



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 12:08 AM UTC

PDB ID : 6YF8 / pdb_00006yf8
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 : 4-5-2 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

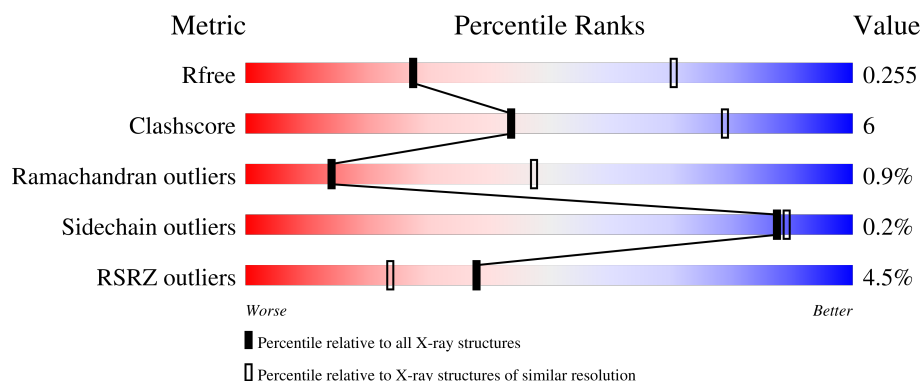
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	5% 81% 12% 7%
1	B	368	5% 79% 14% 8%
1	C	368	7% 72% 18% 10%
1	D	368	5% 73% 16% 10%

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.

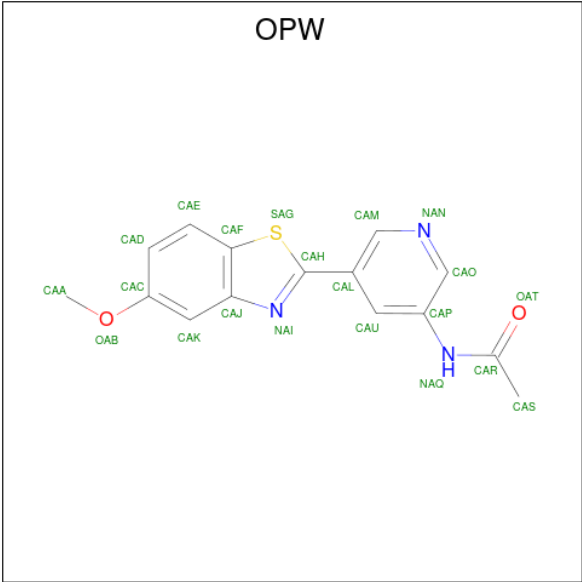
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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

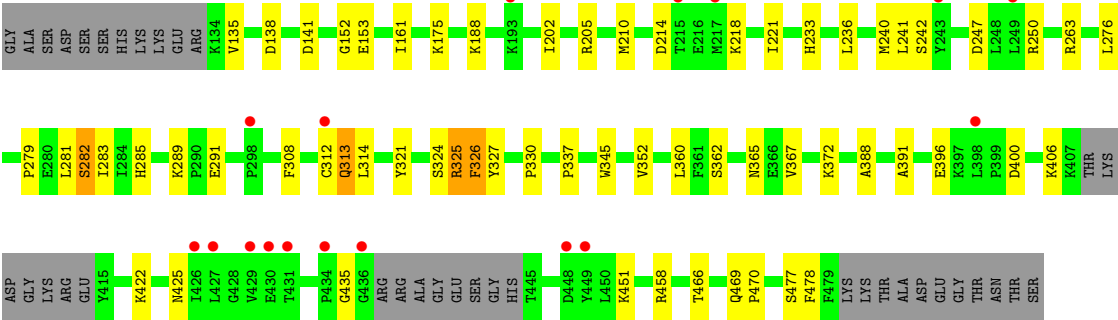
- Molecule 2 is {N}-[5-(5-methoxy-1,3-benzothiazol-2-yl)pyridin-3-yl]ethanamide (CCD ID: OPW) (formula: C₁₅H₁₃N₃O₂S) (labeled as "Ligand of Interest" by depositor).



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		

GLY
THR
ASN
THR
SER

● 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) 99.3 (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 (Not available) , 0.255	Depositor DCC
R_{free} test set	1456 reflections (4.80%)	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 , 34.0	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: PTR, OPW

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	0.14	0/2842	0.42	0/3833
1	B	0.14	0/2808	0.46	0/3789
1	C	0.15	0/2724	0.48	0/3686
1	D	0.30	0/2743	0.58	2/3703 (0.1%)
All	All	0.19	0/11117	0.49	2/15011 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	SER	CA-C-N	-5.06	115.84	122.37
1	D	282	SER	C-N-CA	-5.06	115.84	122.37

