



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:13 PM UTC

PDB ID : 5OQ7 / pdb_00005oq7
Title : Structure of CHK1 8-pt. mutant complex with arylbenzamide LRRK2 inhibitor
Authors : Dokurno, P.; Williamson, D.S.; Acheson-Dossang, P.; Chen, I.; Murray, J.B.; Shaw, T.; Surgenor, A.E.
Deposited on : 2017-08-10
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

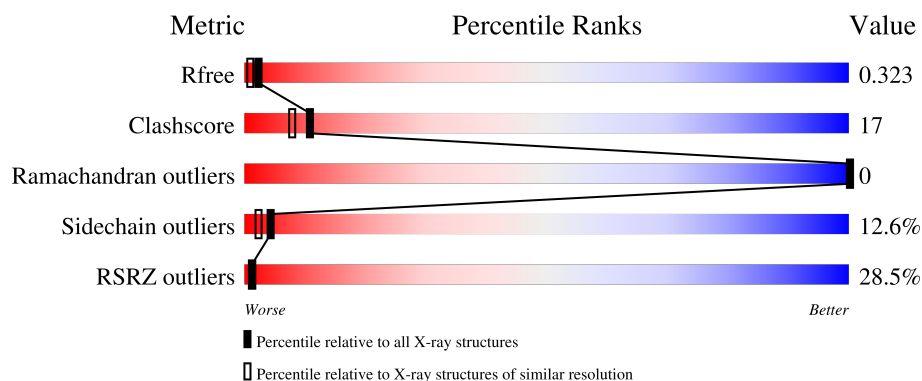
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	297	14% 61% 20% 5% 13%
1	B	297	35% 53% 28% 6% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4374 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 Chk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	1	0
			2076	1332	356	375	13			
1	B	256	Total	C	N	O	S	0	1	0
			2061	1323	353	372	13			

There are 32 discrepancies between the modelled and reference sequences:

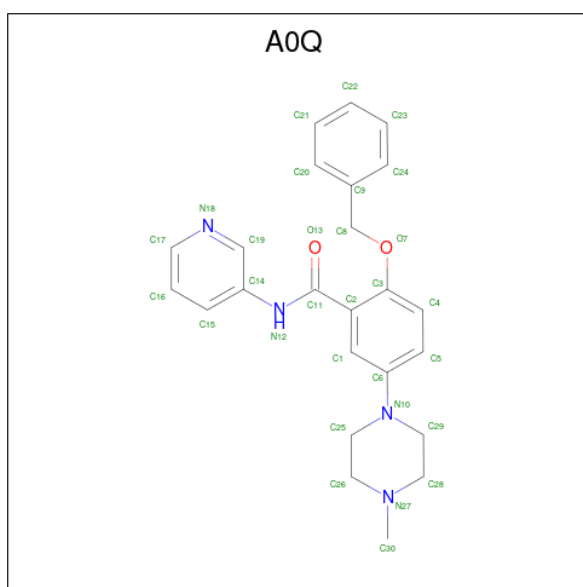
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	LEU	ASN	engineered mutation	UNP O14757
A	68	ILE	VAL	engineered mutation	UNP O14757
A	84	MET	LEU	engineered mutation	UNP O14757
A	86	LEU	TYR	engineered mutation	UNP O14757
A	87	ALA	CYS	engineered mutation	UNP O14757
A	91	SER	GLU	engineered mutation	UNP O14757
A	134	HIS	GLU	engineered mutation	UNP O14757
A	147	ALA	SER	engineered mutation	UNP O14757
A	290	HIS	-	expression tag	UNP O14757
A	291	HIS	-	expression tag	UNP O14757
A	292	HIS	-	expression tag	UNP O14757
A	293	HIS	-	expression tag	UNP O14757
A	294	HIS	-	expression tag	UNP O14757
A	295	HIS	-	expression tag	UNP O14757
A	296	HIS	-	expression tag	UNP O14757
A	297	HIS	-	expression tag	UNP O14757
B	59	LEU	ASN	engineered mutation	UNP O14757
B	68	ILE	VAL	engineered mutation	UNP O14757
B	84	MET	LEU	engineered mutation	UNP O14757
B	86	LEU	TYR	engineered mutation	UNP O14757
B	87	ALA	CYS	engineered mutation	UNP O14757
B	91	SER	GLU	engineered mutation	UNP O14757
B	134	HIS	GLU	engineered mutation	UNP O14757
B	147	ALA	SER	engineered mutation	UNP O14757
B	290	HIS	-	expression tag	UNP O14757

