



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 06:24 AM UTC

PDB ID : 7VDP / pdb_00007vdp
Title : The structure of cyclin-dependent kinase 5 (CDK5) in complex with p25 and Compound 1
Authors : Malojcic, G.; Clugston, S.L.; Daniels, M.; Harmange, J.C.; Ledeborer, M.
Deposited on : 2021-09-07
Resolution : 2.09 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

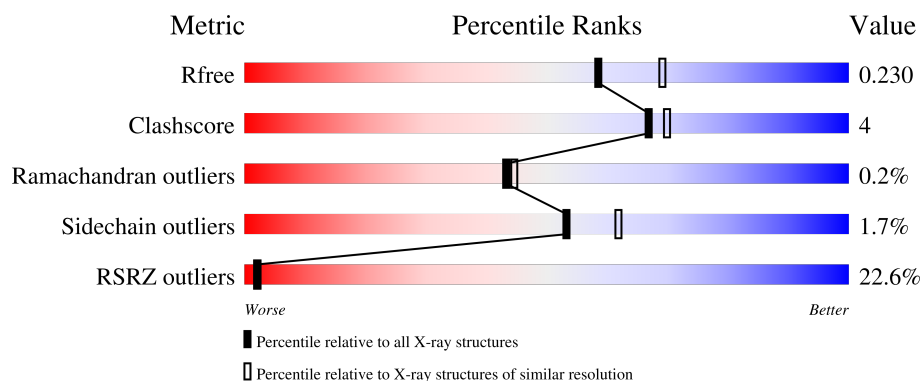
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	292	4% 90% 8% ..
1	B	292	23% 83% 12% ..
2	C	209	2% 69% 29% .
2	D	209	51% 53% 10% 37%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7321 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 Cyclin-dependent-like kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2307	1480	397	419	11			
1	B	279	Total	C	N	O	S	0	0	0
			2248	1447	388	403	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q00535
B	1	SER	-	expression tag	UNP Q00535

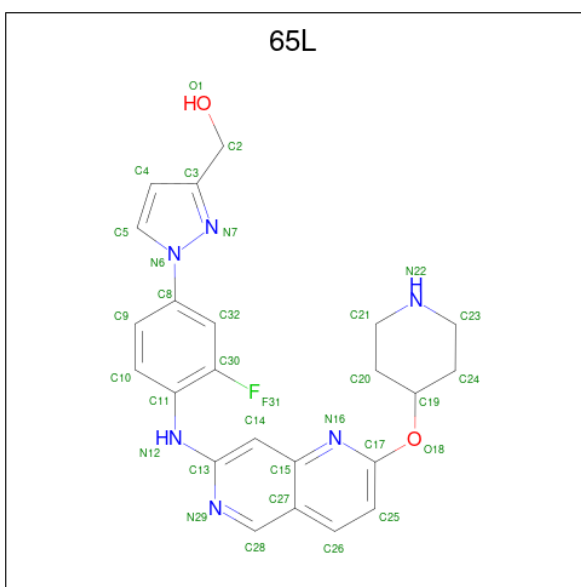
- Molecule 2 is a protein called Cyclin-dependent kinase 5 activator 1, p25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	148	Total	C	N	O	S	0	0	0
			1196	768	197	220	11			
2	D	131	Total	C	N	O	S	0	0	0
			1067	689	174	196	8			

There are 2 discrepancies between the modelled and reference sequences:

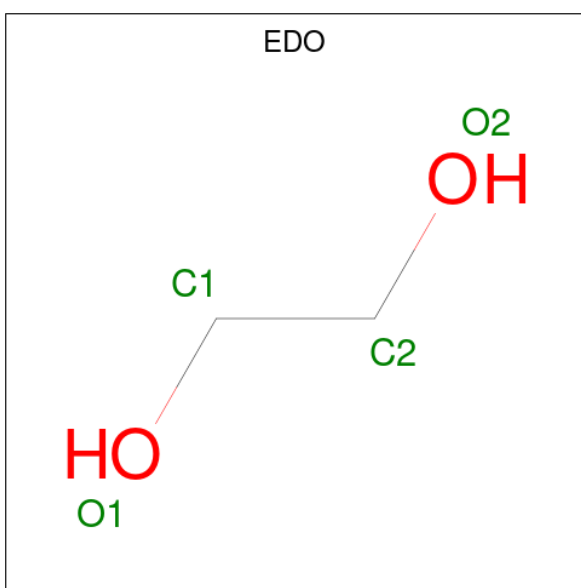
Chain	Residue	Modelled	Actual	Comment	Reference
C	99	MET	-	initiating methionine	UNP Q15078
D	99	MET	-	initiating methionine	UNP Q15078

