



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:07 am BST

PDB ID : 6UWY
Title : DYRK1A bound to a harmine derivative
Authors : Khamrui, S.; Lazarus, M.B.
Deposited on : 2019-11-05
Resolution : 2.95 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

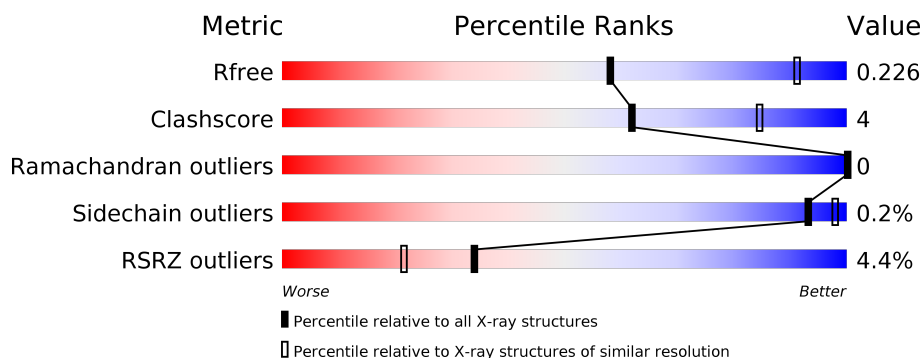
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	361	<div> <div>0%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
1	B	361	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
1	C	361	<div> <div>12%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	D	361	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PG4	C	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11717 atoms, of which 76 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.

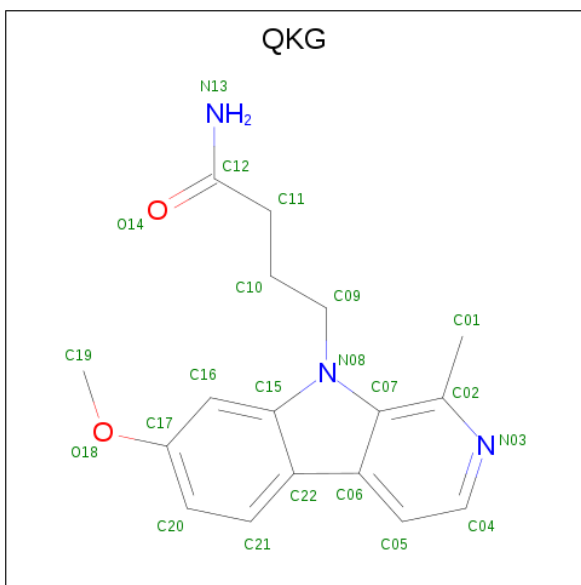
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	P	S	0	1	0
			2845	1828	491	508	1	17			
1	B	348	Total	C	N	O	P	S	0	3	0
			2860	1838	489	514	2	17			
1	C	347	Total	C	N	O	P	S	0	2	0
			2844	1827	488	511	1	17			
1	D	348	Total	C	N	O	P	S	0	3	0
			2862	1838	489	516	2	17			

There are 8 discrepancies between the modelled and reference sequences:

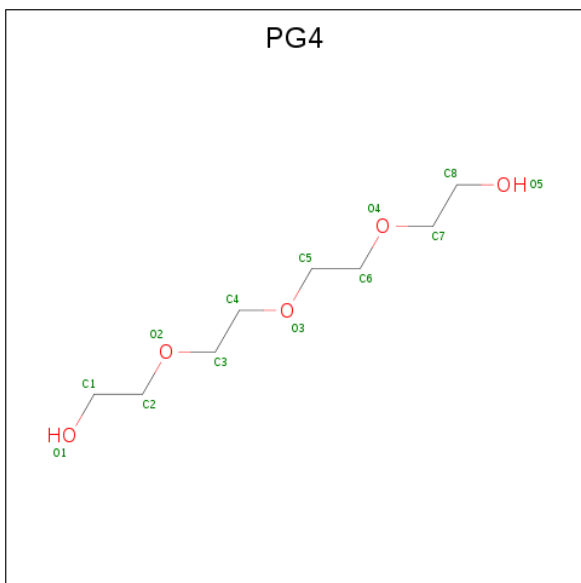
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	expression tag	UNP Q13627
A	126	MET	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
B	126	MET	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
C	126	MET	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627
D	126	MET	-	expression tag	UNP Q13627

- Molecule 2 is 4-(7-methoxy-1-methyl-9H-beta-carbolin-9-yl)butanamide (three-letter code: QKG) (formula: C₁₇H₁₉N₃O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			41	17	19	3	2		
2	B	1	Total	C	H	N	O	0	0
			41	17	19	3	2		
2	C	1	Total	C	H	N	O	0	0
			41	17	19	3	2		
2	D	1	Total	C	H	N	O	0	0
			41	17	19	3	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 13 8 5	0	0
3	D	1	Total C O 10 6 4	0	0
3	D	1	Total C O 13 8 5	0	0

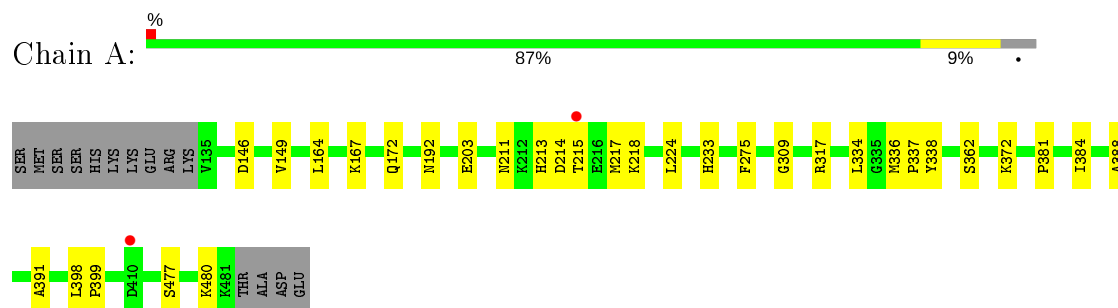
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	3	Total O 3 3	0	0

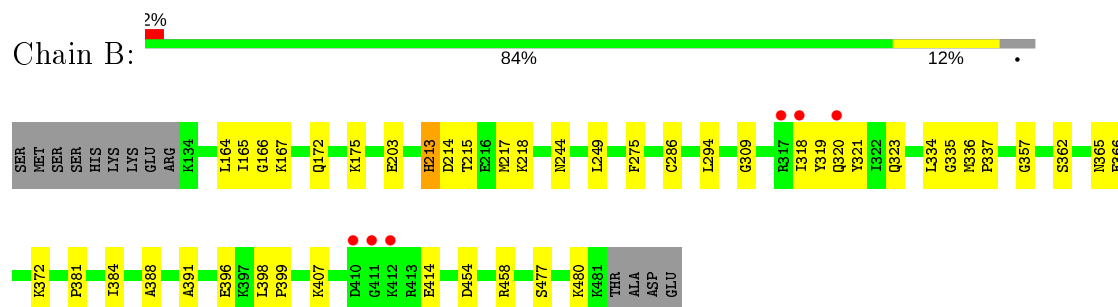
3 Residue-property plots [i](#)

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.