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	291	HIS	-	expression tag	UNP O14757
B	292	HIS	-	expression tag	UNP O14757
B	293	HIS	-	expression tag	UNP O14757
B	294	HIS	-	expression tag	UNP O14757
B	295	HIS	-	expression tag	UNP O14757
B	296	HIS	-	expression tag	UNP O14757
B	297	HIS	-	expression tag	UNP O14757

- Molecule 2 is 5-(4-methylpiperazin-1-yl)-2-phenylmethoxy- {N}-pyridin-3-yl-benzamide (CCD ID: A0Q) (formula: C₂₄H₂₆N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	24	4	2		
2	B	1	Total	C	N	O	0	0
			30	24	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	86	Total	O	0	0
			86	86		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.21Å 66.25Å 109.32Å 90.00° 100.76° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.00-2.10) 98.8 (40.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.255 , 0.324 0.260 , 0.323	Depositor DCC
R_{free} test set	1836 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4374	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 28.24 % 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 1.9077e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A0Q

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	1.22	4/2128 (0.2%)	1.21	7/2884 (0.2%)
1	B	1.10	5/2112 (0.2%)	1.25	14/2860 (0.5%)
All	All	1.16	9/4240 (0.2%)	1.23	21/5744 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	PRO	C-O	6.35	1.31	1.23
1	B	243	HIS	C-O	-5.47	1.17	1.24
1	B	175	ALA	CA-C	5.44	1.59	1.53
1	A	198	LEU	N-CA	5.42	1.52	1.46
1	A	201	MET	C-O	-5.42	1.17	1.24
1	B	196	ILE	N-CA	-5.32	1.40	1.46
1	A	211	PRO	CA-C	5.13	1.58	1.53
1	A	196	ILE	CA-CB	5.11	1.60	1.54
1	B	241	LEU	CA-C	5.08	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	CYS	CA-C-N	10.59	130.80	119.05
1	A	48	CYS	C-N-CA	10.59	130.80	119.05
1	B	256	ILE	N-CA-CB	7.81	115.42	110.50
1	B	132	LYS	N-CA-C	-7.57	101.41	108.22
1	B	62	LEU	N-CA-C	7.51	120.51	108.41
1	B	180	LYS	N-CA-C	6.78	119.67	111.40
1	B	50	GLU	N-CA-C	-6.77	103.83	111.07
1	B	132	LYS	CB-CA-C	6.10	118.27	110.22
1	A	62	LEU	N-CA-C	5.69	117.95	109.25
1	B	168	CYS	N-CA-C	5.63	116.83	108.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	N-CA-C	-5.36	101.71	109.59
1	A	49	PRO	N-CA-C	5.29	120.89	113.53
1	B	68	ILE	N-CA-C	5.27	116.21	109.30
1	B	187	GLU	CA-C-N	-5.25	114.26	119.56
1	B	187	GLU	C-N-CA	-5.25	114.26	119.56
1	A	182	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	25	LEU	N-CA-C	-5.18	101.52	109.76
1	B	175	ALA	CA-C-N	5.15	125.19	119.32
1	B	175	ALA	C-N-CA	5.15	125.19	119.32
1	B	186	ALA	N-CA-C	5.13	116.87	111.28
1	B	248	GLU	N-CA-C	5.09	116.91	111.36

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	2067	52	1
1	B	2061	0	2057	86	1
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	91	0	0	18	1
3	B	86	0	0	58	0
All	All	4374	0	4124	138	2

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 17.