- Molecule 3 is [1-[3-fluoranyl-4-[(2-piperidin-4-yloxy-1,6-naphthyridin-7-yl)amino]phenyl]pyrazol-3-yl]methanol (CCD ID: 65L) (formula: C₂₃H₂₃FN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 23	F 1	N 6	O 2	0	0
3	B	1	Total 32	C 23	F 1	N 6	O 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	Cl	0	0
			6	6		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	183	Total	O	0	0
			183	183		
8	B	86	Total	O	0	0
			86	86		
8	C	97	Total	O	0	0
			97	97		
8	D	6	Total	O	0	0
			6	6		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.37Å 118.37Å 155.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.79 – 2.09 51.79 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.79-2.09) 99.9 (51.79-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.229 0.207 , 0.230	Depositor DCC
R_{free} test set	3645 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PEG, CL, EDO, GOL, 65L

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	1.03	0/2360	1.29	1/3193 (0.0%)
1	B	1.02	0/2299	1.31	2/3109 (0.1%)
2	C	1.05	0/1224	1.40	0/1660
2	D	1.00	0/1091	1.45	0/1479
All	All	1.02	0/6974	1.34	3/9441 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	245	THR	CA-CB-OG1	-5.26	101.72	109.60
1	B	220	GLY	CA-C-O	-5.02	117.87	122.24

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	2307	0	2324	19	0
1	B	2248	0	2280	24	0
2	C	1196	0	1185	1	0
2	D	1067	0	1060	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	0	1	0
3	B	32	0	0	0	0
4	A	28	0	42	4	0
4	C	12	0	18	0	0
5	A	14	0	20	2	0
6	A	6	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	0	0
8	A	183	0	0	3	0
8	B	86	0	0	1	0
8	C	97	0	0	0	0
8	D	6	0	0	1	0
All	All	7321	0	6937	51	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 4.

