



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:54 AM EDT

PDB ID : 6YF8
Title : DYRK1A with PST001
Authors : Rothweiler, U.
Deposited on : 2020-03-26
Resolution : 3.20 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

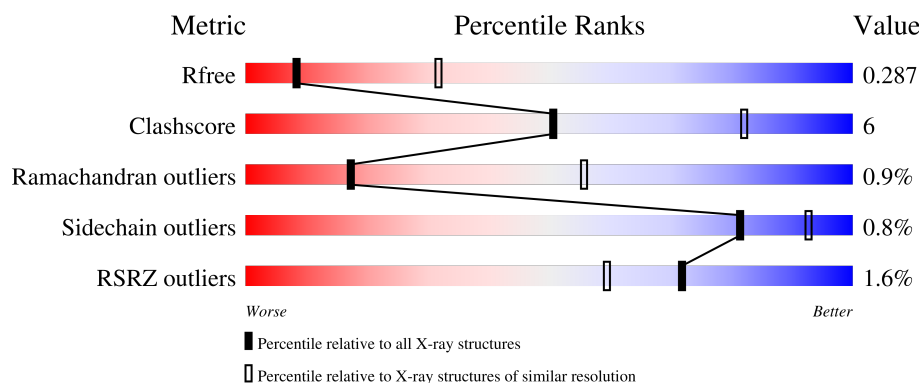
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	368	<div> <div>0%</div> <div>81% 12% 7%</div> </div>
1	B	368	<div> <div>0%</div> <div>80% 12% 8%</div> </div>
1	C	368	<div> <div>3%</div> <div>71% 18% 10%</div> </div>
1	D	368	<div> <div>2%</div> <div>73% 16% 10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11014 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.

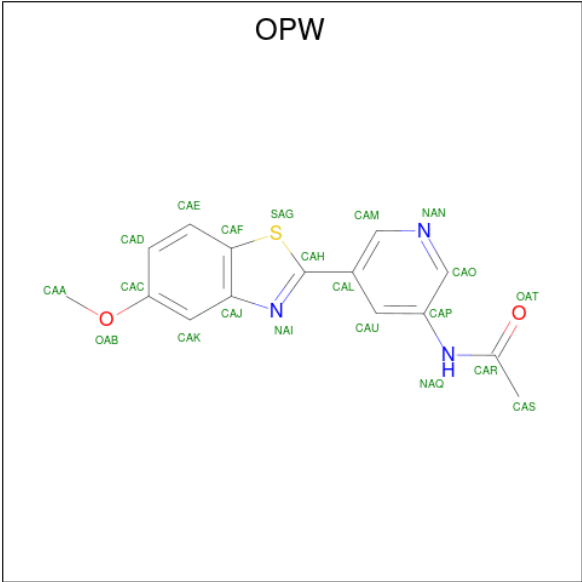
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2794	1798	477	501	1	17			
1	B	340	Total	C	N	O	P	S	0	0	0
			2761	1777	471	495	1	17			
1	C	333	Total	C	N	O	P	S	0	0	0
			2678	1724	452	484	1	17			
1	D	331	Total	C	N	O	P	S	0	0	0
			2697	1744	451	484	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is {N}-[5-(5-methoxy-1,3-benzothiazol-2-yl)pyridin-3-yl]ethanamide (three-letter code: OPW) (formula: C₁₅H₁₃N₃O₂S) (labeled as "Ligand of Interest" by depositor).

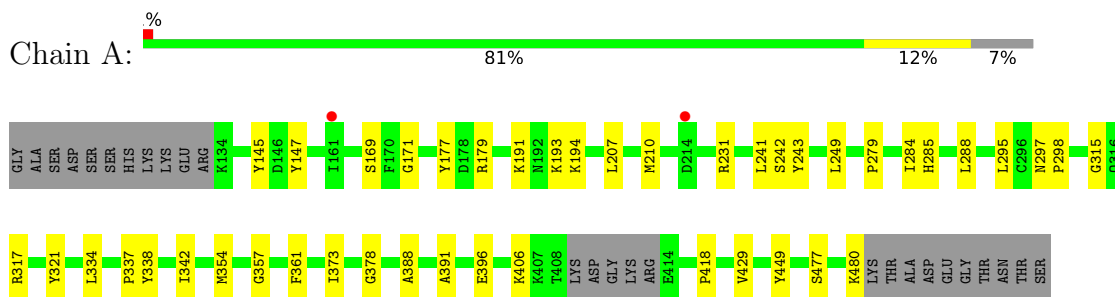


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	15	3	2	1		
2	B	1	Total	C	N	O	S	0	0
			21	15	3	2	1		
2	C	1	Total	C	N	O	S	0	0
			21	15	3	2	1		
2	D	1	Total	C	N	O	S	0	0
			21	15	3	2	1		

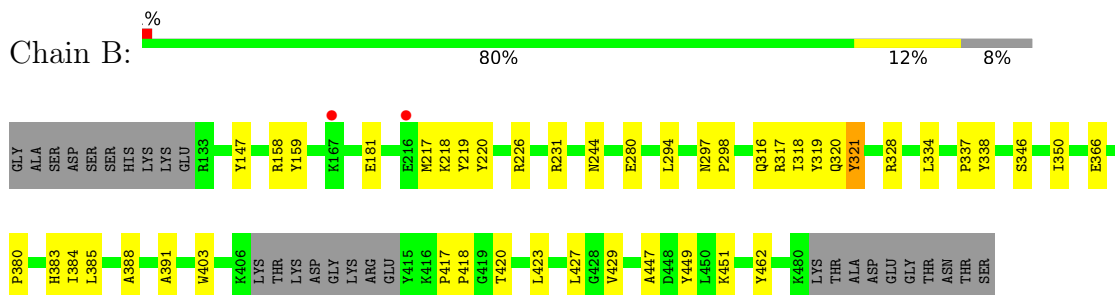
3 Residue-property plots [i](#)

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.