All (138) 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:B:110:PHE:HB2	3:B:416:HOH:O	1.29	1.27
1:B:178:LEU:HA	3:B:415:HOH:O	1.49	1.13
1:B:153:THR:HG22	3:B:427:HOH:O	1.48	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:THR:O	3:B:401:HOH:O	1.65	1.11
1:B:117:GLY:N	3:B:403:HOH:O	1.96	0.99
1:B:256:ILE:HA	3:B:401:HOH:O	1.64	0.98
1:B:190:ASP:HA	3:B:409:HOH:O	1.62	0.97
1:B:208:TRP:CD1	3:B:408:HOH:O	2.16	0.96
1:B:129:ARG:NH1	3:B:404:HOH:O	1.96	0.95
1:B:62:LEU:HA	3:B:405:HOH:O	1.73	0.88
1:B:114:LEU:HD12	3:B:410:HOH:O	1.71	0.88
1:B:93:PHE:O	3:B:402:HOH:O	1.94	0.85
1:B:106:ASP:HB3	3:B:456:HOH:O	1.78	0.82
1:B:102:MET:SD	3:B:456:HOH:O	2.38	0.80
1:A:139:ASP:O	3:A:401:HOH:O	1.99	0.80
1:A:73:HIS:HA	1:A:81:TYR:O	1.81	0.80
1:A:42:MET:N	1:A:78:ASN:O	2.15	0.79
1:A:118:VAL:HB	3:A:404:HOH:O	1.84	0.78
1:B:107:ALA:HA	3:B:416:HOH:O	1.84	0.77
1:B:184:PHE:CD1	3:B:415:HOH:O	2.38	0.75
1:A:55:GLU:HG3	3:A:476:HOH:O	1.87	0.75
1:A:38:LYS:NZ	1:A:55:GLU:OE2	2.19	0.75
1:A:268:PRO:HB2	3:A:408:HOH:O	1.85	0.75
1:B:255:THR:C	3:B:401:HOH:O	2.16	0.74
1:B:110:PHE:CE2	3:B:456:HOH:O	2.40	0.74
1:A:15:LEU:HD11	1:A:25:LEU:HB2	1.69	0.74
1:B:256:ILE:CA	3:B:401:HOH:O	2.26	0.72
1:B:259:ILE:CG1	3:B:401:HOH:O	2.39	0.71
1:A:149:PHE:HB2	3:A:476:HOH:O	1.91	0.70
1:B:161:GLU:OE1	1:B:185:HIS:ND1	2.18	0.70
1:B:111:PHE:HA	3:B:476:HOH:O	1.92	0.70
1:B:113:GLN:O	3:B:403:HOH:O	2.11	0.68
1:B:110:PHE:HA	3:B:414:HOH:O	1.94	0.68
1:B:208:TRP:HD1	3:B:408:HOH:O	1.67	0.67
1:B:132:LYS:HB2	3:B:467:HOH:O	1.95	0.66
1:B:144:LEU:C	1:B:144:LEU:HD23	2.21	0.66
1:B:146:ILE:HD11	3:B:410:HOH:O	1.97	0.65
1:A:105:PRO:HD3	3:A:482:HOH:O	1.98	0.64
1:A:170:THR:HG22	1:A:172:PRO:HD2	1.81	0.63
1:A:165:ASN:HD22	1:A:165:ASN:C	2.06	0.63
1:A:269:LEU:O	3:A:402:HOH:O	2.15	0.62
1:B:175:ALA:N	3:B:407:HOH:O	2.30	0.62
1:B:186:ALA:HB3	3:B:442:HOH:O	1.99	0.61
1:B:62:LEU:HD23	3:B:405:HOH:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HG13	3:B:401:HOH:O	1.98	0.61
1:B:144:LEU:HD13	3:B:414:HOH:O	2.00	0.60
1:B:121:LEU:HA	3:B:450:HOH:O	2.00	0.60
1:B:259:ILE:HD12	3:B:401:HOH:O	2.01	0.60
1:B:124:ILE:CG1	3:B:450:HOH:O	2.49	0.60
1:A:182:ARG:HH11	1:A:182:ARG:HG2	1.67	0.60
1:A:12:VAL:HG13	1:A:13:GLN:HG2	1.83	0.60
1:B:49:PRO:HA	1:B:52:ILE:HG22	1.84	0.59
1:B:248:GLU:HA	3:B:411:HOH:O	2.02	0.59
1:A:40:VAL:HG23	1:A:80:GLN:HB2	1.85	0.58
1:B:253:ARG:NH1	3:B:411:HOH:O	2.37	0.57
1:B:138:LEU:HD12	1:B:144:LEU:HA	1.86	0.57
1:B:75:ARG:CB	1:B:80:GLN:NE2	2.68	0.56
1:B:176:PRO:HG2	3:B:411:HOH:O	2.06	0.56
1:B:127:THR:HG21	1:B:186:ALA:HB1	1.87	0.55
1:A:37:VAL:HG13	1:A:83:PHE:CD2	2.42	0.55
1:B:208:TRP:NE1	3:B:408:HOH:O	2.32	0.54
1:B:259:ILE:CD1	3:B:401:HOH:O	2.56	0.54
1:A:115:MET:HA	3:A:404:HOH:O	2.06	0.54
1:B:184:PHE:CG	3:B:415:HOH:O	2.61	0.54
1:A:207:PRO:HB2	1:A:208:TRP:CE3	2.43	0.53
1:B:164:LEU:HD11	1:B:186:ALA:CB	2.38	0.53
1:A:213:ASP:HA	3:A:443:HOH:O	2.09	0.53
1:A:144:LEU:C	1:A:144:LEU:HD23	2.34	0.53
1:A:198:LEU:C	3:A:403:HOH:O	2.51	0.53
