



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 02:14 AM UTC

PDB ID : 5HIE / pdb_00005hie
Title : BRAF Kinase domain b3aC loop deletion mutant in complex with dabrafenib
Authors : Whalen, D.M.; Foster, S.A.; Ozen, A.; Wongchenko, M.; Yin, J.; Schaefer, G.; Mayfield, J.; Chmielecki, J.; Stephens, P.; Albacker, L.; Yan, Y.; Song, K.; Hatzivassiliou, G.; Eigenbrot, C.; Yu, C.; Shaw, A.S.; Manning, G.; Skelton, N.J.; Hymowitz, S.G.; Malek, S.
Deposited on : 2016-01-11
Resolution : 3.00 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](#) ①) 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

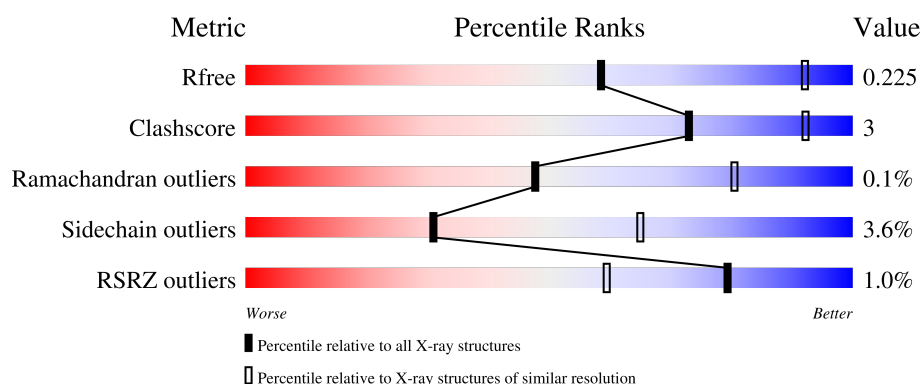
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	302	
1	B	302	
1	C	302	
1	D	302	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8400 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			2076	1332	365	366	13			
1	B	259	Total	C	N	O	S	0	0	0
			2074	1330	363	368	13			
1	C	253	Total	C	N	O	S	0	0	0
			2029	1303	353	360	13			
1	D	253	Total	C	N	O	S	0	1	0
			2032	1305	353	360	14			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	initiating methionine	UNP P15056
A	421	ASP	-	expression tag	UNP P15056
A	422	ARG	-	expression tag	UNP P15056
A	423	GLY	-	expression tag	UNP P15056
A	424	SER	-	expression tag	UNP P15056
A	425	HIS	-	expression tag	UNP P15056
A	426	HIS	-	expression tag	UNP P15056
A	427	HIS	-	expression tag	UNP P15056
A	428	HIS	-	expression tag	UNP P15056
A	429	HIS	-	expression tag	UNP P15056
A	430	HIS	-	expression tag	UNP P15056
A	431	GLY	-	expression tag	UNP P15056
A	?	-	ASN	deletion	UNP P15056
A	?	-	VAL	deletion	UNP P15056
A	?	-	THR	deletion	UNP P15056
A	?	-	ALA	deletion	UNP P15056
A	?	-	PRO	deletion	UNP P15056
B	420	MET	-	initiating methionine	UNP P15056
B	421	ASP	-	expression tag	UNP P15056
B	422	ARG	-	expression tag	UNP P15056
B	423	GLY	-	expression tag	UNP P15056

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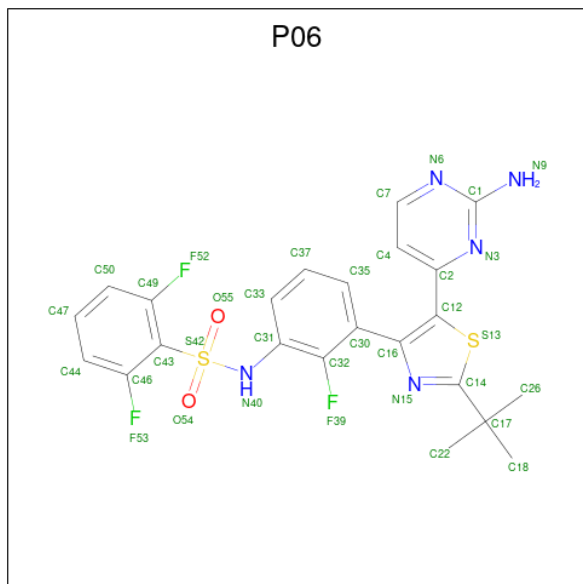
Chain	Residue	Modelled	Actual	Comment	Reference
B	424	SER	-	expression tag	UNP P15056
B	425	HIS	-	expression tag	UNP P15056
B	426	HIS	-	expression tag	UNP P15056
B	427	HIS	-	expression tag	UNP P15056
B	428	HIS	-	expression tag	UNP P15056
B	429	HIS	-	expression tag	UNP P15056
B	430	HIS	-	expression tag	UNP P15056
B	431	GLY	-	expression tag	UNP P15056
B	?	-	ASN	deletion	UNP P15056
B	?	-	VAL	deletion	UNP P15056
B	?	-	THR	deletion	UNP P15056
B	?	-	ALA	deletion	UNP P15056
B	?	-	PRO	deletion	UNP P15056
C	420	MET	-	initiating methionine	UNP P15056
C	421	ASP	-	expression tag	UNP P15056
C	422	ARG	-	expression tag	UNP P15056
C	423	GLY	-	expression tag	UNP P15056
C	424	SER	-	expression tag	UNP P15056
C	425	HIS	-	expression tag	UNP P15056
C	426	HIS	-	expression tag	UNP P15056
C	427	HIS	-	expression tag	UNP P15056
C	428	HIS	-	expression tag	UNP P15056
C	429	HIS	-	expression tag	UNP P15056
C	430	HIS	-	expression tag	UNP P15056
C	431	GLY	-	expression tag	UNP P15056
C	?	-	ASN	deletion	UNP P15056
C	?	-	VAL	deletion	UNP P15056
C	?	-	THR	deletion	UNP P15056
C	?	-	ALA	deletion	UNP P15056
C	?	-	PRO	deletion	UNP P15056
D	420	MET	-	initiating methionine	UNP P15056
D	421	ASP	-	expression tag	UNP P15056
D	422	ARG	-	expression tag	UNP P15056
D	423	GLY	-	expression tag	UNP P15056
D	424	SER	-	expression tag	UNP P15056
D	425	HIS	-	expression tag	UNP P15056
D	426	HIS	-	expression tag	UNP P15056
D	427	HIS	-	expression tag	UNP P15056
D	428	HIS	-	expression tag	UNP P15056
D	429	HIS	-	expression tag	UNP P15056
D	430	HIS	-	expression tag	UNP P15056
D	431	GLY	-	expression tag	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP P15056
D	?	-	VAL	deletion	UNP P15056
D	?	-	THR	deletion	UNP P15056
D	?	-	ALA	deletion	UNP P15056
D	?	-	PRO	deletion	UNP P15056

