Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:23 PM BST

PDB ID	:	4EWH
Title	:	Co-crystal structure of ACK1 with inhibitor
Authors	:	Liu, J.; Walker, N.; Wang, Z.
Deposited on	:	2012-04-27
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

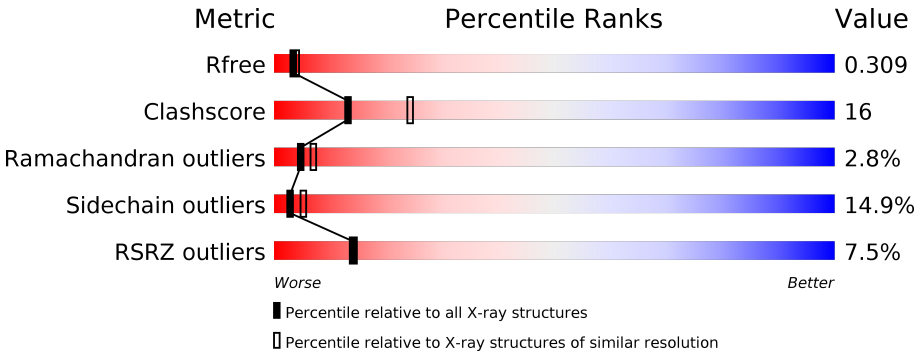
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	275	7% 63% 26% 11%
1	B	275	8% 60% 29% 9% .

2 Entry composition

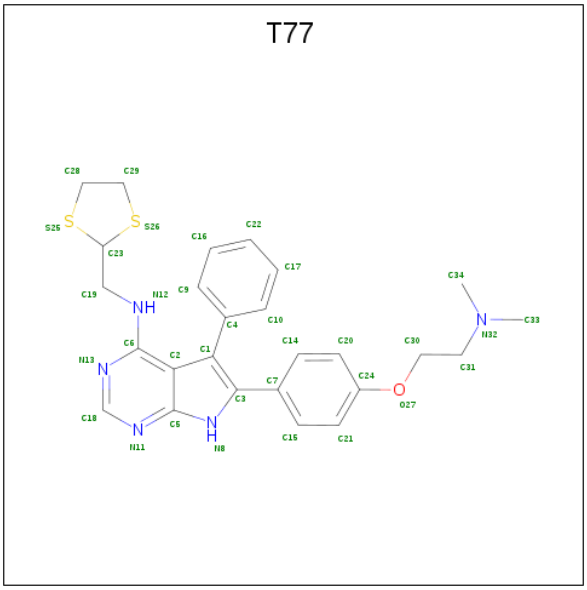
There are 3 unique types of molecules in this entry. The entry contains 4502 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Activated CDC42 kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	274	Total	C	N	O	P	S	0	0	0
			2202	1401	390	395	1	15			
1	A	275	Total	C	N	O	P	S	0	0	0
			2209	1405	391	397	1	15			

- Molecule 2 is 6-{4-[2-(dimethylamino)ethoxy]phenyl}-N-(1,3-dithiolan-2-ylmethyl)-5-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-amine (three-letter code: T77) (formula: $C_{26}H_{29}N_5OS_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			34	26	5	1	2		
2	A	1	Total	C	N	O	S	0	0
			34	26	5	1	2		

- Molecule 3 is water.

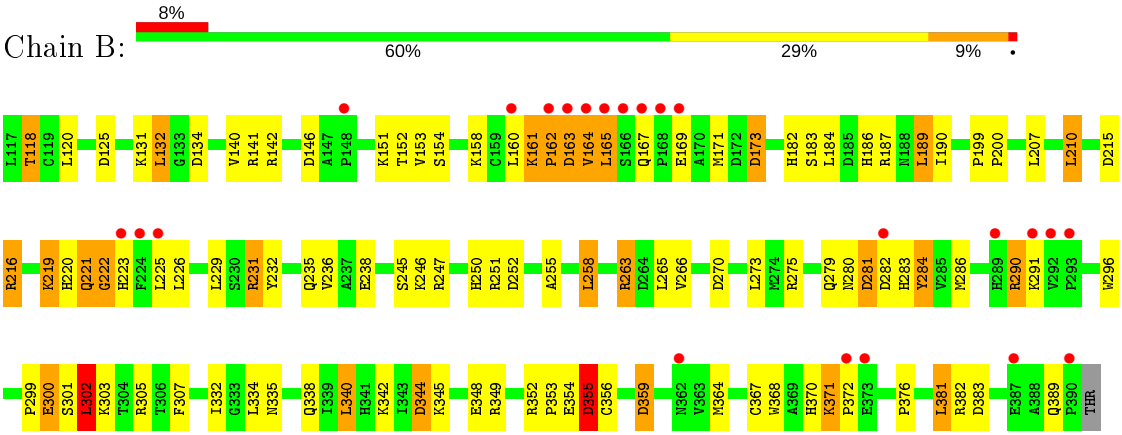
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	16	Total O 16 16	0	0
3	A	7	Total O 7 7	0	0

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.