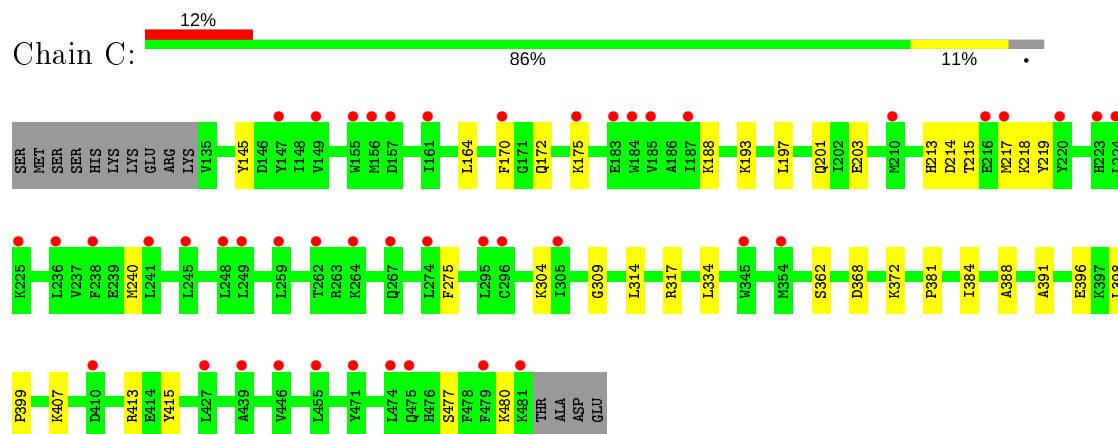
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



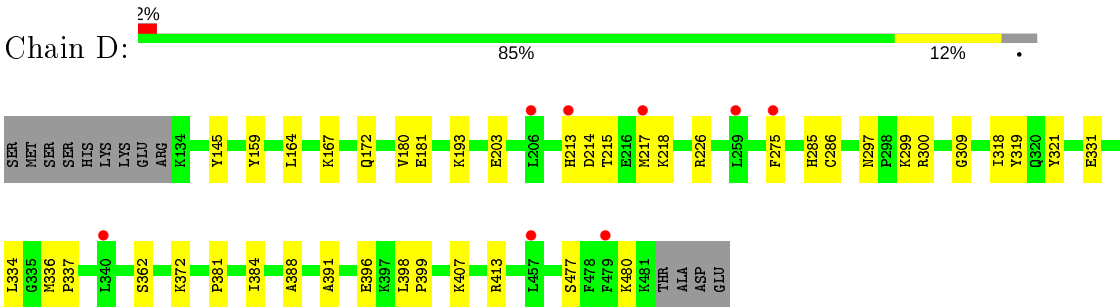
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.04Å 65.22Å 138.76Å 90.00° 114.86° 90.00°	Depositor
Resolution (Å)	119.80 – 2.95 125.90 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (119.80-2.95) 99.9 (125.90-2.95)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.195 , 0.227 0.196 , 0.226	Depositor DCC
R_{free} test set	2325 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: PG4, QKG, PTR

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	0.25	0/2897	0.44	0/3903
1	B	0.25	0/2902	0.46	0/3913
1	C	0.25	0/2899	0.44	0/3909
1	D	0.25	0/2904	0.44	0/3916
All	All	0.25	0/11602	0.44	0/15641

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	319	TYR	Peptide

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	2845	0	2851	23	0
1	B	2860	0	2848	32	0
1	C	2844	0	2839	24	0
1	D	2862	0	2848	27	0
2	A	22	19	0	0	0
2	B	22	19	0	0	0
2	C	22	19	0	0	0
2	D	22	19	0	0	0
3	A	36	0	49	0	0
3	B	36	0	49	0	0
3	C	23	0	31	0	0
3	D	36	0	49	0	0
4	A	8	0	0	0	0
4	B	3	0	0	0	0
All	All	11641	76	11564	102	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 (102) 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:203:GLU:HB2	1:C:309:GLY:HA2	1.60	0.82
1:B:166:GLY:HA2	1:D:180:VAL:O	1.84	0.77
1:D:214:ASP:O	1:D:215:THR:HG23	1.85	0.76
1:C:213:HIS:O	1:C:218:LYS:HD3	1.86	0.75
1:B:213:HIS:O	1:B:218:LYS:HD3	1.90	0.72
1:A:214:ASP:O	1:A:215:THR:HG23	1.90	0.71
1:A:146:ASP:HB3	1:A:172:GLN:OE1	1.89	0.71
1:B:414:GLU:OE1	1:D:299:LYS:NZ	2.24	0.70
1:B:214:ASP:O	1:B:215:THR:HG23	1.92	0.70
1:A:213:HIS:O	1:A:218:LYS:HD3	1.95	0.67
1:D:213:HIS:O	1:D:218:LYS:HD3	1.95	0.66
1:A:149:VAL:HG23	1:A:172:GLN:HE22	1.61	0.66
1:B:167:LYS:HD2	1:D:181:GLU:OE2	1.96	0.65
1:B:320:GLN:HE22	1:B:335:GLY:HA2	1.61	0.65
1:B:396:GLU:OE2	1:B:407:LYS:HE3	1.97	0.64
1:B:320:GLN:HE22	1:B:335:GLY:CA	2.11	0.64
1:C:214:ASP:O	1:C:215:THR:HG23	1.97	0.63
1:B:164:LEU:HD11	1:B:172:GLN:HB3	1.80	0.63
1:C:170:PHE:CD1	1:C:188:LYS:HE3	2.34	0.62
1:C:219:TYR:O	1:C:304:LYS:NZ	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:GLU:OE1	1:D:407:LYS:HG3	2.02	0.59
1:B:203:GLU:HB2	1:B:309:GLY:HA2	1.85	0.58
1:B:477:SER:HA	1:B:480:LYS:HD3	1.86	0.58
1:C:145:TYR:CZ	1:C:193:LYS:HD2	2.40	0.57
1:C:477:SER:HA	1:C:480:LYS:HD3	1.86	0.57
1:A:203:GLU:HB2	1:A:309:GLY:HA2	1.86	0.57
1:C:145:TYR:CE2	1:C:193:LYS:HD2	2.41	0.55
1:B:321[A]:PTR:O3P	1:B:366:GLU:HG3	2.07	0.55
1:C:219:TYR:C	1:C:304:LYS:HZ3	2.10	0.55
1:B:334:LEU:HB3	1:B:388:ALA:HB1	1.89	0.54
1:A:477:SER:HA	1:A:480:LYS:HD3	1.88	0.54
1:D:336:MET:HB3	1:D:337:PRO:HD2	1.89	0.54
1:B:336:MET:HB3	1:B:337:PRO:HD2	1.89	0.53
1:D:331:GLU:HA	1:D:336:MET:HE2	1.91	0.53
1:B:321[A]:PTR:O3P	1:B:366:GLU:CG	2.56	0.53
1:D:164:LEU:HD11	1:D:172:GLN:HB3	1.89	0.52
1:A:211:ASN:HD21	1:A:224:LEU:H	1.55	0.52
1:A:164:LEU:HD11	1:A:172:GLN:HB3	1.91	0.52
1:D:334:LEU:HB3	1:D:388:ALA:HB1	1.91	0.52
1:C:398:LEU:HB3	1:C:399:PRO:HD2	1.92	0.51
1:C:175:LYS:HG3	1:C:240:MET:HE3	1.93	0.51
1:B:164:LEU:CD1	1:B:172:GLN:HB3	2.41	0.51
1:D:321[A]:PTR:HE2	1:D:321[A]:PTR:O3P	2.10	0.51
1:A:336:MET:HB3	1:A:337:PRO:HD2	1.91	0.51
1:B:318:ILE:HG21	1:B:337:PRO:HA	1.91	0.51
1:D:413:ARG:HD2	1:D:413:ARG:O	2.09	0.51
1:A:398:LEU:HB3	1:A:399:PRO:HD2	1.92	0.50
1:D:477:SER:HA	1:D:480:LYS:HD3	1.92	0.50
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.92	0.50
1:C:217:MET:HB3	1:C:275:PHE:HB2	1.92	0.50
1:D:318:ILE:HG13	1:D:319:TYR:CD2	2.46	0.50
1:D:398:LEU:HB3	1:D:399:PRO:HD2	1.93	0.49
1:D:167:LYS:HG2	1:D:172:GLN:HG2	1.94	0.49
1:B:320:GLN:NE2	1:B:335:GLY:HA2	2.26	0.49
1:C:362:SER:O	1:C:372:LYS:HE3	2.13	0.49
1:A:215:THR:O	1:A:218:LYS:HG2	2.12	0.48
1:B:286:CYS:O	1:B:323:GLN:HG2	2.13	0.48
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.95	0.48
1:D:164:LEU:CD1	1:D:172:GLN:HB3	2.43	0.48
1:C:314:LEU:HD12	1:C:314:LEU:O	2.13	0.47
1:A:362:SER:O	1:A:372:LYS:HE3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:HG23	1:A:172:GLN:NE2	2.28	0.47
1:C:334:LEU:HB3	1:C:388:ALA:HB1	1.97	0.46
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.97	0.46
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.98	0.46
1:B:381:PRO:HD2	1:B:384:ILE:HD12	1.97	0.46
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.97	0.46
1:A:381:PRO:HD2	1:A:384:ILE:HD12	1.97	0.46
1:C:164:LEU:HD11	1:C:172:GLN:HB3	1.99	0.45
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.98	0.45
1:D:362:SER:O	1:D:372:LYS:HE3	2.16	0.45
1:A:214:ASP:O	1:A:215:THR:CG2	2.63	0.45
1:B:362:SER:O	1:B:372:LYS:HE3	2.17	0.45
1:A:317:ARG:HG3	1:A:317:ARG:O	2.16	0.45
1:A:217:MET:HB3	1:A:275:PHE:HB2	1.97	0.45
1:C:396:GLU:OE2	1:C:407:LYS:HE3	2.17	0.44
1:B:244:ASN:HA	1:B:294:LEU:HA	2.00	0.44
1:D:145:TYR:CE2	1:D:193:LYS:HD2	2.52	0.44
1:D:203:GLU:HB2	1:D:309:GLY:HA2	1.99	0.44
1:C:219:TYR:C	1:C:304:LYS:NZ	2.71	0.43
1:C:413:ARG:O	1:C:413:ARG:HD2	2.19	0.43
1:B:217:MET:HB3	1:B:275:PHE:HB2	2.00	0.43
1:C:197:LEU:O	1:C:201:GLN:HG3	2.19	0.42
1:B:365:ASN:HD21	1:D:299:LYS:HB3	1.85	0.42
1:D:381:PRO:HD2	1:D:384:ILE:HD12	2.01	0.42
1:A:167:LYS:HG2	1:A:172:GLN:HG2	2.02	0.42
1:A:192:ASN:HB2	1:A:233:HIS:CE1	2.55	0.42
1:A:164:LEU:CD1	1:A:172:GLN:HB3	2.50	0.41
1:B:167:LYS:HG2	1:B:172:GLN:HG2	2.03	0.41
1:B:249:LEU:HD22	1:B:357:GLY:HA2	2.02	0.41
1:B:321[A]:PTR:HE1	1:B:321[A]:PTR:O1P	2.20	0.41
1:D:285:HIS:O	1:D:286:CYS:HB2	2.21	0.41
1:B:165:ILE:HD11	1:B:175:LYS:HB2	2.02	0.41
1:C:170:PHE:CE1	1:C:188:LYS:HD2	2.56	0.41
1:C:368:ASP:OD1	1:C:415:TYR:OH	2.15	0.41
1:C:381:PRO:HD2	1:C:384:ILE:HD12	2.01	0.41
1:D:159:TYR:OH	1:D:226:ARG:HD2	2.21	0.41
1:D:297:ASN:HB3	1:D:300:ARG:HB2	2.01	0.41
1:A:317:ARG:HD2	1:A:338:TYR:CZ	2.56	0.41
1:B:249:LEU:HD23	1:B:249:LEU:HA	1.94	0.40
1:D:217:MET:HB3	1:D:275:PHE:HB2	2.02	0.40
1:B:454:ASP:O	1:B:458[B]:ARG:HG3	2.21	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	345/361 (96%)	336 (97%)	9 (3%)	0	100	100
1	B	347/361 (96%)	337 (97%)	10 (3%)	0	100	100
1	C	346/361 (96%)	333 (96%)	13 (4%)	0	100	100
1	D	347/361 (96%)	338 (97%)	9 (3%)	0	100	100
All	All	1385/1444 (96%)	1344 (97%)	41 (3%)	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	306/320 (96%)	306 (100%)	0	100	100
1	B	305/320 (95%)	304 (100%)	1 (0%)	92	97
1	C	306/320 (96%)	305 (100%)	1 (0%)	92	97
1	D	306/320 (96%)	306 (100%)	0	100	100
All	All	1223/1280 (96%)	1221 (100%)	2 (0%)	93	98