1:B:116:ALA:HB3	3:B:403:HOH:O	2.09	0.52
1:B:256:ILE:HA	1:B:259:ILE:HD12	1.91	0.52
1:A:238:PRO:HD3	1:A:264:TRP:CD1	2.45	0.52
1:B:248:GLU:O	1:B:250:PRO:HD3	2.10	0.52
1:A:167:MET:HG2	1:A:178:LEU:HD13	1.91	0.51
1:B:96:ILE:CG2	1:B:101:GLY:HA2	2.41	0.51
1:A:79:ILE:HG22	1:A:81:TYR:CE1	2.47	0.50
1:B:124:ILE:CD1	3:B:405:HOH:O	2.60	0.49
1:B:196:ILE:HA	3:B:455:HOH:O	2.12	0.49
1:B:110:PHE:CA	3:B:414:HOH:O	2.57	0.49
1:B:124:ILE:HD11	3:B:405:HOH:O	2.13	0.48
1:B:126:ILE:HB	3:B:450:HOH:O	2.13	0.48
1:B:166:LYS:NZ	1:B:168:CYS:HB3	2.29	0.48
1:B:168:CYS:HA	3:B:474:HOH:O	2.14	0.48
1:B:145:LYS:NZ	3:B:417:HOH:O	2.46	0.48
1:A:199:THR:HA	3:A:403:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HG21	1:B:81:TYR:CZ	2.49	0.47
1:A:190:ASP:HB2	3:A:433:HOH:O	2.14	0.47
1:B:164:LEU:HD11	1:B:186:ALA:HB2	1.96	0.47
1:A:42:MET:C	1:A:78:ASN:HB3	2.40	0.47
1:B:96:ILE:HG23	1:B:101:GLY:HA2	1.97	0.47
1:B:26:ALA:HB3	1:B:35:VAL:HG12	1.97	0.46
1:A:12:VAL:CG1	1:A:25:LEU:HD22	2.45	0.46
1:B:110:PHE:CD2	3:B:456:HOH:O	2.66	0.46
1:B:186:ALA:CB	3:B:442:HOH:O	2.62	0.46
1:A:130:ASP:HB2	1:A:151:LEU:HD12	1.97	0.45
1:B:166:LYS:HZ2	1:B:168:CYS:HB3	1.80	0.45
1:B:222:LYS:HD3	1:B:248:GLU:OE2	2.16	0.45
1:A:52:ILE:HD13	1:A:52:ILE:HA	1.79	0.45
1:A:97:GLU:HB3	1:A:100:ILE:HG13	1.98	0.45
1:B:67:VAL:HB	3:B:460:HOH:O	2.17	0.45
1:B:230:PRO:HD2	1:B:231:TRP:NE1	2.32	0.45
1:B:238:PRO:HD3	1:B:264:TRP:CD1	2.52	0.45
1:A:74:ARG:O	1:A:81:TYR:HD1	1.99	0.44
1:A:190:ASP:CB	3:A:433:HOH:O	2.65	0.44
1:B:137:LEU:O	1:B:145:LYS:N	2.49	0.44
1:A:73:HIS:CA	1:A:81:TYR:O	2.60	0.44
1:A:178:LEU:HD22	1:A:184:PHE:CZ	2.52	0.44
1:A:42:MET:CE	1:A:78:ASN:OD1	2.66	0.43
1:B:84:MET:HE2	1:B:84:MET:HB2	1.78	0.43
1:A:242:LEU:HD11	3:A:403:HOH:O	2.18	0.43
1:A:227:TYR:N	3:A:415:HOH:O	2.48	0.43
1:A:12:VAL:HG13	1:A:13:GLN:HE21	1.84	0.43
1:B:229:ASN:OD1	3:B:406:HOH:O	2.21	0.43
1:A:75:ARG:HA	1:A:79:ILE:O	2.19	0.43
1:A:197:VAL:HG12	3:A:421:HOH:O	2.18	0.42
1:A:210:GLN:HE21	1:A:212:SER:HB3	1.84	0.42
1:A:256:ILE:HD13	3:A:404:HOH:O	2.18	0.42
1:A:132:LYS:NZ	3:A:417:HOH:O	2.51	0.42
1:A:178:LEU:CD1	1:A:178:LEU:C	2.92	0.42
1:B:25:LEU:HD23	1:B:86:LEU:HD13	2.01	0.42
1:B:203:ALA:HB2	1:B:234:ILE:HD11	2.01	0.42
1:A:97:GLU:CD	1:A:100:ILE:HG12	2.44	0.42
1:B:124:ILE:HG13	3:B:450:HOH:O	2.18	0.42
1:B:211:PRO:HD3	3:B:408:HOH:O	2.20	0.42
1:B:164:LEU:HD23	3:B:434:HOH:O	2.20	0.41
1:B:53:LYS:O	1:B:57[A]:CYS:SG	2.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HG3	1:B:143:ASN:OD1	2.20	0.41
1:A:174:VAL:O	1:A:211:PRO:HG3	2.20	0.41
1:B:178:LEU:HD23	1:B:184:PHE:CE2	2.55	0.41
1:B:42:MET:HE3	1:B:49:PRO:HA	2.01	0.41
1:A:113:GLN:HE22	1:A:143:ASN:HD22	1.67	0.41
1:B:119:VAL:CG2	1:B:256:ILE:HG21	2.51	0.41
1:B:124:ILE:HG12	3:B:450:HOH:O	2.17	0.41
1:A:174:VAL:HG22	1:A:178:LEU:HG	2.03	0.41
1:B:107:ALA:CA	3:B:416:HOH:O	2.57	0.41
1:A:42:MET:HE2	1:A:78:ASN:HA	2.03	0.41
1:A:165:ASN:C	1:A:165:ASN:ND2	2.74	0.40
1:B:155:PHE:HB3	3:B:434:HOH:O	2.20	0.40

