Full wwPDB X-ray Structure Validation Report (i)

May 22, 2025 – 05:21 PM EDT

PDB ID	:	9NA5 / pdb_00009na5
Title	:	IRAK4 in Complex with Compound 24
Authors	:	Ferrao, R.; Lansdon, E.B.
Deposited on	:	2025-02-11
Resolution	:	1.73 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 (i) 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 (i)) were used in the production of this report:

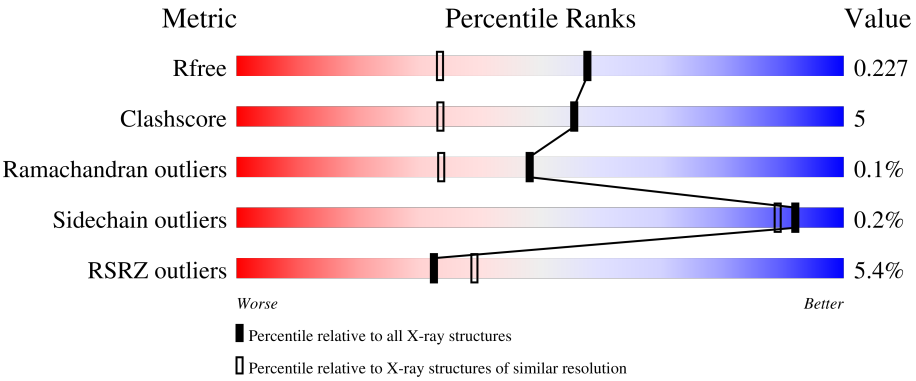
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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 <=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	304	4% 85% 11% .
1	B	304	5% 85% 8% 7%
1	C	304	3% 87% 9% .
1	D	304	8% 80% 13% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10186 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

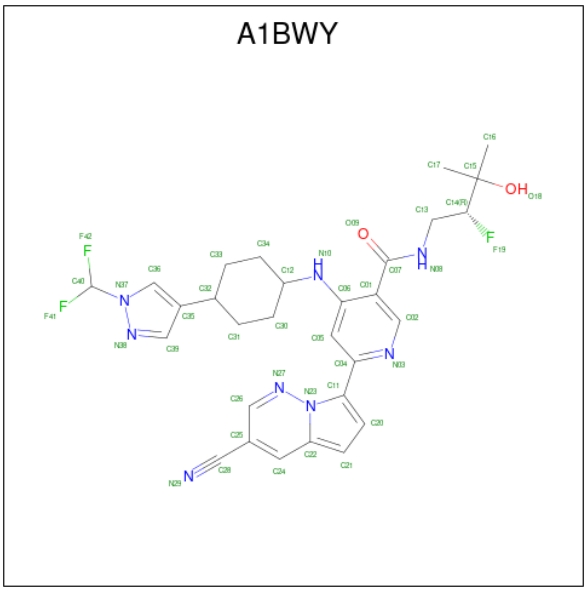
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	P	S	0	2	0
			2294	1437	382	457	3	15			
1	B	284	Total	C	N	O	P	S	0	1	0
			2247	1407	376	447	3	14			
1	C	291	Total	C	N	O	P	S	0	3	0
			2296	1438	383	457	3	15			
1	D	285	Total	C	N	O	P	S	0	2	0
			2254	1416	376	444	3	15			

There are 12 discrepancies between the modelled and reference sequences:

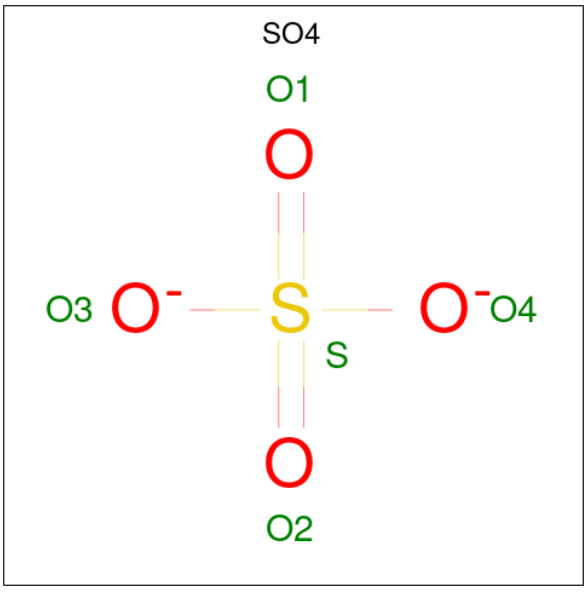
Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	expression tag	UNP Q9NWZ3
A	158	ALA	-	expression tag	UNP Q9NWZ3
A	159	MET	-	expression tag	UNP Q9NWZ3
B	157	GLY	-	expression tag	UNP Q9NWZ3
B	158	ALA	-	expression tag	UNP Q9NWZ3
B	159	MET	-	expression tag	UNP Q9NWZ3
C	157	GLY	-	expression tag	UNP Q9NWZ3
C	158	ALA	-	expression tag	UNP Q9NWZ3
C	159	MET	-	expression tag	UNP Q9NWZ3
D	157	GLY	-	expression tag	UNP Q9NWZ3
D	158	ALA	-	expression tag	UNP Q9NWZ3
D	159	MET	-	expression tag	UNP Q9NWZ3

- Molecule 2 is (6P)-6-[(8R)-3-cyanopyrrolo[1,2-b]pyridazin-7-yl]-4-({(1s,4S)-4-[1-(difluoromethyl)-1H-pyrazol-4-yl]cyclohexyl}amino)-N-[(2S)-2-fluoro-3-hydroxy-3-methylbutyl]pyridine-3-carboxamide (CCD ID: A1BWY) (formula: $C_{29}H_{31}F_3N_8O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			42	29	3	8	2		
2	B	1	Total	C	F	N	O	0	0
			42	29	3	8	2		
2	C	1	Total	C	F	N	O	0	0
			42	29	3	8	2		
2	D	1	Total	C	F	N	O	0	0
			42	29	3	8	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

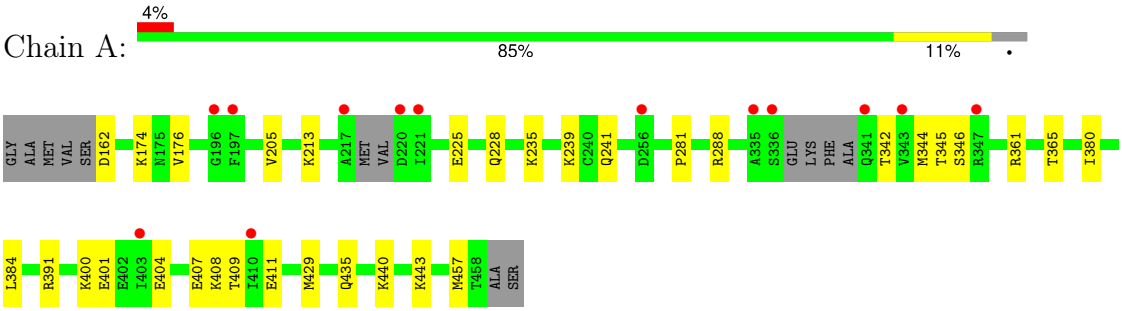
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	242	Total O 242 242	0	0
4	B	203	Total O 203 203	0	0
4	C	251	Total O 251 251	0	0
4	D	176	Total O 176 176	0	0

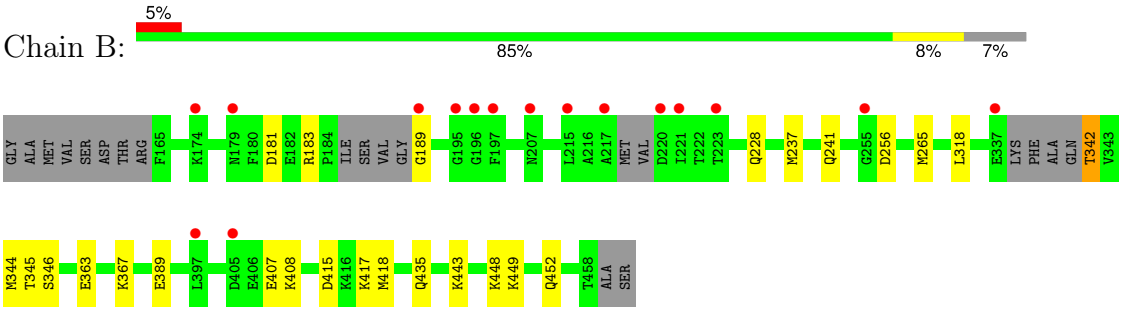
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