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

Mol	Chain	Res	Type
1	B	213	HIS
1	C	317	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	320	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	PTR	C	321	1	15,16,17	1.15	1 (6%)	19,22,24	0.98	2 (10%)
1	PTR	D	321[B]	-	15,16,17	1.17	1 (6%)	19,22,24	0.78	0
1	PTR	A	321	1	15,16,17	1.24	1 (6%)	19,22,24	0.89	1 (5%)
1	PTR	D	321[A]	-	15,16,17	1.16	1 (6%)	19,22,24	0.73	1 (5%)
1	PTR	B	321[A]	-	15,16,17	1.26	1 (6%)	19,22,24	0.64	0
1	PTR	B	321[B]	-	15,16,17	1.35	1 (6%)	19,22,24	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	D	321[B]	-	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321[A]	-	-	0/10/11/13	0/1/1/1
1	PTR	B	321[A]	-	-	3/10/11/13	0/1/1/1
1	PTR	B	321[B]	-	-	3/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321[B]	PTR	OH-CZ	-4.44	1.30	1.40
1	D	321[A]	PTR	OH-CZ	-4.11	1.31	1.40
1	B	321[A]	PTR	OH-CZ	-4.06	1.31	1.40
1	A	321	PTR	OH-CZ	-4.06	1.31	1.40
1	C	321	PTR	OH-CZ	-4.01	1.31	1.40
1	D	321[B]	PTR	OH-CZ	-3.73	1.32	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	CG-CB-CA	2.61	119.38	114.10
1	A	321	PTR	CG-CB-CA	2.13	118.42	114.10
1	C	321	PTR	CB-CA-C	2.11	115.43	111.47
1	D	321[A]	PTR	O3P-P-OH	2.07	111.70	105.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	321	PTR	O-C-CA-CB
1	D	321[B]	PTR	N-CA-CB-CG
1	D	321[B]	PTR	C-CA-CB-CG
1	A	321	PTR	O-C-CA-CB
1	B	321[A]	PTR	O-C-CA-CB
1	B	321[A]	PTR	C-CA-CB-CG
1	B	321[B]	PTR	O-C-CA-CB
1	B	321[B]	PTR	N-CA-CB-CG
1	B	321[B]	PTR	C-CA-CB-CG
1	B	321[A]	PTR	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	321[A]	PTR	1	0
1	B	321[A]	PTR	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
3	PG4	D	503	-	9,9,12	0.52	0	8,8,11	0.26	0
3	PG4	A	504	-	12,12,12	0.54	0	11,11,11	0.13	0
3	PG4	C	503	-	9,9,12	0.52	0	8,8,11	0.22	0
3	PG4	B	504	-	12,12,12	0.53	0	11,11,11	0.26	0
3	PG4	A	503	-	12,12,12	0.52	0	11,11,11	0.23	0
3	PG4	B	502	-	12,12,12	0.53	0	11,11,11	0.22	0
3	PG4	A	502	-	9,9,12	0.52	0	8,8,11	0.24	0
3	PG4	C	502	-	12,12,12	0.53	0	11,11,11	0.21	0
2	QKG	A	501	-	22,24,24	1.84	8 (36%)	24,34,34	1.45	4 (16%)
2	QKG	C	501	-	22,24,24	1.86	8 (36%)	24,34,34	1.46	4 (16%)
3	PG4	D	502	-	12,12,12	0.54	0	11,11,11	0.18	0
3	PG4	B	503	-	9,9,12	0.52	0	8,8,11	0.24	0
2	QKG	D	501	-	22,24,24	1.85	7 (31%)	24,34,34	1.48	4 (16%)
3	PG4	D	504	-	12,12,12	0.53	0	11,11,11	0.19	0
2	QKG	B	501	-	22,24,24	1.89	7 (31%)	24,34,34	1.47	4 (16%)