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	32	0
1	C	2678	0	2601	43	0
1	D	2697	0	2681	44	0
2	A	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	134	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 (134) 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:D:210:MET:HE2	1:D:283:ILE:HD13	1.66	0.78
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:D:325:ARG:O	1:D:326:PHE:C	2.36	0.66
1:A:169:SER:O	1:A:191:LYS:NZ	2.27	0.66
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: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:B:370:MET:HE2	1:B:374:VAL:HG23	1.85	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:B:346:SER:O	1:B:350:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:325:ARG:C	1:D:327:TYR:N	2.68	0.51
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:B:210:MET:HE1	1:B:308:PHE:CE2	2.45	0.51
1:C:463:ASP:HB3	1:C:466:THR:OG1	2.12	0.50
1:D:362:SER:O	1:D:372:LYS:NZ	2.36	0.50
1:D:458:ARG:NH2	1:D:466:THR:O	2.37	0.49
1:D:152:GLY:O	1:D:153:GLU:C	2.55	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:B:297:ASN:CG	1:B:298:PRO:HD2	2.37	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:D:175:LYS:HE2	1:D:240:MET:HE2	1.94	0.48
1:A:378:GLY:HA2	1:A:418:PRO:HB3	1.95	0.48
1:C:341:ALA:O	1:C:467:ARG:NH1	2.46	0.48
1:B:210:MET:HE3	1:B:283:ILE:HD13	1.96	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:MET:HE3	1:B:373:ILE:HB	1.97	0.47
1:D:210:MET:HE2	1:D:283:ILE:CD1	2.42	0.47
1:B:317:ARG:HG3	1:B:338:TYR:CE2	2.51	0.46
1:C:259:LEU:H	1:C:444:HIS:HE2	1.60	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
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: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:A:207:LEU:HA	1:A:210:MET:HE3	2.00	0.44
1:B:280:GLU:N	1:B:280:GLU:OE2	2.50	0.44
1:B:218:LYS:C	1:B:220:TYR:H	2.26	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:D:285:HIS:HD1	1:D:285:HIS:C	2.25	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:D:210:MET:HE1	1:D:308:PHE:CE2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:210:MET:CE	1:D:283:ILE:HD13	2.44	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: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:A:171:GLY:HA2	1:A:191:LYS:HZ2	1.85	0.41
1:C:333:LEU:HD13	1:C:370:MET:HE2	2.03	0.41
1:C:365:ASN:HB3	1:D:138:ASP:OD1	2.21	0.41
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%)	14	47
1	C	326/368 (89%)	308 (94%)	13 (4%)	5 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	324/368 (88%)	304 (94%)	16 (5%)	4 (1%)	10	42
All	All	1322/1472 (90%)	1252 (95%)	58 (4%)	12 (1%)	14	47

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
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%)	301 (100%)	0	100	100
1	B	296/324 (91%)	296 (100%)	0	100	100
1	C	282/324 (87%)	282 (100%)	0	100	100
1	D	291/324 (90%)	289 (99%)	2 (1%)	76	83
All	All	1170/1296 (90%)	1168 (100%)	2 (0%)	87	89

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

Mol	Chain	Res	Type
1	D	312	CYS
1	D	313	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	A	383	HIS
1	A	404	ASN
1	A	469	GLN
1	A	475	GLN
1	B	251	ASN
1	B	320	GLN
1	B	387	GLN
1	B	476	HIS
1	C	198	ASN
1	C	297	ASN
1	C	313	GLN
1	C	365	ASN
1	C	383	HIS
1	D	213	HIS
1	D	260	ASN
1	D	313	GLN
1	D	365	ASN

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	1.32	1 (6%)	17,22,24	0.52	0
1	PTR	D	321	1	15,16,17	1.21	1 (6%)	17,22,24	0.47	0
1	PTR	A	321	1	15,16,17	1.28	1 (6%)	17,22,24	0.61	0

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	1.19	1 (6%)	17,22,24	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	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	C	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	-4.42	1.30	1.40
1	D	321	PTR	OH-CZ	-4.34	1.30	1.40
1	C	321	PTR	OH-CZ	-4.26	1.31	1.40
1	A	321	PTR	OH-CZ	-4.19	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A	501	-	23,23,23	1.73	4 (17%)	32,32,32	2.56	12 (37%)
2	OPW	C	501	-	23,23,23	1.75	4 (17%)	32,32,32	2.65	10 (31%)
2	OPW	D	501	-	23,23,23	1.75	4 (17%)	32,32,32	2.66	11 (34%)
2	OPW	B	501	-	23,23,23	1.77	4 (17%)	32,32,32	2.58	12 (37%)