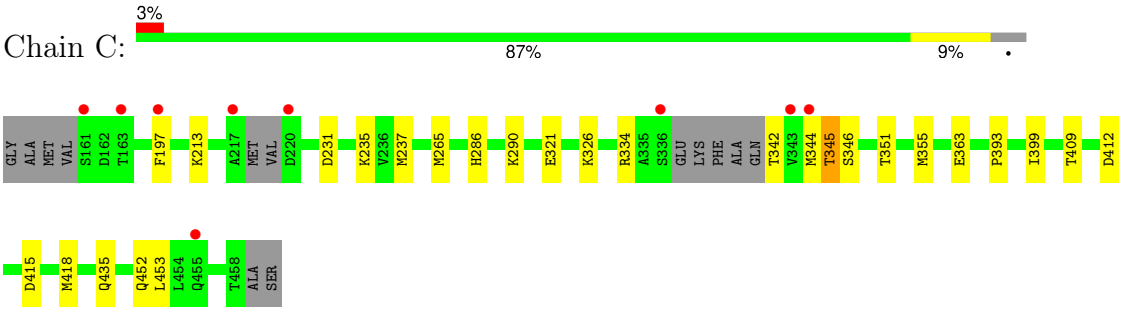
• Molecule 1: Interleukin-1 receptor-associated kinase 4



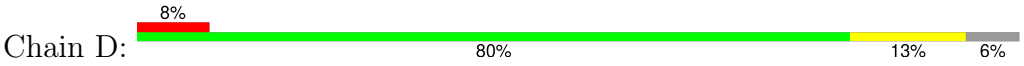
• Molecule 1: Interleukin-1 receptor-associated kinase 4

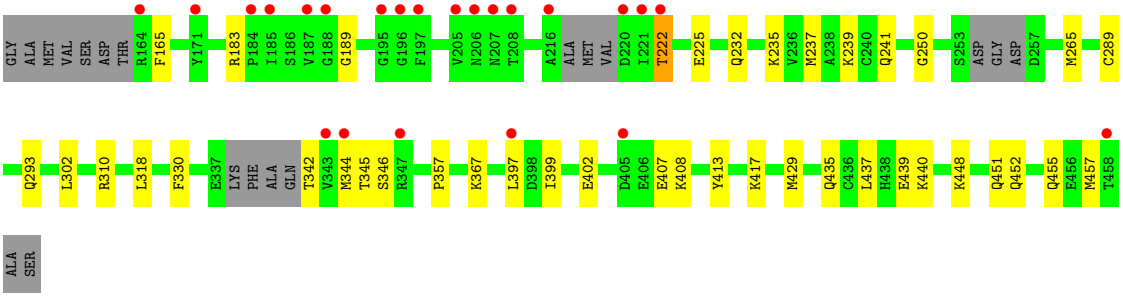


• Molecule 1: Interleukin-1 receptor-associated kinase 4



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




GLY ALA MET VAL SER ASP THR R164 F165 Y171 R183 P184 I185 S186 V187 G188 G189 G195 G196 F197 V205 N206 N207 T208 A216 ALA MET VAL D220 I221 T222 E225 Q232 K235 V236 M237 A238 K239 C240 Q241 G250 S253 ASP GLY ASP D257 M265 C289
Q293 L302 R310 L318 F330 E337 LYS PHE ALA GLN T342 V343 M344 T345 S346 R347 P357 K367 L397 D398 I399 E402 D405 E406 E407 K408 Y413 K417 M429 Q435 C436 L437 H438 E439 K440 K448 Q451 Q452 Q455 E456 M457 T458
ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.26Å 141.64Å 111.26Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	48.50 – 1.73 48.50 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.50-1.73) 89.7 (48.50-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	7673 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10186	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1029e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, A1BWY, SO4, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/2303	0.53	0/3102
1	B	0.30	0/2250	0.51	0/3030
1	C	0.33	0/2309	0.53	0/3112
1	D	0.31	0/2263	0.51	0/3047
All	All	0.32	0/9125	0.52	0/12291

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	D	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	D	310	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2294	0	2248	20	0
1	B	2247	0	2198	21	0
1	C	2296	0	2254	16	0
1	D	2254	0	2221	28	0
2	A	42	0	0	0	0
2	B	42	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	0	0
3	A	10	0	0	0	0
3	B	15	0	0	1	0
3	C	10	0	0	0	0
3	D	20	0	0	2	0
4	A	242	0	0	6	0
4	B	203	0	0	6	0
4	C	251	0	0	1	0
4	D	176	0	0	3	0
All	All	10186	0	8921	84	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 5.

