



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:30 PM UTC

PDB ID : 5K72 / pdb_00005k72
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 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

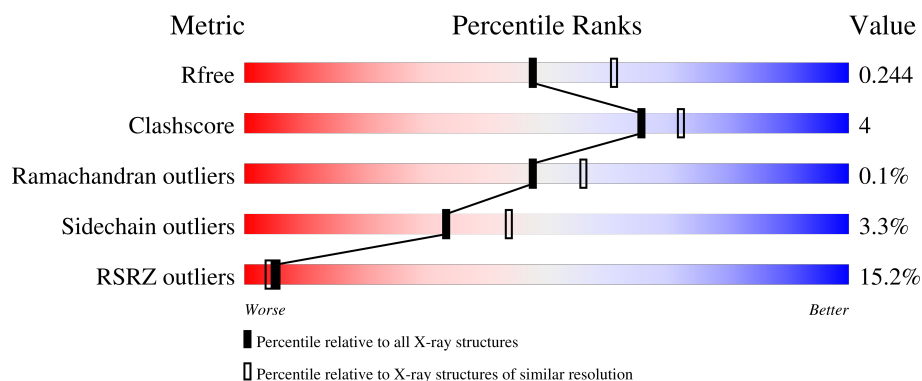
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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 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	301	7% 81% 10% • 7%
1	B	301	6% 79% 8% • 11%
1	C	301	22% 78% 13% • 7%
1	D	301	21% 78% 14% • 8%

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 (CCD ID: SO4) (formula: O₄S).



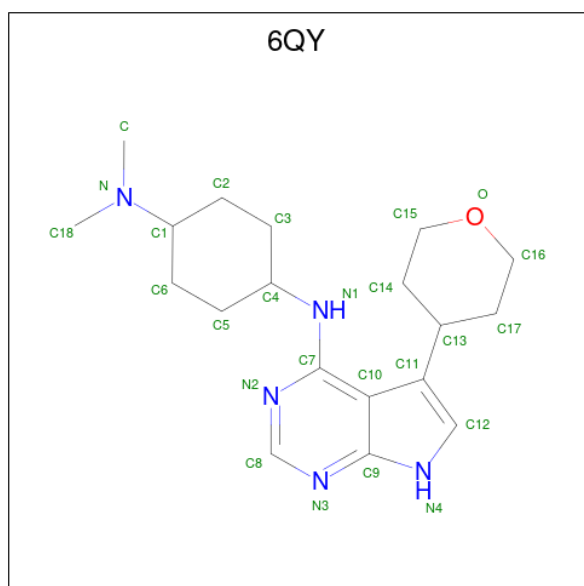
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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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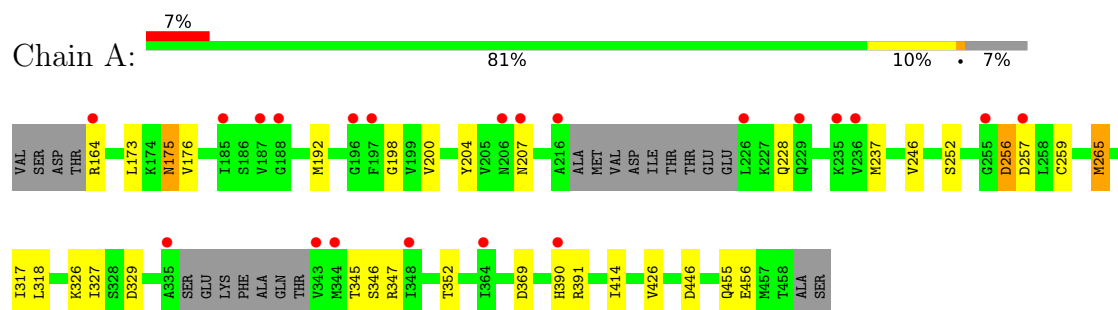
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	78	Total 78	O 78	0	0
4	D	70	Total 70	O 70	0	0

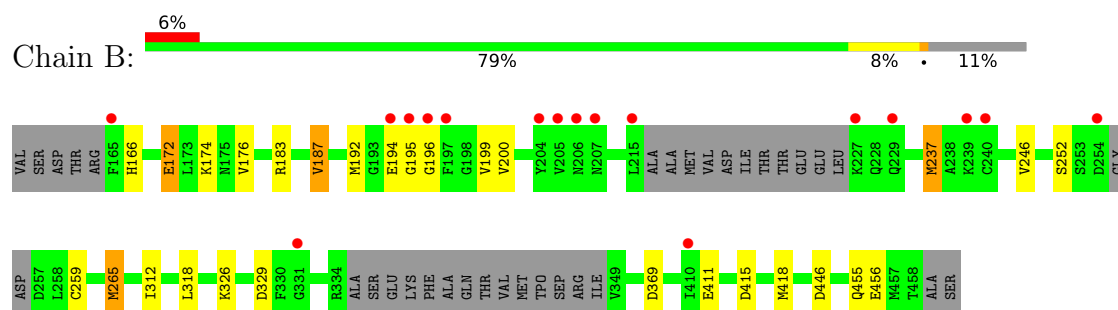
3 Residue-property plots [i](#)

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.