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	A	501	-	-	4/10/10/10	0/3/3/3
2	OPW	C	501	-	-	4/10/10/10	0/3/3/3
2	OPW	D	501	-	-	4/10/10/10	0/3/3/3
2	OPW	B	501	-	-	4/10/10/10	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OPW	CAR-NAQ	5.45	1.46	1.36
2	B	501	OPW	CAR-NAQ	5.44	1.46	1.36
2	D	501	OPW	CAR-NAQ	5.43	1.46	1.36
2	C	501	OPW	CAR-NAQ	5.28	1.45	1.36
2	C	501	OPW	CAL-CAH	3.81	1.53	1.47
2	B	501	OPW	CAL-CAH	3.42	1.52	1.47
2	D	501	OPW	CAL-CAH	3.40	1.52	1.47
2	B	501	OPW	CAH-SAG	-3.11	1.70	1.76
2	A	501	OPW	CAL-CAH	3.10	1.52	1.47
2	D	501	OPW	CAH-SAG	-3.04	1.70	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OPW	CAH-SAG	-2.95	1.70	1.76
2	C	501	OPW	CAH-SAG	-2.88	1.70	1.76
2	D	501	OPW	CAP-NAQ	2.25	1.46	1.41
2	A	501	OPW	CAP-NAQ	2.18	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 (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	OPW	CAF-SAG-CAH	7.69	97.60	88.97
2	D	501	OPW	CAF-SAG-CAH	7.35	97.21	88.97
2	B	501	OPW	CAF-SAG-CAH	7.31	97.17	88.97
2	A	501	OPW	CAF-SAG-CAH	6.72	96.51	88.97
2	C	501	OPW	SAG-CAH-NAI	-6.04	106.26	115.54
2	D	501	OPW	SAG-CAH-NAI	-5.78	106.67	115.54
2	B	501	OPW	SAG-CAH-NAI	-5.68	106.82	115.54
2	A	501	OPW	SAG-CAH-NAI	-5.32	107.37	115.54
2	A	501	OPW	CAS-CAR-NAQ	5.00	122.47	114.95
2	D	501	OPW	CAL-CAH-SAG	4.95	128.87	120.32
2	C	501	OPW	CAL-CAH-SAG	4.82	128.65	120.32
2	D	501	OPW	CAS-CAR-NAQ	4.75	122.09	114.95
2	C	501	OPW	CAS-CAR-NAQ	4.54	121.78	114.95
2	B	501	OPW	CAS-CAR-NAQ	4.53	121.76	114.95
2	A	501	OPW	CAL-CAH-SAG	4.52	128.12	120.32
2	B	501	OPW	CAL-CAH-SAG	4.25	127.67	120.32
2	B	501	OPW	CAO-NAN-CAM	3.84	122.73	117.51
2	A	501	OPW	CAO-NAN-CAM	3.67	122.50	117.51
2	D	501	OPW	CAO-NAN-CAM	3.67	122.49	117.51
2	C	501	OPW	CAO-NAN-CAM	3.56	122.35	117.51
2	D	501	OPW	CAE-CAF-SAG	3.54	135.72	127.36
2	C	501	OPW	CAE-CAF-SAG	3.51	135.65	127.36
2	C	501	OPW	CAJ-CAF-SAG	-3.39	104.74	109.75
2	A	501	OPW	CAE-CAF-SAG	3.37	135.31	127.36
2	B	501	OPW	CAE-CAF-SAG	3.30	135.14	127.36
2	A	501	OPW	OAT-CAR-NAQ	-3.25	118.61	123.06
2	D	501	OPW	CAJ-CAF-SAG	-3.21	105.00	109.75
2	D	501	OPW	OAT-CAR-NAQ	-3.20	118.68	123.06
2	C	501	OPW	OAT-CAR-NAQ	-3.13	118.77	123.06
2	B	501	OPW	CAJ-CAF-SAG	-3.02	105.29	109.75
2	D	501	OPW	CAL-CAM-NAN	-2.99	119.05	123.50
2	A	501	OPW	CAL-CAM-NAN	-2.99	119.05	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	OPW	OAT-CAR-NAQ	-2.96	119.00	123.06
2	A	501	OPW	CAU-CAL-CAM	2.92	120.92	117.92
2	B	501	OPW	CAL-CAM-NAN	-2.86	119.25	123.50
2	A	501	OPW	CAJ-CAF-SAG	-2.83	105.56	109.75
2	D	501	OPW	CAU-CAL-CAM	2.55	120.55	117.92
2	B	501	OPW	CAP-NAQ-CAR	-2.49	123.33	127.98
2	C	501	OPW	CAL-CAM-NAN	-2.48	119.81	123.50
2	B	501	OPW	CAU-CAL-CAM	2.35	120.34	117.92
2	C	501	OPW	CAJ-NAI-CAH	2.30	117.07	110.53
2	D	501	OPW	CAJ-NAI-CAH	2.26	116.96	110.53
2	B	501	OPW	CAJ-NAI-CAH	2.19	116.76	110.53
2	A	501	OPW	CAJ-NAI-CAH	2.13	116.57	110.53
2	A	501	OPW	CAL-CAU-CAP	-2.13	117.70	120.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