- Molecule 2 is Dabrafenib (CCD ID: P06) (formula: $C_{23}H_{20}F_3N_5O_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		
2	B	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		
2	C	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		
2	D	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	14	Total	O	0	0
			14	14		
3	C	6	Total	O	0	0
			6	6		

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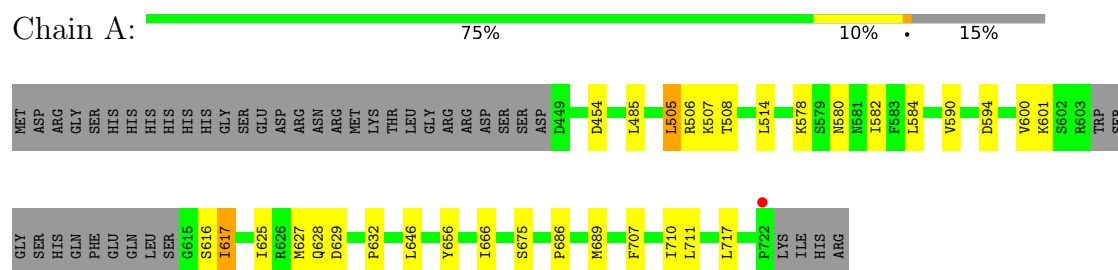
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	9	Total	O	0	0
			9	9		

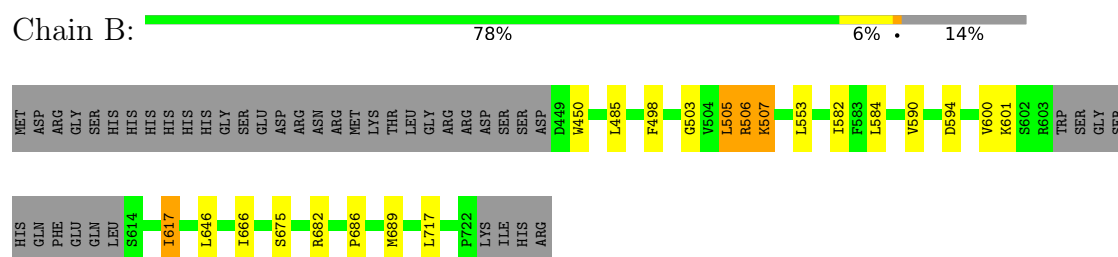
3 Residue-property plots

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.

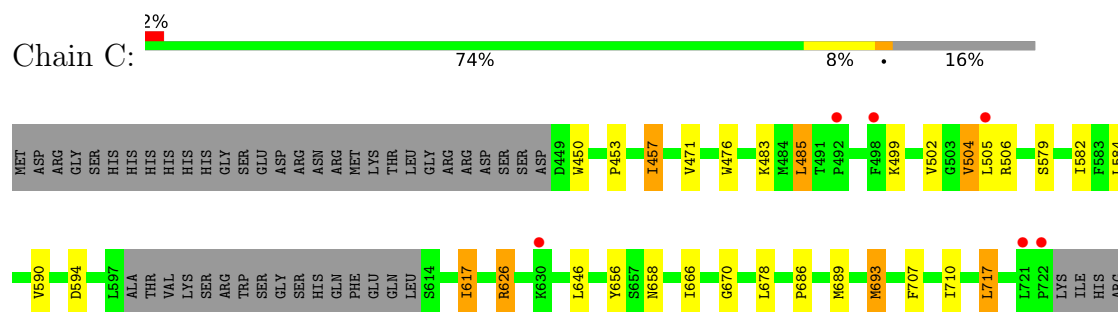
- Molecule 1: Serine/threonine-protein kinase B-raf



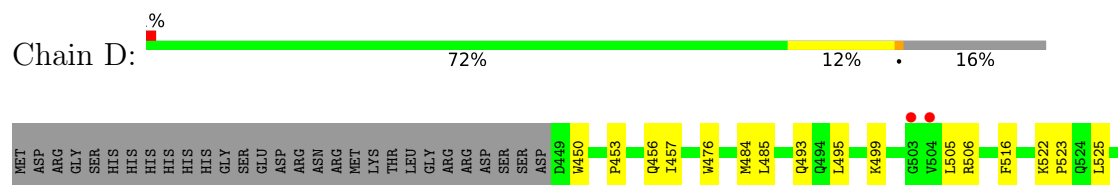
- Molecule 1: Serine/threonine-protein kinase B-raf

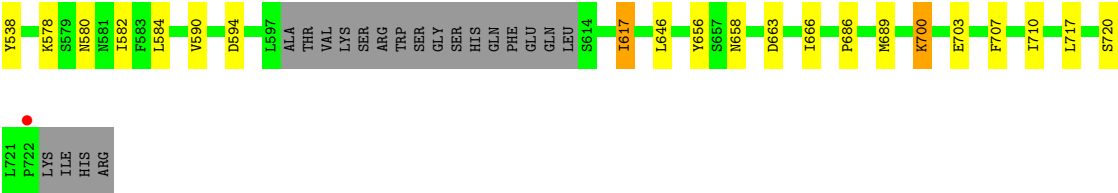


- Molecule 1: Serine/threonine-protein kinase B-raf



- Molecule 1: Serine/threonine-protein kinase B-raf





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.41Å 127.79Å 83.14Å 90.00° 105.79° 90.00°	Depositor
Resolution (Å)	35.28 – 3.00 35.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.28-3.00) 97.9 (35.28-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.194 , 0.221 0.199 , 0.225	Depositor DCC
R_{free} test set	1305 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8400	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P06