All (84) 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:213:LYS:NZ	4:A:603:HOH:O	2.26	0.68
1:D:232:GLN:HE21	1:D:232:GLN:HA	1.59	0.67
1:B:448:LYS:O	1:B:452:GLN:HG2	1.96	0.65
1:B:407:GLU:HB3	1:B:408:LYS:HE3	1.80	0.64
1:A:225:GLU:HA	1:A:228:GLN:HG3	1.79	0.64
1:A:435:GLN:NE2	4:A:607:HOH:O	2.31	0.62
1:D:357:PRO:HG3	1:D:439:GLU:OE2	1.99	0.62
1:C:197:PHE:CD1	1:C:213:LYS:HE3	2.35	0.61
1:D:265:MET:HE2	1:D:265:MET:HA	1.81	0.61
1:D:435:GLN:NE2	4:D:601:HOH:O	2.33	0.61
1:B:189:GLY:N	4:B:603:HOH:O	2.35	0.60
1:D:448:LYS:O	1:D:452:GLN:HG3	2.02	0.59
1:D:451:GLN:O	1:D:455:GLN:HG3	2.05	0.57
1:B:265:MET:HA	1:B:265:MET:HE2	1.87	0.56
1:B:237:MET:HA	1:B:237:MET:HE2	1.88	0.54
1:B:367:LYS:NZ	3:B:502:SO4:O4	2.40	0.54
1:D:237[A]:MET:HA	1:D:237[A]:MET:HE2	1.90	0.54
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ILE:HA	1:D:402:GLU:HG3	1.90	0.54
1:C:237:MET:HE2	1:C:237:MET:HA	1.91	0.53
1:D:183:ARG:HB2	1:D:189:GLY:HA3	1.90	0.53
1:D:232:GLN:HE22	1:D:235:LYS:NZ	2.05	0.53
1:D:407:GLU:O	1:D:408:LYS:HG3	2.09	0.53
1:A:400:LYS:HE2	1:A:404:GLU:HG3	1.91	0.53
1:C:409:THR:HG22	1:C:412:ASP:OD2	2.09	0.52
1:C:235:LYS:N	1:C:235:LYS:HD3	2.25	0.52
1:D:232:GLN:HA	1:D:232:GLN:NE2	2.24	0.52
1:B:389:GLU:H	1:B:389:GLU:CD	2.18	0.52
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.93	0.51
1:C:344:MET:SD	1:C:363:GLU:HG2	2.52	0.50
1:D:367:LYS:NZ	3:D:505:SO4:O1	2.44	0.50
1:B:344:MET:SD	1:B:363:GLU:HG2	2.52	0.50
1:A:429:MET:HB2	1:A:457:MET:SD	2.52	0.50
1:A:174:LYS:NZ	4:A:614:HOH:O	2.46	0.49
1:A:361:ARG:HD2	4:A:785:HOH:O	2.12	0.49
1:D:408:LYS:HD3	1:D:413:TYR:OH	2.12	0.49
1:B:228:GLN:NE2	4:B:612:HOH:O	2.45	0.49
1:C:231:ASP:O	1:C:235:LYS:HE2	2.13	0.48
1:D:222:THR:OG1	1:D:225:GLU:HG3	2.15	0.47
1:A:401:GLU:HA	1:A:401:GLU:OE1	2.14	0.47
1:A:281:PRO:HD3	1:C:321:GLU:HG3	1.95	0.47
1:D:417:LYS:HE2	4:D:632:HOH:O	2.14	0.47
1:A:440:LYS:CD	1:A:443:LYS:HE3	2.45	0.47
1:D:289:CYS:O	1:D:293:GLN:HG3	2.15	0.47
1:B:417:LYS:HE2	4:B:628:HOH:O	2.14	0.47
1:B:449:LYS:HB2	1:B:449:LYS:HE2	1.69	0.46
1:A:407:GLU:O	1:A:408:LYS:HD3	2.15	0.46
1:D:397:LEU:HD21	1:D:437:LEU:HD22	1.96	0.46
1:D:265:MET:HG3	1:D:318:LEU:HB3	1.98	0.46
1:D:440:LYS:HG2	3:D:503:SO4:O1	2.16	0.46
1:C:452:GLN:HG3	1:C:453:LEU:N	2.30	0.45
1:A:241:GLN:OE1	4:A:601:HOH:O	2.20	0.45
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.98	0.45
1:A:235:LYS:HG3	4:A:658:HOH:O	2.16	0.45
1:B:448:LYS:HD3	1:B:448:LYS:HA	1.75	0.45
1:D:429:MET:HB2	1:D:457:MET:SD	2.57	0.44
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.82	0.44
1:A:162:ASP:OD2	1:A:239:LYS:HE3	2.17	0.44
1:B:344:MET:HB3	1:B:344:MET:HE3	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:GLN:NE2	4:B:614:HOH:O	2.51	0.43
1:C:334:ARG:NH2	1:C:345:TPO:O1P	2.36	0.43
1:B:183:ARG:H	1:B:183:ARG:HG2	1.55	0.43
1:B:342:TPO:HA	4:B:605:HOH:O	2.18	0.43
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.00	0.43
1:C:351:THR:O	1:C:355:MET:HG3	2.18	0.43
1:A:176:VAL:HG11	1:A:205:VAL:HG22	2.00	0.43
1:D:232:GLN:HE22	1:D:235:LYS:HZ2	1.66	0.43
1:C:393:PRO:HG2	1:C:399:ILE:HG13	2.00	0.43
1:D:241:GLN:NE2	4:D:608:HOH:O	2.52	0.43
1:C:286:HIS:NE2	1:C:290:LYS:HD2	2.34	0.42
1:A:344:MET:HE3	1:A:344:MET:HB3	1.56	0.42
1:B:241:GLN:HB2	4:B:749:HOH:O	2.20	0.42
1:D:239:LYS:HA	1:D:239:LYS:HE2	2.01	0.42
1:B:181:ASP:OD1	1:B:183:ARG:HG2	2.19	0.42
1:A:409:THR:HG23	1:A:411:GLU:N	2.35	0.42
1:B:265:MET:HG3	1:B:318:LEU:HB3	2.02	0.42
1:D:344:MET:HB3	1:D:344:MET:HE3	1.64	0.42
1:D:237[B]:MET:HE2	1:D:237[B]:MET:HB2	1.98	0.41
1:C:265:MET:SD	1:C:326:LYS:HD2	2.61	0.41
1:C:344:MET:HE3	1:C:344:MET:HB3	1.76	0.41
1:A:440:LYS:HB2	1:A:443:LYS:HG3	2.03	0.40
1:B:443:LYS:HD3	1:B:443:LYS:HA	1.82	0.40
1:A:384:LEU:HB3	1:A:391:ARG:NH1	2.37	0.40
1:C:435:GLN:NE2	4:C:614:HOH:O	2.53	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	284/304 (93%)	279 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	275/304 (90%)	268 (98%)	6 (2%)	1 (0%)	30 16
1	C	286/304 (94%)	280 (98%)	6 (2%)	0	100 100
1	D	277/304 (91%)	273 (99%)	4 (1%)	0	100 100
All	All	1122/1216 (92%)	1100 (98%)	21 (2%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ASP

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	250/260 (96%)	249 (100%)	1 (0%)	89 85
1	B	244/260 (94%)	244 (100%)	0	100 100
1	C	251/260 (96%)	251 (100%)	0	100 100
1	D	246/260 (95%)	245 (100%)	1 (0%)	89 85
All	All	991/1040 (95%)	989 (100%)	2 (0%)	92 89

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

Mol	Chain	Res	Type
1	A	365	THR
1	D	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	306	HIS
1	A	438	HIS

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Mol	Chain	Res	Type
1	B	178	ASN
1	B	305	ASN
1	C	179	ASN
1	D	232	GLN
1	D	293	GLN
1	D	305	ASN
1	D	306	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	345	1	8,10,11	1.24	0	10,14,16	1.67	1 (10%)
1	TPO	D	345	1	8,10,11	1.21	0	10,14,16	1.50	1 (10%)
1	TPO	A	342	1	8,10,11	1.18	0	10,14,16	1.93	1 (10%)
1	SEP	B	346	1	8,9,10	1.62	1 (12%)	7,12,14	0.66	0
1	TPO	D	342	1	8,10,11	1.28	0	10,14,16	2.01	1 (10%)
1	TPO	B	342	1	8,10,11	1.23	0	10,14,16	1.74	1 (10%)
1	SEP	D	346	1	8,9,10	1.64	1 (12%)	7,12,14	0.98	0
1	SEP	A	346	1	8,9,10	1.63	1 (12%)	7,12,14	0.95	0
1	SEP	C	346	1	8,9,10	1.68	1 (12%)	7,12,14	0.85	0
1	TPO	A	345	1	8,10,11	1.09	0	10,14,16	1.80	1 (10%)
1	TPO	C	342	1	8,10,11	1.21	0	10,14,16	1.85	1 (10%)
1	TPO	B	345	1	8,10,11	1.20	0	10,14,16	1.67	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	A	342	1	-	4/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	D	342	1	-	2/9/11/13	-
1	TPO	B	342	1	-	2/9/11/13	-
1	SEP	D	346	1	-	5/6/8/10	-
1	SEP	A	346	1	-	3/6/8/10	-
1	SEP	C	346	1	-	5/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	2/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	346	SEP	P-O1P	3.67	1.61	1.50
1	D	346	SEP	P-O1P	3.59	1.61	1.50
1	A	346	SEP	P-O1P	3.56	1.61	1.50
1	B	346	SEP	P-O1P	3.51	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	342	TPO	P-OG1-CB	-5.87	107.37	123.33
1	A	342	TPO	P-OG1-CB	-5.62	108.06	123.33
1	C	342	TPO	P-OG1-CB	-5.26	109.04	123.33
1	B	342	TPO	P-OG1-CB	-4.89	110.03	123.33
1	A	345	TPO	P-OG1-CB	-4.62	110.78	123.33
1	B	345	TPO	P-OG1-CB	-4.45	111.24	123.33
1	C	345	TPO	P-OG1-CB	-4.25	111.77	123.33
1	D	345	TPO	P-OG1-CB	-3.84	112.89	123.33