All (51) 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)
2:D:249:LEU:HD21	2:D:254:LYS:HE3	1.78	0.66
2:D:261:CYS:SG	8:D:404:HOH:O	2.53	0.66
1:B:157:CYS:HB2	1:B:177:LYS:HB3	1.81	0.63
1:B:153:ILE:HD12	2:D:276:ASN:HA	1.82	0.62
1:B:21:ALA:HB3	1:B:32:LEU:HD13	1.85	0.57
2:D:249:LEU:HD21	2:D:254:LYS:CE	2.38	0.54
1:A:61:LYS:NZ	8:A:403:HOH:O	2.41	0.53
1:B:43:GLY:O	1:B:46:SER:OG	2.27	0.52
1:A:260:ARG:HB2	5:A:310:PEG:H12	1.91	0.52
1:B:287:SER:O	1:B:288:ASP:OD1	2.27	0.52
1:A:12:GLU:HA	1:A:17:THR:HA	1.93	0.50
3:A:301:65L:C10	4:A:302:EDO:H12	2.41	0.49
1:A:136:ARG:HA	4:A:307:EDO:H11	1.94	0.49
1:B:78:LEU:N	1:B:78:LEU:HD23	2.28	0.48
2:D:208:CYS:HA	2:D:212:ILE:HD13	1.96	0.48
1:B:256:ASN:OD1	1:B:256:ASN:N	2.47	0.48
1:A:241:MET:HE3	8:A:469:HOH:O	2.14	0.47
1:B:53:CYS:SG	2:D:265:ILE:HG12	2.53	0.47
1:A:78:LEU:HD12	1:A:78:LEU:N	2.29	0.47
1:B:159:SER:HB2	2:D:239:ASN:O	2.14	0.47
1:A:135:ASN:O	4:A:307:EDO:H22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HD23	2:D:258:TRP:CD1	2.49	0.47
1:B:50:ARG:NH1	1:B:148:ALA:O	2.47	0.47
1:B:30:VAL:HG23	1:B:32:LEU:CD1	2.46	0.46
1:A:40:ASP:OD2	1:B:36:ARG:NH2	2.49	0.46
1:A:162:VAL:HG21	1:A:179:TYR:OH	2.17	0.45
1:B:98:LEU:O	1:B:254:LYS:HE3	2.15	0.45
1:B:34:ARG:CG	1:B:75:LYS:HD2	2.47	0.45
2:D:255:GLU:O	2:D:259:ASP:HB2	2.17	0.45
2:D:151:LEU:HD22	2:D:289:LEU:HD23	2.00	0.44
1:B:196:ALA:HB1	1:B:255:LEU:HG	1.98	0.44
1:B:120:ARG:O	2:D:273:LEU:HD11	2.17	0.44
1:B:35:VAL:HG13	1:B:44:VAL:HG12	2.00	0.43
1:A:136:ARG:N	1:A:136:ARG:HD2	2.32	0.43
1:A:36:ARG:CZ	1:B:36:ARG:HD2	2.49	0.43
1:B:60:HIS:O	8:B:401:HOH:O	2.21	0.43
2:D:190:TRP:CE3	2:D:190:TRP:HA	2.54	0.43
1:B:127:LEU:CD2	1:B:142:LEU:HD11	2.48	0.43
1:A:39:ASP:HB2	1:A:42:GLU:HA	2.01	0.43
2:D:228:THR:HG21	2:D:260:ARG:HD2	2.01	0.42
1:A:44:VAL:N	1:A:45:PRO:CD	2.83	0.42
1:A:257:ALA:HA	5:A:310:PEG:H11	2.02	0.42
1:B:116:PHE:O	1:B:120:ARG:HG2	2.19	0.42
1:A:36:ARG:CD	1:B:36:ARG:CZ	2.98	0.42
2:C:246:LYS:HB3	2:C:247:PRO:HD3	2.01	0.42
1:A:180:SER:HB2	8:A:554:HOH:O	2.20	0.42
1:A:136:ARG:HA	4:A:307:EDO:C1	2.50	0.41
1:B:44:VAL:HB	1:B:45:PRO:HD3	2.03	0.41
1:A:213:LYS:O	1:A:217:ARG:HB2	2.21	0.41
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.96	0.40
2:D:206:MET:HE3	2:D:206:MET:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	283/292 (97%)	270 (95%)	12 (4%)	1 (0%)	30	28
1	B	273/292 (94%)	262 (96%)	10 (4%)	1 (0%)	30	28
2	C	146/209 (70%)	146 (100%)	0	0	100	100
2	D	125/209 (60%)	122 (98%)	3 (2%)	0	100	100
All	All	827/1002 (82%)	800 (97%)	25 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	VAL
1	B	163	VAL

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	256/260 (98%)	252 (98%)	4 (2%)	55	64
1	B	249/260 (96%)	245 (98%)	4 (2%)	55	64
2	C	138/187 (74%)	137 (99%)	1 (1%)	76	83
2	D	124/187 (66%)	120 (97%)	4 (3%)	34	38
All	All	767/894 (86%)	754 (98%)	13 (2%)	53	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	42	GLU
1	A	141	LYS
1	A	232	LYS
1	B	78	LEU
1	B	102	ILE

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	153	ILE
2	C	293	SER
2	D	170	SER
2	D	186	LEU
2	D	206	MET
2	D	283	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	206	ASN
1	A	256	ASN
1	B	27	HIS
1	B	85	GLN
1	B	282	GLN
2	C	188	GLN
2	C	266	ASN
2	D	188	GLN
2	D	239	ASN
2	D	266	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](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