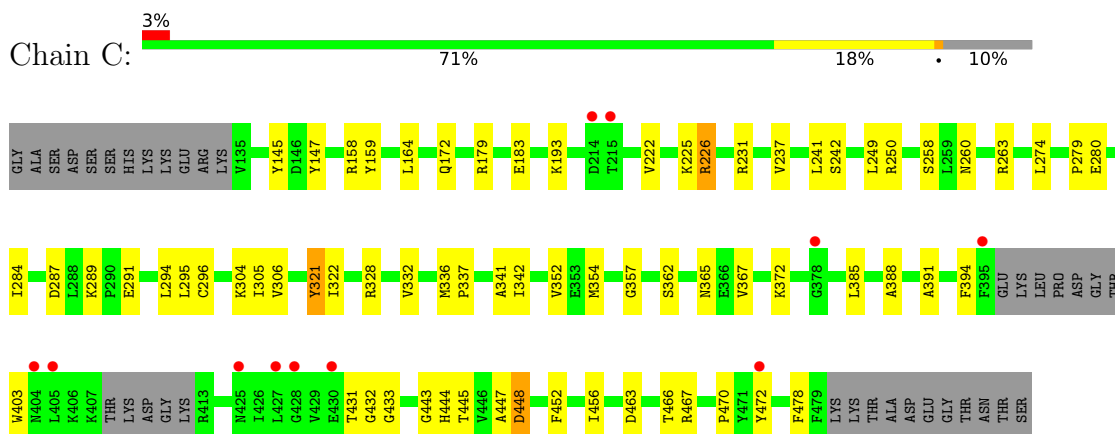
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



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

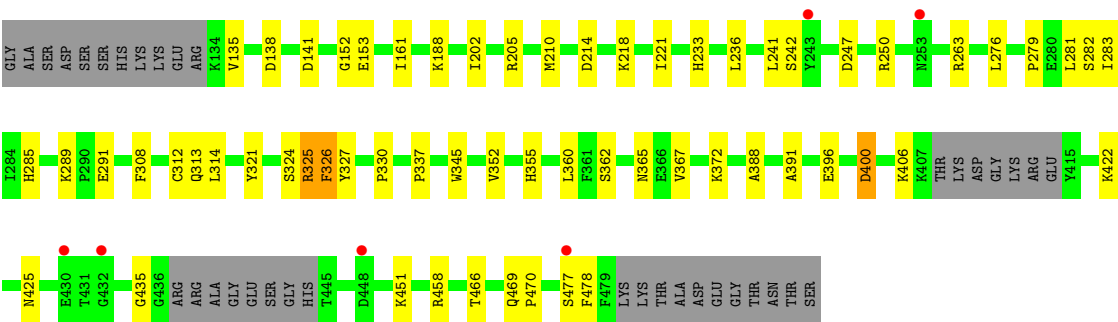


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.00Å 88.04Å 229.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 3.20 48.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.30-3.20) 99.4 (48.30-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.249 , 0.283 0.250 , 0.287	Depositor DCC
R_{free} test set	1456 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11014	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: OPW, 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	0/2842	0.46	0/3833
1	B	0.26	0/2808	0.48	0/3789
1	C	0.26	0/2724	0.49	0/3686
1	D	0.31	0/2743	0.52	0/3703
All	All	0.27	0/11117	0.49	0/15011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2794	0	2787	25	0
1	B	2761	0	2745	28	0
1	C	2678	0	2601	42	0
1	D	2697	0	2681	40	0
2	A	21	0	0	1	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	1	0
All	All	11014	0	10814	124	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 6.