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	342	TPO	N-CA-CB-OG1
1	A	342	TPO	C-CA-CB-CG2
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	CB-OG-P-O1P
1	A	346	SEP	CB-OG-P-O2P
1	B	342	TPO	C-CA-CB-CG2
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	346	SEP	N-CA-CB-OG
1	C	346	SEP	C-CA-CB-OG
1	C	346	SEP	CB-OG-P-O1P
1	C	346	SEP	CB-OG-P-O2P
1	C	346	SEP	CB-OG-P-O3P
1	D	342	TPO	C-CA-CB-CG2
1	D	345	TPO	N-CA-CB-OG1
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	D	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	D	346	SEP	CB-OG-P-O3P
1	C	342	TPO	C-CA-CB-CG2
1	D	346	SEP	CB-OG-P-O1P
1	A	342	TPO	CB-OG1-P-O3P
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CA-CB-OG1-P
1	C	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CA-CB-OG1-P
1	C	342	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	A	342	TPO	N-CA-CB-CG2
1	B	342	TPO	N-CA-CB-CG2
1	D	342	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	345	TPO	1	0
1	B	342	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
2	A1BWY	B	501	-	39,46,46	1.00	2 (5%)	48,67,67	1.50	9 (18%)
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.12	0
2	A1BWY	D	501	-	39,46,46	0.99	1 (2%)	48,67,67	1.39	6 (12%)
3	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.26	0
3	SO4	C	503	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	D	504	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	B	504	-	4,4,4	0.20	0	6,6,6	0.24	0
3	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	D	503	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.35	0
3	SO4	B	503	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	D	505	-	4,4,4	0.25	0	6,6,6	0.11	0
2	A1BWY	A	501	-	39,46,46	1.05	1 (2%)	48,67,67	1.65	8 (16%)
2	A1BWY	C	501	-	39,46,46	0.87	1 (2%)	48,67,67	1.61	8 (16%)
3	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.18	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
2	A1BWY	D	501	-	-	8/22/43/43	0/5/5/5
2	A1BWY	C	501	-	-	5/22/43/43	0/5/5/5
2	A1BWY	A	501	-	-	3/22/43/43	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1BWY	B	501	-	-	4/22/43/43	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1BWY	F19-C14	-3.15	1.34	1.40
2	A	501	A1BWY	F19-C14	-2.99	1.34	1.40
2	D	501	A1BWY	F19-C14	-2.78	1.35	1.40
2	C	501	A1BWY	F19-C14	-2.19	1.36	1.40
2	B	501	A1BWY	C26-N27	2.05	1.36	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	A1BWY	C21-C20-C11	5.19	111.02	107.61
2	C	501	A1BWY	C21-C20-C11	4.85	110.80	107.61
2	A	501	A1BWY	C21-C20-C11	4.49	110.56	107.61
2	A	501	A1BWY	F41-C40-F42	4.46	111.09	105.40
2	D	501	A1BWY	C21-C20-C11	4.33	110.46	107.61
2	A	501	A1BWY	F42-C40-N37	-3.98	104.95	109.62
2	C	501	A1BWY	C24-C25-C28	3.96	123.03	119.66
2	D	501	A1BWY	F41-C40-F42	3.87	110.35	105.40
2	C	501	A1BWY	F41-C40-F42	3.78	110.23	105.40
2	D	501	A1BWY	C06-N10-C12	-3.44	118.95	124.60
2	A	501	A1BWY	C31-C30-C12	-3.35	107.81	111.49
2	B	501	A1BWY	F41-C40-F42	3.33	109.66	105.40
2	B	501	A1BWY	F19-C14-C13	3.01	110.86	108.06
2	A	501	A1BWY	F41-C40-N37	-2.95	106.15	109.62
2	D	501	A1BWY	F41-C40-N37	-2.81	106.33	109.62
2	C	501	A1BWY	C26-C25-C28	-2.71	117.16	120.05
2	B	501	A1BWY	C31-C30-C12	-2.66	108.57	111.49
2	C	501	A1BWY	C01-C06-N10	-2.64	118.75	121.08
2	C	501	A1BWY	C34-C12-N10	-2.60	106.58	110.77
2	C	501	A1BWY	C31-C30-C12	-2.51	108.74	111.49
2	B	501	A1BWY	C24-C25-C26	2.44	120.27	118.13
2	B	501	A1BWY	C25-C24-C22	-2.32	118.02	120.39
2	B	501	A1BWY	C33-C34-C12	-2.30	108.97	111.49
2	B	501	A1BWY	C34-C12-N10	-2.30	107.07	110.77
2	C	501	A1BWY	C25-C24-C22	-2.29	118.05	120.39
2	A	501	A1BWY	C35-C36-N37	-2.24	104.90	107.59
2	B	501	A1BWY	C06-N10-C12	-2.14	121.08	124.60
2	A	501	A1BWY	C24-C25-C26	2.13	120.00	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	A1BWY	F42-C40-N37	-2.10	107.15	109.62
2	D	501	A1BWY	C34-C12-N10	-2.04	107.50	110.77
2	A	501	A1BWY	C24-C25-C28	2.04	121.39	119.66

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1BWY	N03-C04-C11-N23
2	B	501	A1BWY	N03-C04-C11-N23
2	C	501	A1BWY	N03-C04-C11-N23
2	D	501	A1BWY	N03-C04-C11-N23
2	A	501	A1BWY	C02-C01-C07-O09
2	C	501	A1BWY	C02-C01-C07-O09
2	B	501	A1BWY	C02-C01-C07-O09
2	D	501	A1BWY	C02-C01-C07-O09
2	A	501	A1BWY	C02-C01-C07-N08
2	C	501	A1BWY	C02-C01-C07-N08
2	D	501	A1BWY	C02-C01-C07-N08
2	D	501	A1BWY	C05-C04-C11-N23
2	D	501	A1BWY	C30-C12-N10-C06
2	D	501	A1BWY	C34-C12-N10-C06
2	B	501	A1BWY	C02-C01-C07-N08
2	C	501	A1BWY	N03-C04-C11-C20
2	D	501	A1BWY	N03-C04-C11-C20
2	C	501	A1BWY	C05-C04-C11-N23
2	B	501	A1BWY	N03-C04-C11-C20
2	D	501	A1BWY	C05-C04-C11-C20

There are no ring outliers.

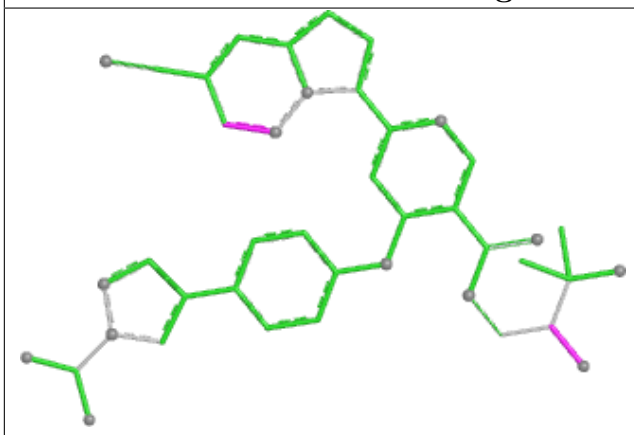
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	SO4	1	0
3	D	503	SO4	1	0
3	D	505	SO4	1	0

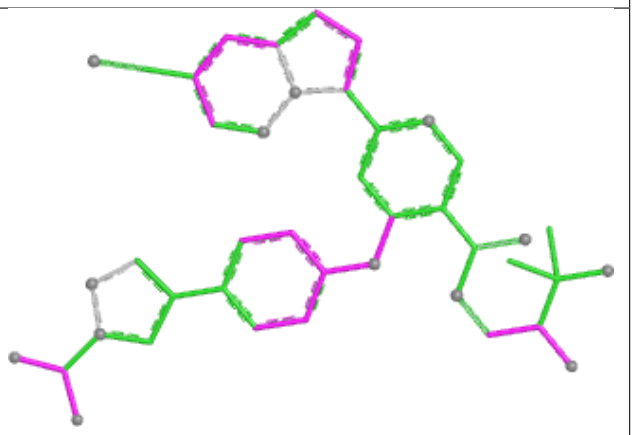
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