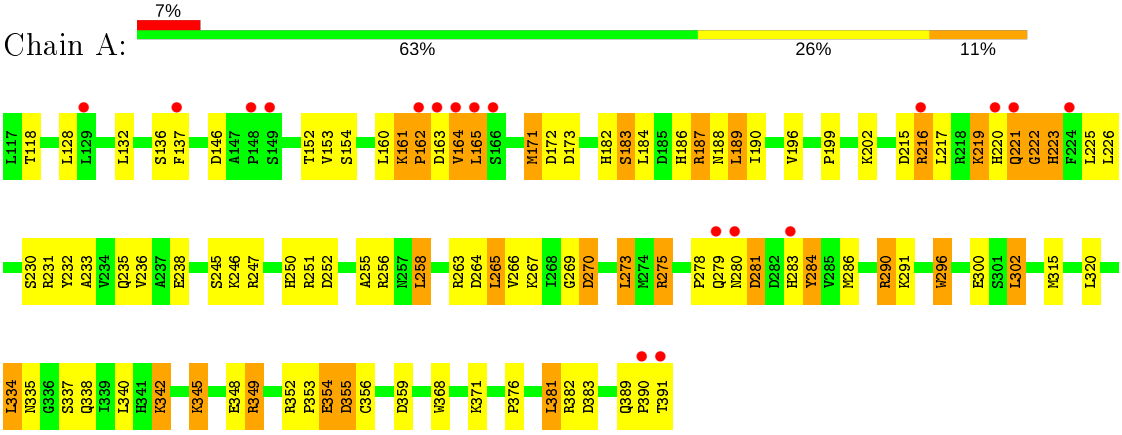
- Molecule 1: Activated CDC42 kinase 1

Chain B:



- Molecule 1: Activated CDC42 kinase 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	201.20Å 42.48Å 71.03Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50 60.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (100.00-2.50) 99.7 (60.46-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.256 , 0.313 0.251 , 0.309	Depositor DCC
R_{free} test set	1083 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: T77, PTR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	2/2245 (0.1%)	1.05	11/3038 (0.4%)
1	B	0.93	1/2238 (0.0%)	1.06	14/3028 (0.5%)
All	All	0.92	3/4483 (0.1%)	1.05	25/6066 (0.4%)

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	A	0	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	TRP	CE3-CZ3	5.08	1.47	1.38
1	A	300	GLU	CD-OE1	-5.02	1.20	1.25
1	B	296	TRP	CE3-CZ3	5.01	1.47	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	134	ASP	CB-CG-OD2	7.04	124.63	118.30
1	A	383	ASP	CB-CG-OD2	6.87	124.49	118.30
1	B	383	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	344	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	125	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	281	ASP	CB-CG-OD2	6.39	124.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	355	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	282	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	273	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	349	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	146	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	349	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	281	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	264	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	340	LEU	CA-CB-CG	5.80	128.65	115.30
1	B	210	LEU	CB-CG-CD1	5.74	120.76	111.00
1	A	215	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	359	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	173	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	302	LEU	CB-CG-CD2	-5.56	101.54	111.00
1	A	355	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	146	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	172	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	215	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	270	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	GLN	Peptide
1	B	163	ASP	Peptide
1	B	389	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2202	67	1
1	B	2202	0	2195	75	1
2	A	34	0	29	4	0
2	B	34	0	29	5	0
3	A	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	0	1	0
All	All	4502	0	4455	146	1

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 16.