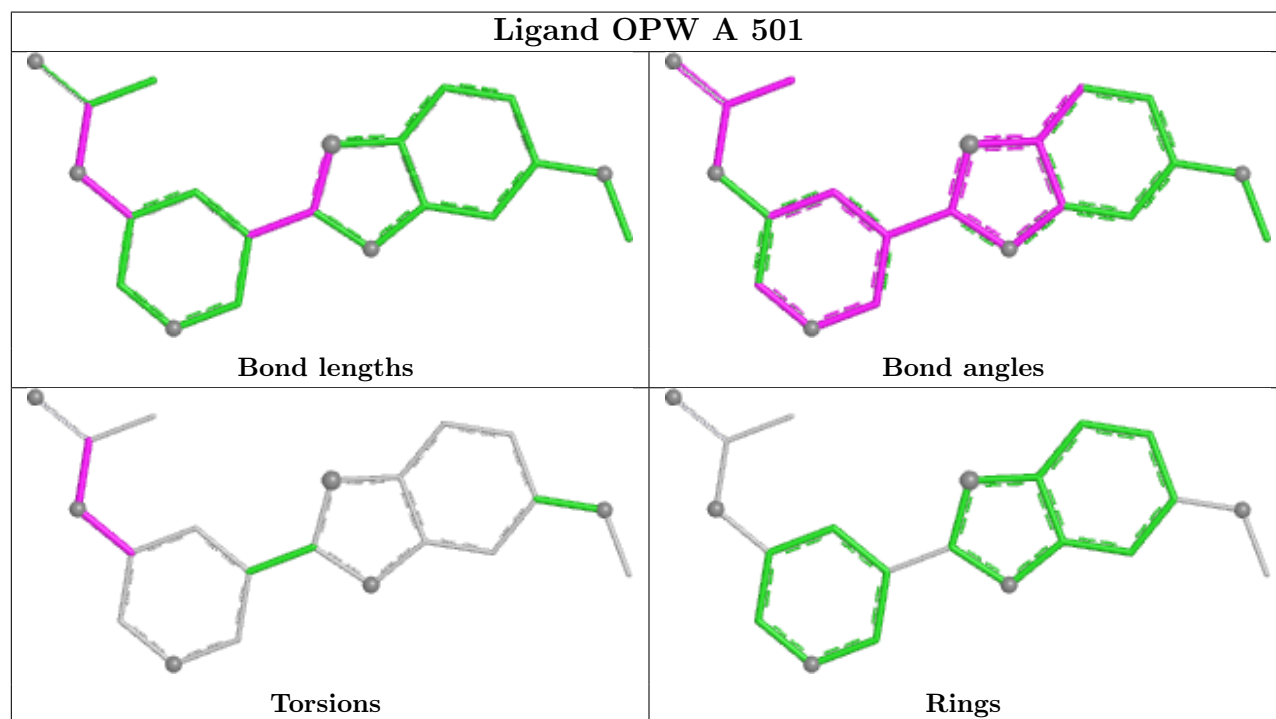
Mol	Chain	Res	Type	Atoms
2	A	501	OPW	CAS-CAR-NAQ-CAP
2	B	501	OPW	CAS-CAR-NAQ-CAP
2	C	501	OPW	CAS-CAR-NAQ-CAP
2	D	501	OPW	CAS-CAR-NAQ-CAP
2	A	501	OPW	OAT-CAR-NAQ-CAP
2	B	501	OPW	OAT-CAR-NAQ-CAP
2	C	501	OPW	OAT-CAR-NAQ-CAP
2	D	501	OPW	OAT-CAR-NAQ-CAP
2	B	501	OPW	CAO-CAP-NAQ-CAR
2	B	501	OPW	CAU-CAP-NAQ-CAR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