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$
4	EDO	A	305	-	3,3,3	0.10	0	2,2,2	0.13	0
7	GOL	A	317	-	5,5,5	0.10	0	5,5,5	0.28	0
4	EDO	C	403	-	3,3,3	0.03	0	2,2,2	0.12	0
4	EDO	C	402	-	3,3,3	0.07	0	2,2,2	0.13	0
5	PEG	A	310	-	6,6,6	0.18	0	5,5,5	0.24	0
3	65L	B	301	-	36,36,36	0.82	2 (5%)	45,50,50	2.42	12 (26%)
4	EDO	A	303	-	3,3,3	0.09	0	2,2,2	0.16	0
4	EDO	A	304	-	3,3,3	0.09	0	2,2,2	0.13	0
3	65L	A	301	-	36,36,36	0.82	1 (2%)	45,50,50	2.45	12 (26%)
4	EDO	C	401	-	3,3,3	0.25	0	2,2,2	0.14	0
4	EDO	A	302	-	3,3,3	0.25	0	2,2,2	0.61	0
4	EDO	A	307	-	3,3,3	0.08	0	2,2,2	0.28	0
4	EDO	A	306	-	3,3,3	0.07	0	2,2,2	0.17	0
5	PEG	A	309	-	6,6,6	0.19	0	5,5,5	0.13	0
4	EDO	A	308	-	3,3,3	0.04	0	2,2,2	0.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	305	-	-	0/1/1/1	-
7	GOL	A	317	-	-	0/4/4/4	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	C	402	-	-	1/1/1/1	-
5	PEG	A	310	-	-	3/4/4/4	-
3	65L	B	301	-	-	0/14/22/22	0/5/5/5
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
3	65L	A	301	-	-	1/14/22/22	0/5/5/5
4	EDO	C	401	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	306	-	-	1/1/1/1	-
5	PEG	A	309	-	-	3/4/4/4	-
4	EDO	A	308	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	65L	N6-N7	2.93	1.40	1.36
3	B	301	65L	N6-N7	2.80	1.40	1.36
3	B	301	65L	C15-N16	-2.06	1.34	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	65L	C3-N7-N6	8.34	108.94	104.89
3	A	301	65L	C17-N16-C15	7.56	121.51	115.85
3	B	301	65L	C17-N16-C15	7.38	121.37	115.85
3	B	301	65L	C3-N7-N6	7.23	108.40	104.89
3	A	301	65L	C5-N6-N7	-5.59	106.87	111.66
3	B	301	65L	C28-N29-C13	5.49	122.97	117.81
3	B	301	65L	C5-N6-N7	-4.99	107.38	111.66
3	A	301	65L	C28-N29-C13	4.63	122.16	117.81
3	B	301	65L	C8-N6-N7	4.46	125.35	119.93
3	A	301	65L	C17-O18-C19	2.93	120.84	117.82
3	B	301	65L	C17-O18-C19	2.78	120.69	117.82
3	A	301	65L	C14-C15-N16	2.77	122.84	118.78
3	B	301	65L	C5-C4-C3	2.77	107.65	105.47
3	A	301	65L	C8-N6-N7	2.65	123.14	119.93
3	A	301	65L	C5-C4-C3	2.61	107.52	105.47
3	B	301	65L	C32-C30-C11	-2.59	120.78	123.43
3	A	301	65L	O18-C17-N16	2.48	121.76	119.69
3	A	301	65L	C25-C17-N16	-2.40	120.71	125.11
3	B	301	65L	C14-C15-N16	2.37	122.25	118.78
3	A	301	65L	C14-C13-N29	-2.34	119.85	122.93
3	B	301	65L	O18-C17-N16	2.24	121.56	119.69
3	B	301	65L	C27-C28-N29	-2.21	120.69	124.25
3	B	301	65L	C25-C17-N16	-2.13	121.20	125.11
3	A	301	65L	C26-C25-C17	2.02	120.25	117.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