All (2) 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:A:181:ARG:NH2	1:B:32:GLU:OE2[1_554]	1.69	0.51
3:A:426:HOH:O	3:A:480:HOH:O[2_555]	2.19	0.01

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	256/297 (86%)	249 (97%)	7 (3%)	0	100	100
1	B	251/297 (84%)	243 (97%)	8 (3%)	0	100	100
All	All	507/594 (85%)	492 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/259 (86%)	196 (88%)	28 (12%)	4	2
1	B	224/259 (86%)	196 (88%)	28 (12%)	4	2
All	All	448/518 (86%)	392 (88%)	56 (12%)	4	2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	GLN
1	A	14	THR
1	A	15	LEU
1	A	23	VAL
1	A	27	VAL
1	A	35	VAL
1	A	37	VAL
1	A	39	ILE
1	A	40	VAL
1	A	42	MET
1	A	52	ILE
1	A	60	LYS
1	A	68	ILE
1	A	79	ILE
1	A	84	MET
1	A	88	SER
1	A	100	ILE
1	A	141	ARG
1	A	145	LYS
1	A	165	ASN
1	A	166	LYS
1	A	174	VAL
1	A	178	LEU
1	A	181	ARG
1	A	182	ARG
1	A	232	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	239	LEU
1	B	8	ASP
1	B	11	LEU
1	B	14	THR
1	B	17	GLU
1	B	23	VAL
1	B	24	GLN
1	B	25	LEU
1	B	27	VAL
1	B	35	VAL
1	B	39	ILE
1	B	52	ILE
1	B	96	ILE
1	B	99	ASP
1	B	100	ILE
1	B	127	THR
1	B	138	LEU
1	B	141	ARG
1	B	144	LEU
1	B	171	LEU
1	B	174	VAL
1	B	198	LEU
1	B	205	GLU
1	B	215	CYS
1	B	219	SER
1	B	223	GLU
1	B	229	ASN
1	B	239	LEU
1	B	251	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	66	ASN
1	A	80	GLN
1	A	143	ASN
1	A	158	ASN
1	A	165	ASN
1	A	210	GLN
1	B	24	GLN
1	B	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	GLN
1	B	158	ASN
1	B	210	GLN
1	B	229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A0Q	B	301	-	33,33,33	0.93	1 (3%)	44,44,44	1.86	12 (27%)
2	A0Q	A	301	-	33,33,33	1.15	3 (9%)	44,44,44	1.21	4 (9%)