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	PG4	D	503	-	-	5/7/7/10	-
3	PG4	A	504	-	-	3/10/10/10	-
3	PG4	C	503	-	-	6/7/7/10	-
3	PG4	B	504	-	-	5/10/10/10	-
3	PG4	A	503	-	-	5/10/10/10	-
3	PG4	B	502	-	-	3/10/10/10	-
3	PG4	A	502	-	-	5/7/7/10	-
3	PG4	C	502	-	-	3/10/10/10	-
2	QKG	A	501	-	-	2/8/8/8	0/3/3/3
2	QKG	C	501	-	-	2/8/8/8	0/3/3/3
3	PG4	D	502	-	-	3/10/10/10	-
3	PG4	B	503	-	-	5/7/7/10	-
2	QKG	D	501	-	-	5/8/8/8	0/3/3/3
3	PG4	D	504	-	-	1/10/10/10	-
2	QKG	B	501	-	-	3/8/8/8	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	QKG	C05-C04	4.36	1.42	1.36
2	C	501	QKG	C05-C04	4.35	1.42	1.36
2	B	501	QKG	C05-C04	4.27	1.42	1.36
2	A	501	QKG	C05-C04	4.18	1.42	1.36
2	C	501	QKG	C02-N03	3.79	1.35	1.32
2	A	501	QKG	C02-N03	3.75	1.35	1.32
2	D	501	QKG	C02-N03	3.65	1.35	1.32
2	B	501	QKG	C02-N03	3.63	1.35	1.32
2	D	501	QKG	C02-C07	2.91	1.47	1.43
2	A	501	QKG	C16-C15	2.88	1.46	1.40
2	C	501	QKG	C16-C15	2.86	1.46	1.40
2	D	501	QKG	C21-C20	2.77	1.42	1.36
2	B	501	QKG	C12-N13	2.65	1.41	1.32
2	B	501	QKG	C21-C20	2.65	1.42	1.36
2	C	501	QKG	C21-C20	2.64	1.42	1.36
2	A	501	QKG	C21-C20	2.59	1.42	1.36
2	A	501	QKG	C02-C07	2.42	1.46	1.43
2	D	501	QKG	C12-N13	2.41	1.40	1.32
2	B	501	QKG	C02-C07	2.38	1.46	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	QKG	C02-C07	2.32	1.46	1.43
2	B	501	QKG	C16-C15	2.29	1.45	1.40
2	D	501	QKG	O18-C17	2.28	1.42	1.37
2	A	501	QKG	O18-C17	2.27	1.42	1.37
2	D	501	QKG	C16-C15	2.25	1.45	1.40
2	A	501	QKG	C12-N13	2.25	1.40	1.32
2	C	501	QKG	O18-C17	2.23	1.42	1.37
2	C	501	QKG	C12-N13	2.19	1.39	1.32
2	B	501	QKG	O18-C17	2.15	1.42	1.37
2	A	501	QKG	C16-C17	2.09	1.40	1.37
2	C	501	QKG	C16-C17	2.04	1.40	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	QKG	O14-C12-N13	-3.58	112.74	122.50
2	C	501	QKG	O14-C12-N13	-3.53	112.85	122.50
2	A	501	QKG	O14-C12-N13	-3.53	112.88	122.50
2	D	501	QKG	O14-C12-N13	-3.37	113.31	122.50
2	C	501	QKG	C11-C12-N13	3.29	126.76	116.51
2	B	501	QKG	C11-C12-N13	3.26	126.67	116.51
2	A	501	QKG	C11-C12-N13	3.24	126.59	116.51
2	D	501	QKG	C11-C12-N13	2.93	125.63	116.51
2	D	501	QKG	C04-C05-C06	-2.60	117.52	119.77
2	B	501	QKG	C04-C05-C06	-2.52	117.59	119.77
2	C	501	QKG	C04-C05-C06	-2.52	117.60	119.77
2	A	501	QKG	C04-C05-C06	-2.45	117.65	119.77
2	D	501	QKG	C04-N03-C02	2.27	121.08	118.33
2	B	501	QKG	C04-N03-C02	2.21	121.00	118.33
2	A	501	QKG	C04-N03-C02	2.18	120.98	118.33
2	C	501	QKG	C04-N03-C02	2.17	120.96	118.33

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	QKG	C10-C09-N08-C15
2	C	501	QKG	C10-C09-N08-C07
2	A	501	QKG	C10-C09-N08-C15
2	A	501	QKG	C10-C09-N08-C07
2	B	501	QKG	C10-C09-N08-C15
2	B	501	QKG	C10-C09-N08-C07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	QKG	C09-C10-C11-C12
2	D	501	QKG	C10-C09-N08-C15
2	D	501	QKG	C10-C09-N08-C07
3	A	502	PG4	O2-C3-C4-O3
3	C	503	PG4	O2-C3-C4-O3
3	B	503	PG4	O2-C3-C4-O3
3	C	503	PG4	O1-C1-C2-O2
3	A	503	PG4	O4-C7-C8-O5
3	C	502	PG4	O4-C7-C8-O5
3	B	502	PG4	O4-C7-C8-O5
3	A	502	PG4	O1-C1-C2-O2
3	D	502	PG4	O4-C7-C8-O5
3	D	503	PG4	O2-C3-C4-O3
2	B	501	QKG	N08-C09-C10-C11
3	C	502	PG4	O1-C1-C2-O2
3	D	502	PG4	O1-C1-C2-O2
3	D	503	PG4	O1-C1-C2-O2
3	B	504	PG4	O1-C1-C2-O2
3	B	503	PG4	O1-C1-C2-O2
3	B	503	PG4	O3-C5-C6-O4
3	B	502	PG4	O1-C1-C2-O2
3	B	504	PG4	O2-C3-C4-O3
3	D	503	PG4	O3-C5-C6-O4
3	D	504	PG4	O4-C7-C8-O5
3	B	504	PG4	C4-C3-O2-C2
3	B	503	PG4	C1-C2-O2-C3
3	D	503	PG4	C6-C5-O3-C4
3	A	503	PG4	C4-C3-O2-C2
3	B	504	PG4	C5-C6-O4-C7
3	A	504	PG4	C8-C7-O4-C6
3	C	503	PG4	C6-C5-O3-C4
3	C	503	PG4	C1-C2-O2-C3
3	B	503	PG4	C4-C3-O2-C2
3	A	502	PG4	C6-C5-O3-C4
3	D	503	PG4	C3-C4-O3-C5
3	A	502	PG4	C3-C4-O3-C5
2	D	501	QKG	C10-C11-C12-O14
3	A	503	PG4	C1-C2-O2-C3
3	C	503	PG4	C3-C4-O3-C5
3	D	502	PG4	C6-C5-O3-C4
2	D	501	QKG	C10-C11-C12-N13
3	A	504	PG4	O3-C5-C6-O4

Continued on next page...

