Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2025 – 04:09 PM JST

PDB ID	:	9LVR / pdb_00009lvr
Title	:	Crystal structure of SARS-CoV-2 3CL protease in complex with compound 1
Authors	:	Unoh, Y.; Hirai, K.; Uehara, S.; Kawashima, S.; Nobori, H.; Sato, J.; Shibayama, H.; Hori, A.; Nakahara, K.; Kurahashi, K.; Takamatsu, M.; Yamamoto, S.; Zhang, O.; Tanimura, M.; Dodo, R.; Maruyama, Y.; Sawa, H.; Watari, R.; Miyano, T.; Kato, T.; Sato, T.; Tachibana, Y.
Deposited on	:	2025-02-12
Resolution	:	2.20 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:

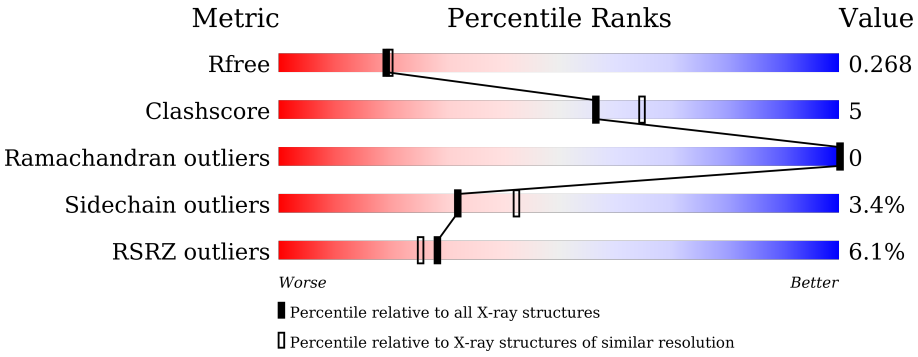
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	9% 76% 13% • 10%
1	B	329	2% 79% 10% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4619 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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2211	1403	368	418	22			
1	B	297	Total	C	N	O	S	0	1	0
			2269	1437	382	428	22			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P0DTD1
A	-21	GLY	-	expression tag	UNP P0DTD1
A	-20	SER	-	expression tag	UNP P0DTD1
A	-19	SER	-	expression tag	UNP P0DTD1
A	-18	HIS	-	expression tag	UNP P0DTD1
A	-17	HIS	-	expression tag	UNP P0DTD1
A	-16	HIS	-	expression tag	UNP P0DTD1
A	-15	HIS	-	expression tag	UNP P0DTD1
A	-14	HIS	-	expression tag	UNP P0DTD1
A	-13	HIS	-	expression tag	UNP P0DTD1
A	-12	HIS	-	expression tag	UNP P0DTD1
A	-11	HIS	-	expression tag	UNP P0DTD1
A	-10	HIS	-	expression tag	UNP P0DTD1
A	-9	HIS	-	expression tag	UNP P0DTD1
A	-8	SER	-	expression tag	UNP P0DTD1
A	-7	SER	-	expression tag	UNP P0DTD1
A	-6	GLY	-	expression tag	UNP P0DTD1
A	-5	LEU	-	expression tag	UNP P0DTD1
A	-4	VAL	-	expression tag	UNP P0DTD1
A	-3	PRO	-	expression tag	UNP P0DTD1
A	-2	ARG	-	expression tag	UNP P0DTD1
A	-1	GLY	-	expression tag	UNP P0DTD1
A	0	SER	-	expression tag	UNP P0DTD1
B	-22	MET	-	initiating methionine	UNP P0DTD1
B	-21	GLY	-	expression tag	UNP P0DTD1