All (124) 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:A:396:GLU:HG3	1:A:406:LYS:HG2	1.64	0.80
1:C:222:VAL:HG11	1:C:306:VAL:HG23	1.65	0.77
1:A:279:PRO:HG3	1:D:337:PRO:HG3	1.67	0.76
1:D:247:ASP:HA	1:D:250:ARG:HG3	1.66	0.76
1:C:274:LEU:HD13	1:C:470:PRO:HB2	1.69	0.74
1:A:337:PRO:HG3	1:D:279:PRO:HG3	1.69	0.74
1:C:159:TYR:OH	1:C:226:ARG:NH1	2.22	0.72
1:D:281:LEU:O	1:D:313:GLN:NE2	2.23	0.71
1:D:325:ARG:O	1:D:327:TYR:N	2.24	0.71
1:A:477:SER:HA	1:A:480:LYS:HG2	1.73	0.70
1:C:296:CYS:SG	1:C:304:LYS:NZ	2.63	0.69
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.74	0.68
1:B:317:ARG:NH2	1:C:280:GLU:OE1	2.29	0.66
1:C:365:ASN:HD22	1:D:138:ASP:HA	1.60	0.66
1:D:451:LYS:HE3	1:D:477:SER:HB2	1.80	0.64
1:D:289:LYS:HD3	1:D:291:GLU:HG2	1.80	0.63
1:C:322:ILE:O	1:C:328:ARG:NH1	2.30	0.63
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.81	0.62
1:D:325:ARG:O	1:D:326:PHE:C	2.36	0.62
1:B:447:ALA:O	1:B:451:LYS:HD3	2.01	0.60
1:B:159:TYR:OH	1:B:226:ARG:HD2	2.03	0.59
1:C:284:ILE:HG21	1:C:342:ILE:HD11	1.84	0.59
1:D:362:SER:O	1:D:372:LYS:NZ	2.36	0.58
1:B:317:ARG:HH12	1:B:320:GLN:HG2	1.67	0.58
1:C:249:LEU:HD22	1:C:357:GLY:HA2	1.86	0.57
1:C:231:ARG:HG2	1:C:231:ARG:HH11	1.69	0.57
1:C:362:SER:O	1:C:372:LYS:NZ	2.30	0.57
1:A:169:SER:O	1:A:191:LYS:NZ	2.27	0.57
1:B:346:SER:O	1:B:350:ILE:HG13	2.04	0.57
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.88	0.56
1:C:260:ASN:HD21	1:C:443:GLY:HA3	1.71	0.55
1:D:289:LYS:CE	1:D:324:SER:OG	2.55	0.55
1:C:249:LEU:HD21	1:C:354:MET:HA	1.90	0.54
1:A:297:ASN:OD1	1:A:298:PRO:HD2	2.07	0.54
1:B:328:ARG:NH1	1:B:366:GLU:OE2	2.41	0.53
1:B:321:PTR:O2P	1:B:328:ARG:NH2	2.32	0.53
1:D:202:ILE:HG13	1:D:205:ARG:HH11	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:HIS:CE1	1:B:384:ILE:HG12	2.46	0.51
1:C:431:THR:O	1:C:433:GLY:N	2.40	0.51
1:A:334:LEU:HB3	1:A:388:ALA:HB1	1.93	0.51
1:B:147:TYR:OH	1:B:231:ARG:NH1	2.44	0.51
1:C:463:ASP:HB3	1:C:466:THR:OG1	2.12	0.50
1:A:171:GLY:HA2	1:A:191:LYS:HZ2	1.76	0.50
1:D:458:ARG:NH2	1:D:466:THR:O	2.37	0.49
1:A:145:TYR:CD2	1:A:193:LYS:HG3	2.48	0.49
1:A:249:LEU:HD22	1:A:357:GLY:HA2	1.94	0.49
1:A:147:TYR:OH	1:A:231:ARG:NH1	2.45	0.49
1:B:244:ASN:HA	1:B:294:LEU:HA	1.94	0.49
1:C:452:PHE:CZ	1:C:456:ILE:HD11	2.48	0.49
1:D:352:VAL:HG11	1:D:360:LEU:HD13	1.94	0.49
1:B:317:ARG:NH1	1:B:320:GLN:HG2	2.27	0.49
1:B:218:LYS:O	1:B:220:TYR:N	2.46	0.49
1:A:429:VAL:HG22	1:A:449:TYR:HB3	1.94	0.49
1:C:158:ARG:O	1:C:179:ARG:HG3	2.13	0.48
1:D:152:GLY:N	1:D:161:ILE:O	2.32	0.48
1:A:378:GLY:HA2	1:A:418:PRO:HB3	1.95	0.48
1:D:210:MET:CE	1:D:283:ILE:HD13	2.44	0.48
1:C:341:ALA:O	1:C:467:ARG:NH1	2.46	0.48
1:A:284:ILE:HG21	1:A:342:ILE:HD11	1.96	0.47
1:D:289:LYS:HD3	1:D:291:GLU:CG	2.44	0.47
1:B:429:VAL:HG22	1:B:449:TYR:HB3	1.97	0.47
1:D:281:LEU:O	1:D:282:SER:HB2	2.14	0.47
1:C:321:PTR:O1P	1:C:328:ARG:NH2	2.47	0.47
1:C:328:ARG:HG2	1:C:332:VAL:HG23	1.96	0.47
1:C:336:MET:HB3	1:C:337:PRO:HD2	1.96	0.47
1:D:325:ARG:C	1:D:327:TYR:N	2.68	0.47
1:B:317:ARG:HG3	1:B:338:TYR:CE2	2.51	0.46
1:A:315:GLY:HA2	1:D:314:LEU:O	2.15	0.46
1:D:289:LYS:HE3	1:D:324:SER:OG	2.16	0.46
1:A:177:TYR:CD2	1:A:179:ARG:HD2	2.51	0.46
1:C:445:THR:O	1:C:448:ASP:OD1	2.33	0.46
1:B:317:ARG:HD3	1:B:337:PRO:HA	1.97	0.46
1:C:365:ASN:ND2	1:D:138:ASP:HA	2.30	0.46
1:B:337:PRO:HB3	1:C:279:PRO:HG3	1.98	0.45
1:D:221:ILE:HD12	1:D:308:PHE:HZ	1.81	0.45
1:D:188:LYS:HB3	1:D:236:LEU:HB2	1.98	0.45
1:D:241:LEU:H	2:D:501:OPW:CAD	2.29	0.45
1:C:352:VAL:HG22	1:C:456:ILE:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HE2	1:B:319:TYR:CZ	2.52	0.45
1:C:328:ARG:HG2	1:C:332:VAL:CG2	2.46	0.45
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.98	0.45
1:D:152:GLY:O	1:D:153:GLU:C	2.55	0.45
1:C:365:ASN:HD21	1:D:135:VAL:HG11	1.81	0.44
1:D:263:ARG:HG3	1:D:478:PHE:CE2	2.52	0.44
1:A:249:LEU:HD21	1:A:354:MET:HA	1.98	0.44
1:B:280:GLU:N	1:B:280:GLU:OE2	2.50	0.44
1:D:210:MET:HE3	1:D:283:ILE:HD13	2.00	0.44
1:B:297:ASN:CG	1:B:298:PRO:HD2	2.37	0.44
1:D:365:ASN:HD21	1:D:367:VAL:HB	1.83	0.44
1:A:317:ARG:HG3	1:A:338:TYR:CE2	2.53	0.44
1:B:380:PRO:HG3	1:B:462:TYR:CE1	2.52	0.44
1:C:258:SER:HB2	1:C:444:HIS:CE1	2.52	0.44
1:C:385:LEU:HD22	1:C:403:TRP:CG	2.53	0.44
1:D:396:GLU:HG3	1:D:406:LYS:HB2	2.00	0.44
1:C:289:LYS:HD3	1:C:291:GLU:HG3	2.00	0.43
1:C:241:LEU:HB2	1:C:294:LEU:HD23	2.00	0.43
1:D:214:ASP:HA	1:D:218:LYS:NZ	2.34	0.43
1:A:242:SER:N	1:A:295:LEU:O	2.43	0.43
1:D:400:ASP:OD1	1:D:400:ASP:N	2.50	0.43
1:C:241:LEU:HB3	1:C:295:LEU:O	2.19	0.43
1:A:285:HIS:HB3	1:A:288:LEU:HD11	2.01	0.43
1:D:276:LEU:HD22	1:D:283:ILE:HB	1.99	0.43
1:A:241:LEU:H	2:A:501:OPW:CAD	2.32	0.43
1:B:334:LEU:HB3	1:B:388:ALA:HB1	2.01	0.43
1:D:141:ASP:OD1	1:D:233:HIS:NE2	2.52	0.43
1:B:417:PRO:HA	1:B:418:PRO:HD3	1.87	0.42
1:A:361:PHE:CE1	1:A:373:ILE:HA	2.55	0.42
1:B:423:LEU:HG	1:B:427:LEU:CD1	2.49	0.42
1:C:263:ARG:HG3	1:C:478:PHE:CE1	2.55	0.42
1:D:469:GLN:HB3	1:D:470:PRO:HD2	2.02	0.42
1:B:385:LEU:HD23	1:B:403:TRP:CG	2.55	0.41
1:B:158:ARG:HH21	1:B:181:GLU:HG2	1.85	0.41
1:A:207:LEU:HA	1:A:210:MET:HE3	2.02	0.41
1:C:367:VAL:HA	1:C:394:PHE:HE1	1.86	0.41
1:D:330:PRO:HD3	1:D:345:TRP:CE2	2.56	0.41
1:B:316:GLN:HG3	1:B:318:ILE:HD11	2.03	0.41
1:C:164:LEU:HD11	1:C:172:GLN:HB3	2.03	0.41
1:B:383:HIS:HD1	1:C:472:TYR:HH	1.69	0.41
1:C:365:ASN:HB3	1:D:138:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TYR:O	1:C:172:GLN:NE2	2.43	0.40
1:C:183:GLU:OE2	1:C:225:LYS:NZ	2.50	0.40
1:C:226:ARG:NH1	1:C:237:VAL:HG11	2.36	0.40
1:D:422:LYS:HB2	1:D:425:ASN:OD1	2.21	0.40
1:C:222:VAL:HG12	1:C:305:ILE:O	2.20	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	337/368 (92%)	324 (96%)	13 (4%)	0	100	100
1	B	335/368 (91%)	316 (94%)	16 (5%)	3 (1%)	17	56
1	C	326/368 (89%)	308 (94%)	13 (4%)	5 (2%)	10	44
1	D	324/368 (88%)	304 (94%)	16 (5%)	4 (1%)	13	49
All	All	1322/1472 (90%)	1252 (95%)	58 (4%)	12 (1%)	17	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	MET
1	B	219	TYR
1	C	432	GLY
1	D	326	PHE
1	C	287	ASP
1	C	447	ALA
1	C	448	ASP
1	D	435	GLY
1	B	420	THR
1	D	242	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	325	ARG
1	C	242	SER