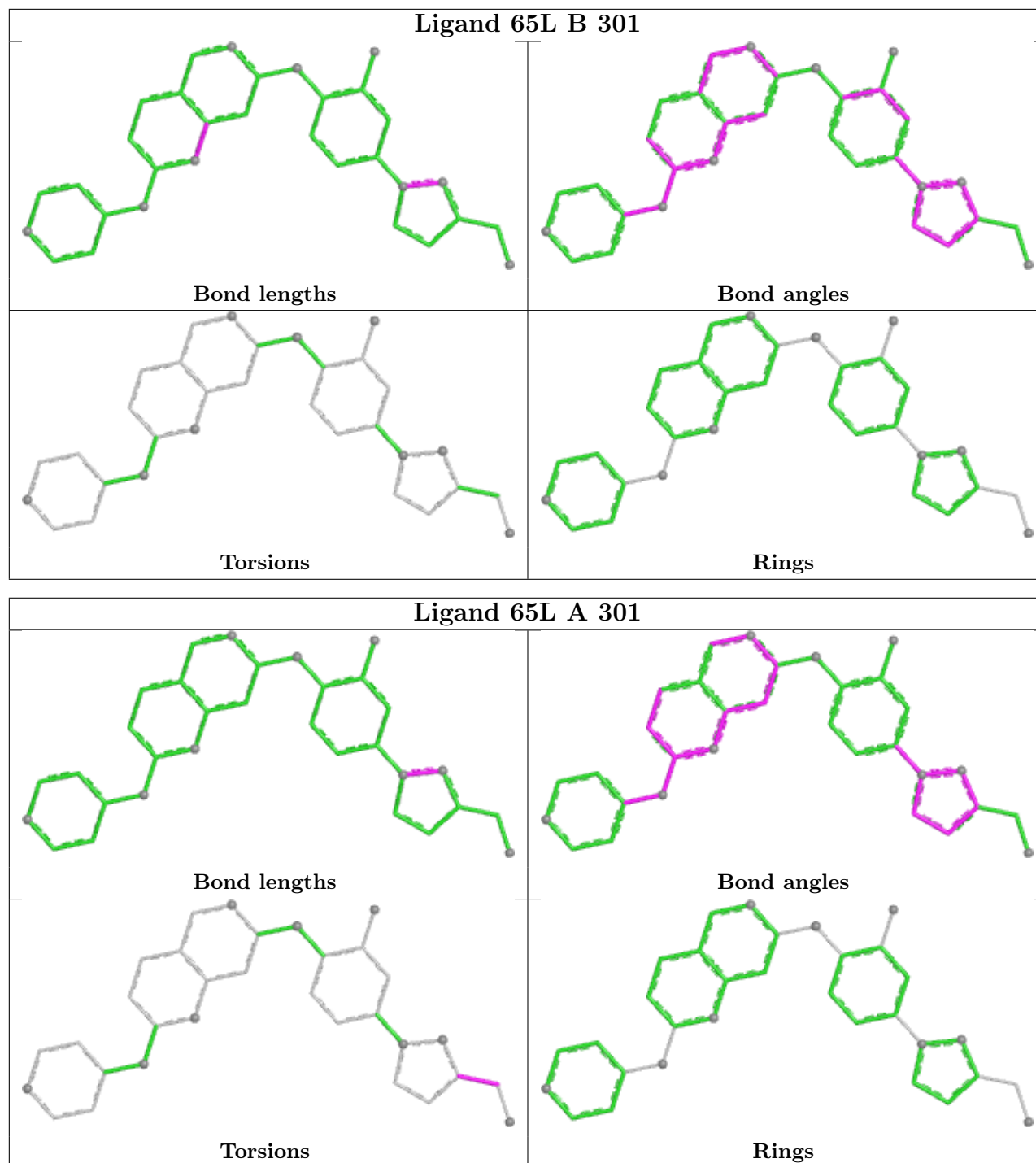
Mol	Chain	Res	Type	Atoms
3	A	301	65L	O1-C2-C3-N7
5	A	309	PEG	O1-C1-C2-O2
5	A	309	PEG	O2-C3-C4-O4
5	A	310	PEG	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
4	C	402	EDO	O1-C1-C2-O2
5	A	309	PEG	C1-C2-O2-C3
5	A	310	PEG	C1-C2-O2-C3
4	C	401	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
5	A	310	PEG	C4-C3-O2-C2
4	A	306	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	310	PEG	2	0
3	A	301	65L	1	0
4	A	302	EDO	1	0
4	A	307	EDO	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.