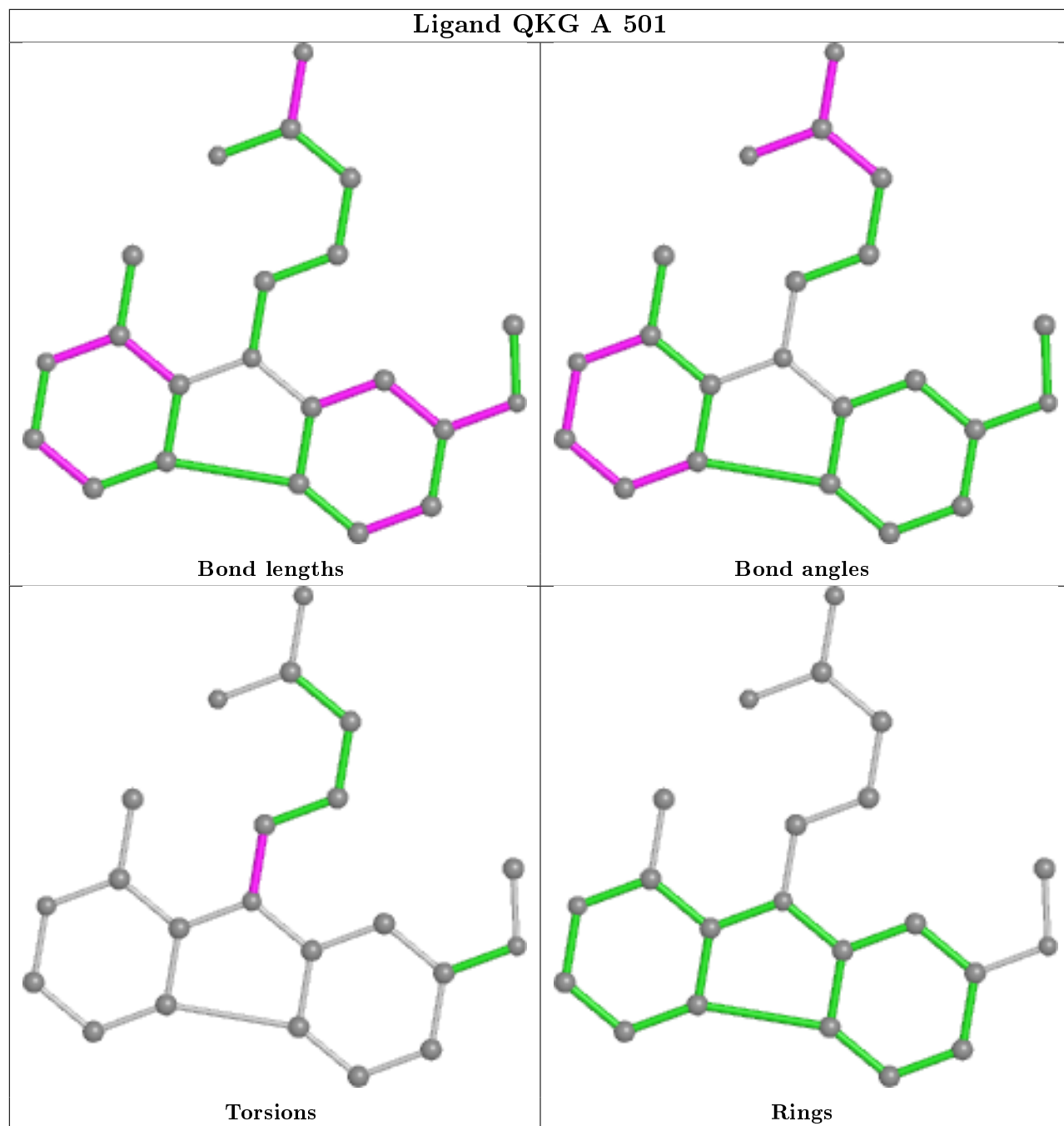
Continued from previous page...

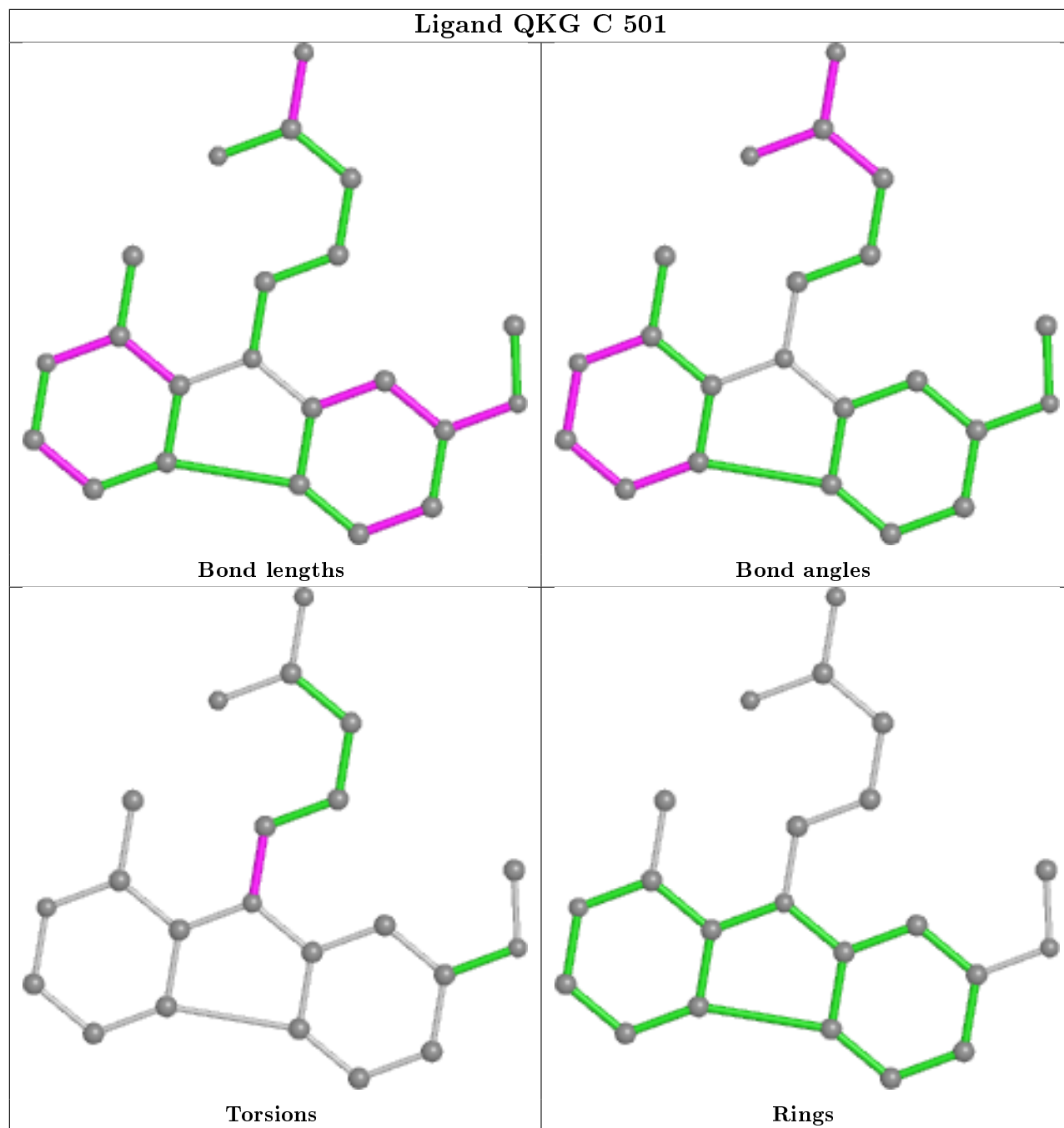
Mol	Chain	Res	Type	Atoms
3	B	502	PG4	C6-C5-O3-C4
3	A	503	PG4	C6-C5-O3-C4
3	A	503	PG4	C5-C6-O4-C7
3	C	502	PG4	C6-C5-O3-C4
3	A	502	PG4	C1-C2-O2-C3
3	A	504	PG4	C6-C5-O3-C4
3	B	504	PG4	C8-C7-O4-C6
3	C	503	PG4	O3-C5-C6-O4