All (146) 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:235:GLN:HE21	1:A:266:VAL:HG12	1.34	0.92
1:A:186:HIS:HD2	1:A:188:ASN:H	1.17	0.92
1:B:235:GLN:NE2	1:B:266:VAL:HG12	1.87	0.89
1:B:216:ARG:CG	1:B:216:ARG:HH11	1.87	0.88
1:B:235:GLN:HE21	1:B:266:VAL:HG12	1.37	0.86
1:A:118:THR:HG21	1:A:182:HIS:CD2	2.14	0.83
1:A:235:GLN:NE2	1:A:266:VAL:HG12	1.93	0.83
1:B:118:THR:HG21	1:B:182:HIS:CD2	2.15	0.80
1:A:251:ARG:NH1	1:A:284:PTR:HE2	1.95	0.80
1:A:186:HIS:CD2	1:A:188:ASN:H	2.01	0.78
1:B:216:ARG:HG2	1:B:216:ARG:HH11	1.48	0.78
1:A:250:HIS:HD2	1:A:252:ASP:H	1.34	0.75
1:A:335:ASN:H	1:A:338:GLN:HE21	1.33	0.75
1:B:160:LEU:HG	1:B:162:PRO:HD3	1.70	0.74
1:A:118:THR:HG21	1:A:182:HIS:HD2	1.54	0.73
1:B:342:LYS:HE2	1:B:348:GLU:OE2	1.90	0.72
1:A:232:TYR:O	1:A:236:VAL:HG23	1.90	0.71
1:A:251:ARG:HH12	1:A:284:PTR:HE2	1.52	0.71
1:A:160:LEU:HG	1:A:162:PRO:HD3	1.74	0.70
1:B:349:ARG:NH1	1:B:368:TRP:O	2.25	0.70
1:A:161:LYS:N	1:A:162:PRO:HD3	2.08	0.69
1:A:186:HIS:HB3	1:A:189:LEU:HD22	1.73	0.69
1:B:161:LYS:N	1:B:162:PRO:HD3	2.07	0.68
1:A:182:HIS:O	1:A:183:SER:CB	2.41	0.68
1:A:216:ARG:HH11	1:A:216:ARG:CG	2.07	0.67
1:A:279:GLN:NE2	1:A:279:GLN:HA	2.09	0.67
1:A:349:ARG:NH1	1:A:368:TRP:O	2.28	0.67
1:B:250:HIS:HE1	1:B:270:ASP:O	1.77	0.67
1:B:299:PRO:O	1:B:300:GLU:C	2.33	0.67
1:B:216:ARG:NH1	1:B:216:ARG:HG2	2.11	0.66
1:A:247:ARG:NH1	1:A:278:PRO:O	2.23	0.66
1:B:118:THR:HG21	1:B:182:HIS:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLN:NE2	1:B:279:GLN:HA	2.09	0.65
1:B:376:PRO:HB2	1:B:381:LEU:HD13	1.77	0.65
1:B:171:MET:CE	1:A:171:MET:CE	2.73	0.65
1:B:335:ASN:H	1:B:338:GLN:HE21	1.43	0.64
1:B:186:HIS:HB3	1:B:189:LEU:HD22	1.80	0.63
1:A:163:ASP:C	1:A:165:LEU:H	2.00	0.63
1:A:250:HIS:CD2	1:A:252:ASP:H	2.16	0.62
1:B:302:LEU:HB3	1:B:340:LEU:HD13	1.82	0.61
2:B:401:T77:C4	2:B:401:T77:H15	2.30	0.61
1:B:160:LEU:HG	1:B:162:PRO:CD	2.30	0.61
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.66	0.60
1:B:171:MET:HE2	1:A:171:MET:CE	2.32	0.60
2:B:401:T77:H15	2:B:401:T77:C9	2.32	0.60
2:A:401:T77:H15	2:A:401:T77:C4	2.31	0.60
1:A:160:LEU:HG	1:A:162:PRO:CD	2.31	0.59
1:A:182:HIS:O	1:A:183:SER:HB3	2.02	0.59
1:A:251:ARG:NH1	1:A:284:PTR:CE2	2.63	0.59
1:B:344:ASP:OD2	1:B:370:HIS:HE1	1.85	0.59
1:B:250:HIS:HD2	1:B:252:ASP:H	1.50	0.59
1:A:342:LYS:HE2	1:A:348:GLU:OE2	2.02	0.59
1:B:163:ASP:C	1:B:165:LEU:H	2.07	0.58
1:B:275:ARG:CZ	1:B:284:PTR:HE1	2.34	0.58
1:A:118:THR:CG2	1:A:182:HIS:CD2	2.87	0.57
1:A:246:LYS:O	1:A:247:ARG:HB2	2.03	0.57
1:B:120:LEU:HB2	1:A:118:THR:HG23	1.85	0.57
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.69	0.57
1:A:163:ASP:C	1:A:165:LEU:N	2.57	0.57
1:A:221:GLN:O	1:A:222:GLY:C	2.43	0.56
1:A:335:ASN:H	1:A:338:GLN:NE2	2.01	0.56
1:B:184:LEU:HB2	3:B:509:HOH:O	2.06	0.56
1:B:182:HIS:O	1:B:183:SER:CB	2.55	0.55
1:B:286:MET:SD	1:B:290:ARG:HG3	2.46	0.55
1:B:246:LYS:O	1:B:247:ARG:HB2	2.06	0.54
1:A:196:VAL:HB	1:A:202:LYS:HB2	1.90	0.54
1:B:171:MET:CE	1:A:171:MET:HE2	2.38	0.54
1:A:280:ASN:O	1:A:281:ASP:HB2	2.09	0.53
1:B:163:ASP:C	1:B:165:LEU:N	2.62	0.53
1:B:251:ARG:HG2	1:B:307:PHE:CD1	2.42	0.53
1:B:221:GLN:O	1:B:222:GLY:C	2.46	0.53
1:B:303:LYS:HG3	1:B:340:LEU:HD11	1.91	0.53