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	A0Q	B	301	-	-	0/17/27/27	0/4/4/4
2	A0Q	A	301	-	-	0/17/27/27	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A0Q	C2-C11	3.64	1.57	1.50
2	A	301	A0Q	C29-N10	3.18	1.52	1.46
2	A	301	A0Q	C6-N10	2.60	1.46	1.38
2	B	301	A0Q	C25-N10	2.06	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	A0Q	C1-C6-N10	-6.16	114.68	121.33
2	A	301	A0Q	C29-N10-C25	3.54	119.53	111.57
2	B	301	A0Q	C29-N10-C25	3.36	119.13	111.57
2	B	301	A0Q	C4-C5-C6	-3.17	116.29	120.30
2	B	301	A0Q	C2-C11-N12	3.13	122.52	116.03
2	A	301	A0Q	C3-C2-C11	-2.96	120.91	126.24
2	B	301	A0Q	C25-C26-N27	-2.92	106.17	110.86
2	B	301	A0Q	O13-C11-C2	-2.79	115.92	121.03
2	A	301	A0Q	C17-N18-C19	2.78	121.72	116.85
2	B	301	A0Q	C8-O7-C3	2.75	123.20	117.76
2	B	301	A0Q	C17-N18-C19	2.63	121.46	116.85
2	B	301	A0Q	C28-N27-C26	2.59	113.67	109.54
2	B	301	A0Q	C30-N27-C26	2.40	115.21	110.63
2	B	301	A0Q	C29-C28-N27	-2.31	107.15	110.86
2	A	301	A0Q	C2-C11-N12	2.01	120.20	116.03
2	B	301	A0Q	C30-N27-C28	2.00	114.45	110.63

There are no chirality outliers.