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	287/292 (98%)	0.28	13 (4%) 38 40	29, 41, 79, 123	0
1	B	279/292 (95%)	1.25	68 (24%) 2 2	37, 68, 125, 161	0
2	C	148/209 (70%)	0.14	4 (2%) 56 59	31, 41, 63, 76	0
2	D	131/209 (62%)	3.42	106 (80%) 0 0	99, 134, 158, 174	0
All	All	845/1002 (84%)	1.06	191 (22%) 2 2	29, 53, 142, 174	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	LEU	10.5
2	D	222	LEU	8.3
2	D	207	LEU	7.6
2	D	203	PHE	7.5
2	D	212	ILE	7.4
2	D	224	ALA	7.2
2	D	211	VAL	7.1
2	D	236	TYR	7.0
1	B	15	TYR	6.6
2	D	285	VAL	6.1
2	D	241	ILE	6.0
1	B	21	ALA	5.8
2	D	178	LEU	5.8
2	D	235	SER	5.7
2	D	225	VAL	5.6
2	D	169	LEU	5.6
2	D	227	LEU	5.6
2	D	258	TRP	5.6
2	D	151	LEU	5.5
2	D	152	LEU	5.3
2	D	175	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	176	LEU	5.1
2	D	166	LEU	5.0
2	D	229	CYS	4.9
2	D	275	ILE	4.9
2	D	177	TRP	4.8
2	D	231	TYR	4.8
2	D	232	LEU	4.7
1	A	162	VAL	4.6
1	A	16	GLY	4.6
1	B	178	LEU	4.5
2	D	204	LEU	4.5
2	D	201	VAL	4.4
2	D	265	ILE	4.4
2	D	243	TYR	4.4
2	D	281	TYR	4.4
2	D	237	MET	4.3
1	B	30	VAL	4.3
2	D	283	THR	4.3
2	D	289	LEU	4.2
2	D	264	VAL	4.2
1	A	11	GLY	4.2
2	D	239	ASN	4.1
2	D	248	PHE	4.1
2	D	257	PHE	4.0
2	D	273	LEU	4.0
2	D	174	PRO	4.0
2	D	195	PHE	4.0
2	D	205	TYR	3.9
2	D	202	VAL	3.9
2	D	181	VAL	3.9
2	D	250	VAL	3.9
1	B	29	ILE	3.9
1	A	160	ALA	3.9
1	A	156	ARG	3.8
2	D	245	LEU	3.8
1	B	10	ILE	3.7
2	C	146	ALA	3.7
1	B	26	THR	3.7
1	B	70	LEU	3.7
2	D	148	THR	3.7
2	D	230	LEU	3.6
2	D	267	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	210	ASP	3.6
2	D	200	ASN	3.6
1	B	7	LEU	3.6
1	B	43	GLY	3.5
2	D	196	ILE	3.5
2	D	171	PRO	3.5
2	D	247	PRO	3.5
1	B	32	LEU	3.5
2	D	277	ALA	3.5
2	D	268	MET	3.4
1	B	58	LEU	3.4
2	D	168	HIS	3.4
1	B	245	THR	3.4
1	B	78	LEU	3.3
1	B	17	THR	3.3
2	D	228	THR	3.3
2	D	272	MET	3.3
1	A	155	VAL	3.3
1	B	18	VAL	3.3
2	D	271	LYS	3.3
1	B	49	LEU	3.2
1	B	76	LEU	3.2
2	D	259	ASP	3.1
2	D	165	ARG	3.1
2	D	244	PRO	3.1
2	D	208	CYS	3.1
2	D	249	LEU	3.1
2	D	242	SER	3.1
2	D	282	PHE	3.1
1	B	44	VAL	3.1
2	D	206	MET	3.1
1	B	16	GLY	3.1
2	D	198	PRO	3.1
2	D	269	SER	3.1
1	B	4	TYR	3.0
2	D	286	PHE	3.0
2	D	220	HIS	3.0
1	B	31	ALA	3.0
2	D	263	SER	3.0
2	D	197	THR	3.0
1	B	56	LYS	3.0
1	B	251	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	219	ASP	2.9
1	B	249	VAL	2.9
1	A	41	ASP	2.9
2	C	241	ILE	2.9
1	B	22	LYS	2.9
2	D	262	LEU	2.9
1	A	39	ASP	2.9
1	B	39	ASP	2.9
1	B	79	VAL	2.9
1	B	66	LEU	2.8
2	D	293	SER	2.8
2	D	256	ALA	2.8
1	B	20	LYS	2.8
1	B	72	SER	2.8
1	B	75	LYS	2.8
2	D	147	SER	2.8
1	A	12	GLU	2.8
1	B	37	LEU	2.8
1	B	69	VAL	2.8
2	D	261	CYS	2.8
1	A	158	TYR	2.7
1	B	77	THR	2.7
2	D	279	PRO	2.7
2	D	223	GLN	2.7
1	B	3	LYS	2.7
1	B	286	PHE	2.7
2	D	234	TYR	2.7
1	B	52	ILE	2.7
1	B	65	ARG	2.7
1	B	246	THR	2.7
1	B	63	ILE	2.7
2	D	190	TRP	2.7
2	D	213	SER	2.6
1	B	9	LYS	2.6
1	B	244	ALA	2.6
2	D	199	ALA	2.6
2	D	185	LEU	2.6
2	D	180	SER	2.6
1	B	24	ARG	2.6
2	D	290	LYS	2.6
2	D	209	ARG	2.6
2	D	233	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	2.6
2	D	278	ASP	2.6
2	D	253	CYS	2.5
2	D	270	SER	2.5
1	B	262	LEU	2.5
1	B	74	LYS	2.4
2	D	276	ASN	2.4
1	B	142	LEU	2.4
2	D	187	LEU	2.4
1	B	53	CYS	2.4
1	A	43	GLY	2.3
1	B	19	PHE	2.3
1	A	291	PRO	2.3
2	C	284	GLN	2.3
1	B	154	PRO	2.3
1	B	6	LYS	2.3
1	B	288	ASP	2.3
1	B	248	LEU	2.3
1	B	224	GLU	2.2
2	D	240	GLU	2.2
2	D	238	GLY	2.2
1	B	25	GLU	2.2
1	B	54	LEU	2.2
1	B	64	VAL	2.2
2	D	260	ARG	2.2
2	D	172	THR	2.2
1	B	55	LEU	2.1
2	D	153	ARG	2.1
2	D	186	LEU	2.1
1	B	285	TYR	2.1
2	C	239	ASN	2.1
1	B	151	PHE	2.1
1	B	153	ILE	2.1
1	B	122	VAL	2.1
2	D	170	SER	2.1
2	D	251	GLU	2.1
1	B	223	THR	2.1
2	D	274	GLN	2.0
1	A	289	PHE	2.0
1	B	82	PHE	2.0
1	B	247	SER	2.0
1	B	250	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	265	ASN	2.0
2	D	179	ARG	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(Å ²)	Q<0.9
4	EDO	A	308	4/4	0.66	0.24	69,76,80,83	0
4	EDO	A	306	4/4	0.74	0.16	92,92,95,97	0
4	EDO	C	403	4/4	0.77	0.17	72,73,73,75	0
7	GOL	A	317	6/6	0.79	0.15	72,74,75,77	0
5	PEG	A	310	7/7	0.80	0.18	48,58,62,64	0
4	EDO	A	307	4/4	0.83	0.20	70,73,74,75	0
4	EDO	A	304	4/4	0.84	0.16	82,84,84,85	0
5	PEG	A	309	7/7	0.84	0.18	58,60,66,66	0
4	EDO	A	302	4/4	0.85	0.23	43,47,52,56	0
4	EDO	A	305	4/4	0.86	0.20	60,60,61,61	0
4	EDO	C	402	4/4	0.88	0.21	71,74,75,77	0
3	65L	B	301	32/32	0.89	0.12	53,69,74,76	0
6	CL	A	315	1/1	0.89	0.16	75,75,75,75	0
4	EDO	A	303	4/4	0.89	0.14	58,64,66,67	0
6	CL	A	312	1/1	0.90	0.26	63,63,63,63	0
4	EDO	C	401	4/4	0.93	0.27	42,43,43,44	0
6	CL	C	404	1/1	0.93	0.16	73,73,73,73	0
6	CL	A	314	1/1	0.93	0.13	64,64,64,64	0
3	65L	A	301	32/32	0.95	0.08	32,39,55,61	0
6	CL	A	316	1/1	0.95	0.15	87,87,87,87	0
6	CL	A	313	1/1	0.96	0.11	54,54,54,54	0