1:A:235:GLN:HE21	1:A:266:VAL:CG1	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HB3	1:A:220:HIS:CD2	2.43	0.52
1:B:250:HIS:CD2	1:B:252:ASP:H	2.27	0.52
1:A:216:ARG:NH1	1:A:216:ARG:CG	2.73	0.52
1:B:251:ARG:NH1	1:B:286:MET:HE2	2.25	0.51
1:B:353:PRO:HB2	1:B:356:CYS:HB2	1.92	0.51
1:A:280:ASN:O	1:A:280:ASN:OD1	2.28	0.51
1:B:216:ARG:NH1	1:B:216:ARG:CG	2.57	0.51
1:B:229:LEU:O	1:B:232:TYR:HB2	2.11	0.50
1:A:250:HIS:HE1	1:A:270:ASP:O	1.94	0.50
1:A:265:LEU:HD13	1:A:267:LYS:HE2	1.94	0.50
1:A:187:ARG:O	1:A:267:LYS:HD3	2.12	0.50
1:B:335:ASN:H	1:B:338:GLN:NE2	2.10	0.50
1:B:354:GLU:O	1:B:355:ASP:HB2	2.11	0.50
1:B:299:PRO:O	1:B:302:LEU:N	2.46	0.49
1:B:232:TYR:O	1:B:236:VAL:HG23	2.13	0.48
1:B:275:ARG:CZ	1:B:284:PTR:CE1	2.91	0.48
1:A:376:PRO:HG2	1:A:381:LEU:CD1	2.44	0.48
1:B:255:ALA:HA	1:B:258:LEU:HD22	1.95	0.48
1:B:118:THR:CG2	1:B:182:HIS:CD2	2.92	0.48
1:A:345:LYS:NZ	3:A:503:HOH:O	2.46	0.47
2:A:401:T77:H15	2:A:401:T77:C9	2.44	0.47
2:A:401:T77:H11	2:A:401:T77:H1	1.48	0.47
1:B:286:MET:CG	1:B:290:ARG:HG3	2.44	0.47
1:A:354:GLU:O	1:A:355:ASP:HB2	2.14	0.46
1:A:376:PRO:HG2	1:A:381:LEU:HD13	1.98	0.46
2:A:401:T77:H23	2:A:401:T77:C10	2.28	0.46
1:B:250:HIS:CE1	1:B:270:ASP:O	2.64	0.46
1:B:251:ARG:NH1	1:B:286:MET:CE	2.78	0.46
1:A:173:ASP:OD2	1:A:290:ARG:NH2	2.40	0.45
1:B:280:ASN:OD1	1:B:280:ASN:O	2.34	0.45
1:A:263:ARG:HG3	1:A:263:ARG:NH1	2.31	0.45
1:B:162:PRO:HD2	1:B:163:ASP:H	1.81	0.45
1:A:233:ALA:HB1	1:A:320:LEU:HD11	1.99	0.45
1:B:335:ASN:OD1	1:B:338:GLN:HG3	2.16	0.45
1:B:164:VAL:HG21	1:B:199:PRO:HB3	1.99	0.45
1:A:128:LEU:HD11	1:A:202:LYS:HE2	1.99	0.44
1:B:231:ARG:O	1:B:235:GLN:HG3	2.17	0.44
1:B:284:PTR:HE2	1:B:286:MET:HA	1.99	0.44
1:A:255:ALA:HA	1:A:258:LEU:HD22	1.99	0.44
1:B:142:ARG:HH11	1:B:207:LEU:HD21	1.83	0.44
1:A:286:MET:CG	1:A:290:ARG:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:T77:H1	2:B:401:T77:H11	1.54	0.44
1:A:275:ARG:HE	1:A:275:ARG:HB3	1.57	0.44
1:B:300:GLU:O	1:B:303:LYS:N	2.51	0.44
1:B:219:LYS:HB3	1:B:220:HIS:CD2	2.53	0.43
2:B:401:T77:C10	2:B:401:T77:H23	2.31	0.43
1:B:290:ARG:O	1:B:305:ARG:NH2	2.51	0.43
1:B:162:PRO:HB2	1:B:167:GLN:HG3	2.01	0.43
1:B:173:ASP:OD2	1:B:290:ARG:NH2	2.42	0.43
1:B:280:ASN:O	1:B:281:ASP:HB2	2.18	0.43
1:A:220:HIS:O	1:A:223:HIS:HB3	2.19	0.43
1:B:182:HIS:O	1:B:183:SER:HB3	2.19	0.43
1:A:184:LEU:HD23	1:A:184:LEU:N	2.33	0.42
1:A:296:TRP:O	1:A:315:MET:HG2	2.19	0.42
1:A:290:ARG:HG2	1:A:290:ARG:H	1.64	0.42
1:A:302:LEU:HB3	1:A:340:LEU:HD13	2.00	0.42
1:A:190:ILE:HG12	1:A:269:GLY:HA2	2.01	0.42
1:B:263:ARG:NH1	1:B:263:ARG:HG3	2.34	0.42
1:A:164:VAL:HG21	1:A:199:PRO:HB3	2.01	0.42
1:B:132:LEU:HG	2:B:401:T77:C7	2.50	0.41
1:B:190:ILE:HA	1:B:190:ILE:HD13	1.90	0.41
1:B:199:PRO:HA	1:B:200:PRO:HA	1.90	0.41
1:B:364:MET:O	1:B:367:CYS:HB2	2.20	0.41
1:A:334:LEU:N	1:A:334:LEU:CD1	2.83	0.41
1:A:137:PHE:C	1:A:137:PHE:CD1	2.94	0.41
1:A:280:ASN:CG	1:A:280:ASN:O	2.58	0.41
1:A:353:PRO:HB2	1:A:356:CYS:HB2	2.03	0.41
1:B:131:LYS:HA	1:B:141:ARG:HG2	2.02	0.41
1:B:371:LYS:O	1:B:372:PRO:C	2.59	0.41
1:B:140:VAL:HG22	1:B:158:LYS:HG2	2.03	0.41
1:B:275:ARG:HE	1:B:275:ARG:HB3	1.64	0.41
1:B:300:GLU:O	1:B:301:SER:C	2.59	0.40
1:A:162:PRO:HD2	1:A:163:ASP:H	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:O	1:A:337:SER:OG[4_555]	2.05	0.15