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	0.74	0/2123	1.34	8/2861 (0.3%)
1	B	0.74	0/2118	1.29	2/2855 (0.1%)
1	C	0.76	1/2073 (0.0%)	1.36	4/2795 (0.1%)
1	D	0.75	0/2079	1.34	3/2803 (0.1%)
All	All	0.75	1/8393 (0.0%)	1.33	17/11314 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	693	MET	SD-CE	-5.87	1.64	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	507	LYS	N-CA-C	6.29	118.13	111.28
1	C	453	PRO	CA-C-N	6.18	128.89	120.54
1	C	453	PRO	C-N-CA	6.18	128.89	120.54
1	D	663	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	506	ARG	CA-C-N	5.54	127.71	120.28
1	A	506	ARG	C-N-CA	5.54	127.71	120.28
1	B	506	ARG	CA-C-N	5.45	131.95	121.54
1	B	506	ARG	C-N-CA	5.45	131.95	121.54
1	A	508	THR	CA-C-N	5.38	131.81	121.54
1	A	508	THR	C-N-CA	5.38	131.81	121.54
1	A	628	GLN	N-CA-C	-5.37	106.69	113.18
1	D	700	LYS	CA-C-N	5.30	127.70	120.54
1	D	700	LYS	C-N-CA	5.30	127.70	120.54
1	A	454	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	717	LEU	CA-C-N	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	717	LEU	C-N-CA	5.03	127.02	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2076	0	2128	13	0
1	B	2074	0	2120	12	0
1	C	2029	0	2068	15	0
1	D	2032	0	2073	17	0
2	A	35	0	20	3	0
2	B	35	0	20	1	0
2	C	35	0	20	2	0
2	D	35	0	20	2	0
3	A	20	0	0	1	0
3	B	14	0	0	0	0
3	C	6	0	0	0	0
3	D	9	0	0	0	0
All	All	8400	0	8469	54	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 3.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:TRP:HE1	1:C:506:ARG:HE	1.20	0.89
1:C:594:ASP:H	2:C:801:P06:H17	1.27	0.81
1:A:627:MET:HG3	1:A:632:PRO:HG3	1.73	0.69
1:B:594:ASP:H	2:B:801:P06:H17	1.43	0.67
1:D:594:ASP:H	2:D:801:P06:H17	1.41	0.66
1:A:594:ASP:H	2:A:801:P06:H17	1.44	0.64
1:C:626:ARG:HD2	1:C:670:GLY:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:TRP:CD1	1:B:506:ARG:HD3	2.36	0.60
1:D:495:LEU:HD22	1:D:525:LEU:HD21	1.86	0.58
1:A:617:ILE:HD13	1:A:666:ILE:HG13	1.90	0.54
1:C:457:ILE:HD12	1:C:476:TRP:HB2	1.90	0.53
1:D:617:ILE:HD13	1:D:666:ILE:HG13	1.90	0.53
1:D:522:LYS:HA	1:D:523:PRO:C	2.33	0.53
1:C:678:LEU:HG	1:C:693:MET:CE	2.40	0.52
1:B:617:ILE:HD13	1:B:666:ILE:HG13	1.90	0.52
1:C:617:ILE:HD13	1:C:666:ILE:HG13	1.91	0.52
1:B:646:LEU:HD22	1:B:689:MET:HE1	1.91	0.52
1:D:516:PHE:HB2	2:D:801:P06:H19	1.92	0.51
1:A:675:SER:O	1:D:658:ASN:HB2	2.12	0.50
1:D:495:LEU:HG	1:D:499:LYS:HE2	1.93	0.50
1:B:498:PHE:HE2	1:B:505:LEU:HD13	1.77	0.50
1:B:503:GLY:O	1:B:507:LYS:HB2	2.12	0.50
1:D:646:LEU:HD22	1:D:689:MET:HE1	1.92	0.49
1:D:538:TYR:HB3	1:D:580:ASN:HD22	1.78	0.48
1:A:505:LEU:HD23	2:A:801:P06:H20	1.96	0.48
1:A:646:LEU:HD22	1:A:689:MET:HE1	1.95	0.48
1:C:646:LEU:HD22	1:C:689:MET:HE1	1.96	0.47
1:B:582:ILE:HG23	1:B:590:VAL:HG13	1.97	0.46
1:A:582:ILE:HG23	1:A:590:VAL:HG13	1.97	0.46
1:A:686:PRO:HG2	1:A:717:LEU:HD21	1.98	0.46
1:C:678:LEU:HG	1:C:693:MET:HE2	1.97	0.46
1:C:582:ILE:HG23	1:C:590:VAL:HG13	1.98	0.45
1:C:707:PHE:HA	1:C:710:ILE:HB	2.00	0.44
1:B:686:PRO:HG2	1:B:717:LEU:HD21	1.99	0.44
1:D:686:PRO:HG2	1:D:717:LEU:HD21	1.99	0.44
1:A:514:LEU:HD11	2:A:801:P06:H2	1.99	0.44
1:D:582:ILE:HG23	1:D:590:VAL:HG13	1.99	0.43
1:D:450:TRP:HE1	1:D:506:ARG:HD2	1.84	0.43
1:C:483:LYS:HG2	1:C:485:LEU:HD23	1.99	0.43
1:A:707:PHE:HA	1:A:710:ILE:HB	1.99	0.42
1:B:553:LEU:HD11	1:B:682:ARG:NH2	2.34	0.42
1:C:471:VAL:HG21	2:C:801:P06:N15	2.35	0.42
1:C:686:PRO:HG2	1:C:717:LEU:HD21	2.02	0.42
1:D:453:PRO:HB2	1:D:456:GLN:HG3	2.02	0.41
1:A:616:SER:HA	3:A:912:HOH:O	2.19	0.41
1:B:498:PHE:CE2	1:B:505:LEU:HD13	2.54	0.41
1:D:700:LYS:HE2	1:D:703:GLU:HG2	2.02	0.41
1:A:601:LYS:NZ	1:B:601:LYS:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:MET:HE1	1:D:523:PRO:HD2	2.03	0.40
1:B:675:SER:O	1:C:658:ASN:HB2	2.21	0.40
1:C:502:VAL:HG12	1:C:504:VAL:HG23	2.02	0.40
1:D:457:ILE:HD12	1:D:476:TRP:HB2	2.02	0.40
1:D:707:PHE:HA	1:D:710:ILE:HB	2.03	0.40
1:A:625:ILE:HG23	1:A:666:ILE:HG23	2.04	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	255/302 (84%)	248 (97%)	7 (3%)	0	100	100
1	B	255/302 (84%)	243 (95%)	11 (4%)	1 (0%)	30	65
1	C	249/302 (82%)	238 (96%)	11 (4%)	0	100	100
1	D	250/302 (83%)	241 (96%)	9 (4%)	0	100	100
All	All	1009/1208 (84%)	970 (96%)	38 (4%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	507	LYS