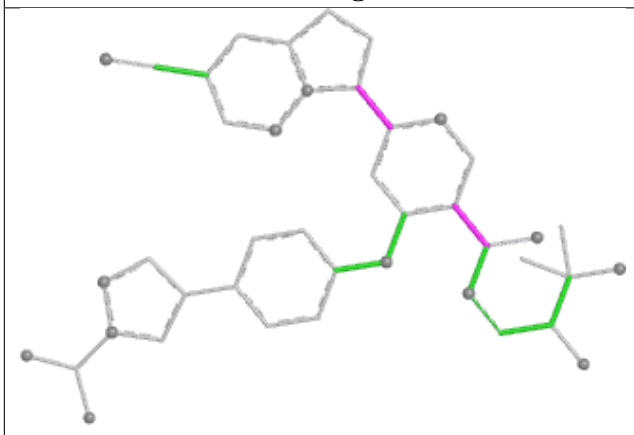
Ligand A1BWY B 501



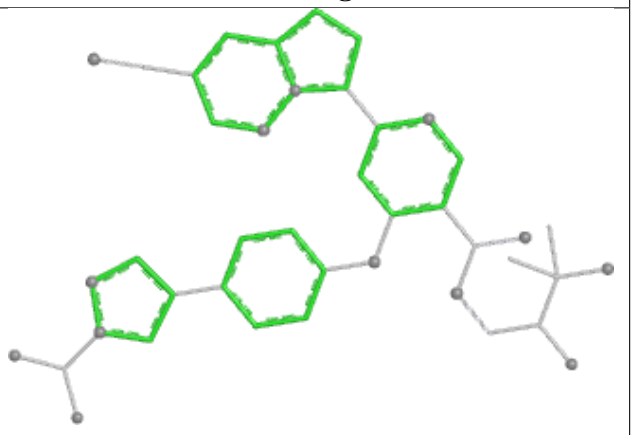
Bond lengths



Bond angles

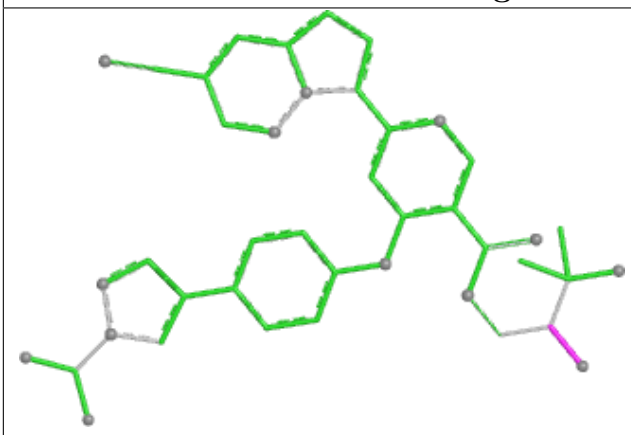


Torsions



Rings

Ligand A1BWY D 501



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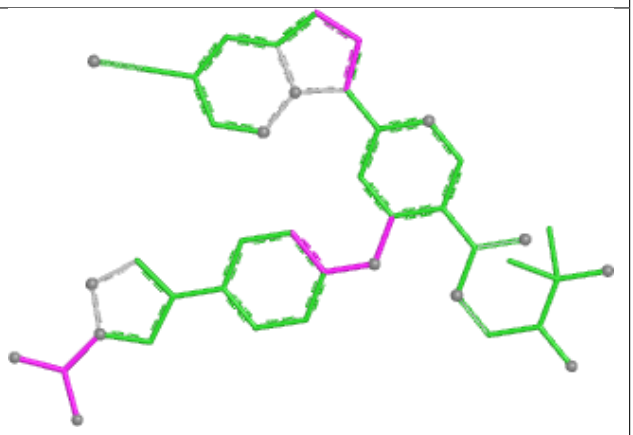
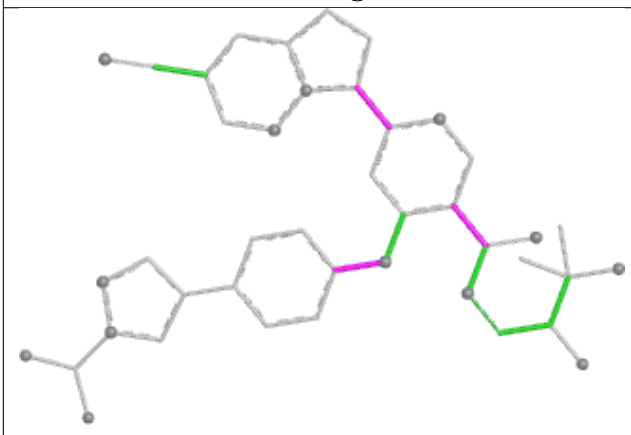


Bond angles



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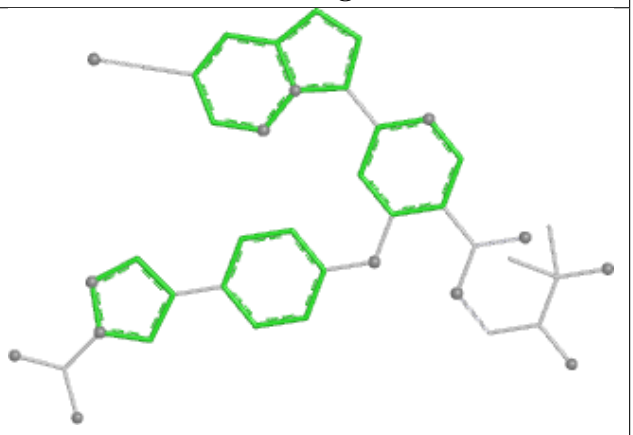
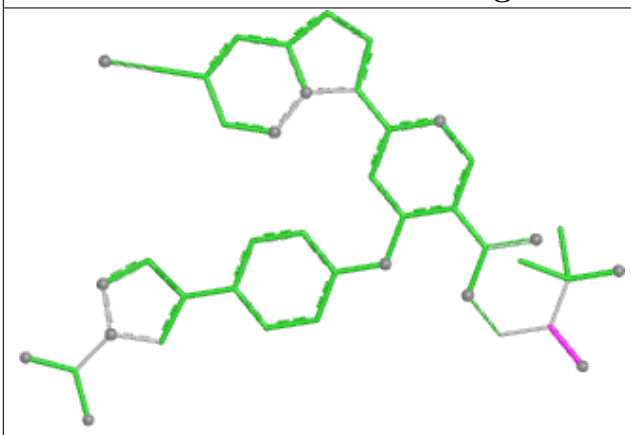
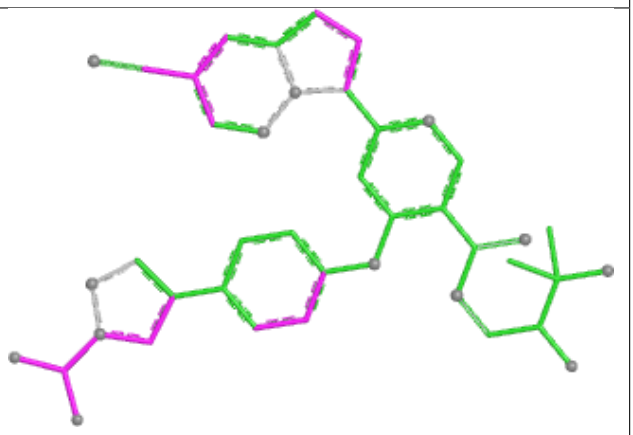