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	272/275 (99%)	243 (89%)	20 (7%)	9 (3%)	4 5
1	B	271/275 (98%)	241 (89%)	24 (9%)	6 (2%)	6 10
All	All	543/550 (99%)	484 (89%)	44 (8%)	15 (3%)	5 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	PRO
1	B	223	HIS
1	A	162	PRO
1	A	223	HIS
1	A	390	PRO
1	A	221	GLN
1	A	222	GLY
1	B	221	GLN
1	B	164	VAL
1	B	222	GLY
1	A	164	VAL
1	A	217	LEU
1	A	183	SER
1	B	161	LYS
1	A	161	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	238/238 (100%)	202 (85%)	36 (15%)	3 5
1	B	237/238 (100%)	202 (85%)	35 (15%)	3 5
All	All	475/476 (100%)	404 (85%)	71 (15%)	3 5

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	THR
1	B	132	LEU
1	B	151	LYS
1	B	152	THR
1	B	153	VAL
1	B	154	SER
1	B	165	LEU
1	B	169	GLU
1	B	187	ARG
1	B	189	LEU
1	B	210	LEU
1	B	216	ARG
1	B	219	LYS
1	B	225	LEU
1	B	226	LEU
1	B	231	ARG
1	B	238	GLU
1	B	245	SER
1	B	258	LEU
1	B	263	ARG
1	B	265	LEU
1	B	273	LEU
1	B	283	HIS
1	B	290	ARG
1	B	291	LYS
1	B	300	GLU
1	B	302	LEU
1	B	334	LEU
1	B	345	LYS
1	B	352	ARG
1	B	355	ASP
1	B	359	ASP
1	B	371	LYS
1	B	381	LEU
1	B	382	ARG

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Mol	Chain	Res	Type
1	A	132	LEU
1	A	136	SER
1	A	152	THR
1	A	153	VAL
1	A	154	SER
1	A	165	LEU
1	A	171	MET
1	A	187	ARG
1	A	189	LEU
1	A	216	ARG
1	A	219	LYS
1	A	225	LEU
1	A	226	LEU
1	A	230	SER
1	A	231	ARG
1	A	238	GLU
1	A	245	SER
1	A	256	ARG
1	A	258	LEU
1	A	265	LEU
1	A	273	LEU
1	A	275	ARG
1	A	283	HIS
1	A	290	ARG
1	A	291	LYS
1	A	302	LEU
1	A	334	LEU
1	A	342	LYS
1	A	345	LYS
1	A	352	ARG
1	A	354	GLU
1	A	359	ASP
1	A	371	LYS
1	A	381	LEU
1	A	382	ARG
1	A	391	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	HIS
1	B	188	ASN

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Mol	Chain	Res	Type
1	B	220	HIS
1	B	235	GLN
1	B	250	HIS
1	B	279	GLN
1	B	287	GLN
1	B	338	GLN
1	B	358	GLN
1	B	370	HIS
1	A	182	HIS
1	A	186	HIS
1	A	188	ASN
1	A	235	GLN
1	A	250	HIS
1	A	279	GLN
1	A	287	GLN
1	A	338	GLN
1	A	358	GLN
1	A	370	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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	284	1	15,16,17	2.37	2 (13%)	19,22,24	1.36	2 (10%)
1	PTR	A	284	1	15,16,17	2.13	4 (26%)	19,22,24	1.35	3 (15%)