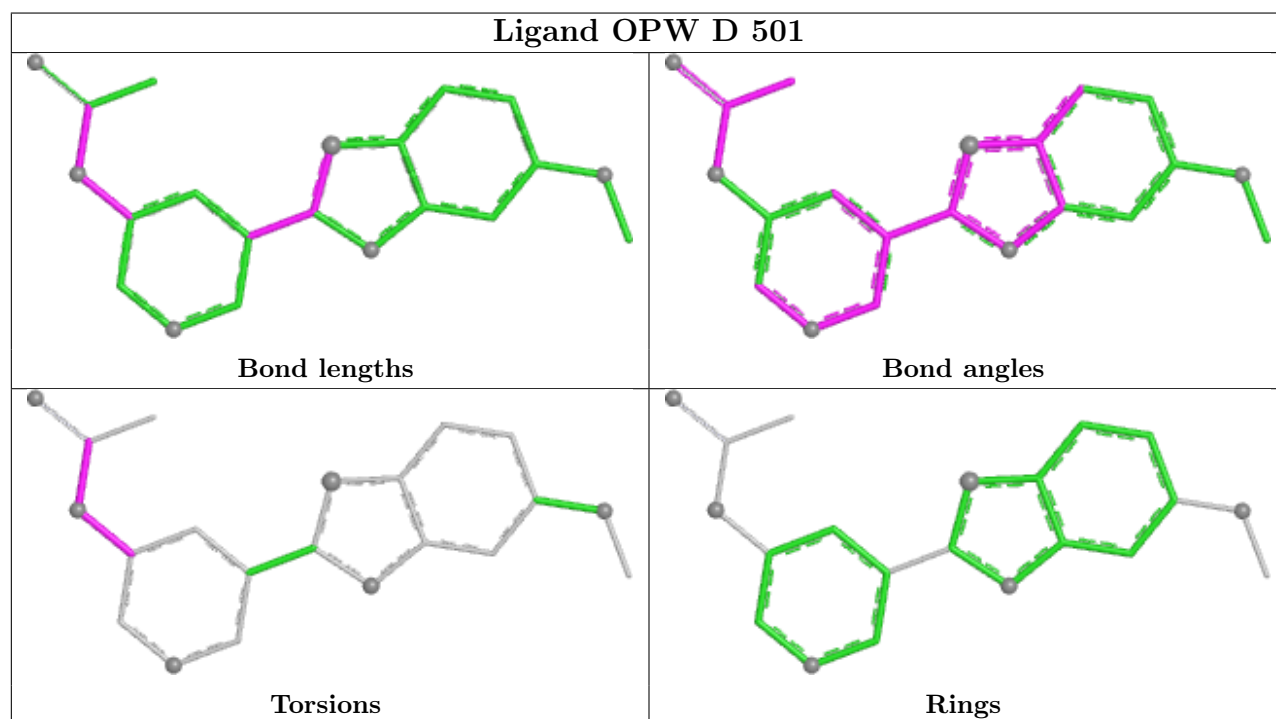
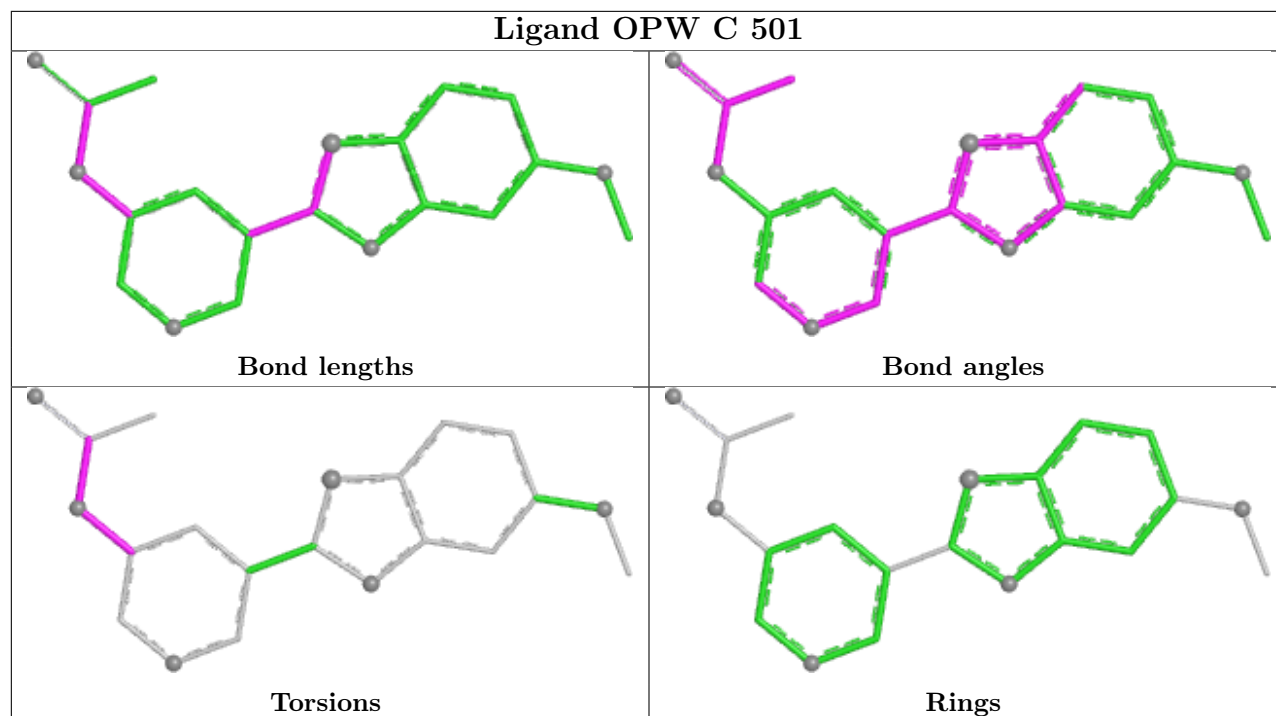
There are no ring outliers.

