2.2
1	B	194	GLU	2.2
1	B	228	GLN	2.2
1	C	252	SER	2.2
1	C	253	SER	2.2
1	C	175	ASN	2.2
1	D	195	GLY	2.2
1	C	164	ARG	2.1
1	C	392	GLU	2.1
1	D	223	THR	2.1
1	C	209	THR	2.1
1	D	347	ARG	2.0
1	B	169	SER	2.0
1	D	203	GLY	2.0
1	D	210	VAL	2.0
1	B	165	PHE	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	SEP	A	346	10/11	0.70	0.20	114,121,131,131	0
1	SEP	C	346	10/11	0.76	0.22	110,117,128,130	0
1	SEP	D	346	10/11	0.77	0.21	124,135,147,147	0
1	TPO	A	345	11/12	0.77	0.15	106,111,115,116	0
1	TPO	C	345	11/12	0.88	0.22	106,110,115,117	0
1	TPO	D	345	11/12	0.89	0.12	120,127,133,136	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

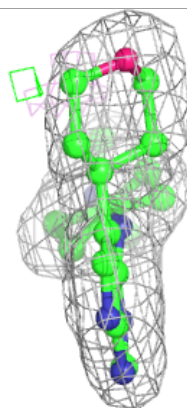
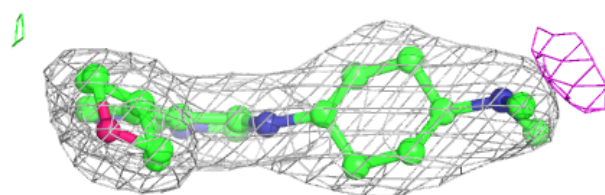
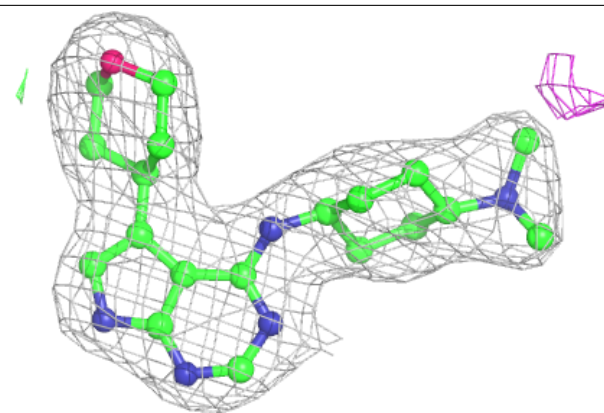
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	502	5/5	0.75	0.21	140,140,140,141	0
2	SO4	A	502	5/5	0.85	0.30	156,157,157,157	0
2	SO4	B	501	5/5	0.88	0.14	89,89,92,93	0
2	SO4	B	503	5/5	0.91	0.12	136,136,136,136	0
2	SO4	A	501	5/5	0.94	0.12	77,77,79,81	0
3	6QY	A	503	25/25	0.95	0.14	35,39,48,51	0
3	6QY	C	501	25/25	0.96	0.12	32,41,46,50	0
3	6QY	D	501	25/25	0.96	0.13	39,45,49,51	0
3	6QY	B	504	25/25	0.96	0.14	33,38,42,44	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.

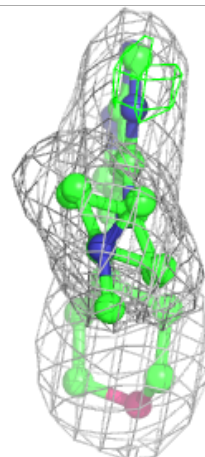
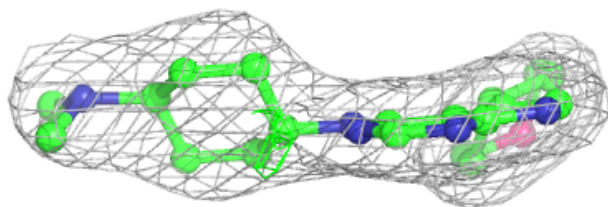
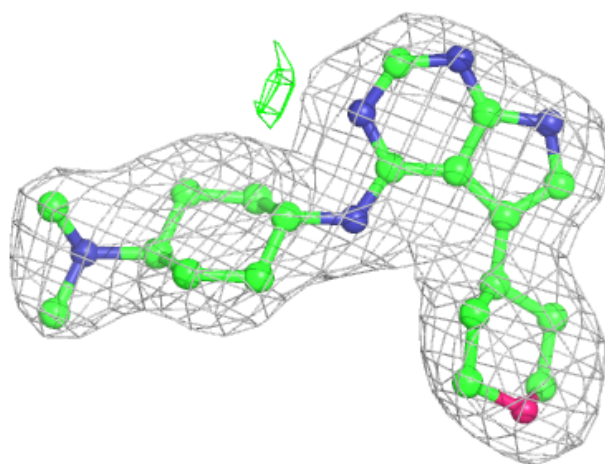
Electron density around 6QY A 503:

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



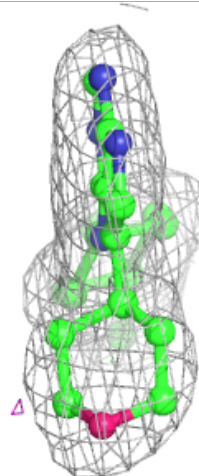
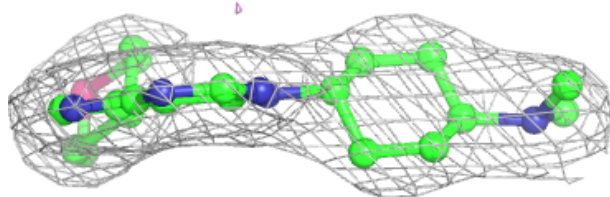
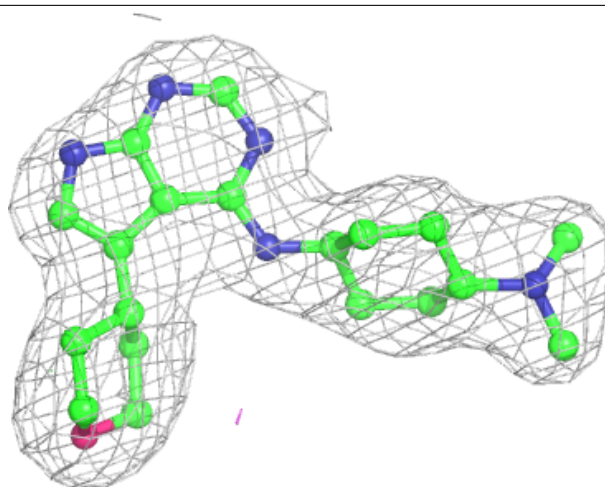
Electron density around 6QY C 501:

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



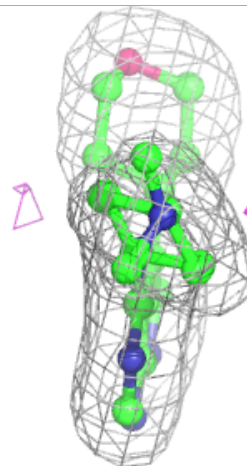
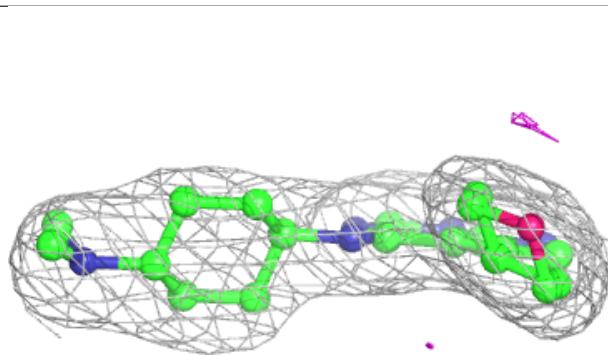
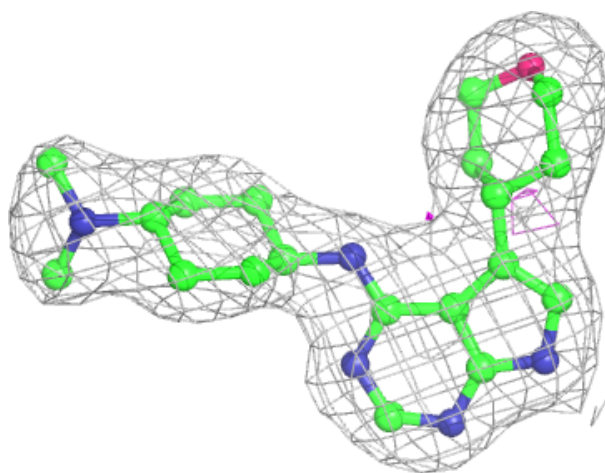
Electron density around 6QY D 501:

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



Electron density around 6QY B 504:

$2mF_o-DF_c$ (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.