Rings

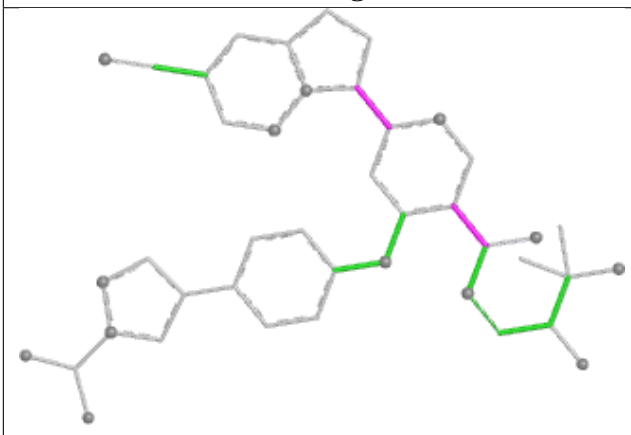
Ligand A1BWY A 501



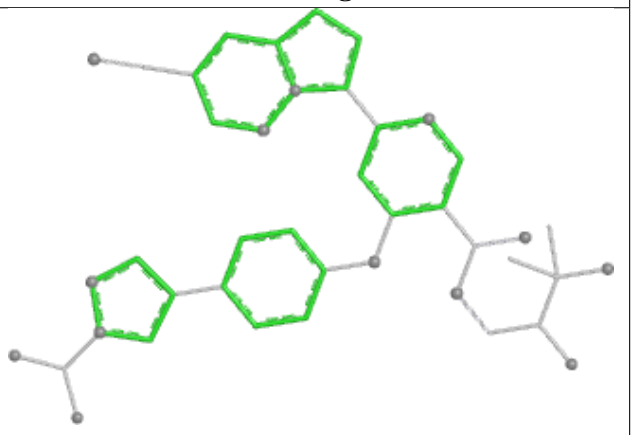
Bond lengths



Bond angles

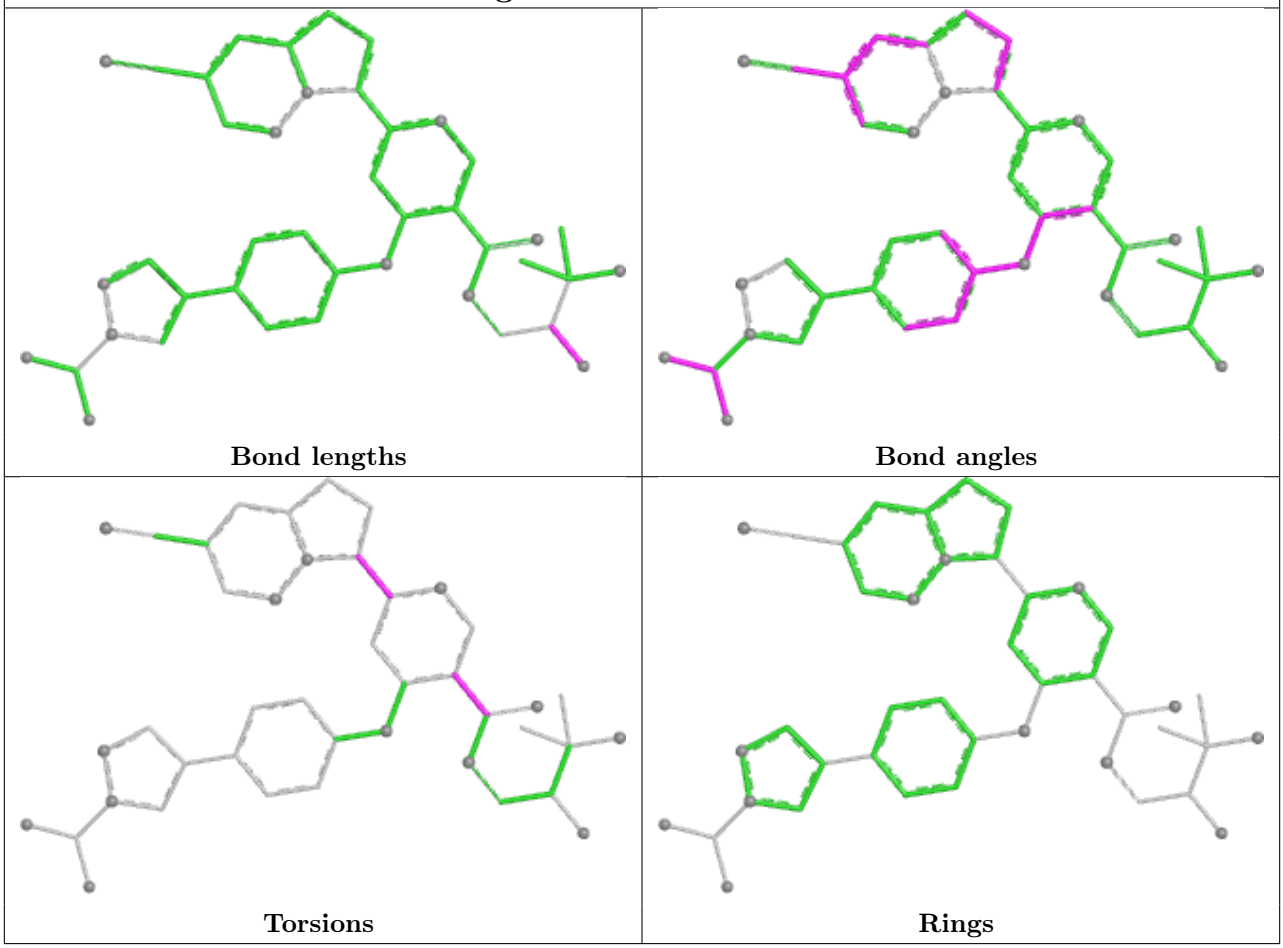


Torsions



Rings

Ligand A1BWY C 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, 95^{th} 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	288/304 (94%)	0.26	13 (4%)	39	46	19, 33, 66, 88	2 (0%)
1	B	281/304 (92%)	0.53	16 (5%)	30	37	22, 38, 67, 82	1 (0%)
1	C	288/304 (94%)	0.23	9 (3%)	51	59	15, 33, 64, 90	3 (1%)
1	D	282/304 (92%)	0.50	23 (8%)	19	24	20, 39, 70, 88	2 (0%)
All	All	1139/1216 (93%)	0.38	61 (5%)	32	39	15, 35, 67, 90	8 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	GLY	4.2
1	B	217	ALA	4.0
1	D	197	PHE	4.0
1	D	187	VAL	4.0
1	B	220	ASP	3.9
1	B	221	ILE	3.7
1	A	221	ILE	3.7
1	C	217	ALA	3.6
1	B	197	PHE	3.5
1	A	341	GLN	3.5
1	D	196	GLY	3.5
1	A	335	ALA	3.5
1	A	220	ASP	3.4
1	D	343	VAL	3.4
1	D	205	VAL	3.3
1	C	161	SER	3.2
1	C	336	SER	3.2
1	D	221	ILE	3.2
1	A	256	ASP	3.2
1	D	220	ASP	3.2
1	A	197	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	255	GLY	3.1
1	B	397	LEU	3.0
1	B	196	GLY	2.9
1	D	207	ASN	2.8
1	B	195	GLY	2.8
1	A	217	ALA	2.8
1	D	188	GLY	2.7
1	D	184	PRO	2.7
1	B	223	THR	2.6
1	A	403	ILE	2.6
1	D	185	ILE	2.6
1	D	344	MET	2.6
1	B	405	ASP	2.6
1	C	343	VAL	2.6
1	D	216	ALA	2.5
1	D	206	ASN	2.5
1	A	336	SER	2.5
1	A	343	VAL	2.5
1	C	220	ASP	2.5
1	D	397	LEU	2.4
1	D	405	ASP	2.4
1	B	179	ASN	2.2
1	C	163	THR	2.2
1	C	197	PHE	2.2
1	B	174	LYS	2.2
1	D	164	ARG	2.2
1	B	207	ASN	2.2
1	D	208	THR	2.2
1	A	347	ARG	2.1
1	D	347	ARG	2.1
1	C	455	GLN	2.1
1	B	215	LEU	2.1
1	B	337	GLU	2.1
1	A	410	ILE	2.1
1	A	196	GLY	2.1
1	B	189	GLY	2.1
1	D	171	TYR	2.1
1	D	458	THR	2.1
1	C	344	MET	2.0
1	D	222	THR	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, 95^{th} 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	TPO	C	342	11/12	0.57	0.20	61,83,103,110	0
1	TPO	B	342	11/12	0.75	0.19	58,76,84,90	0
1	TPO	A	342	11/12	0.78	0.17	72,74,87,88	0
1	TPO	D	342	11/12	0.79	0.17	52,65,77,85	0
1	SEP	D	346	10/11	0.81	0.13	53,73,82,88	0
1	SEP	A	346	10/11	0.82	0.12	55,67,92,99	0
1	SEP	C	346	10/11	0.83	0.13	51,60,80,92	0
1	SEP	B	346	10/11	0.84	0.11	58,66,86,96	0
1	TPO	B	345	11/12	0.92	0.11	48,56,66,67	0
1	TPO	A	345	11/12	0.92	0.10	46,54,64,65	0
1	TPO	D	345	11/12	0.93	0.10	41,52,67,68	0
1	TPO	C	345	11/12	0.93	0.09	44,51,61,61	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, 95^{th} 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	SO4	C	503	5/5	0.56	0.17	66,81,92,103	0
3	SO4	C	502	5/5	0.78	0.12	47,69,73,78	0
3	SO4	A	502	5/5	0.82	0.11	63,65,77,79	0
3	SO4	B	503	5/5	0.83	0.11	48,63,74,77	0
3	SO4	D	504	5/5	0.83	0.10	63,65,72,75	0
3	SO4	A	503	5/5	0.87	0.11	44,55,67,70	0
3	SO4	B	502	5/5	0.88	0.10	57,59,67,77	0
3	SO4	D	503	5/5	0.89	0.10	46,53,64,64	0
2	A1BWY	B	501	42/42	0.93	0.09	25,30,42,54	0
2	A1BWY	D	501	42/42	0.94	0.08	23,29,45,59	0