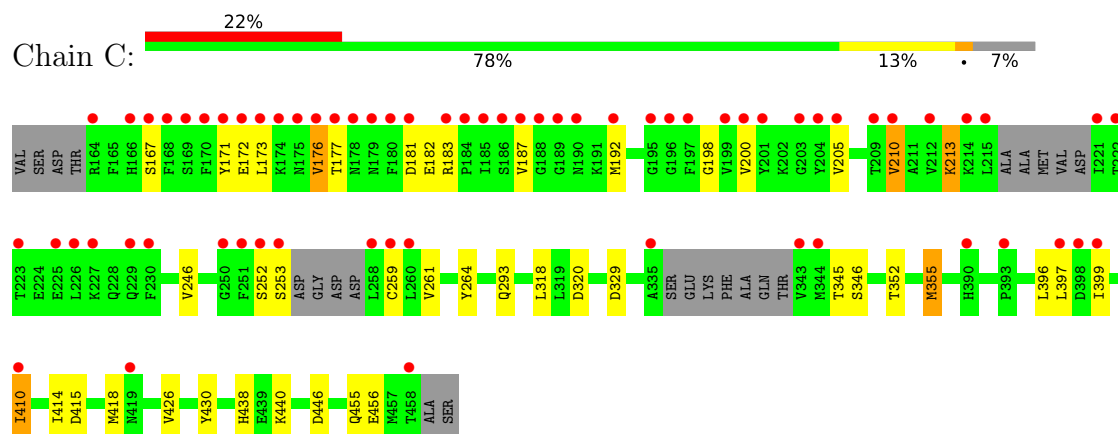
- Molecule 1: Interleukin-1 receptor-associated kinase 4



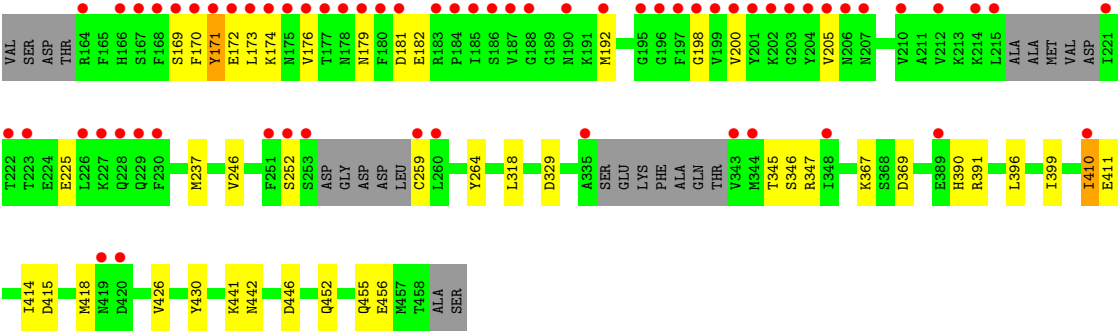
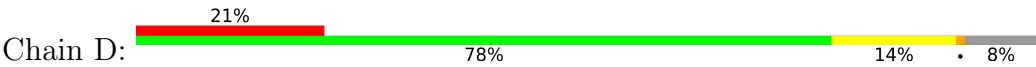
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	145.08Å 140.97Å 87.52Å 90.00° 125.77° 90.00°	Depositor
Resolution (Å)	58.86 – 2.22 58.86 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.0 (58.86-2.22) 99.6 (58.86-2.23)	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 (4.89%)	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)	0.36 , 72.6	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: SO4, 6QY, SEP, 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	1/2220 (0.0%)	1.29	8/2989 (0.3%)
1	B	0.85	3/2145 (0.1%)	1.29	8/2889 (0.3%)
1	C	0.86	1/2226 (0.0%)	1.32	8/2996 (0.3%)
1	D	0.84	0/2218	1.32	9/2985 (0.3%)
All	All	0.85	5/8809 (0.1%)	1.30	33/11859 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	MET	SD-CE	-7.38	1.61	1.79
1	B	265	MET	SD-CE	-6.87	1.62	1.79
1	C	355	MET	SD-CE	-6.41	1.63	1.79
1	B	312	ILE	CG1-CD1	-6.08	1.28	1.51
1	A	265	MET	SD-CE	-5.82	1.65	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	CA-CB-CG	10.11	122.71	112.60
1	D	172	GLU	CB-CG-CD	6.39	123.46	112.60
1	D	181	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	198	GLY	N-CA-C	6.12	119.23	111.09
1	C	181	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	198	GLY	N-CA-C	6.04	119.12	111.09
1	A	446	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	446	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	166	HIS	CA-CB-CG	5.84	119.64	113.80
1	A	256	ASP	N-CA-C	-5.80	106.20	113.28
1	C	446	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	237	MET	CB-CG-SD	5.57	129.41	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	198	GLY	N-CA-C	5.50	118.41	111.09
1	B	195	GLY	N-CA-C	5.46	119.49	110.97
1	D	446	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	411	GLU	CB-CG-CD	5.34	121.68	112.60
1	D	411	GLU	CB-CG-CD	5.34	121.68	112.60
1	A	369	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	171	TYR	CA-CB-CG	-5.29	104.38	113.90
1	C	396	LEU	CA-C-N	5.26	127.33	120.28
1	C	396	LEU	C-N-CA	5.26	127.33	120.28
1	C	456	GLU	CA-C-N	5.25	127.32	120.28
1	C	456	GLU	C-N-CA	5.25	127.32	120.28
1	B	172	GLU	CB-CG-CD	5.19	121.42	112.60
1	D	456	GLU	CA-C-N	5.17	127.20	120.28
1	D	456	GLU	C-N-CA	5.17	127.20	120.28
1	D	369	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	369	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	456	GLU	CA-C-N	5.07	127.07	120.28
1	B	456	GLU	C-N-CA	5.07	127.07	120.28
1	A	456	GLU	CA-C-N	5.02	127.00	120.28
1	A	456	GLU	C-N-CA	5.02	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2205	0	2176	11	0
1	B	2109	0	2084	9	0
1	C	2212	0	2193	28	0
1	D	2204	0	2181	20	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
All	All	9146	0	8634	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (66) 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:HE3	4:C:605:HOH:O	1.57	1.03
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.47	0.96
1:C:192:MET:CE	4:C:605:HOH:O	2.13	0.91
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.59	0.85
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: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:C:352:THR:HA	1:C:355:MET:HE3	1.79	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:D:237:MET:HE1	1:D:246:VAL:HG23	1.84	0.60
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.84	0.59
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:A:192:MET:HE3	1:A:200:VAL:HG12	1.84	0.57
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:O	1:B:176:VAL:HG13	2.05	0.56
1:D:442:ASN:C	4:D:601:HOH:O	2.48	0.56
1:C:210:VAL:HG21	1:C:261:VAL:CG1	2.38	0.54
1:C:192:MET:HE3	1:C:200:VAL:HG12	1.91	0.53
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:C:438:HIS:HD2	1:C:440:LYS:H	1.61	0.48
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:415:ASP:HB3	1:C:418:MET:HE2	2.00	0.44
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:B:415:ASP:HB3	1:B:418:MET:HE2	2.01	0.42
1:C:352:THR:N	1:C:355:MET:HE2	2.34	0.42
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:C:171:TYR:CD1	1:C:171:TYR:C	2.99	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
1:C:352:THR:HA	1:C:355:MET:CE	2.49	0.40
1:D:415:ASP:HB3	1:D:418:MET:HE2	2.03	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%)	30	33
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%)	48	56