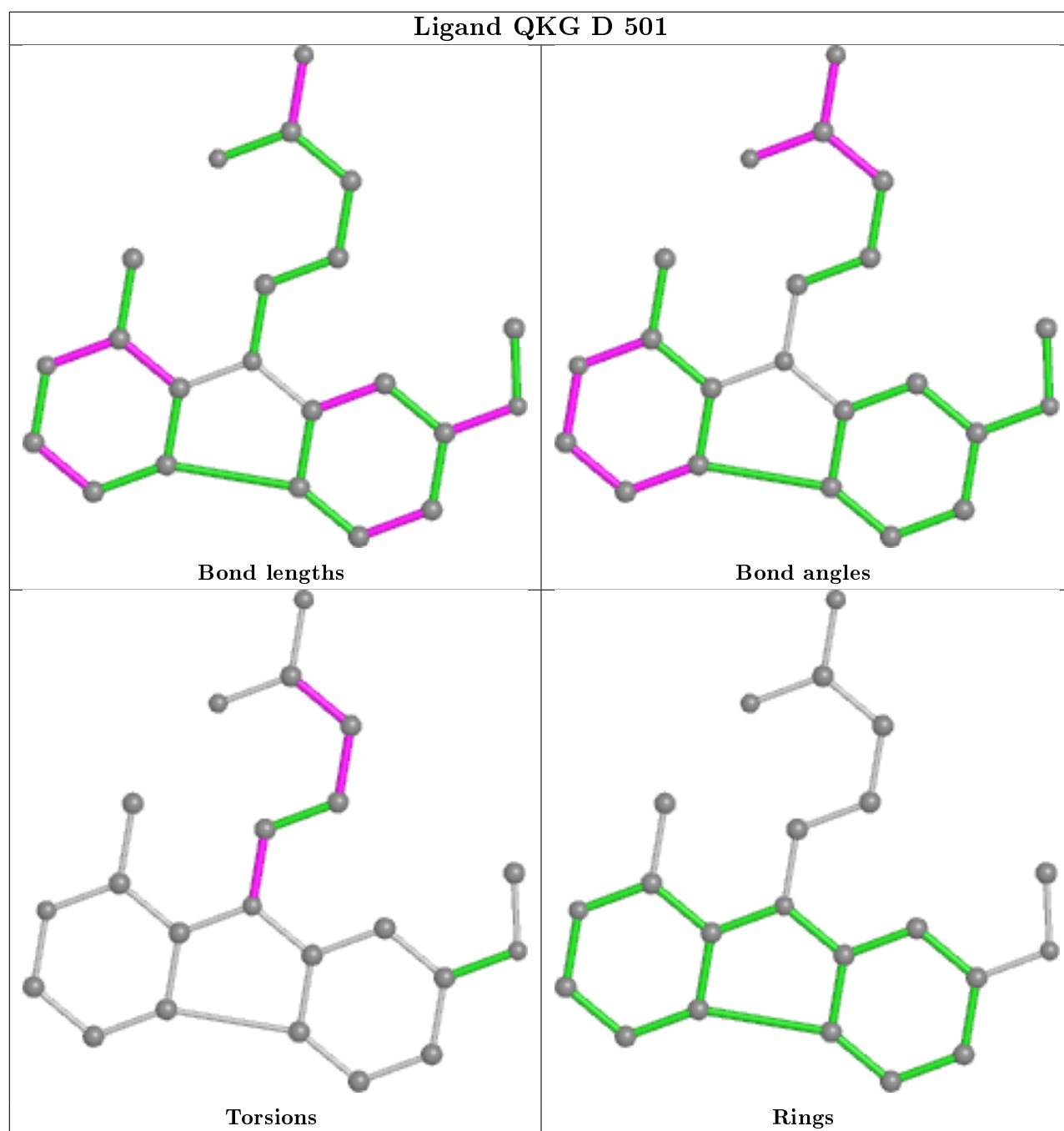
There are no ring outliers.

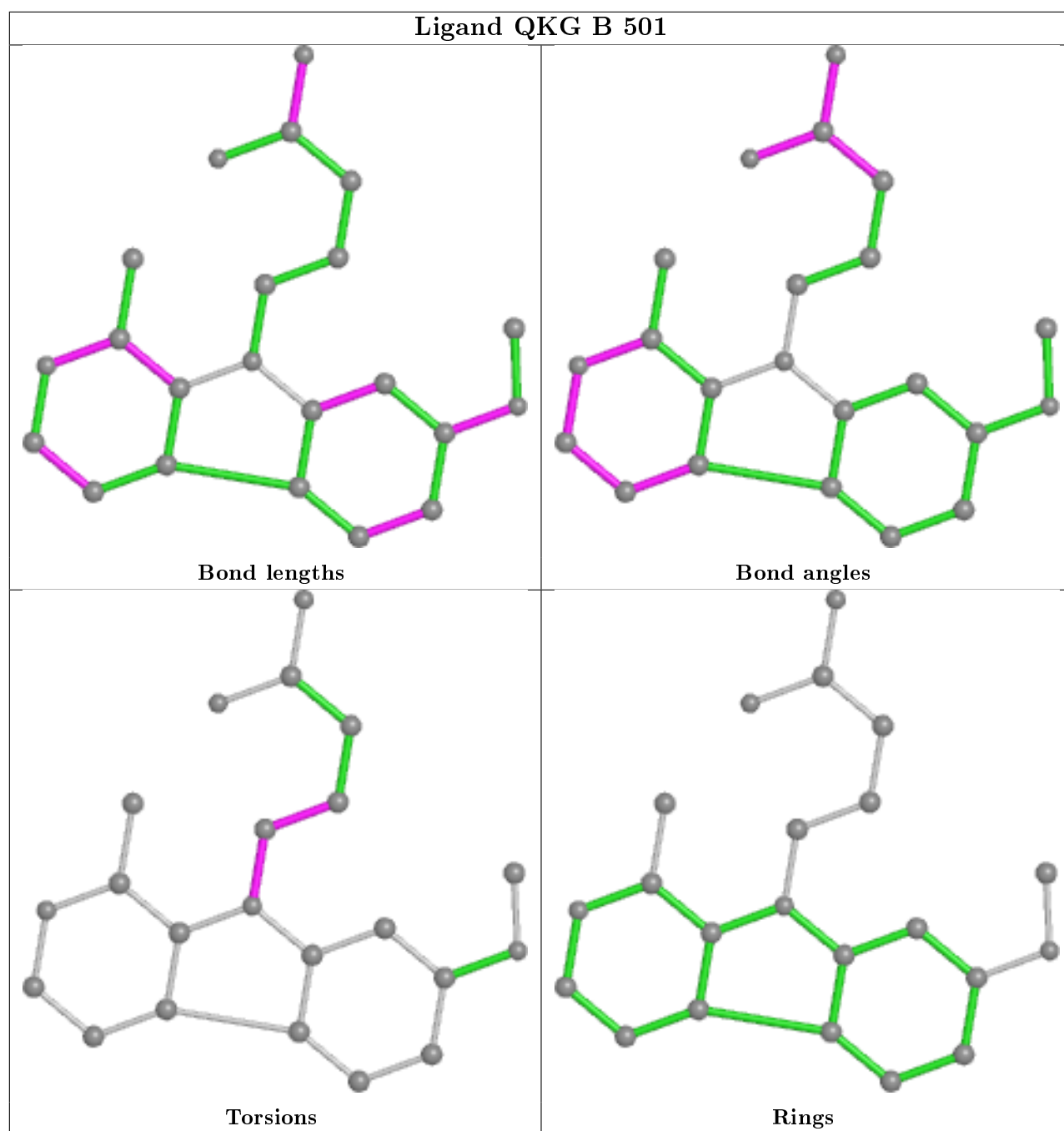
No monomer is involved in short contacts.