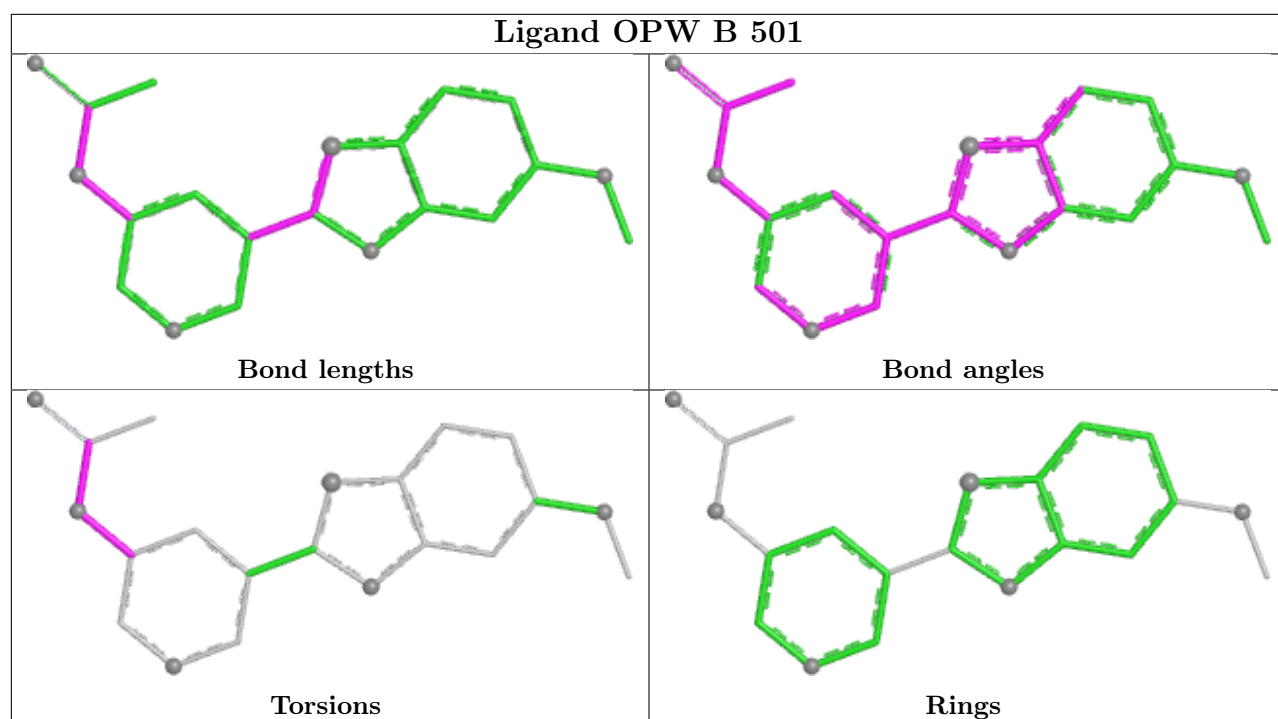
2 monomers are involved in 2 short contacts:

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.







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%)	0.16	2 (0%) 85 73	40, 59, 90, 168	0
1	B	339/368 (92%)	0.47	17 (5%) 34 22	46, 84, 127, 161	0
1	C	332/368 (90%)	0.69	25 (7%) 20 13	47, 86, 149, 210	0
1	D	330/368 (89%)	0.52	17 (5%) 33 21	43, 73, 133, 193	0
All	All	1342/1472 (91%)	0.46	61 (4%) 38 24	40, 75, 133, 210	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	TYR	4.6
1	B	419	GLY	3.8
1	C	446	VAL	3.8
1	D	434	PRO	3.6
1	C	413	ARG	3.4
1	D	436	GLY	3.4
1	C	427	LEU	3.2
1	A	160	GLU	3.2
1	C	378	GLY	3.1
1	C	395	PHE	2.9
1	B	420	THR	2.9
1	D	298	PRO	2.9
1	B	315	GLY	2.9
1	D	193	LYS	2.8
1	D	243	TYR	2.8
1	D	449	TYR	2.8
1	B	417	PRO	2.7
1	B	217	MET	2.7
1	C	405	LEU	2.7
1	D	312	CYS	2.6
1	C	435	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	398	LEU	2.5
1	C	277	ALA	2.5
1	C	219	TYR	2.5
1	B	316	GLN	2.5
1	D	429	VAL	2.5
1	B	143	ASP	2.5
1	D	426	ILE	2.5
1	C	472	TYR	2.5
1	D	427	LEU	2.5
1	D	448	ASP	2.4
1	C	473	ALA	2.4
1	B	292	ASN	2.4
1	C	136	TYR	2.4
1	B	314	LEU	2.4
1	D	249	LEU	2.4
1	A	243	TYR	2.3
1	C	429	VAL	2.3
1	B	243	TYR	2.3
1	D	217	MET	2.2
1	D	215	THR	2.2
1	D	431	THR	2.2
1	B	362	SER	2.2
1	B	299	LYS	2.2
1	C	243	TYR	2.2
1	C	365	ASN	2.2
1	D	398	LEU	2.2
1	C	407	LYS	2.2
1	B	135	VAL	2.2
1	C	449	TYR	2.2
1	B	301	SER	2.2
1	C	448	ASP	2.2
1	C	415	TYR	2.1
1	B	240	MET	2.1
1	C	315	GLY	2.1
1	C	324	SER	2.1
1	C	404	ASN	2.1
1	C	452	PHE	2.0
1	C	426	ILE	2.0
1	C	135	VAL	2.0
1	D	430	GLU	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	0.11	58,63,67,68	0
1	PTR	C	321	16/17	0.92	0.12	76,79,86,88	0
1	PTR	D	321	16/17	0.93	0.09	48,50,56,58	0
1	PTR	B	321	16/17	0.95	0.09	75,79,83,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