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%)	232 (96%)	9 (4%)	30	39
1	B	234/260 (90%)	229 (98%)	5 (2%)	47	61
1	C	243/260 (94%)	231 (95%)	12 (5%)	22	27
1	D	242/260 (93%)	236 (98%)	6 (2%)	42	55
All	All	960/1040 (92%)	928 (97%)	32 (3%)	33	44

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	175	ASN
1	A	228	GLN
1	A	256	ASP
1	A	257	ASP
1	A	329	ASP
1	A	347	ARG
1	A	352	THR
1	A	455	GLN
1	B	174	LYS
1	B	187	VAL
1	B	237	MET
1	B	329	ASP
1	B	455	GLN
1	C	176	VAL
1	C	182	GLU
1	C	183	ARG
1	C	187	VAL
1	C	210	VAL
1	C	213	LYS
1	C	253	SER
1	C	329	ASP
1	C	397	LEU
1	C	399	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	229	GLN
1	A	293	GLN
1	A	394	GLN
1	A	435	GLN
1	A	452	GLN
1	B	293	GLN

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Mol	Chain	Res	Type
1	B	394	GLN
1	B	419	ASN
1	B	435	GLN
1	C	166	HIS
1	C	207	ASN
1	C	229	GLN
1	C	241	GLN
1	C	394	GLN
1	C	435	GLN
1	C	438	HIS
1	C	452	GLN
1	D	166	HIS
1	D	229	GLN
1	D	394	GLN

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	SEP	C	346	1	8,9,10	0.88	0	7,12,14	2.89	1 (14%)
1	SEP	A	346	1	8,9,10	0.76	0	7,12,14	1.97	3 (42%)
1	TPO	D	345	1	8,10,11	1.35	1 (12%)	10,14,16	1.13	0
1	TPO	C	345	1	8,10,11	0.99	0	10,14,16	2.11	2 (20%)
1	TPO	A	345	1	8,10,11	1.09	0	10,14,16	1.34	1 (10%)
1	SEP	D	346	1	8,9,10	0.79	0	7,12,14	1.87	3 (42%)

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	SEP	C	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	C	345	1	-	6/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-

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 (10) 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	4.99	122.97	113.26
1	D	346	SEP	OG-CB-CA	3.30	111.36	108.14
1	C	345	TPO	O2P-P-OG1	3.25	118.50	105.85
1	A	346	SEP	OG-P-O1P	3.16	114.99	106.44
1	A	346	SEP	OG-CB-CA	3.02	111.08	108.14
1	A	345	TPO	O3P-P-OG1	2.84	116.93	105.85
1	D	346	SEP	O3P-P-OG	2.65	113.57	106.67
1	A	346	SEP	O3P-P-OG	2.45	113.05	106.67
1	D	346	SEP	OG-P-O1P	2.24	112.50	106.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CA-CB-OG1-P
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	D	345	TPO	N-CA-CB-OG1

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.41	0	6,6,6	0.30	0
2	SO4	B	503	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.07	0
3	6QY	B	504	-	27,28,28	0.35	0	33,39,39	0.76	2 (6%)
2	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.17	0
3	6QY	D	501	-	27,28,28	0.39	0	33,39,39	0.82	2 (6%)
2	SO4	A	501	-	4,4,4	0.32	0	6,6,6	0.33	0
3	6QY	C	501	-	27,28,28	0.46	0	33,39,39	0.84	2 (6%)
3	6QY	A	503	-	27,28,28	0.45	0	33,39,39	1.61	4 (12%)

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	-	-	0/12/30/30	0/4/4/4
3	6QY	A	503	-	-	6/12/30/30	0/4/4/4
3	6QY	B	504	-	-	0/12/30/30	0/4/4/4
3	6QY	C	501	-	-	0/12/30/30	0/4/4/4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	6QY	C7-N1-C4	7.15	136.25	124.18
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
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	C18-N-C1	-2.16	108.67	112.39
3	B	504	6QY	C7-N1-C4	-2.05	120.72	124.18
3	A	503	6QY	C3-C4-N1	2.03	114.05	110.77
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

There are no chirality outliers.