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	284	1	-	1/10/11/13	0/1/1/1
1	PTR	A	284	1	-	0/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	PTR	P-OH	6.71	1.69	1.59
1	A	284	PTR	P-OH	5.22	1.67	1.59
1	B	284	PTR	OH-CZ	-5.20	1.28	1.40
1	A	284	PTR	OH-CZ	-4.50	1.30	1.40
1	A	284	PTR	P-O2P	-2.27	1.46	1.54
1	A	284	PTR	CE1-CD1	2.27	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	PTR	P-OH-CZ	3.62	135.35	123.75
1	A	284	PTR	P-OH-CZ	2.72	132.48	123.75
1	B	284	PTR	O3P-P-OH	2.36	112.61	105.24
1	A	284	PTR	CB-CA-C	2.12	115.44	111.47
1	A	284	PTR	O2P-P-OH	2.04	111.63	105.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	284	PTR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	284	PTR	3	0
1	A	284	PTR	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	T77	A	401	-	35,38,38	1.36	4 (11%)	35,52,52	2.45	13 (37%)
2	T77	B	401	-	35,38,38	1.47	3 (8%)	35,52,52	2.34	9 (25%)

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	T77	A	401	-	-	5/17/26/26	0/5/5/5
2	T77	B	401	-	-	4/17/26/26	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	T77	C5-N11	5.69	1.44	1.37
2	A	401	T77	C5-N11	4.57	1.43	1.37
2	B	401	T77	C6-C2	-3.56	1.39	1.44
2	A	401	T77	C6-C2	-3.51	1.40	1.44
2	A	401	T77	C1-C2	-2.93	1.38	1.42
2	A	401	T77	C2-C5	-2.37	1.36	1.43
2	B	401	T77	C2-C5	-2.36	1.36	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	T77	C18-N13-C6	8.81	124.15	116.59
2	A	401	T77	C18-N13-C6	7.56	123.07	116.59
2	A	401	T77	C2-C6-N13	-5.05	117.19	121.35
2	B	401	T77	N11-C18-N13	-4.52	121.62	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	T77	C2-C6-N13	-4.12	117.96	121.35
2	B	401	T77	C33-N32-C34	3.92	119.86	109.73
2	A	401	T77	C33-N32-C34	3.81	119.57	109.73
2	A	401	T77	N11-C18-N13	-3.58	123.08	128.68
2	A	401	T77	C16-C9-C4	3.51	124.98	120.56
2	A	401	T77	C19-N12-C6	-3.40	117.20	123.25
2	B	401	T77	C34-N32-C31	3.22	123.51	110.74
2	A	401	T77	C34-N32-C31	3.04	122.79	110.74
2	A	401	T77	C22-C16-C9	-2.86	115.83	120.19
2	B	401	T77	C3-C1-C2	-2.83	104.73	109.09
2	A	401	T77	C3-C1-C2	-2.74	104.86	109.09
2	A	401	T77	C30-C31-N32	-2.65	107.58	114.56
2	B	401	T77	C30-C31-N32	-2.62	107.67	114.56
2	B	401	T77	C30-O27-C24	2.56	124.61	117.93
2	A	401	T77	C29-C28-S25	-2.51	102.38	110.21
2	B	401	T77	C15-C7-C3	-2.36	116.87	120.61
2	A	401	T77	C4-C1-C3	2.17	131.18	126.88
2	A	401	T77	C15-C7-C3	-2.14	117.22	120.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	T77	C30-C31-N32-C34
2	A	401	T77	C2-C1-C4-C9
2	B	401	T77	C30-C31-N32-C34
2	B	401	T77	C1-C3-C7-C15
2	A	401	T77	C1-C3-C7-C15
2	A	401	T77	C1-C3-C7-C14
2	B	401	T77	C1-C3-C7-C14
2	A	401	T77	C23-C19-N12-C6
2	B	401	T77	C23-C19-N12-C6

There are no ring outliers.