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	301/324 (93%)	300 (100%)	1 (0%)	92	96
1	B	296/324 (91%)	296 (100%)	0	100	100
1	C	282/324 (87%)	278 (99%)	4 (1%)	67	86
1	D	291/324 (90%)	287 (99%)	4 (1%)	67	86
All	All	1170/1296 (90%)	1161 (99%)	9 (1%)	81	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	TYR
1	C	145	TYR
1	C	193	LYS
1	C	226	ARG
1	C	250	ARG
1	D	285	HIS
1	D	312	CYS
1	D	355	HIS
1	D	400	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	198	ASN
1	C	365	ASN
1	D	313	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	B	321	1	15,16,17	1.33	1 (6%)	19,22,24	0.50	0
1	PTR	D	321	1	15,16,17	1.23	1 (6%)	19,22,24	0.44	0
1	PTR	C	321	1	15,16,17	1.21	1 (6%)	19,22,24	0.59	0
1	PTR	A	321	1	15,16,17	1.30	1 (6%)	19,22,24	0.59	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	B	321	1	-	2/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	OH-CZ	-4.38	1.30	1.40
1	D	321	PTR	OH-CZ	-4.29	1.30	1.40
1	C	321	PTR	OH-CZ	-4.22	1.31	1.40
1	A	321	PTR	OH-CZ	-4.14	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	C-CA-CB-CG
1	B	321	PTR	N-CA-CB-CG
1	D	321	PTR	CZ-OH-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0
1	C	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	OPW	C	501	-	21,23,23	1.64	3 (14%)	24,32,32	2.57	8 (33%)
2	OPW	B	501	-	21,23,23	1.70	3 (14%)	24,32,32	2.56	8 (33%)
2	OPW	A	501	-	21,23,23	1.67	3 (14%)	24,32,32	2.60	8 (33%)
2	OPW	D	501	-	21,23,23	1.68	3 (14%)	24,32,32	2.59	7 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OPW	C	501	-	-	4/9/10/10	0/3/3/3
2	OPW	B	501	-	-	4/9/10/10	0/3/3/3
2	OPW	A	501	-	-	4/9/10/10	0/3/3/3
2	OPW	D	501	-	-	4/9/10/10	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OPW	CAR-NAQ	5.48	1.46	1.36
2	B	501	OPW	CAR-NAQ	5.47	1.46	1.36
2	D	501	OPW	CAR-NAQ	5.46	1.46	1.36
2	C	501	OPW	CAR-NAQ	5.31	1.45	1.36
2	B	501	OPW	CAH-SAG	-2.67	1.70	1.73
2	D	501	OPW	CAH-SAG	-2.56	1.70	1.73
2	A	501	OPW	CAH-SAG	-2.44	1.70	1.73
2	C	501	OPW	CAH-SAG	-2.34	1.70	1.73
2	D	501	OPW	CAP-NAQ	2.25	1.46	1.41
2	A	501	OPW	CAP-NAQ	2.17	1.46	1.41
2	B	501	OPW	CAP-NAQ	2.16	1.46	1.41
2	C	501	OPW	CAP-NAQ	2.09	1.45	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	OPW	CAH-NAI-CAJ	6.70	117.07	103.78
2	D	501	OPW	CAH-NAI-CAJ	6.64	116.96	103.78
2	B	501	OPW	CAH-NAI-CAJ	6.54	116.76	103.78
2	A	501	OPW	CAH-NAI-CAJ	6.45	116.57	103.78
2	C	501	OPW	CAJ-CAF-SAG	-5.36	104.74	111.85
2	D	501	OPW	CAJ-CAF-SAG	-5.16	105.00	111.85
2	A	501	OPW	CAS-CAR-NAQ	5.11	122.47	114.98
2	B	501	OPW	CAJ-CAF-SAG	-4.95	105.29	111.85
2	D	501	OPW	CAS-CAR-NAQ	4.84	122.09	114.98
2	A	501	OPW	CAJ-CAF-SAG	-4.74	105.56	111.85
2	C	501	OPW	CAS-CAR-NAQ	4.64	121.78	114.98
2	B	501	OPW	CAS-CAR-NAQ	4.62	121.76	114.98
2	B	501	OPW	CAO-NAN-CAM	3.85	122.73	117.48
2	A	501	OPW	CAU-CAL-CAM	3.84	120.92	117.11
2	A	501	OPW	CAO-NAN-CAM	3.68	122.50	117.48
2	D	501	OPW	CAO-NAN-CAM	3.67	122.49	117.48
2	C	501	OPW	CAO-NAN-CAM	3.57	122.35	117.48
2	D	501	OPW	CAU-CAL-CAM	3.46	120.55	117.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	OPW	OAT-CAR-NAQ	-3.37	118.61	123.04
2	D	501	OPW	OAT-CAR-NAQ	-3.32	118.68	123.04
2	B	501	OPW	CAU-CAL-CAM	3.26	120.34	117.11
2	C	501	OPW	OAT-CAR-NAQ	-3.25	118.77	123.04
2	B	501	OPW	OAT-CAR-NAQ	-3.08	119.00	123.04
2	C	501	OPW	CAU-CAL-CAM	2.75	119.84	117.11
2	C	501	OPW	CAF-CAJ-NAI	2.70	114.32	108.04
2	D	501	OPW	CAF-CAJ-NAI	2.63	114.17	108.04
2	B	501	OPW	CAP-NAQ-CAR	-2.56	123.33	127.99
2	A	501	OPW	CAF-CAJ-NAI	2.56	113.99	108.04
2	B	501	OPW	CAF-CAJ-NAI	2.55	113.97	108.04
2	A	501	OPW	CAL-CAU-CAP	-2.26	117.70	121.07
2	C	501	OPW	CAP-NAQ-CAR	-2.02	124.32	127.99