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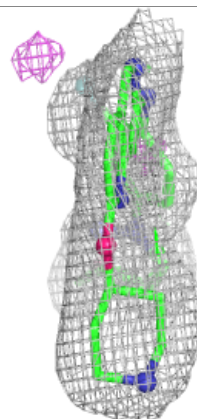
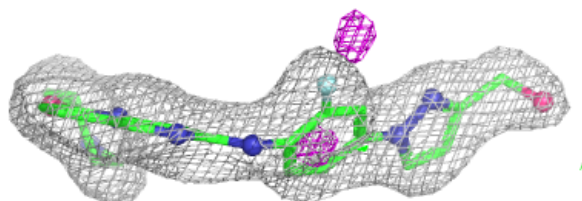
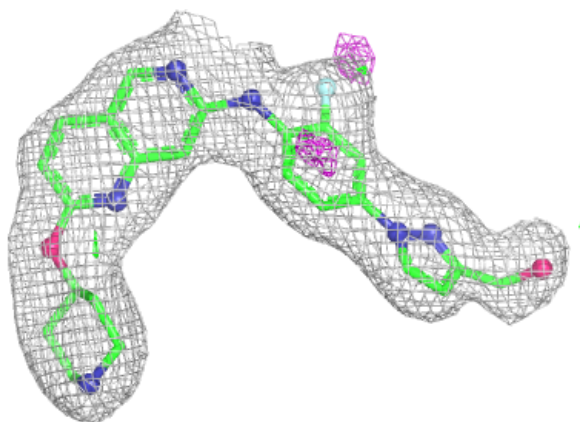
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	311	1/1	0.96	0.10	44,44,44,44	0