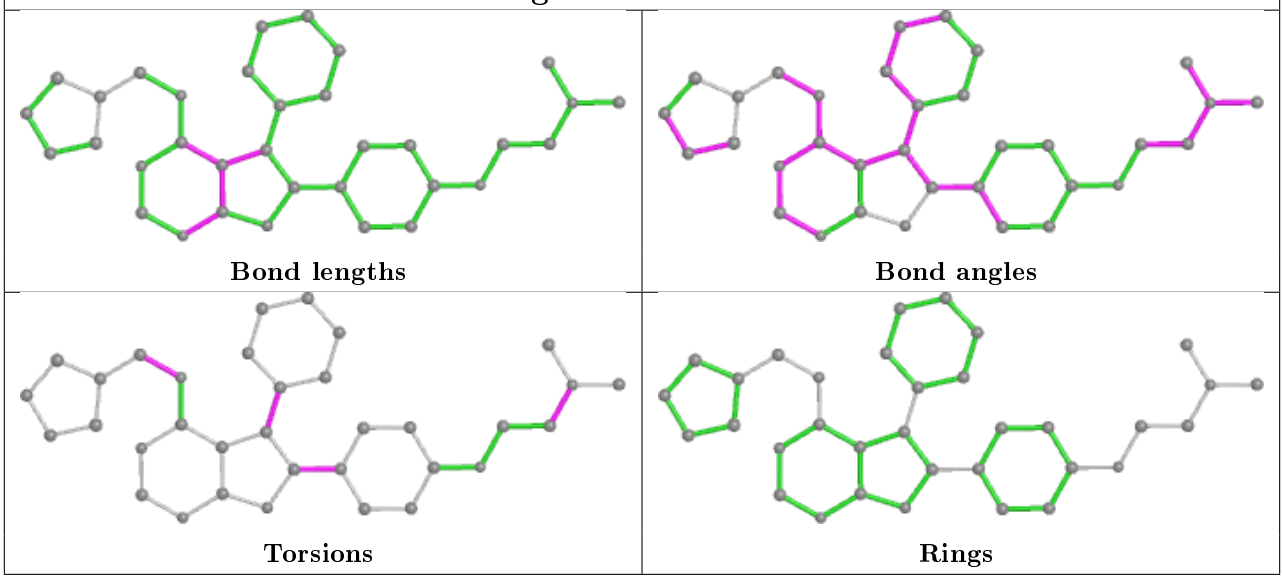
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	T77	4	0
2	B	401	T77	5	0

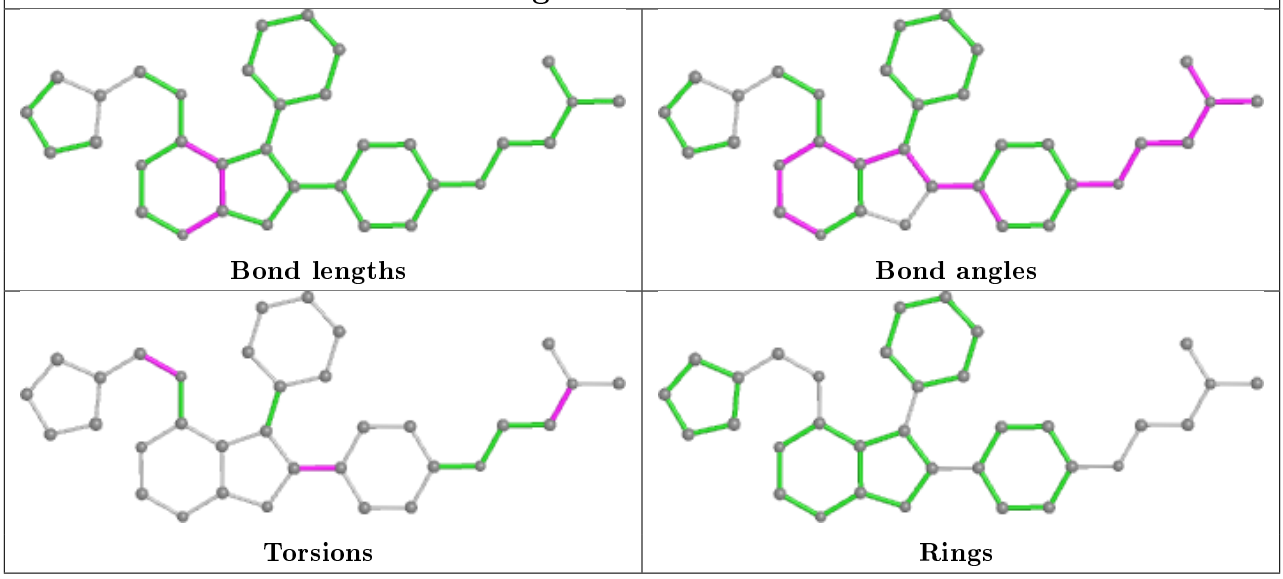
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 T77 A 401