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	228/267 (85%)	219 (96%)	9 (4%)	28	62
1	B	228/267 (85%)	223 (98%)	5 (2%)	45	74
1	C	223/267 (84%)	213 (96%)	10 (4%)	24	59
1	D	224/267 (84%)	216 (96%)	8 (4%)	31	65
All	All	903/1068 (85%)	871 (96%)	32 (4%)	31	65

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

Mol	Chain	Res	Type
1	A	485	LEU
1	A	505	LEU
1	A	578	LYS
1	A	580	ASN
1	A	584	LEU
1	A	600	VAL
1	A	617	ILE
1	A	656	TYR
1	A	711	LEU
1	B	485	LEU
1	B	505	LEU
1	B	584	LEU
1	B	600	VAL
1	B	617	ILE
1	C	457	ILE
1	C	485	LEU
1	C	499	LYS
1	C	504	VAL
1	C	505	LEU
1	C	579	SER
1	C	584	LEU
1	C	617	ILE
1	C	626	ARG
1	C	656	TYR
1	D	485	LEU
1	D	493	GLN
1	D	505	LEU
1	D	578	LYS
1	D	584	LEU
1	D	617	ILE
1	D	656	TYR

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Mol	Chain	Res	Type
1	D	720	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	581	ASN
1	A	628	GLN
1	A	631	ASN
1	B	500	ASN
1	B	581	ASN
1	B	631	ASN
1	C	494	GLN
1	C	540	HIS
1	C	581	ASN
1	C	664	GLN
1	C	709	GLN
1	D	456	GLN
1	D	562	GLN
1	D	580	ASN
1	D	581	ASN
1	D	628	GLN
1	D	631	ASN
1	D	664	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	P06	D	801	-	38,38,38	1.09	2 (5%)	52,58,58	2.63	21 (40%)
2	P06	B	801	-	38,38,38	1.15	4 (10%)	52,58,58	2.66	17 (32%)
2	P06	C	801	-	38,38,38	1.11	3 (7%)	52,58,58	2.58	18 (34%)
2	P06	A	801	-	38,38,38	1.08	2 (5%)	52,58,58	2.53	18 (34%)

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	P06	D	801	-	-	2/25/25/25	0/4/4/4
2	P06	B	801	-	-	1/25/25/25	0/4/4/4
2	P06	C	801	-	-	3/25/25/25	0/4/4/4
2	P06	A	801	-	-	2/25/25/25	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	P06	C16-N15	-3.67	1.32	1.38
2	B	801	P06	C16-N15	-3.38	1.33	1.38
2	A	801	P06	C16-N15	-3.18	1.33	1.38
2	D	801	P06	C16-N15	-3.14	1.33	1.38
2	A	801	P06	C1-N9	2.63	1.39	1.33
2	C	801	P06	C1-N9	2.58	1.39	1.33
2	B	801	P06	C1-N9	2.52	1.38	1.33
2	D	801	P06	C1-N9	2.49	1.38	1.33
2	B	801	P06	S42-N40	2.36	1.67	1.63
2	B	801	P06	C16-C12	2.26	1.39	1.37
2	C	801	P06	C16-C12	2.09	1.39	1.37

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	P06	C16-N15-C14	9.19	119.59	110.55
2	C	801	P06	C16-N15-C14	9.06	119.46	110.55
2	A	801	P06	C16-N15-C14	8.78	119.19	110.55
2	D	801	P06	C16-N15-C14	8.58	118.99	110.55
2	D	801	P06	C2-N3-C1	7.51	121.91	116.37
2	B	801	P06	C2-N3-C1	7.28	121.74	116.37
2	C	801	P06	C2-N3-C1	6.63	121.26	116.37
2	A	801	P06	C7-N6-C1	5.87	122.05	116.21
2	B	801	P06	C7-N6-C1	5.77	121.95	116.21
2	C	801	P06	C7-N6-C1	5.76	121.94	116.21
2	A	801	P06	C2-N3-C1	5.61	120.51	116.37
2	D	801	P06	C7-N6-C1	5.25	121.43	116.21
2	A	801	P06	S13-C14-N15	-5.10	108.53	116.12
2	B	801	P06	S13-C14-N15	-4.81	108.95	116.12
2	C	801	P06	S13-C14-N15	-4.77	109.01	116.12
2	C	801	P06	N6-C1-N3	-4.64	120.53	125.70
2	B	801	P06	N6-C1-N3	-4.59	120.59	125.70
2	D	801	P06	S13-C14-N15	-4.57	109.31	116.12
2	D	801	P06	C4-C2-N3	-4.57	117.59	122.92
2	B	801	P06	C12-C16-N15	-4.52	112.73	115.43
2	D	801	P06	N6-C1-N3	-4.46	120.74	125.70
2	A	801	P06	C12-C16-N15	-4.32	112.84	115.43
2	A	801	P06	N6-C1-N3	-4.27	120.94	125.70
2	D	801	P06	C12-C16-N15	-4.23	112.90	115.43
2	A	801	P06	C4-C7-N6	-4.22	118.80	123.97
2	C	801	P06	C12-C16-N15	-4.20	112.92	115.43
2	B	801	P06	C4-C7-N6	-4.16	118.87	123.97
2	B	801	P06	C4-C2-N3	-4.16	118.07	122.92
2	C	801	P06	C4-C2-N3	-4.02	118.23	122.92
2	D	801	P06	C4-C7-N6	-3.71	119.42	123.97
2	C	801	P06	C4-C7-N6	-3.66	119.49	123.97
2	C	801	P06	C32-C31-N40	-3.56	116.61	120.73
2	A	801	P06	C4-C2-N3	-3.39	118.96	122.92
2	D	801	P06	C32-C31-N40	-3.03	117.23	120.73
2	C	801	P06	C12-C2-N3	2.83	118.96	115.20
2	B	801	P06	C7-C4-C2	2.82	118.75	117.02
2	B	801	P06	C16-C12-S13	-2.80	106.09	109.72
2	B	801	P06	N9-C1-N6	2.75	120.25	117.40
2	B	801	P06	C43-S42-N40	-2.74	103.41	106.66
2	A	801	P06	C32-C31-N40	-2.66	117.66	120.73
2	A	801	P06	F52-C49-C43	2.65	122.44	118.93
2	D	801	P06	C17-C14-S13	2.61	125.88	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	P06	C17-C14-S13	2.59	125.84	121.51
2	C	801	P06	C16-C12-S13	-2.58	106.37	109.72
2	D	801	P06	C7-C4-C2	2.58	118.60	117.02
2	A	801	P06	C7-C4-C2	2.56	118.59	117.02
2	B	801	P06	C32-C31-N40	-2.53	117.81	120.73
2	D	801	P06	O55-S42-C43	-2.51	105.09	108.74
2	D	801	P06	C44-C46-C43	-2.43	119.71	123.50
2	A	801	P06	C18-C17-C14	2.40	112.48	109.24
2	B	801	P06	O55-S42-O54	2.37	122.39	119.52
2	A	801	P06	C43-S42-N40	-2.37	103.85	106.66
2	D	801	P06	N9-C1-N6	2.36	119.84	117.40
2	C	801	P06	F52-C49-C43	2.34	122.02	118.93
2	B	801	P06	C18-C17-C14	2.32	112.37	109.24
2	C	801	P06	N9-C1-N3	2.31	120.68	117.22
2	A	801	P06	C50-C49-C43	-2.29	119.92	123.50
2	D	801	P06	C2-C12-S13	2.29	122.37	118.24
2	D	801	P06	F52-C49-C43	2.29	121.95	118.93
2	A	801	P06	C17-C14-S13	2.28	125.33	121.51
2	D	801	P06	C12-C2-N3	2.27	118.22	115.20
2	A	801	P06	C16-C12-S13	-2.26	106.78	109.72
2	C	801	P06	C7-C4-C2	2.24	118.39	117.02
2	D	801	P06	C50-C49-C43	-2.22	120.03	123.50
2	A	801	P06	C22-C17-C14	2.19	112.19	109.24
2	D	801	P06	C16-C12-S13	-2.16	106.92	109.72
2	C	801	P06	C50-C49-C43	-2.15	120.14	123.50
2	B	801	P06	C50-C49-C43	-2.13	120.17	123.50
2	B	801	P06	C17-C14-S13	2.13	125.07	121.51
2	D	801	P06	C22-C17-C14	2.07	112.03	109.24
2	D	801	P06	C49-C43-C46	2.07	119.42	115.00
2	C	801	P06	F53-C46-C43	2.05	121.64	118.93
2	A	801	P06	C12-C2-N3	2.04	117.91	115.20
2	C	801	P06	C30-C16-C12	2.03	130.62	127.54