All (6) 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

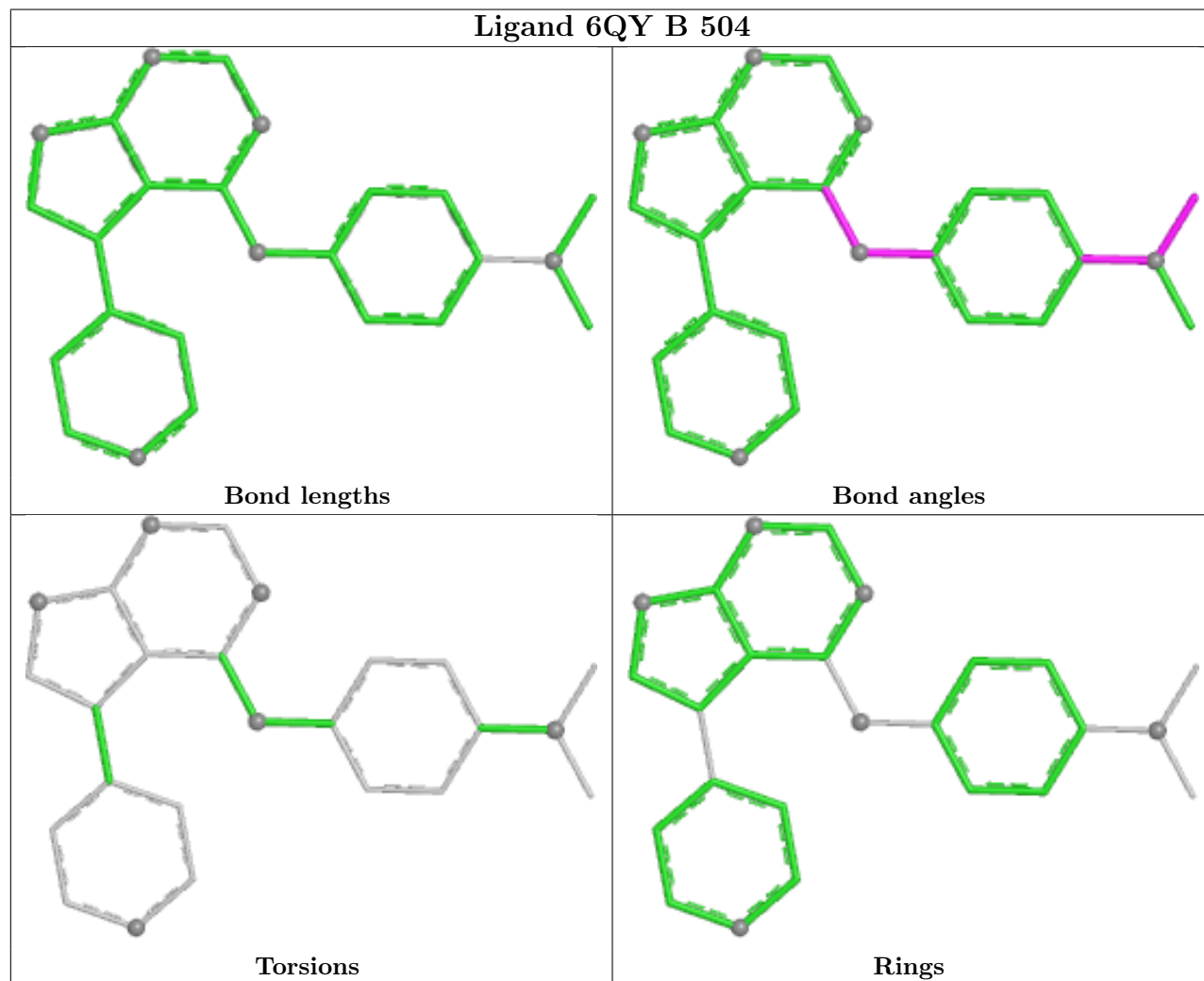
There are no ring outliers.

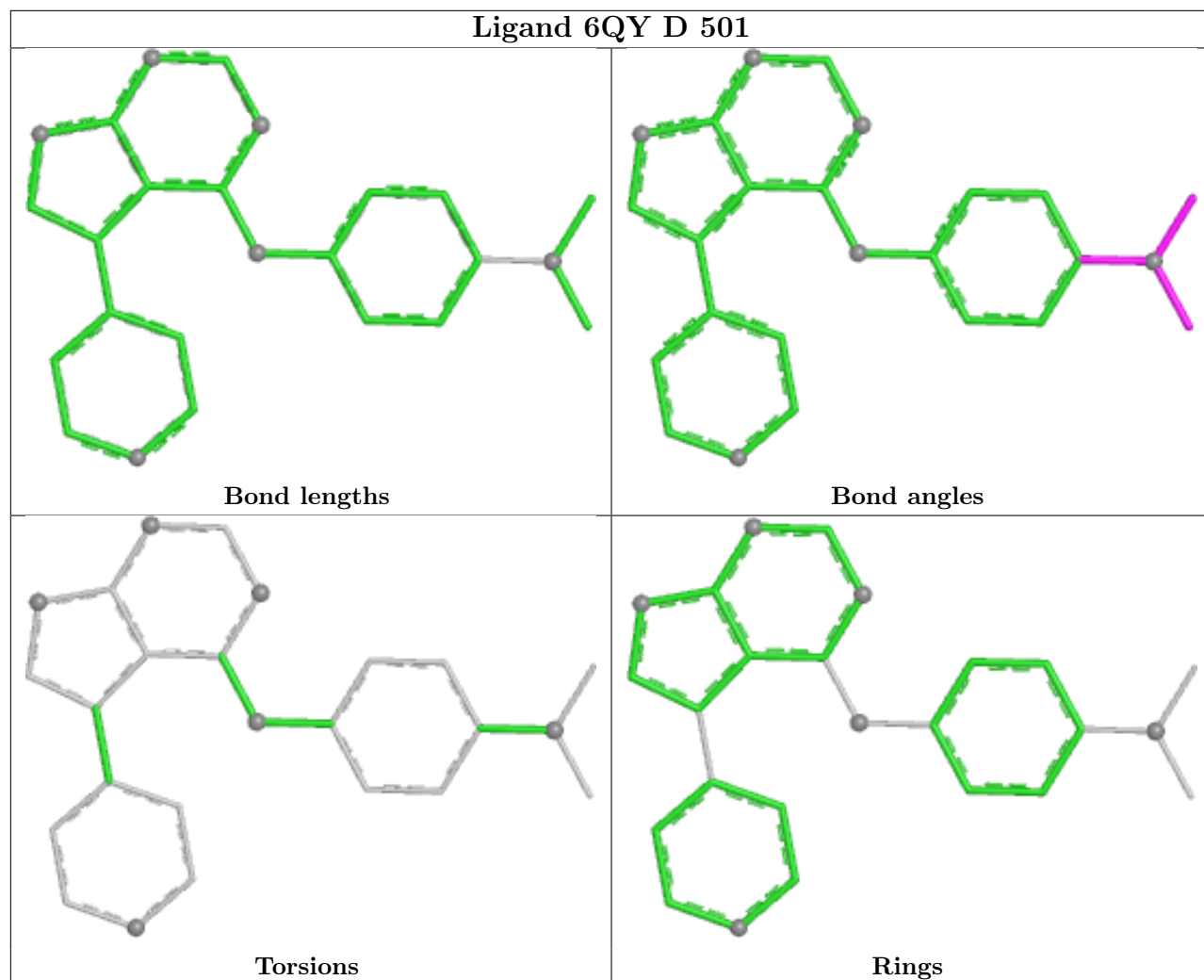
1 monomer is involved in 1 short contact:

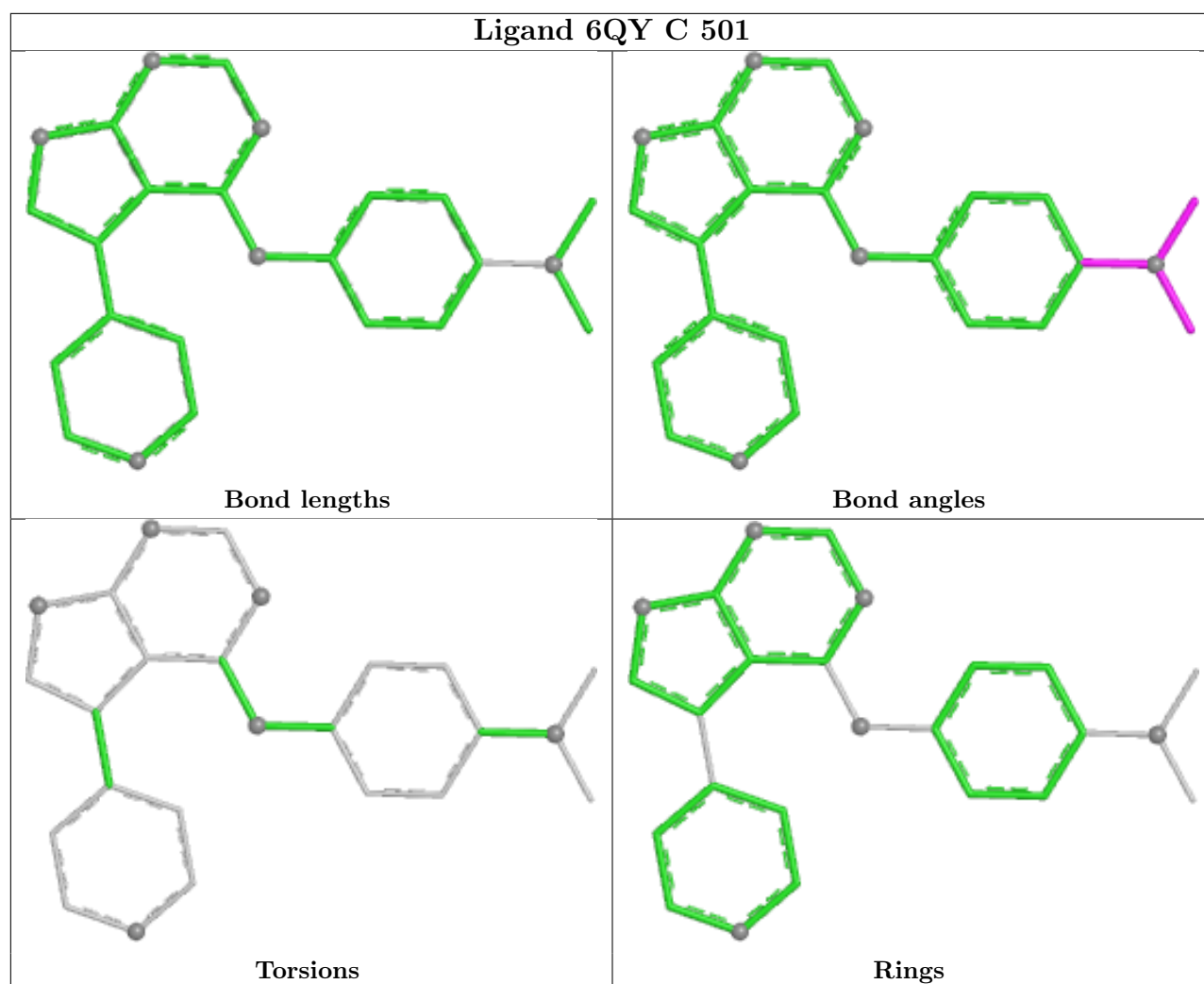
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	6QY	1	0