Ligand T77 B 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	274/275 (99%)	0.49	18 (6%)	18	19	31, 49, 75, 93	0
1	B	273/275 (99%)	0.50	23 (8%)	11	11	30, 49, 75, 93	0
All	All	547/550 (99%)	0.49	41 (7%)	14	14	30, 49, 75, 93	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	VAL	12.3
1	A	164	VAL	10.4
1	A	165	LEU	10.3
1	A	162	PRO	9.2
1	B	165	LEU	8.5
1	A	391	THR	8.4
1	B	293	PRO	5.5
1	B	289	HIS	5.2
1	B	390	PRO	4.8
1	A	166	SER	4.3
1	A	280	ASN	4.0
1	A	221	GLN	4.0
1	B	292	VAL	3.8
1	A	163	ASP	3.7
1	B	223	HIS	3.7
1	A	224	PHE	3.6
1	B	162	PRO	3.5
1	B	225	LEU	3.3
1	A	148	PRO	3.3
1	A	390	PRO	3.2
1	A	279	GLN	3.2
1	B	291	LYS	2.9
1	A	149	SER	2.9
1	B	168	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	224	PHE	2.8
1	A	137	PHE	2.8
1	B	166	SER	2.8
1	B	387	GLU	2.7
1	A	129	LEU	2.7
1	A	220	HIS	2.6
1	B	160	LEU	2.4
1	B	163	ASP	2.3
1	B	167	GLN	2.3
1	A	283	HIS	2.3
1	B	362	ASN	2.2
1	B	169	GLU	2.2
1	B	148	PRO	2.1
1	B	282	ASP	2.1
1	A	216	ARG	2.0
1	B	373	GLU	2.0
1	B	372	PRO	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	PTR	B	284	16/17	0.78	0.19	55,63,64,65	0
1	PTR	A	284	16/17	0.87	0.28	55,62,65,65	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

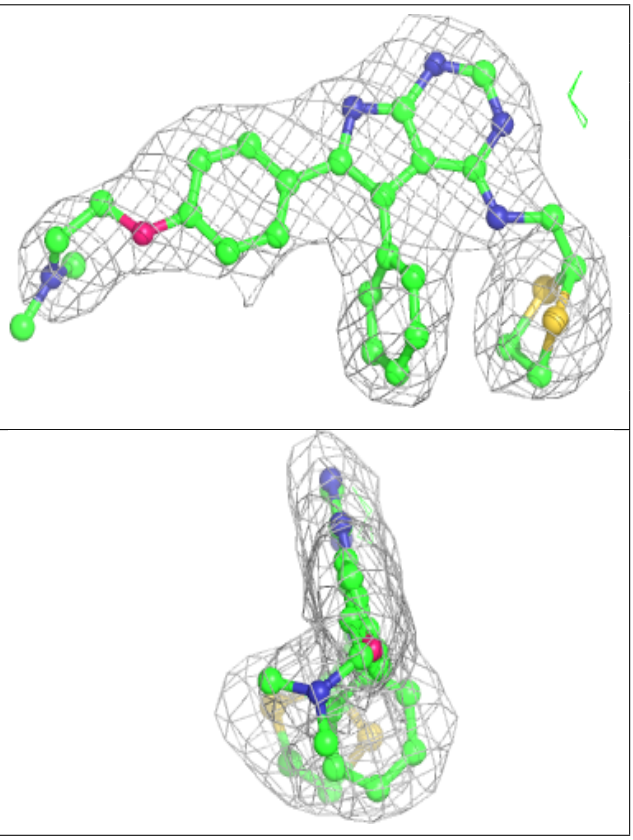
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	T77	A	401	34/34	0.96	0.15	22,34,56,60	0
2	T77	B	401	34/34	0.96	0.14	22,34,56,60	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.

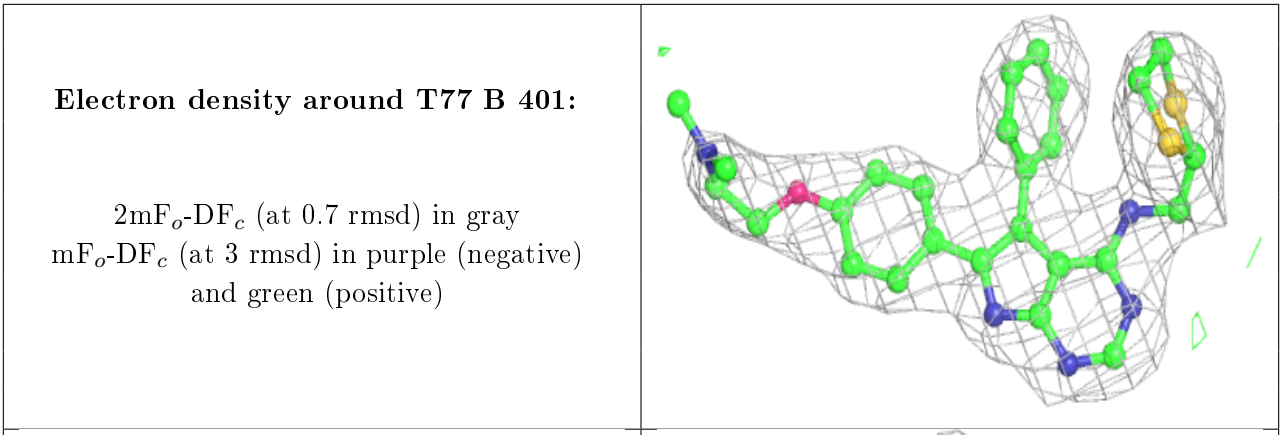
Electron density around T77 A 401:

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



Electron density around T77 B 401:

$2mF_o$-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.