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	346/361 (95%)	0.32	2 (0%) 89 78	51, 74, 127, 177	0
1	B	347/361 (96%)	0.37	6 (1%) 70 53	51, 75, 131, 245	0
1	C	346/361 (95%)	0.73	45 (13%) 3 2	75, 131, 180, 203	0
1	D	347/361 (96%)	0.42	8 (2%) 60 43	60, 94, 145, 192	0
All	All	1386/1444 (95%)	0.46	61 (4%) 34 21	51, 92, 161, 245	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ASP	7.4
1	C	161	ILE	5.1
1	C	479	PHE	4.2
1	B	317	ARG	3.8
1	C	183	GLU	3.7
1	C	156	MET	3.6
1	C	210	MET	3.6
1	C	295	LEU	3.4
1	C	185	VAL	3.3
1	C	248	LEU	3.3
1	C	241	LEU	3.2
1	B	318	ILE	3.2
1	C	224	LEU	3.2
1	C	455	LEU	3.1
1	C	446	VAL	3.0
1	B	320	GLN	3.0
1	C	155	TRP	3.0
1	C	427	LEU	3.0
1	D	479	PHE	3.0
1	C	170	PHE	2.9
1	C	439	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	238	PHE	2.9
1	C	354	MET	2.9
1	C	157	ASP	2.9
1	D	206	LEU	2.8
1	C	410	ASP	2.7
1	C	187	ILE	2.7
1	C	236	LEU	2.7
1	C	225	LYS	2.6
1	C	474	LEU	2.6
1	C	267	GLN	2.6
1	C	175	LYS	2.6
1	C	471	TYR	2.5
1	D	213	HIS	2.5
1	C	475	GLN	2.5
1	C	259	LEU	2.4
1	B	411	GLY	2.4
1	C	149	VAL	2.4
1	C	296	CYS	2.3
1	C	262	THR	2.3
1	C	223	HIS	2.3
1	A	410	ASP	2.3
1	C	264	LYS	2.3
1	C	274	LEU	2.2
1	C	184	TRP	2.2
1	D	275	PHE	2.2
1	C	481	LYS	2.2
1	A	215	THR	2.1
1	C	220	TYR	2.1
1	C	305	ILE	2.1
1	C	217	MET	2.1
1	C	249	LEU	2.1
1	B	412	LYS	2.1
1	C	345	TRP	2.1
1	C	216	GLU	2.1
1	C	245	LEU	2.1
1	C	147	TYR	2.1
1	D	259	LEU	2.0
1	D	457	LEU	2.0
1	D	217	MET	2.0
1	D	340	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	B	321[A]	16/17	0.68	0.36	99,109,113,114	13
1	PTR	B	321[B]	16/17	0.68	0.36	75,106,108,109	13
1	PTR	D	321[B]	16/17	0.83	0.30	88,94,99,99	13
1	PTR	D	321[A]	16/17	0.83	0.30	77,89,94,94	13
1	PTR	C	321	16/17	0.91	0.20	90,112,123,126	0
1	PTR	A	321	16/17	0.94	0.20	100,110,120,120	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

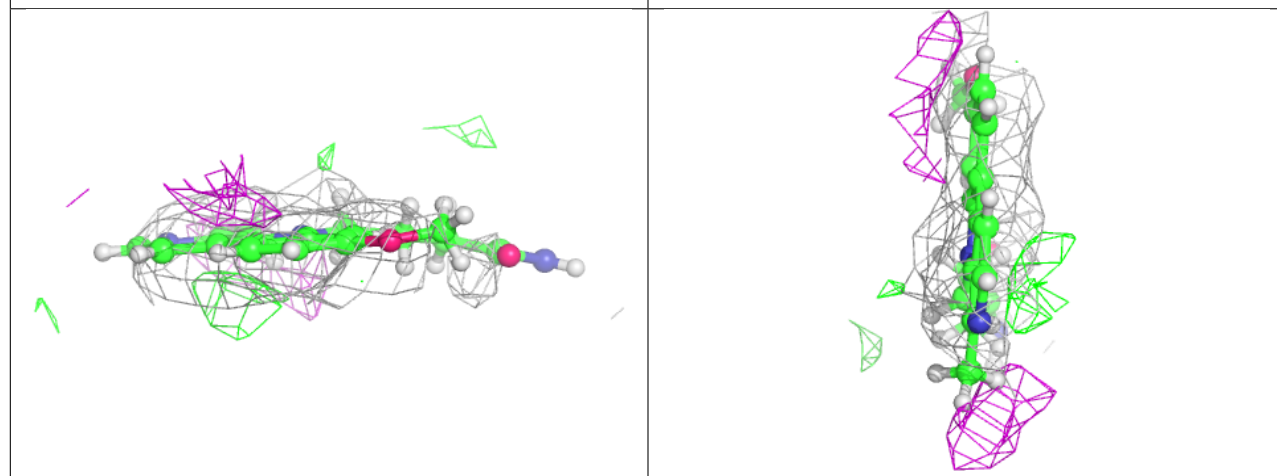
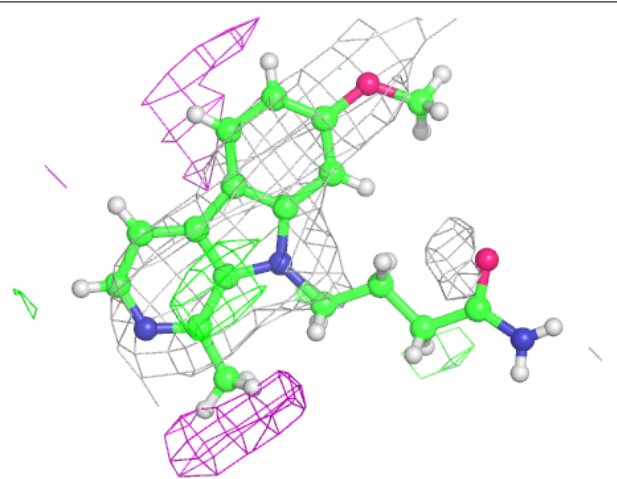
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG4	C	502	13/13	0.65	0.43	134,141,144,144	0
3	PG4	B	503	10/13	0.73	0.23	112,120,126,126	0
3	PG4	B	502	13/13	0.77	0.26	95,105,110,111	0
3	PG4	C	503	10/13	0.77	0.20	103,109,110,111	0
3	PG4	A	502	10/13	0.80	0.19	102,106,114,115	0
3	PG4	B	504	13/13	0.85	0.29	94,102,107,110	0
3	PG4	A	503	13/13	0.85	0.20	95,99,104,105	0
2	QKG	C	501	22/22	0.85	0.51	100,124,156,163	41
3	PG4	A	504	13/13	0.87	0.17	62,68,77,78	0
3	PG4	D	503	10/13	0.88	0.17	104,109,114,115	0
3	PG4	D	502	13/13	0.89	0.22	65,79,93,98	0
3	PG4	D	504	13/13	0.92	0.25	54,59,69,70	0
2	QKG	D	501	22/22	0.94	0.32	68,86,113,125	0
2	QKG	A	501	22/22	0.96	0.31	57,78,112,134	0
2	QKG	B	501	22/22	0.97	0.30	57,74,118,142	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.