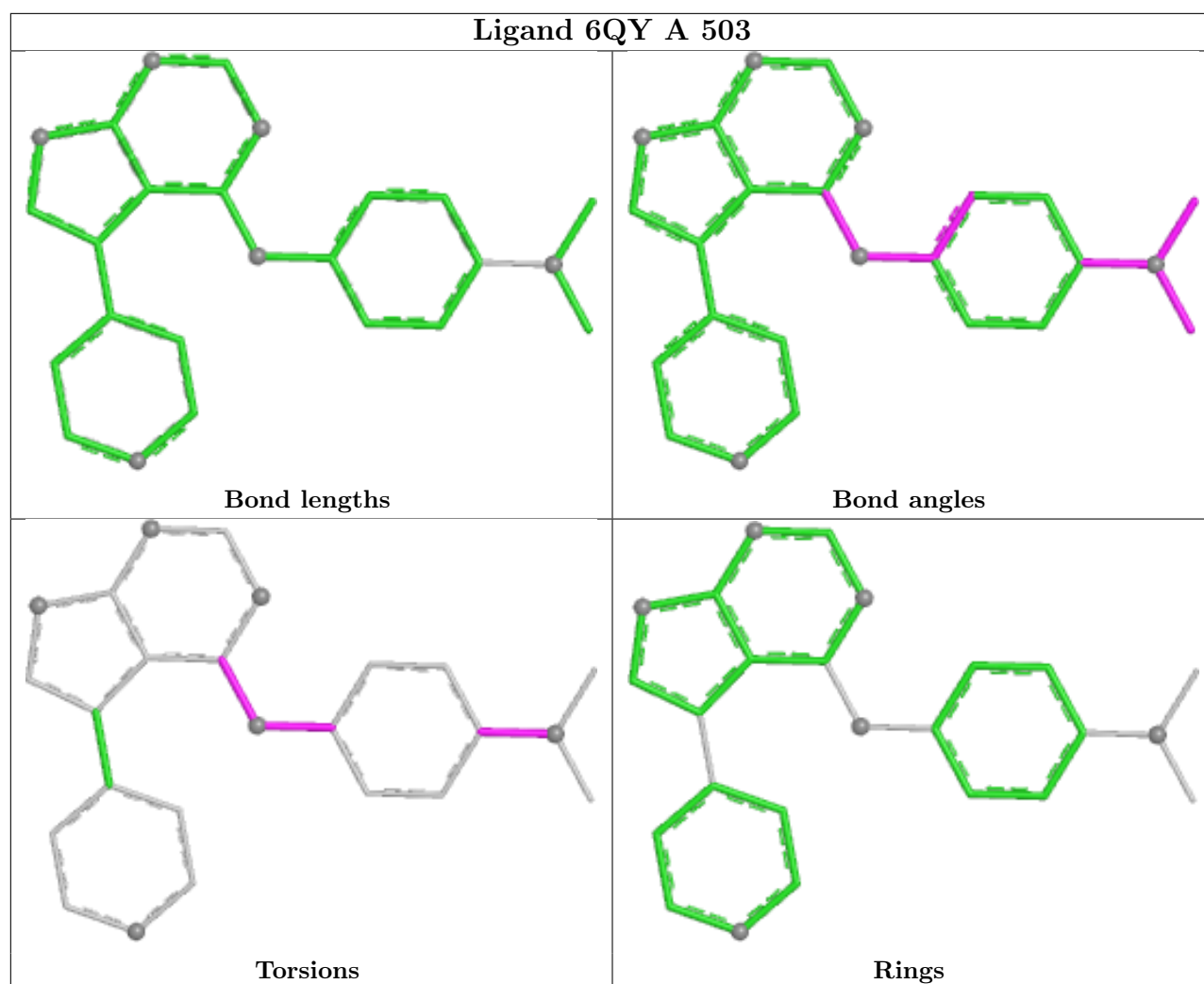
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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%)	0.46	21 (7%) 20 17	31, 55, 98, 133	0
1	B	267/301 (88%)	0.47	17 (6%) 25 22	33, 57, 98, 130	0
1	C	277/301 (92%)	1.10	66 (23%) 2 1	31, 60, 103, 136	0
1	D	276/301 (91%)	1.03	63 (22%) 2 1	32, 61, 111, 158	0
All	All	1097/1204 (91%)	0.77	167 (15%) 5 4	31, 59, 103, 158	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	TYR	8.1
1	C	226	LEU	6.2
1	D	226	LEU	5.7
1	C	399	ILE	5.7
1	C	168	PHE	5.6
1	D	180	PHE	5.6
1	D	179	ASN	5.6
1	C	176	VAL	5.5
1	D	201	TYR	5.4
1	C	253	SER	5.3
1	C	181	ASP	5.3
1	D	253	SER	5.2
1	D	170	PHE	5.1
1	C	171	TYR	5.0
1	C	201	TYR	5.0
1	C	170	PHE	5.0
1	C	251	PHE	5.0
1	C	180	PHE	4.9
1	C	221	ILE	4.9
1	D	181	ASP	4.8
1	C	259	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	176	VAL	4.4
1	D	183	ARG	4.4
1	D	197	PHE	4.3
1	C	203	GLY	4.3
1	C	175	ASN	4.3
1	C	179	ASN	4.3
1	C	173	LEU	4.2
1	D	199	VAL	4.1
1	C	230	PHE	4.1
1	D	177	THR	4.1
1	C	197	PHE	4.0
1	D	343	VAL	4.0
1	C	199	VAL	4.0
1	C	215	LEU	4.0
1	D	173	LEU	4.0
1	D	187	VAL	3.9
1	D	190	ASN	3.9
1	C	222	THR	3.9
1	D	215	LEU	3.9
1	D	168	PHE	3.8
1	C	258	LEU	3.8
1	C	252	SER	3.8
1	D	221	ILE	3.7
1	D	252	SER	3.7
1	D	214	LYS	3.6
1	A	197	PHE	3.6
1	C	214	LYS	3.6
1	C	343	VAL	3.5
1	C	169	SER	3.5
1	D	188	GLY	3.5
1	C	225	GLU	3.5
1	D	205	VAL	3.5
1	A	343	VAL	3.4
1	D	259	CYS	3.4
1	C	223	THR	3.4
1	C	260	LEU	3.3
1	C	205	VAL	3.3
1	A	229	GLN	3.3
1	B	205	VAL	3.3
1	C	250	GLY	3.2
1	D	230	PHE	3.2
1	B	204	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	200	VAL	3.2
1	C	174	LYS	3.2
1	C	190	ASN	3.2
1	C	209	THR	3.2
1	C	164	ARG	3.2
1	D	335	ALA	3.2
1	D	184	PRO	3.2
1	D	223	THR	3.2
1	C	183	ARG	3.1
1	D	186	SER	3.1
1	D	251	PHE	3.1
1	D	344	MET	3.1
1	D	169	SER	3.1
1	C	335	ALA	3.1
1	C	200	VAL	3.1
1	D	204	TYR	3.0
1	D	175	ASN	3.0
1	D	212	VAL	3.0
1	D	167	SER	3.0
1	C	178	ASN	3.0
1	A	390	HIS	2.9
1	C	204	TYR	2.9
1	B	229	GLN	2.9
1	D	178	ASN	2.9
1	C	177	THR	2.9
1	C	187	VAL	2.8
1	C	189	GLY	2.8
1	B	410	ILE	2.8
1	A	257	ASP	2.8
1	D	185	ILE	2.8
1	D	410	ILE	2.8
1	D	192	MET	2.8
1	D	348	ILE	2.7
1	B	195	GLY	2.7
1	D	195	GLY	2.7
1	A	164	ARG	2.7
1	A	216	ALA	2.7
1	C	227	LYS	2.7
1	C	185	ILE	2.7
1	D	203	GLY	2.7
1	B	197	PHE	2.6
1	D	174	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	VAL	2.6
1	B	207	ASN	2.6
1	A	255	GLY	2.6
1	B	165	PHE	2.6
1	A	196	GLY	2.6
1	C	166	HIS	2.6
1	C	393	PRO	2.6
1	A	185	ILE	2.6
1	C	167	SER	2.6
1	B	206	ASN	2.5
1	D	207	ASN	2.5
1	C	458	THR	2.5
1	A	236	VAL	2.5
1	D	210	VAL	2.5
1	B	227	LYS	2.5
1	A	206	ASN	2.5
1	B	331	GLY	2.5
1	C	188	GLY	2.5
1	C	210	VAL	2.4
1	C	212	VAL	2.4
1	D	260	LEU	2.4
1	C	229	GLN	2.4
1	C	196	GLY	2.4
1	A	348	ILE	2.4
1	A	344	MET	2.4
1	D	164	ARG	2.4
1	D	420	ASP	2.4
1	B	196	GLY	2.4
1	C	344	MET	2.4
1	C	410	ILE	2.3
1	C	390	HIS	2.3
1	C	195	GLY	2.3
1	D	198	GLY	2.3
1	C	397	LEU	2.3
1	C	192	MET	2.3
1	C	186	SER	2.3
1	C	172	GLU	2.3
1	A	364	ILE	2.3
1	A	226	LEU	2.3
1	C	419	ASN	2.2
1	B	240	CYS	2.2
1	D	166	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	LYS	2.2
1	D	419	ASN	2.2
1	D	222	THR	2.2
1	B	194	GLU	2.2
1	D	196	GLY	2.2
1	D	229	GLN	2.2
1	B	239	LYS	2.1
1	D	227	LYS	2.1
1	C	184	PRO	2.1
1	A	188	GLY	2.1
1	A	335	ALA	2.1
1	C	398	ASP	2.1
1	D	228	GLN	2.1
1	D	172	GLU	2.1
1	A	207	ASN	2.1
1	B	254	ASP	2.1
1	D	206	ASN	2.1
1	D	389	GLU	2.0
1	B	215	LEU	2.0
1	D	202	LYS	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	0.51	0.14	114,121,131,131	0
1	SEP	D	346	10/11	0.61	0.13	124,135,147,147	0
1	SEP	C	346	10/11	0.73	0.13	110,117,128,130	0
1	TPO	A	345	11/12	0.83	0.13	106,111,115,116	0
1	TPO	C	345	11/12	0.85	0.15	106,110,115,117	0
1	TPO	D	345	11/12	0.88	0.11	120,127,133,136	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