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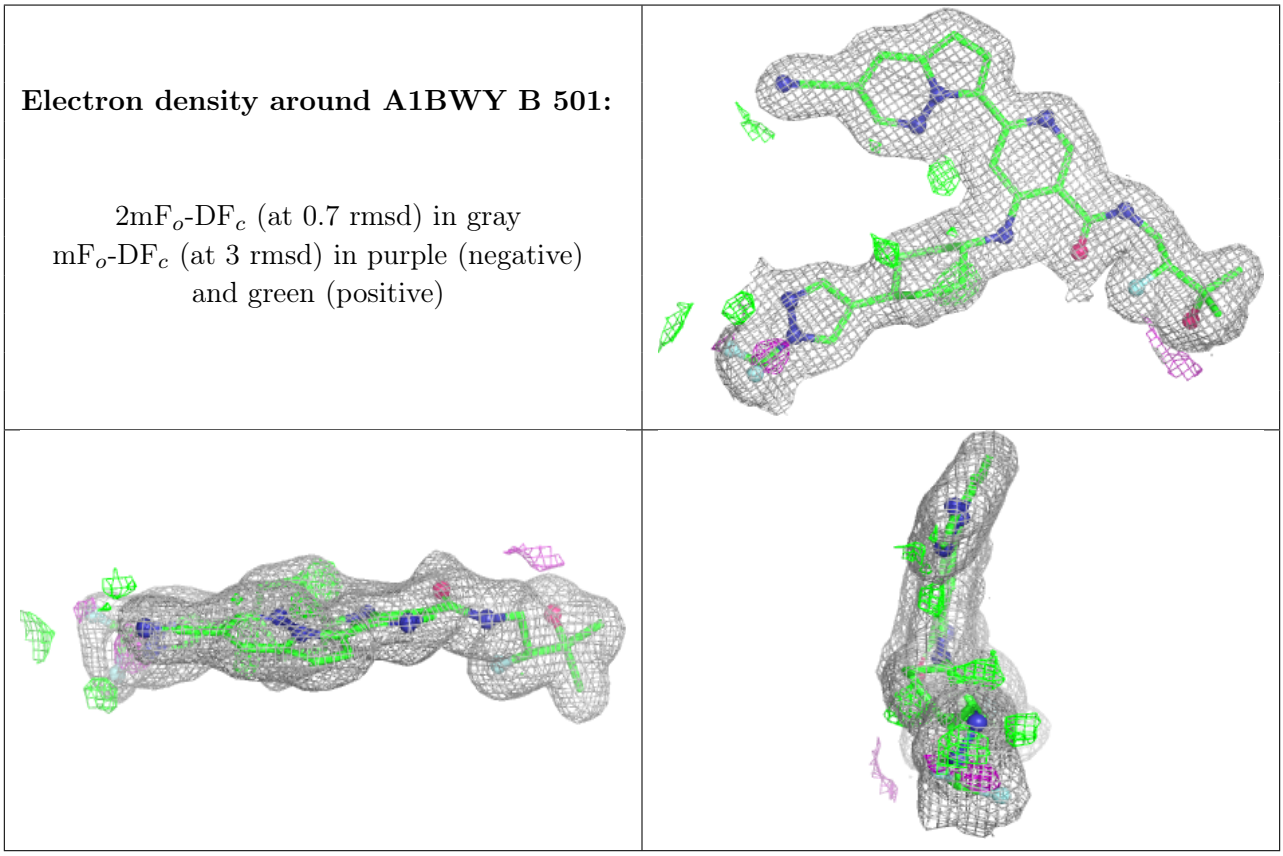
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	502	5/5	0.94	0.08	46,47,59,61	0
2	A1BWY	C	501	42/42	0.95	0.07	16,21,30,42	0
3	SO4	D	505	5/5	0.95	0.07	45,48,55,59	0
3	SO4	B	504	5/5	0.96	0.07	43,49,54,57	0
2	A1BWY	A	501	42/42	0.97	0.05	15,20,33,37	0

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.

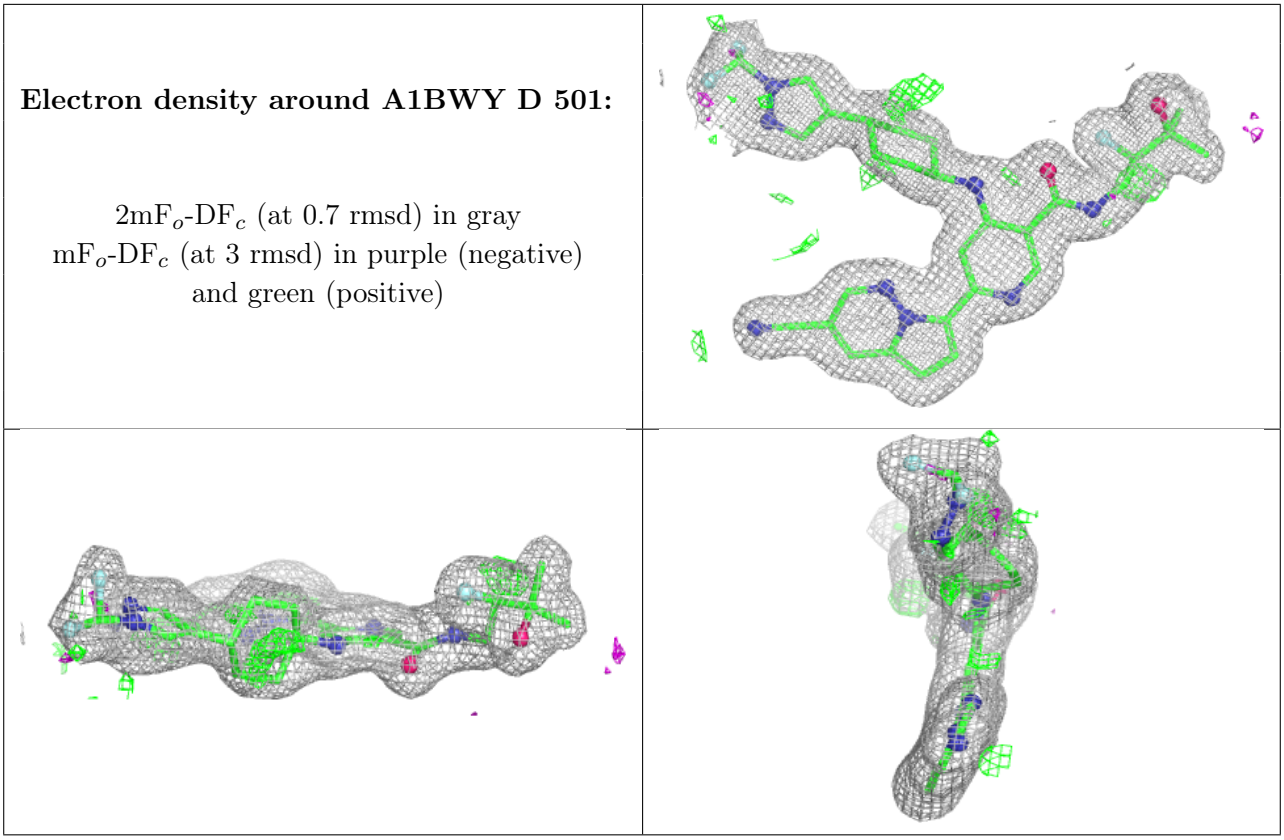
Electron density around A1BWY B 501:

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



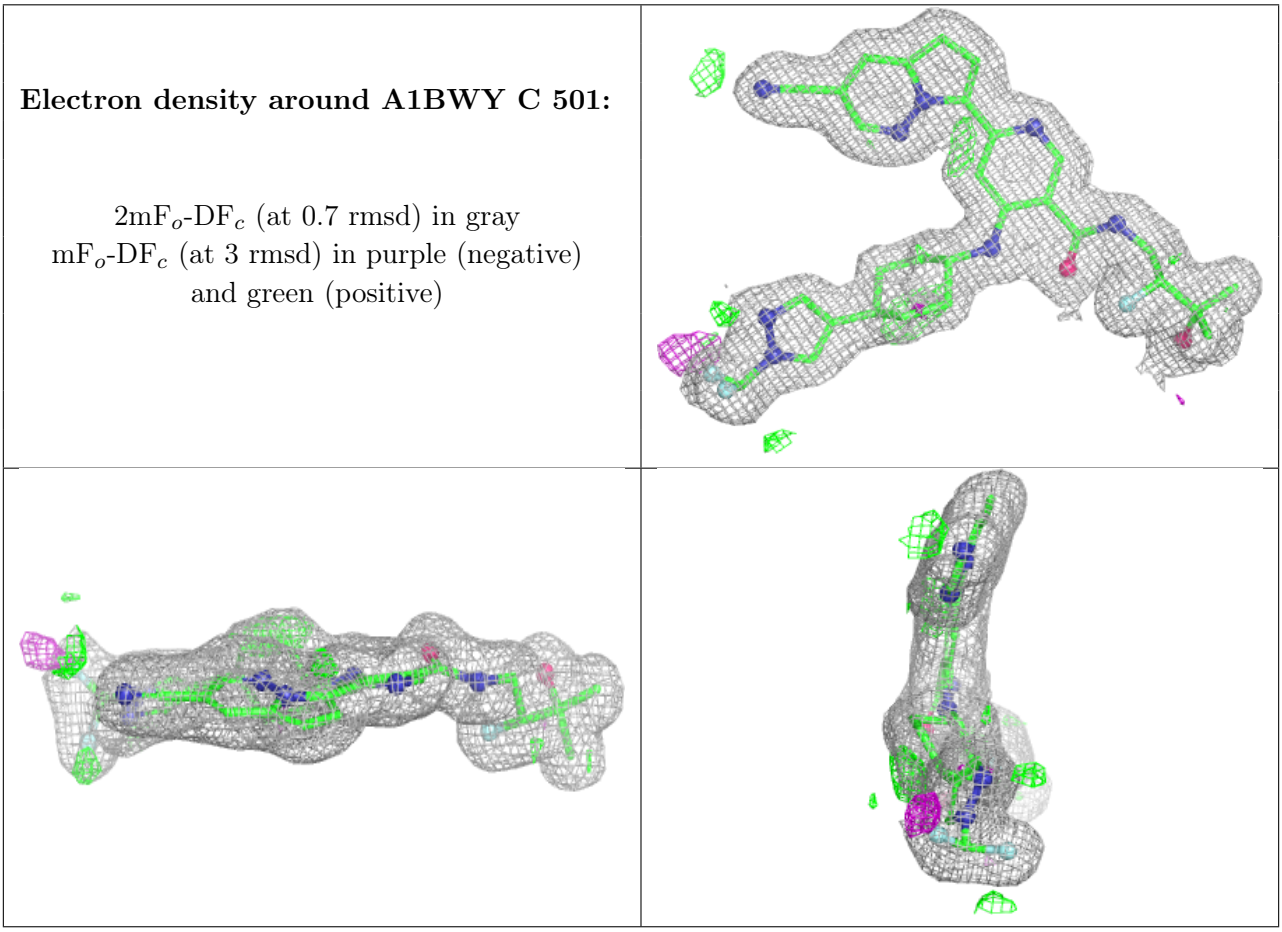
Electron density around A1BWY D 501:

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



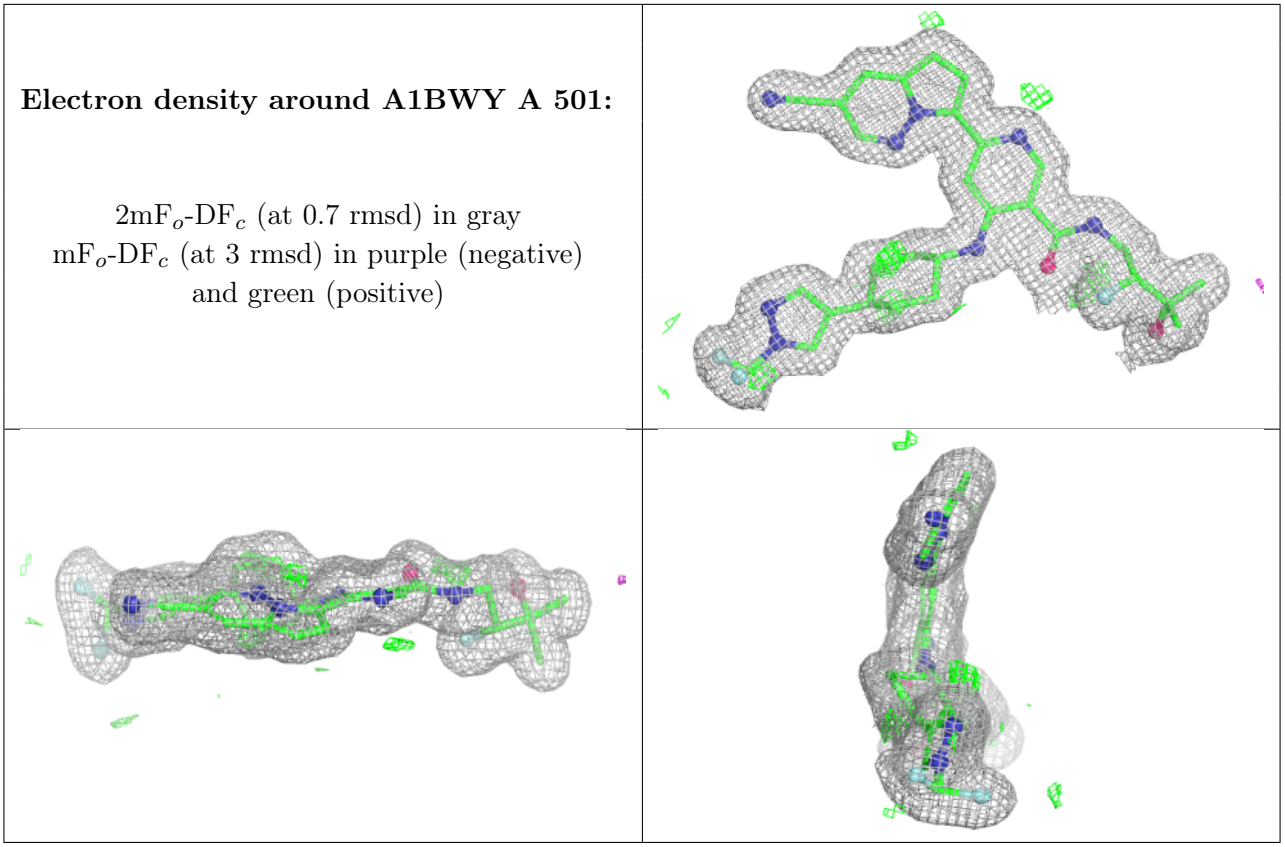
Electron density around A1BWY C 501:

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



Electron density around A1BWY 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.