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	P06	N15-C14-C17-C18
2	C	801	P06	N15-C14-C17-C22
2	C	801	P06	N15-C14-C17-C26
2	D	801	P06	N15-C14-C17-C22
2	A	801	P06	C12-C16-C30-C35

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Mol	Chain	Res	Type	Atoms
2	A	801	P06	C31-N40-S42-O54
2	B	801	P06	C12-C16-C30-C32
2	D	801	P06	C12-C16-C30-C32

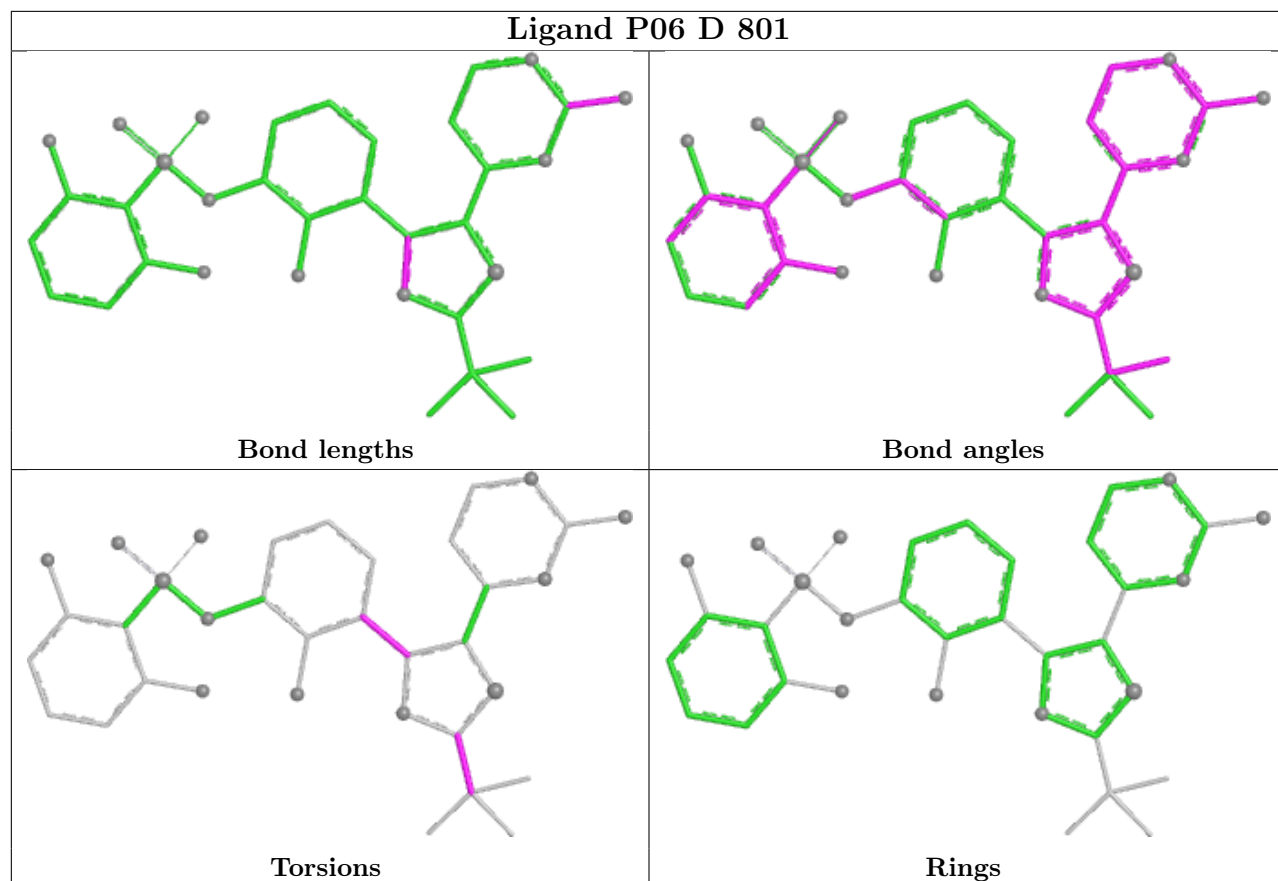
There are no ring outliers.