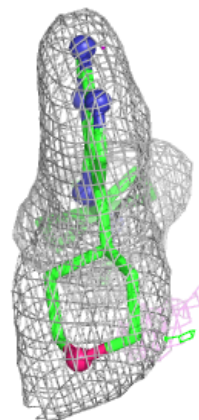
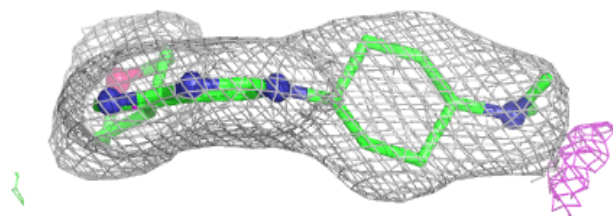
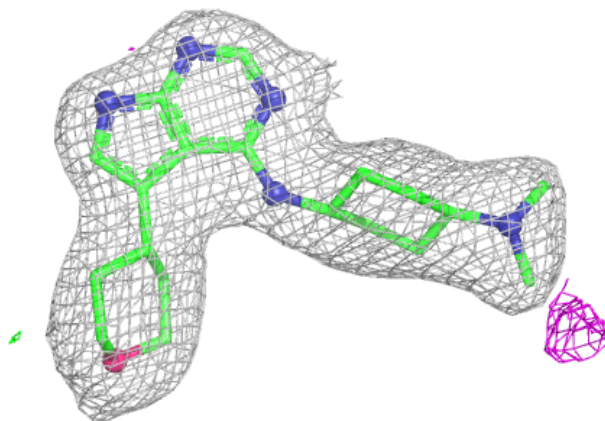
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	503	5/5	0.43	0.10	136,136,136,136	0
2	SO4	B	502	5/5	0.49	0.13	140,140,140,141	0
2	SO4	B	501	5/5	0.73	0.14	89,89,92,93	0
2	SO4	A	502	5/5	0.79	0.13	156,157,157,157	0
2	SO4	A	501	5/5	0.90	0.07	77,77,79,81	0
3	6QY	A	503	25/25	0.95	0.09	35,39,48,51	0
3	6QY	B	504	25/25	0.95	0.08	33,38,42,44	0
3	6QY	C	501	25/25	0.95	0.08	32,41,46,50	0
3	6QY	D	501	25/25	0.95	0.08	39,45,49,51	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.

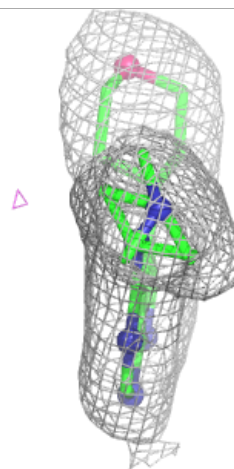
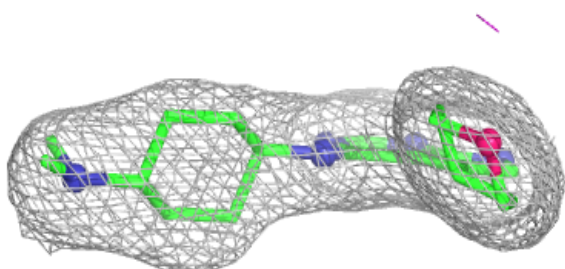
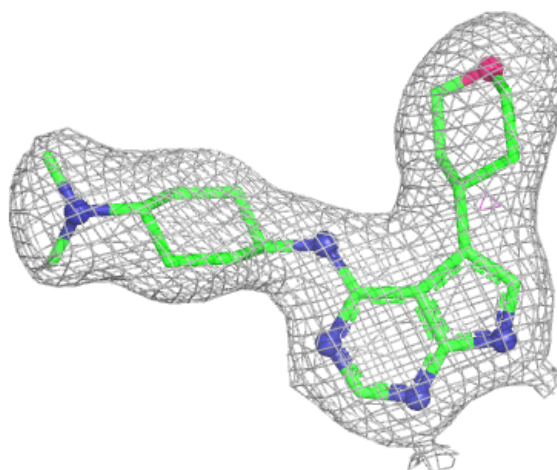
Electron density around 6QY A 503:

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



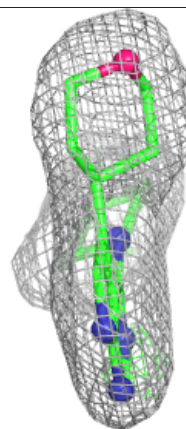
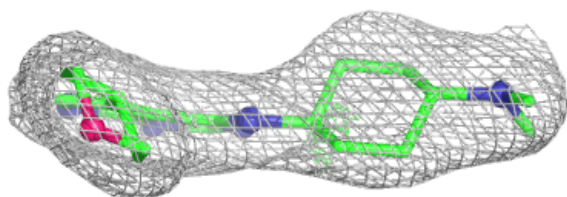
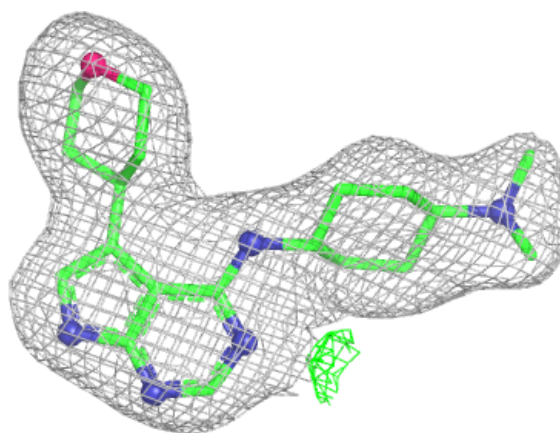
Electron density around 6QY B 504:

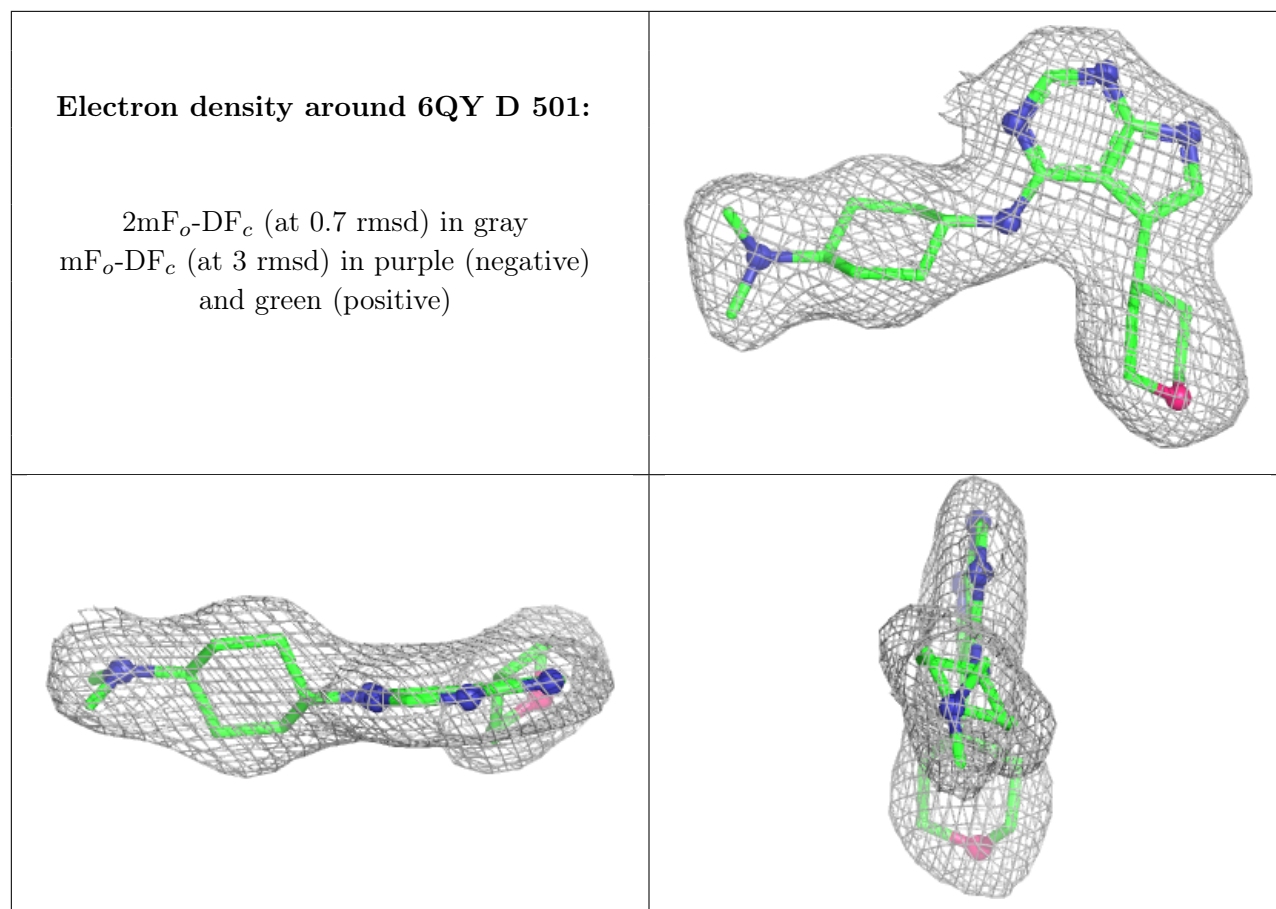
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.