There are no chirality outliers.

All (16) torsion outliers are listed below:

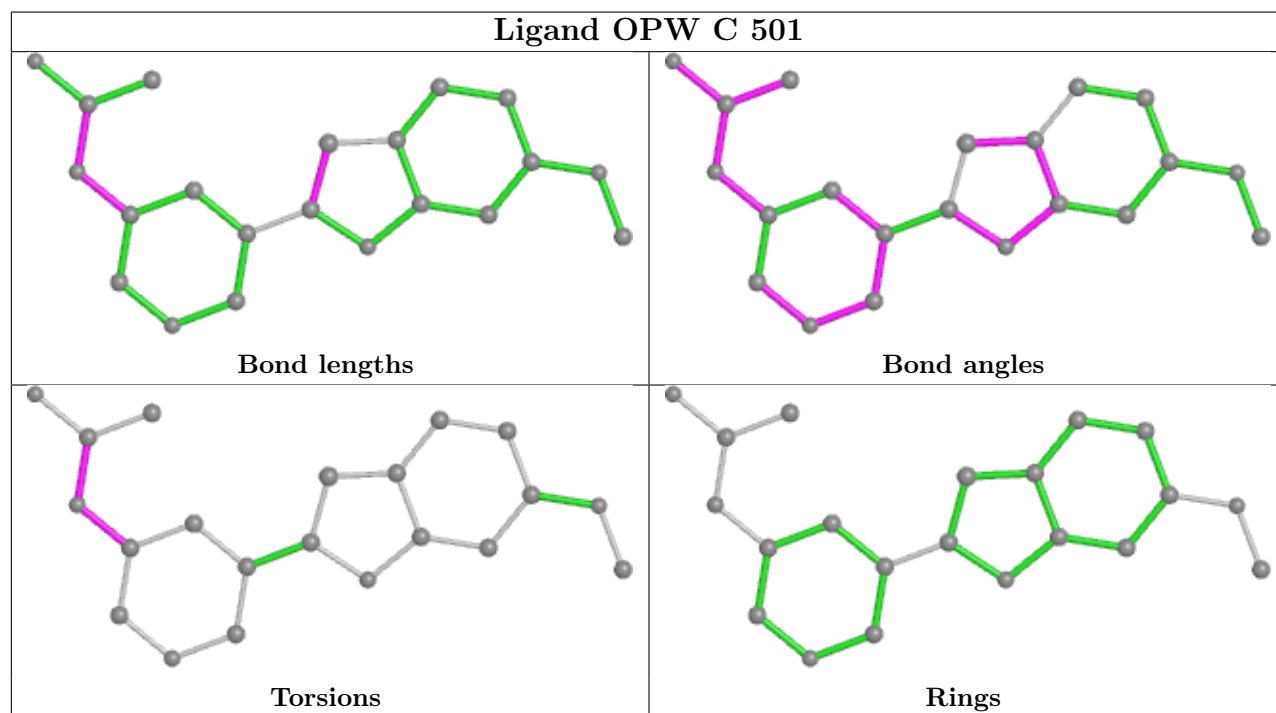
Mol	Chain	Res	Type	Atoms
2	A	501	OPW	CAS-CAR-NAQ-CAP
2	B	501	OPW	CAS-CAR-NAQ-CAP
2	C	501	OPW	CAS-CAR-NAQ-CAP
2	D	501	OPW	CAS-CAR-NAQ-CAP
2	A	501	OPW	OAT-CAR-NAQ-CAP
2	B	501	OPW	OAT-CAR-NAQ-CAP
2	C	501	OPW	OAT-CAR-NAQ-CAP
2	D	501	OPW	OAT-CAR-NAQ-CAP
2	B	501	OPW	CAO-CAP-NAQ-CAR
2	B	501	OPW	CAU-CAP-NAQ-CAR
2	C	501	OPW	CAU-CAP-NAQ-CAR
2	C	501	OPW	CAO-CAP-NAQ-CAR
2	D	501	OPW	CAU-CAP-NAQ-CAR
2	D	501	OPW	CAO-CAP-NAQ-CAR
2	A	501	OPW	CAU-CAP-NAQ-CAR
2	A	501	OPW	CAO-CAP-NAQ-CAR

There are no ring outliers.