4 monomers are involved in 8 short contacts:

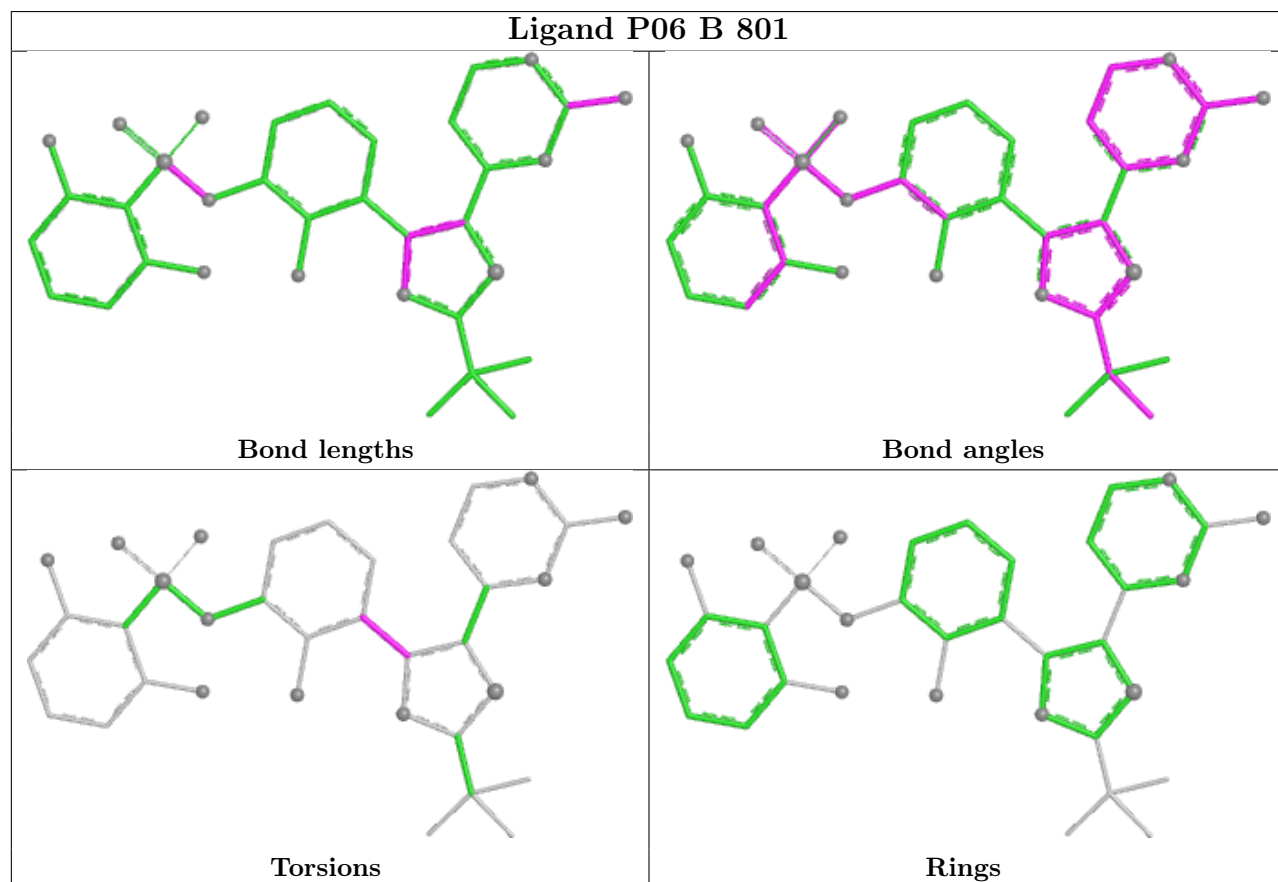
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	P06	2	0
2	B	801	P06	1	0
2	C	801	P06	2	0
2	A	801	P06	3	0

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.