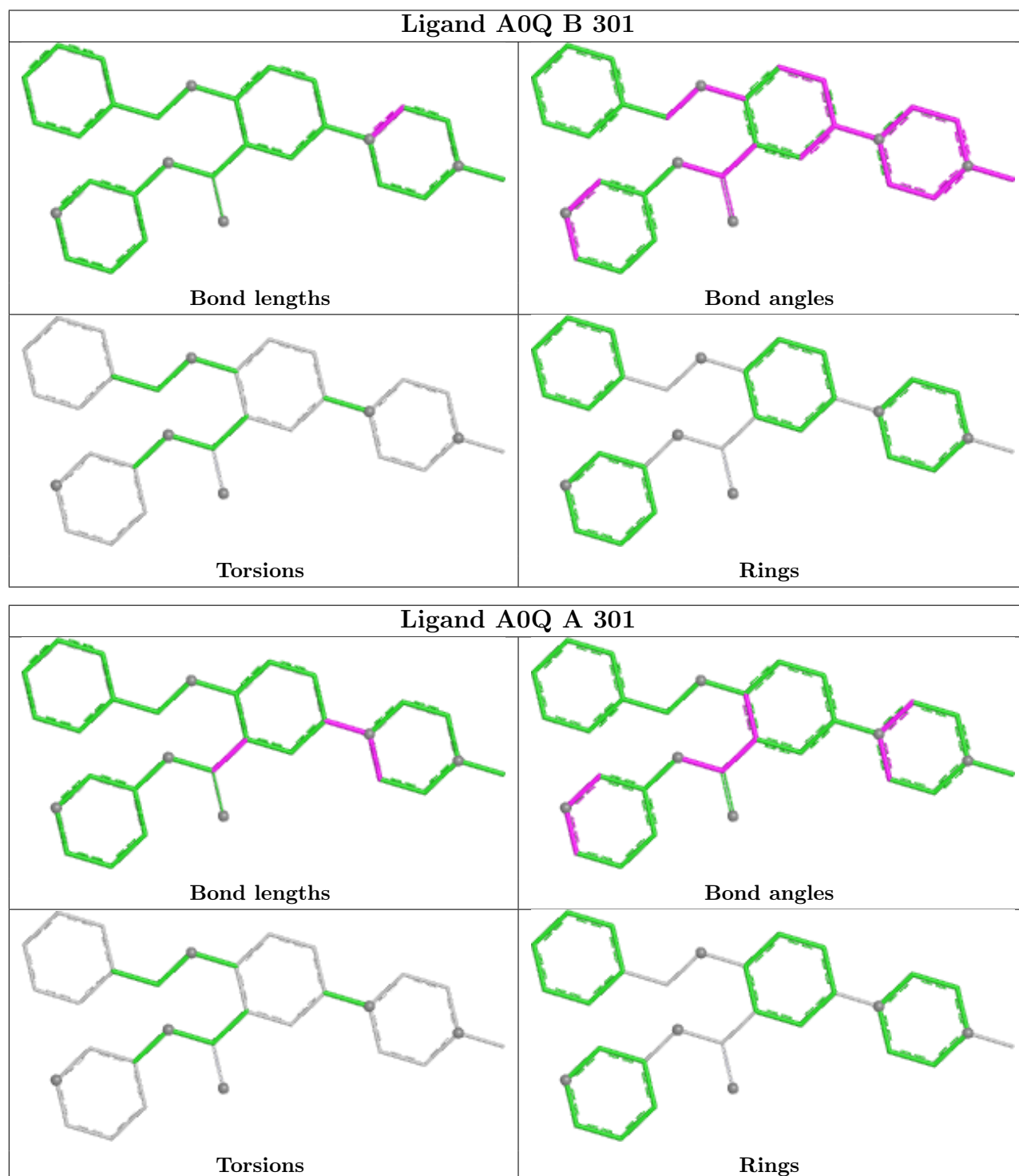
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/297 (87%)	1.06	42 (16%) 4 4	14, 31, 71, 82	1 (0%)
1	B	256/297 (86%)	1.88	105 (41%) 0 1	24, 41, 66, 84	1 (0%)
All	All	515/594 (86%)	1.47	147 (28%) 1 1	14, 37, 69, 84	2 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	LEU	5.6
1	B	96	ILE	5.2
1	B	215	CYS	5.2
1	B	40	VAL	5.1
1	B	100	ILE	4.7
1	B	12	VAL	4.6
1	A	41	ASP	4.5
1	B	173	TYR	4.4
1	A	79	ILE	4.4
1	A	9	TRP	4.3
1	B	269	LEU	4.3
1	A	40	VAL	4.2
1	B	79	ILE	4.2
1	A	30	VAL	4.2
1	A	19	ALA	4.0
1	A	31	THR	3.9
1	B	212	SER	3.7
1	B	219	SER	3.6
1	B	23	VAL	3.6
1	B	49	PRO	3.6
1	B	250	PRO	3.5
1	B	36	ALA	3.5
1	A	27	VAL	3.4
1	B	211	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	GLN	3.4
1	A	12	VAL	3.4
1	A	213	ASP	3.4
1	B	270	LYS	3.4
1	A	36	ALA	3.4
1	B	240	ALA	3.3
1	B	228	LEU	3.3
1	B	217	GLU	3.3
1	A	77	GLY	3.3
1	B	25	LEU	3.3
1	B	134	HIS	3.2
1	B	81	TYR	3.2
1	B	67	VAL	3.2
1	B	82	LEU	3.2
1	A	52	ILE	3.2
1	A	81	TYR	3.2
1	A	83	PHE	3.2
1	B	9	TRP	3.1
1	B	15	LEU	3.1
1	B	27	VAL	3.1
1	B	167	MET	3.1
1	A	11	LEU	3.1
1	B	14	THR	3.1
1	B	93	PHE	3.1
1	B	21	GLY	3.0
1	B	166	LYS	3.0
1	B	11	LEU	3.0
1	B	37	VAL	3.0
1	B	42	MET	3.0
1	B	18	GLY	3.0
1	B	54	LYS	3.0
1	A	20	TYR	3.0
1	B	51	ASN	2.9
1	B	138	LEU	2.9
1	B	189	VAL	2.9
1	B	198	LEU	2.9
1	A	21	GLY	2.9
1	B	141	ARG	2.8
1	B	171	LEU	2.8
1	B	114	LEU	2.8
1	A	14	THR	2.8
1	B	191	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	2.8
1	B	62	LEU	2.8
1	B	168	CYS	2.8
1	B	56	ILE	2.8
1	A	75	ARG	2.8
1	B	120	TYR	2.8
1	A	39	ILE	2.8
1	A	76	GLU	2.7
1	B	223	GLU	2.7
1	B	111	PHE	2.7
1	A	270	LYS	2.7
1	B	218	TYR	2.7
1	B	60	LYS	2.6
1	B	48	CYS	2.6
1	B	181	ARG	2.6
1	B	153	THR	2.6
1	B	237	ALA	2.6
1	A	49	PRO	2.6
1	A	154	VAL	2.6
1	B	98	PRO	2.6
1	A	15	LEU	2.6
1	A	25	LEU	2.6
1	A	48	CYS	2.5
1	B	144	LEU	2.5
1	A	24	GLN	2.5
1	B	175	ALA	2.5
1	B	8	ASP	2.5
1	B	242	LEU	2.5
1	A	42	MET	2.5
1	B	39	ILE	2.5
1	B	52	ILE	2.5
1	A	80	GLN	2.4
1	B	176	PRO	2.4
1	B	229	ASN	2.4
1	B	174	VAL	2.4
1	A	211	PRO	2.4
1	B	78	ASN	2.4
1	B	227	TYR	2.4
1	B	213	ASP	2.4
1	B	84	MET	2.4
1	B	182	ARG	2.3
1	A	72	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	2.3
1	B	118	VAL	2.3
1	A	227	TYR	2.3
1	B	24	GLN	2.3
1	B	241	LEU	2.3
1	B	264	TRP	2.3
1	A	50	GLU	2.2
1	B	259	ILE	2.2
1	B	30	VAL	2.2
1	A	10	ASP	2.2
1	A	144	LEU	2.2
1	B	206	LEU	2.2
1	B	160	ARG	2.2
1	B	267	LYS	2.2
1	A	82	LEU	2.2
1	A	214	SER	2.2
1	B	231	TRP	2.2
1	B	38	LYS	2.2
1	B	70	PHE	2.2
1	B	196	ILE	2.2
1	B	234	ILE	2.2
1	B	151	LEU	2.2
1	B	214	SER	2.2
1	B	251	SER	2.2
1	B	204	GLY	2.1
1	B	34	ALA	2.1
1	B	209	ASP	2.1
1	B	124	ILE	2.1
1	B	90	GLY	2.1
1	B	265	TYR	2.1
1	B	184	PHE	2.1
1	A	232	LYS	2.1
1	B	222	LYS	2.1
1	B	110	PHE	2.1
1	A	8	ASP	2.0
1	B	89	GLY	2.0
1	A	56	ILE	2.0
1	B	208	TRP	2.0
1	B	207	PRO	2.0