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.

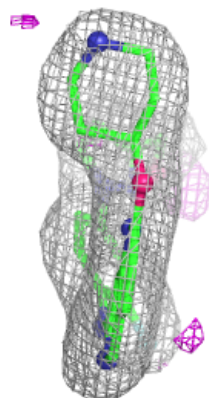
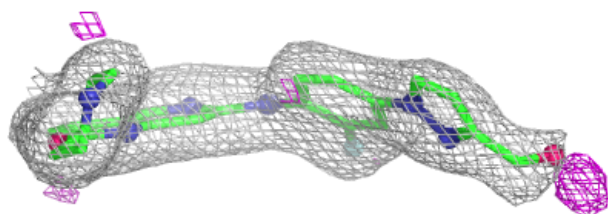
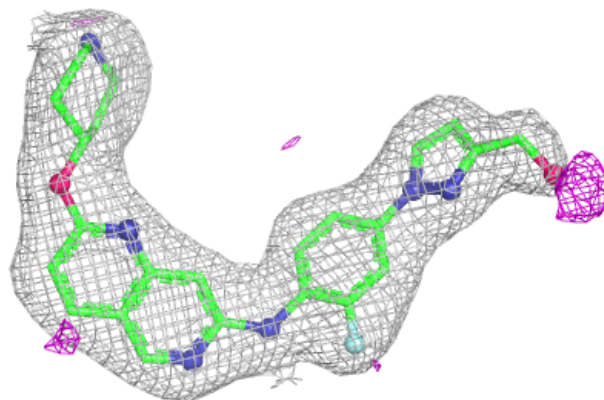
Electron density around 65L B 301:

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 65L 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 ⓘ

There are no such residues in this entry.