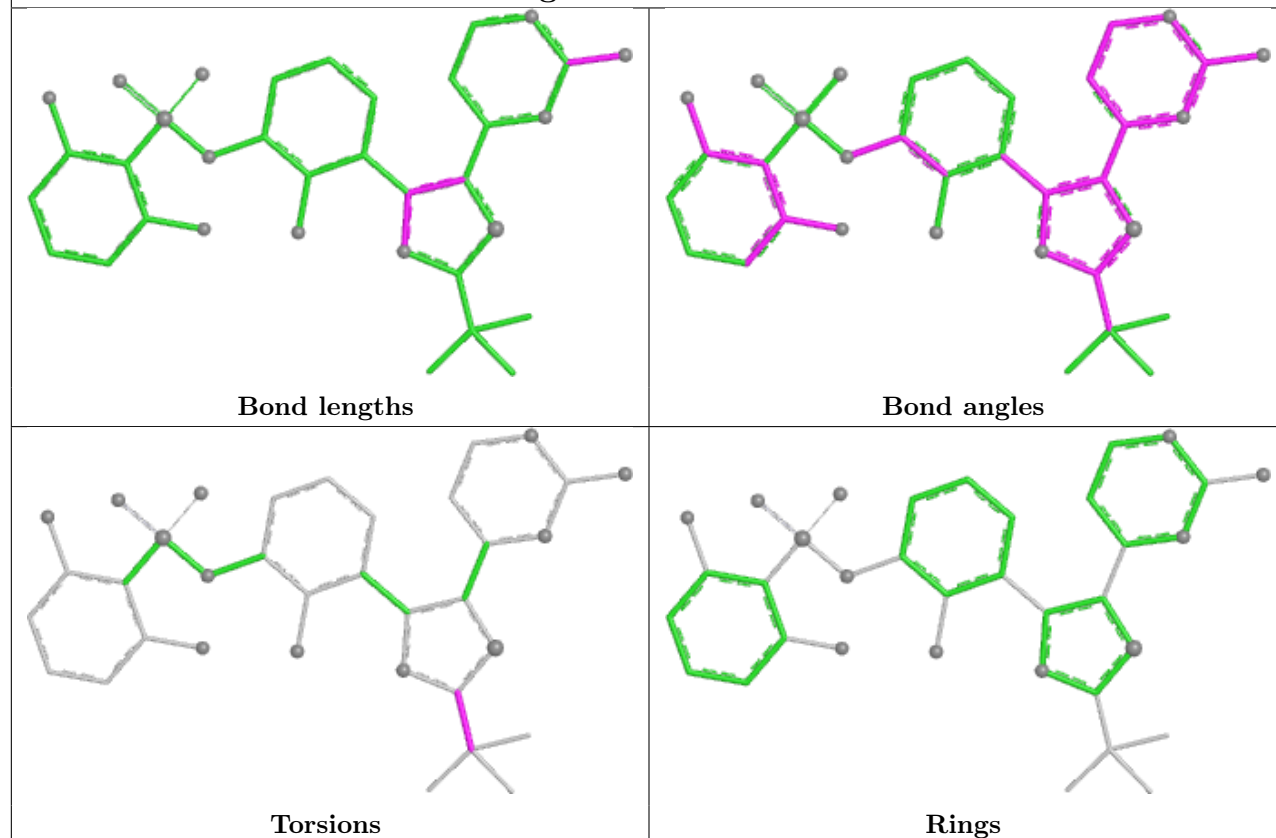
Ligand P06 D 801



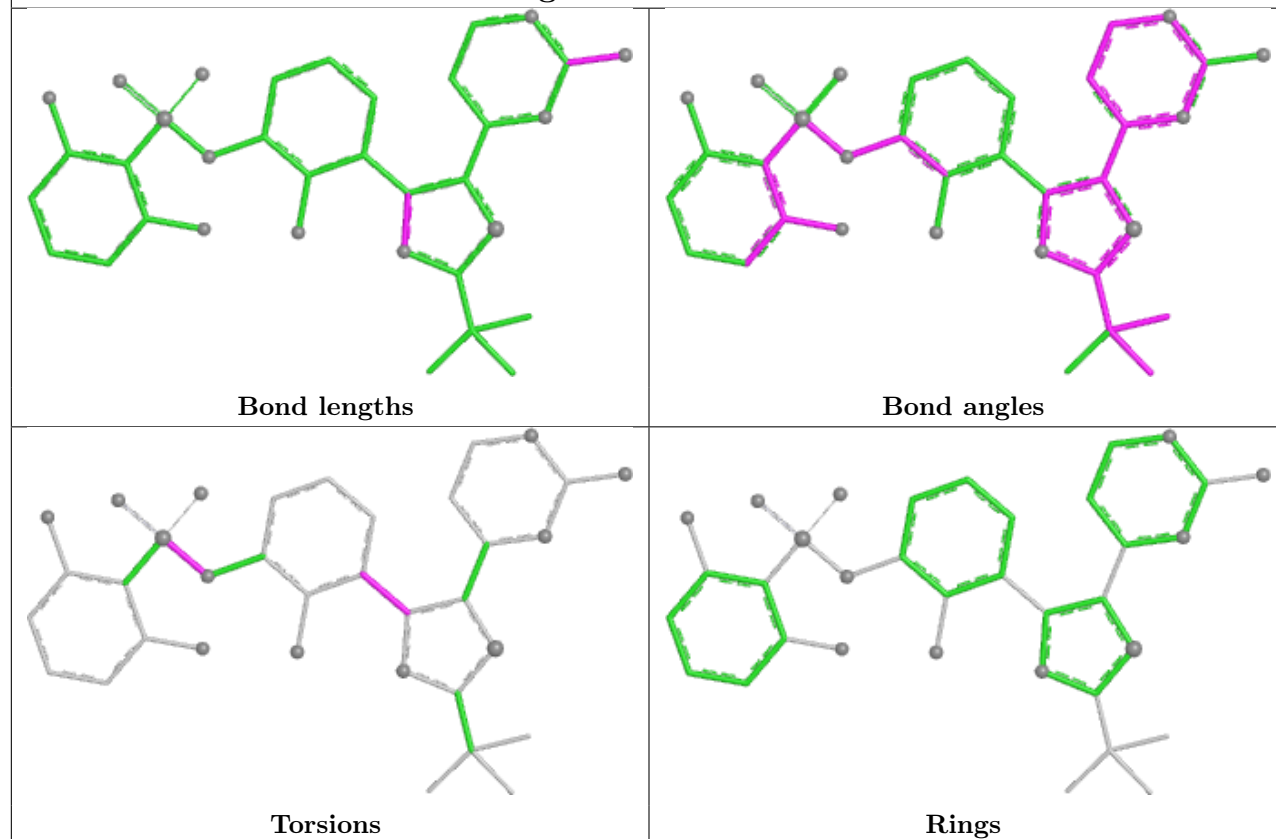
Ligand P06 B 801



Ligand P06 C 801



Ligand P06 A 801



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	258/302 (85%)	-0.40	1 (0%) 88 76	23, 43, 73, 114	1 (0%)
1	B	259/302 (85%)	-0.35	0 100 100	29, 43, 79, 120	0
1	C	253/302 (83%)	0.21	6 (2%) 59 36	36, 72, 120, 138	0
1	D	253/302 (83%)	-0.11	3 (1%) 76 55	32, 51, 93, 125	1 (0%)
All	All	1023/1208 (84%)	-0.16	10 (0%) 79 59	23, 51, 104, 138	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	505	LEU	3.5
1	A	722	PRO	2.8
1	C	722	PRO	2.4
1	D	722	PRO	2.3
1	C	492	PRO	2.2
1	D	503	GLY	2.2
1	D	504	VAL	2.1
1	C	498	PHE	2.1
1	C	721	LEU	2.1
1	C	630	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

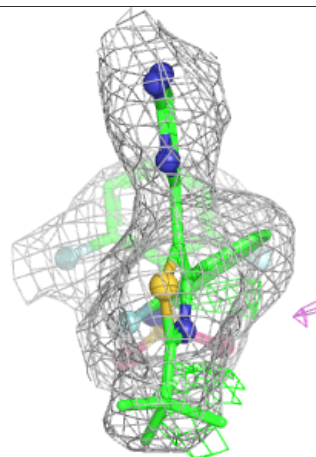
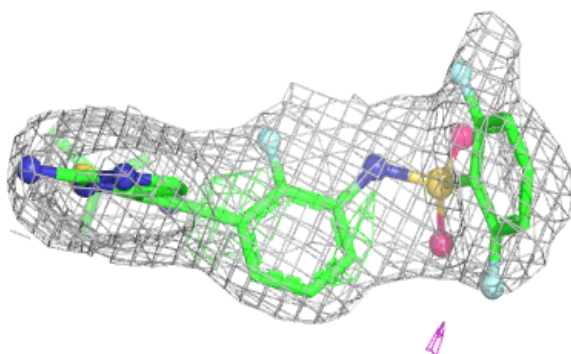
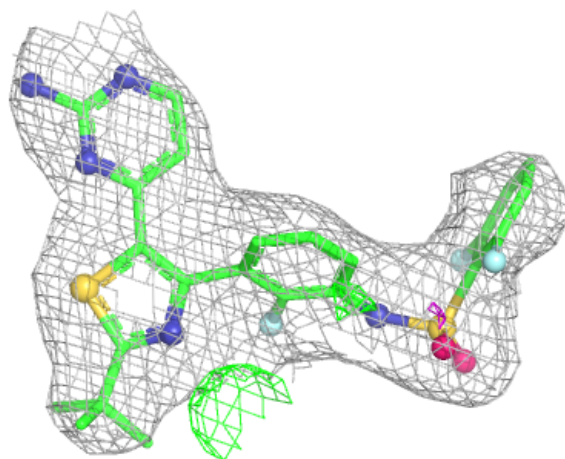
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P06	C	801	35/35	0.93	0.10	50,54,65,68	0
2	P06	A	801	35/35	0.97	0.07	24,34,40,41	0
2	P06	D	801	35/35	0.97	0.06	27,34,40,41	0
2	P06	B	801	35/35	0.98	0.05	27,33,37,40	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.