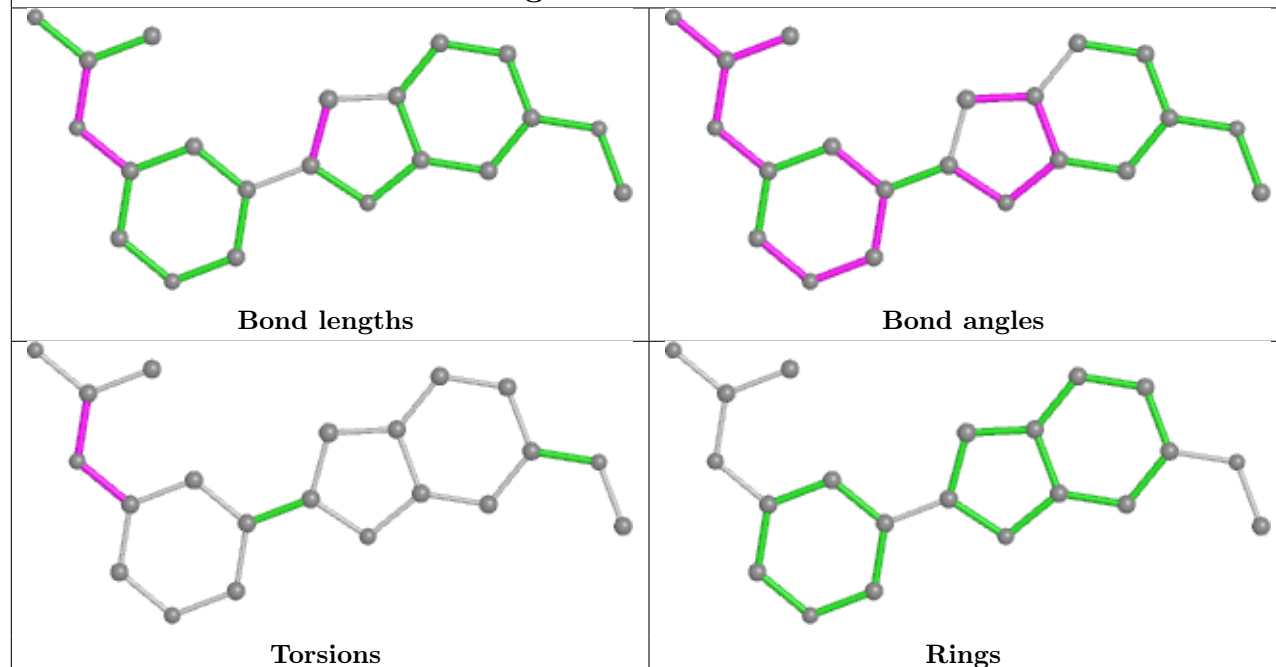
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	OPW	1	0
2	D	501	OPW	1	0

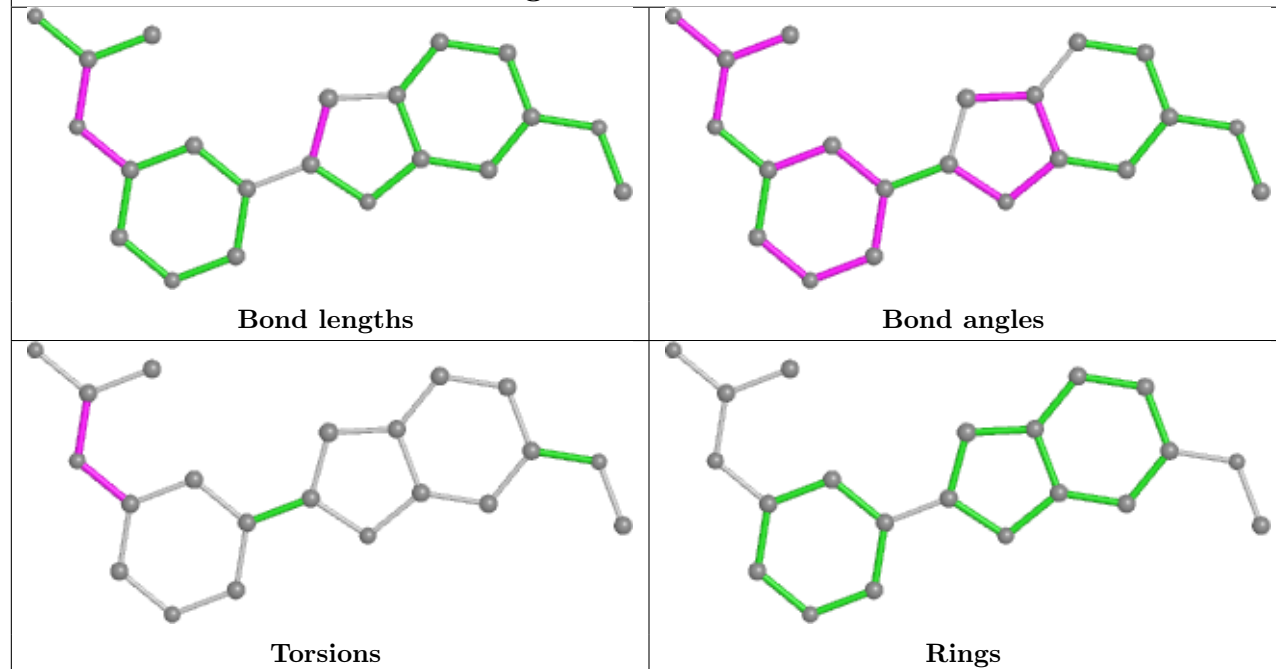
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