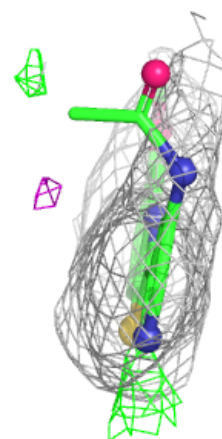
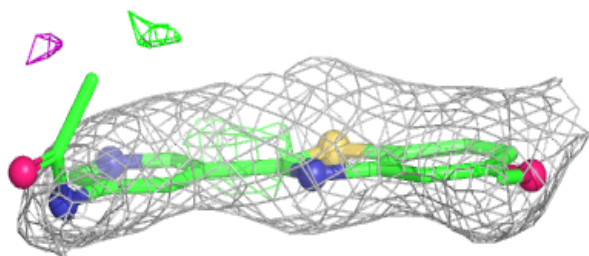
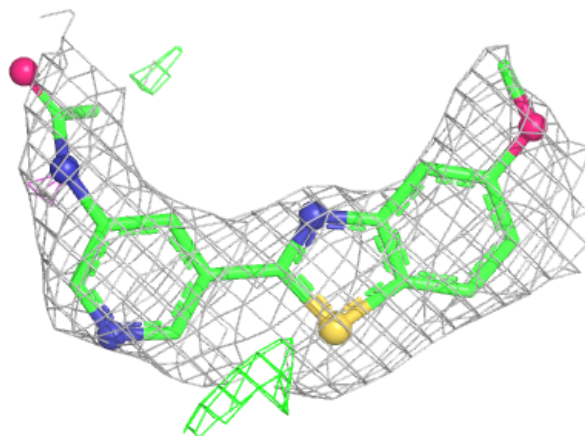
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.80	0.19	78,81,92,94	0
2	OPW	D	501	21/21	0.82	0.17	69,75,90,93	0
2	OPW	A	501	21/21	0.86	0.17	68,73,101,105	0
2	OPW	B	501	21/21	0.86	0.16	67,71,90,93	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.

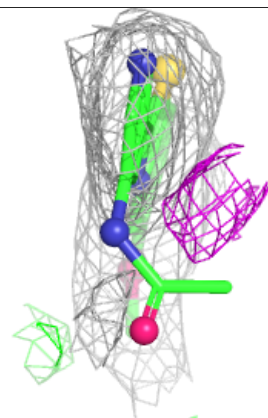
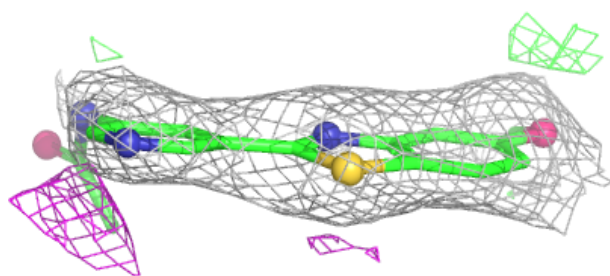
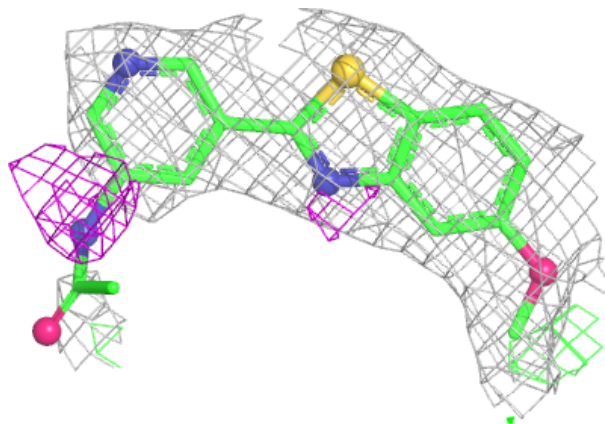
Electron density around OPW C 501:

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



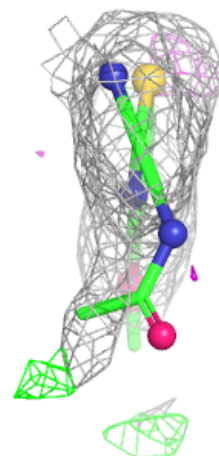
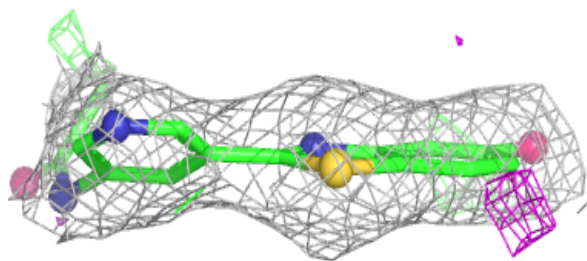
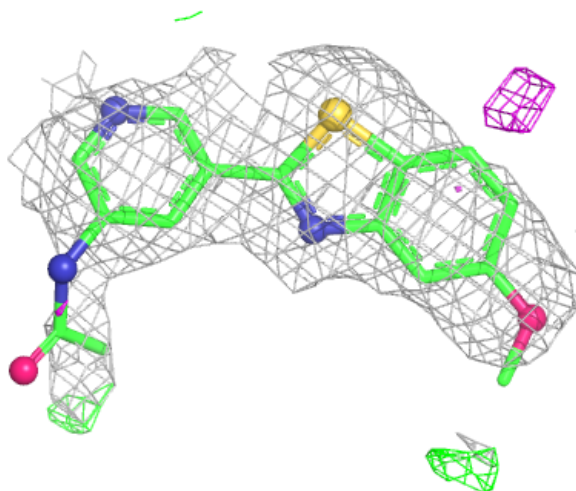
Electron density around OPW D 501:

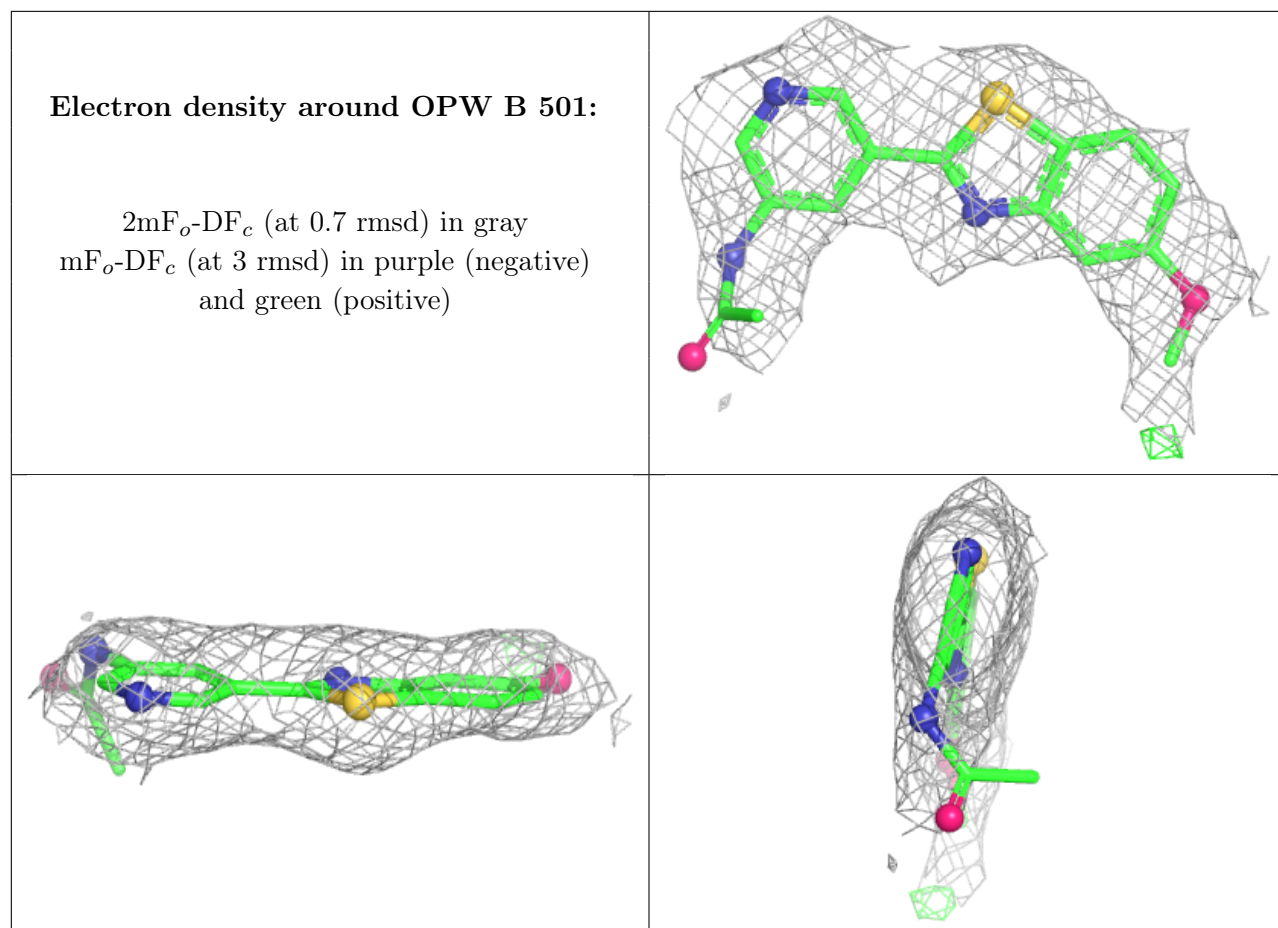
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OPW 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 ⓘ

There are no such residues in this entry.