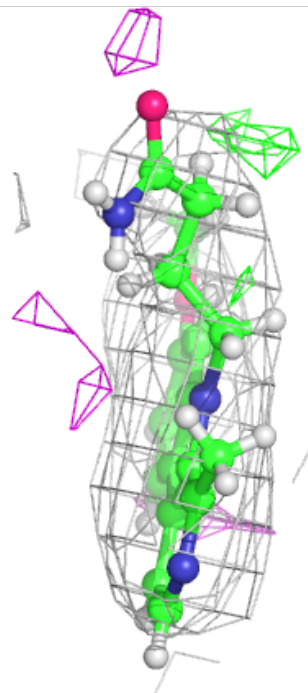
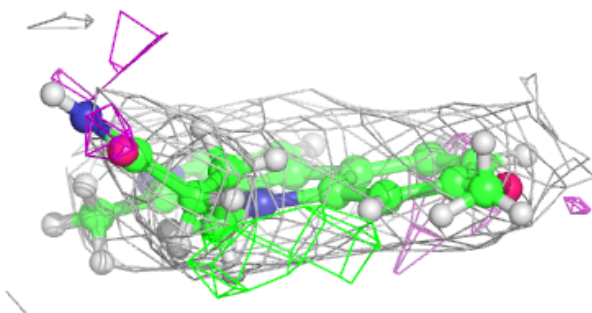
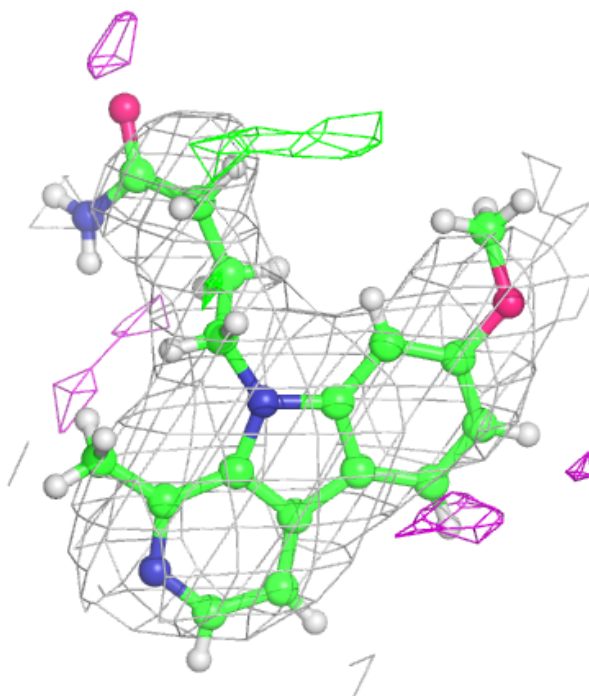
Electron density around QKG C 501:

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



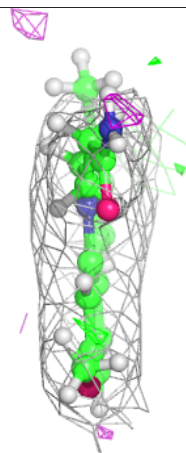
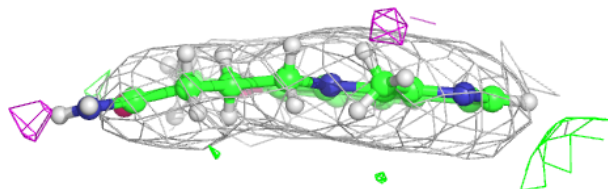
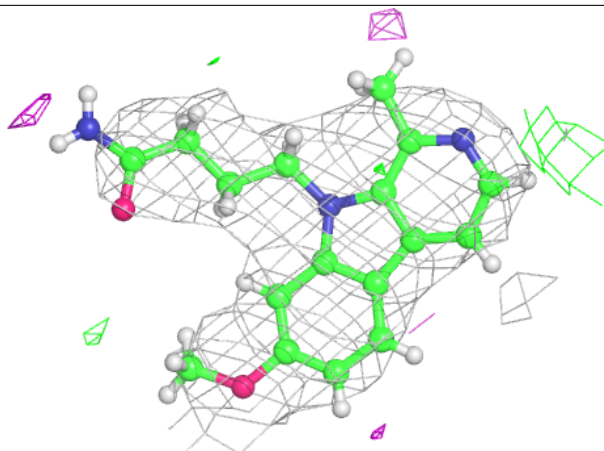
Electron density around QKG D 501:

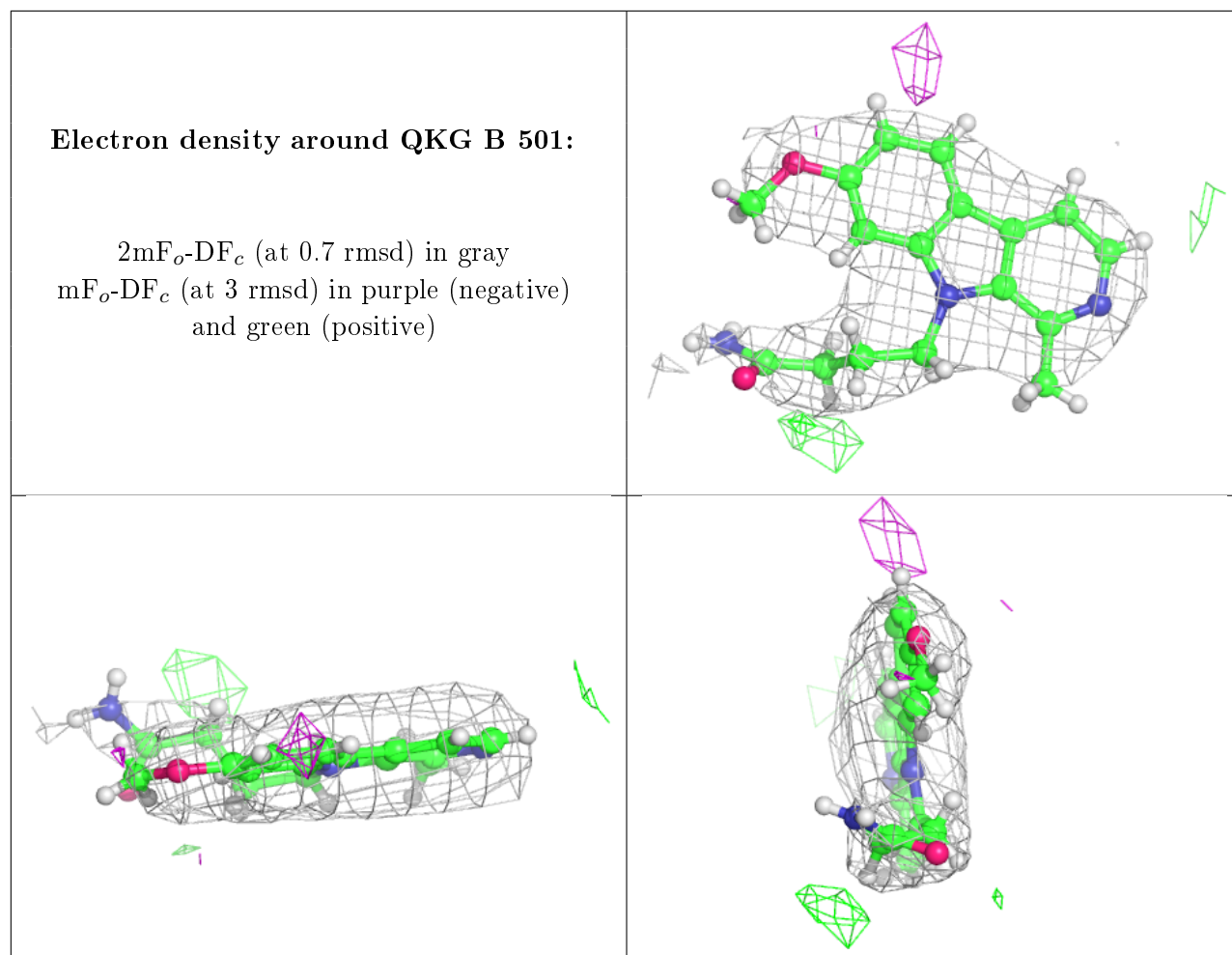
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QKG 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.