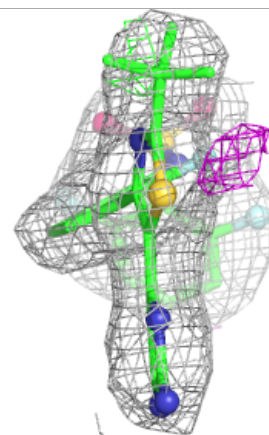
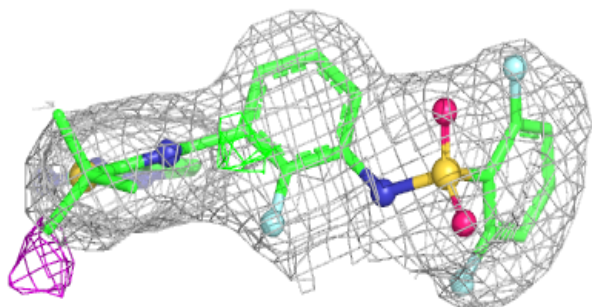
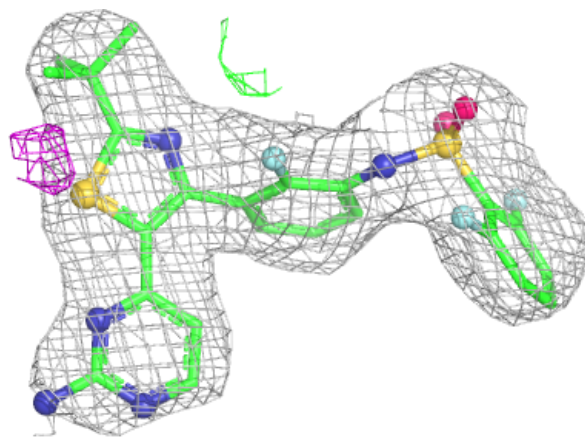
Electron density around P06 C 801:

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



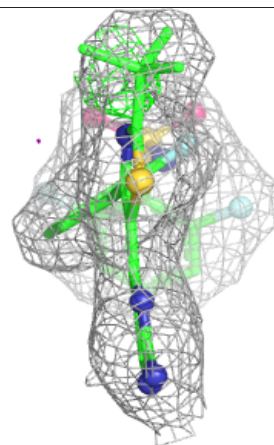
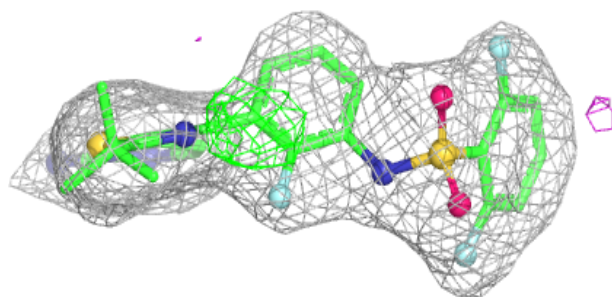
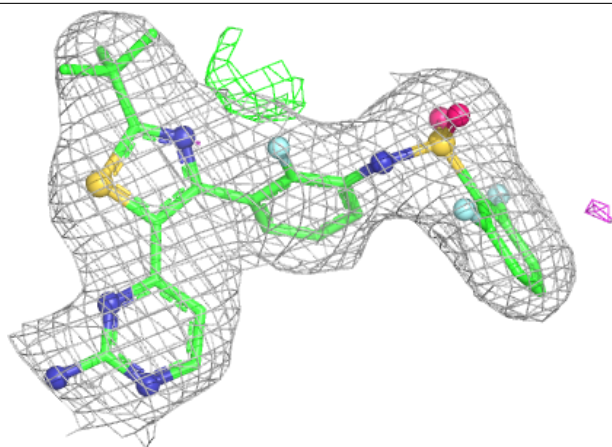
Electron density around P06 A 801:

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



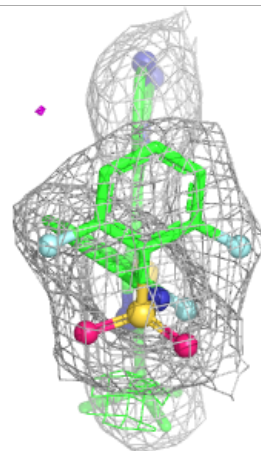
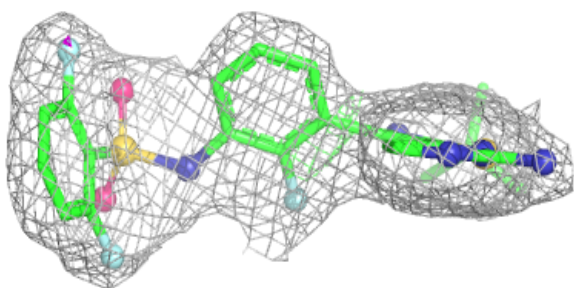
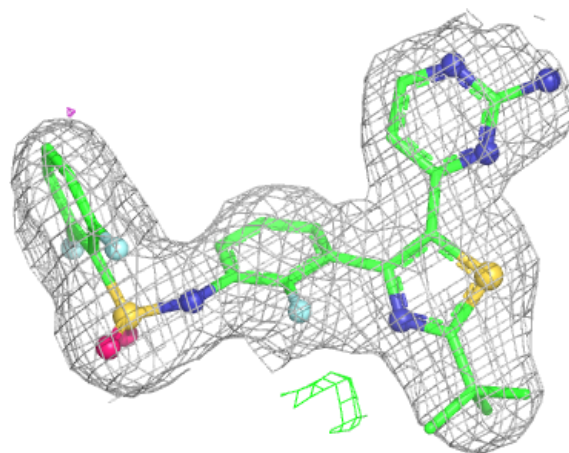
Electron density around P06 D 801:

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



Electron density around P06 B 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.