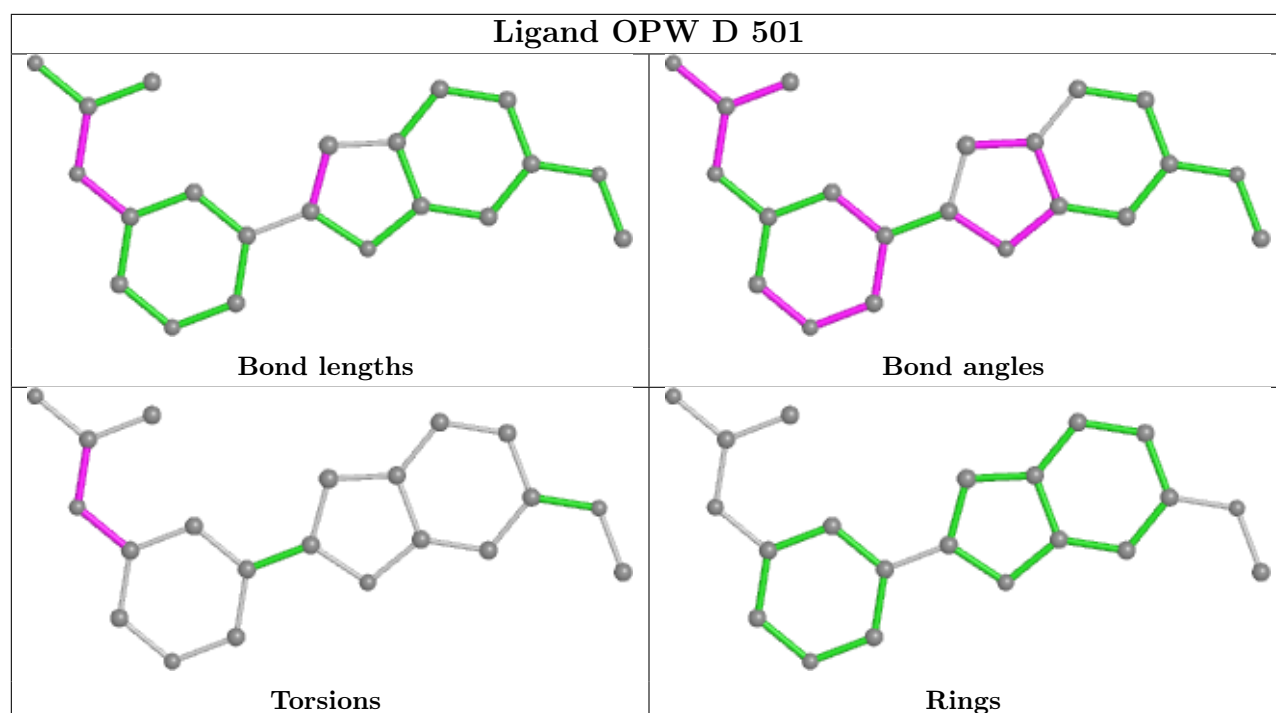


Ligand OPW B 501



Ligand OPW A 501





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	341/368 (92%)	-0.25	2 (0%) 89 83	40, 59, 90, 168	0
1	B	339/368 (92%)	-0.02	2 (0%) 89 83	46, 84, 127, 161	0
1	C	332/368 (90%)	0.13	11 (3%) 46 30	47, 86, 149, 210	0
1	D	330/368 (89%)	0.04	6 (1%) 68 55	43, 73, 133, 193	0
All	All	1342/1472 (91%)	-0.03	21 (1%) 72 59	40, 75, 133, 210	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	378	GLY	4.0
1	C	428	GLY	4.0
1	D	448	ASP	3.5
1	D	430	GLU	3.3
1	C	427	LEU	3.3
1	C	472	TYR	3.0
1	D	477	SER	2.9
1	C	425	ASN	2.6
1	C	214	ASP	2.4
1	C	395	PHE	2.3
1	C	404	ASN	2.3
1	C	405	LEU	2.2
1	A	214	ASP	2.2
1	C	215	THR	2.2
1	D	432	GLY	2.2
1	B	167	LYS	2.1
1	C	430	GLU	2.1
1	A	161	ILE	2.1
1	B	216	GLU	2.0
1	D	253	ASN	2.0
1	D	243	TYR	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	PTR	A	321	16/17	0.92	0.21	58,63,67,68	0
1	PTR	D	321	16/17	0.93	0.15	48,50,56,58	0
1	PTR	C	321	16/17	0.94	0.18	76,79,86,88	0
1	PTR	B	321	16/17	0.95	0.17	75,79,83,84	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

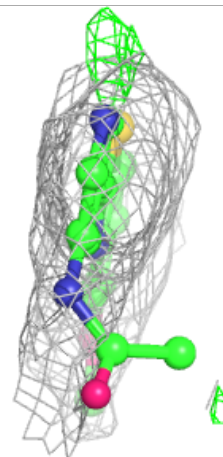
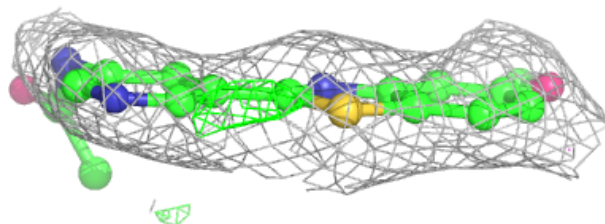
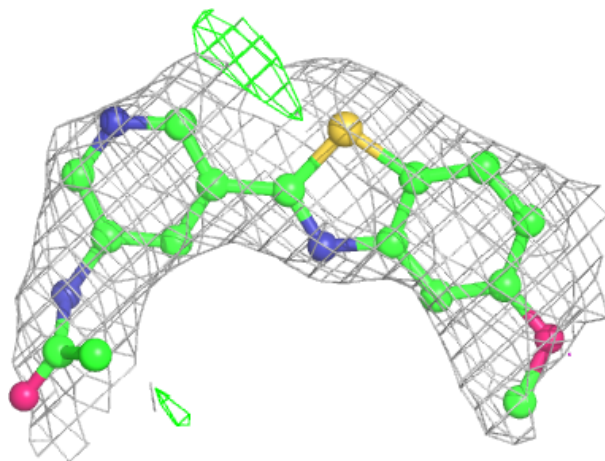
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OPW	C	501	21/21	0.84	0.33	78,81,92,94	0
2	OPW	B	501	21/21	0.88	0.30	67,71,90,93	0
2	OPW	D	501	21/21	0.88	0.32	69,75,90,93	0
2	OPW	A	501	21/21	0.90	0.31	68,73,101,105	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.

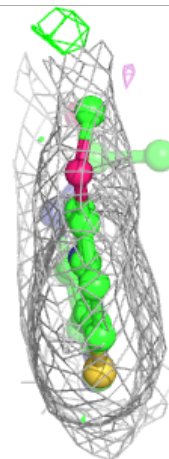
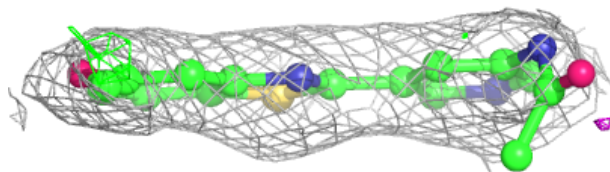
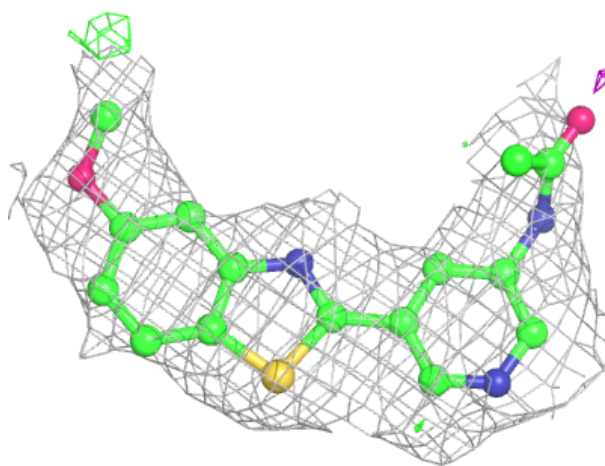
Electron density around OPW C 501:

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



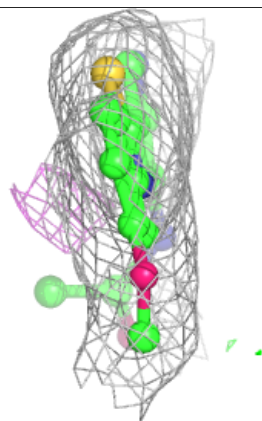
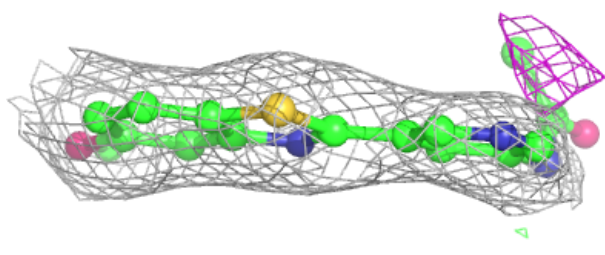
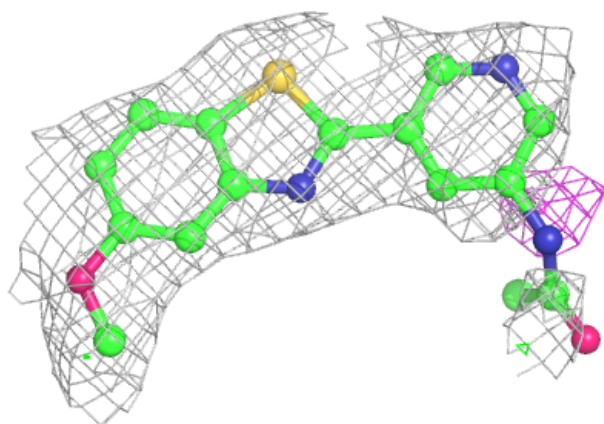
Electron density around OPW B 501:

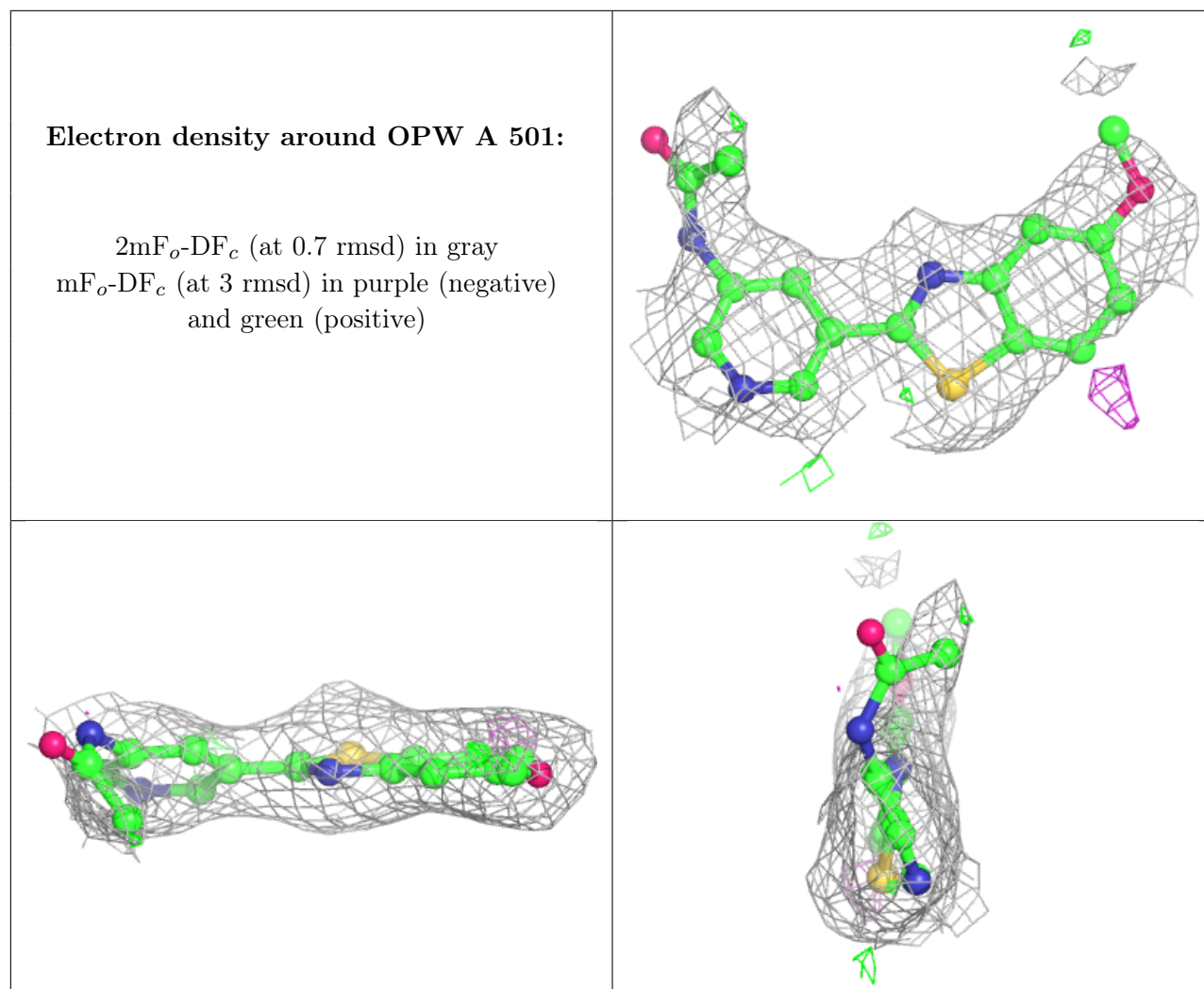
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OPW 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.