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 [i](#)

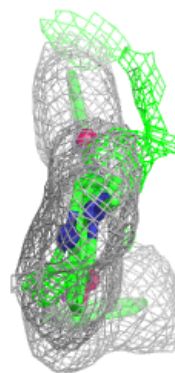
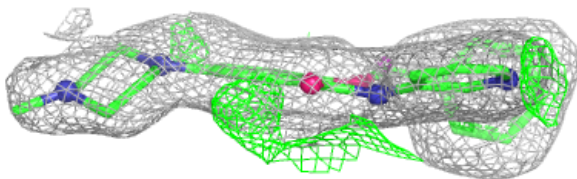
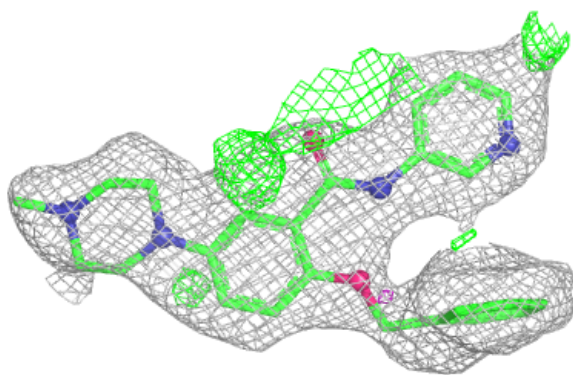
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A0Q	B	301	30/30	0.85	0.13	31,46,56,57	0
2	A0Q	A	301	30/30	0.89	0.12	23,41,51,53	0

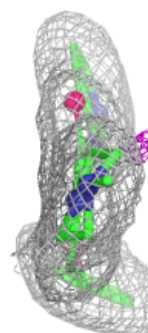
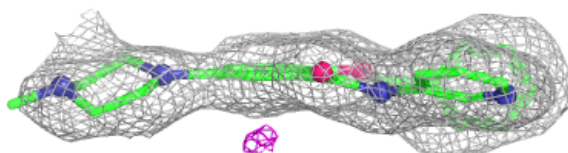
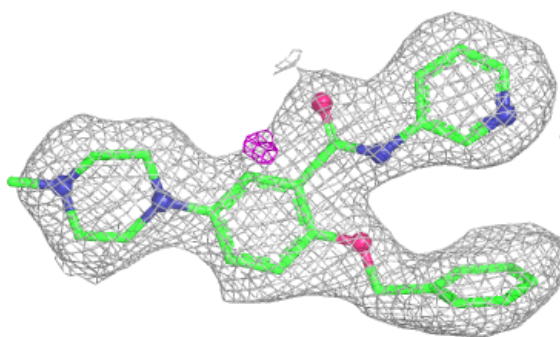
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A0Q B 301:

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

**Electron density around A0Q A 301:**

$2mF_o-DF_c$ (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.