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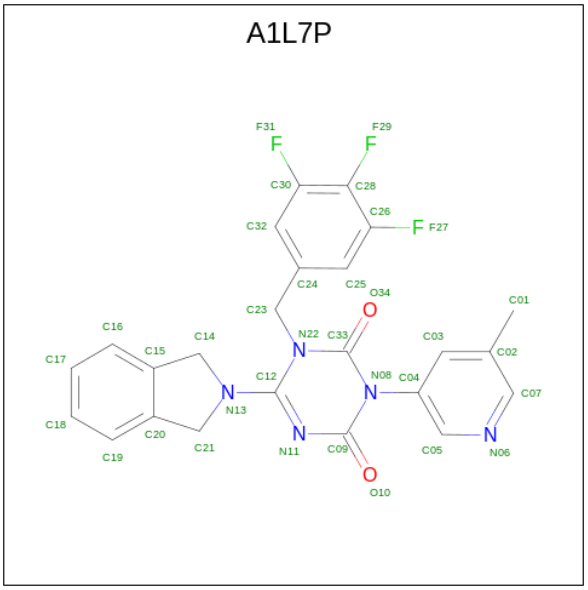
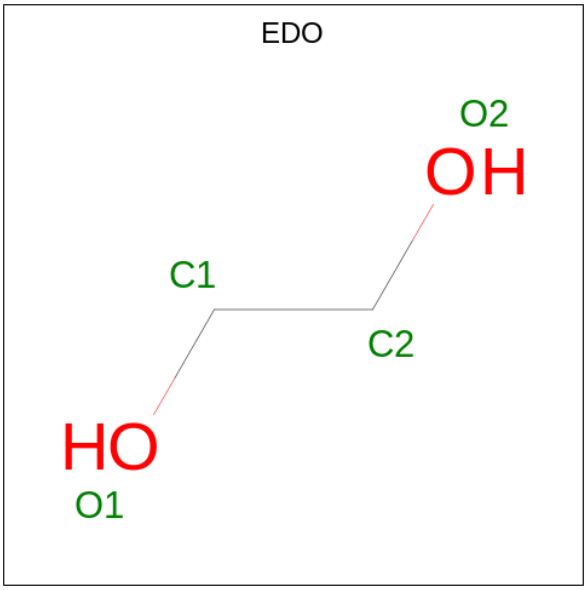
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP P0DTD1
B	-19	SER	-	expression tag	UNP P0DTD1
B	-18	HIS	-	expression tag	UNP P0DTD1
B	-17	HIS	-	expression tag	UNP P0DTD1
B	-16	HIS	-	expression tag	UNP P0DTD1
B	-15	HIS	-	expression tag	UNP P0DTD1
B	-14	HIS	-	expression tag	UNP P0DTD1
B	-13	HIS	-	expression tag	UNP P0DTD1
B	-12	HIS	-	expression tag	UNP P0DTD1
B	-11	HIS	-	expression tag	UNP P0DTD1
B	-10	HIS	-	expression tag	UNP P0DTD1
B	-9	HIS	-	expression tag	UNP P0DTD1
B	-8	SER	-	expression tag	UNP P0DTD1
B	-7	SER	-	expression tag	UNP P0DTD1
B	-6	GLY	-	expression tag	UNP P0DTD1
B	-5	LEU	-	expression tag	UNP P0DTD1
B	-4	VAL	-	expression tag	UNP P0DTD1
B	-3	PRO	-	expression tag	UNP P0DTD1
B	-2	ARG	-	expression tag	UNP P0DTD1
B	-1	GLY	-	expression tag	UNP P0DTD1
B	0	SER	-	expression tag	UNP P0DTD1

- Molecule 2 is 6-(1,3-dihydroisoindol-2-yl)-3-(5-methylpyridin-3-yl)-1-[[3,4,5-tris(fluoranyl)phenyl]methyl]-1,3,5-triazine-2,4-dione (CCD ID: A1L7P) (formula: $C_{24}H_{18}F_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	24	3	5	2		
2	B	1	Total	C	F	N	O	0	0
			34	24	3	5	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

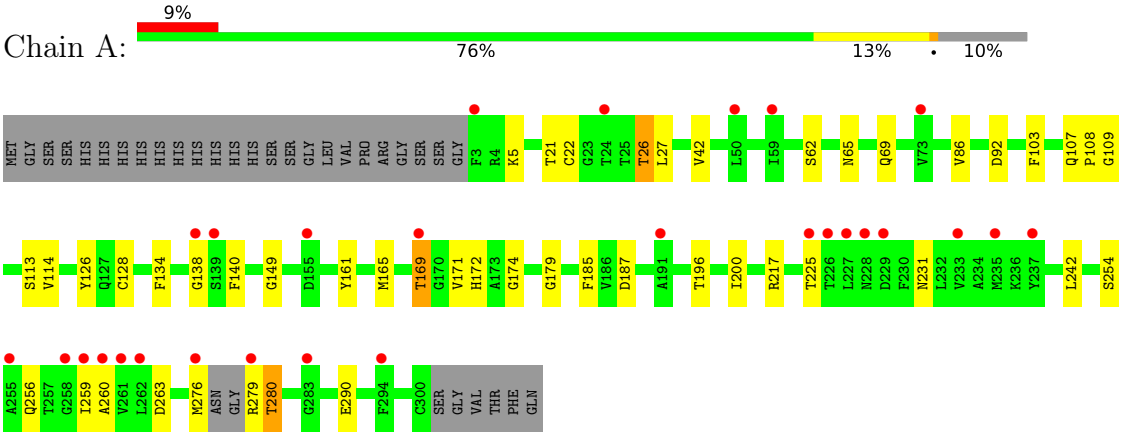
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	40	Total	O	0	0
			40	40		

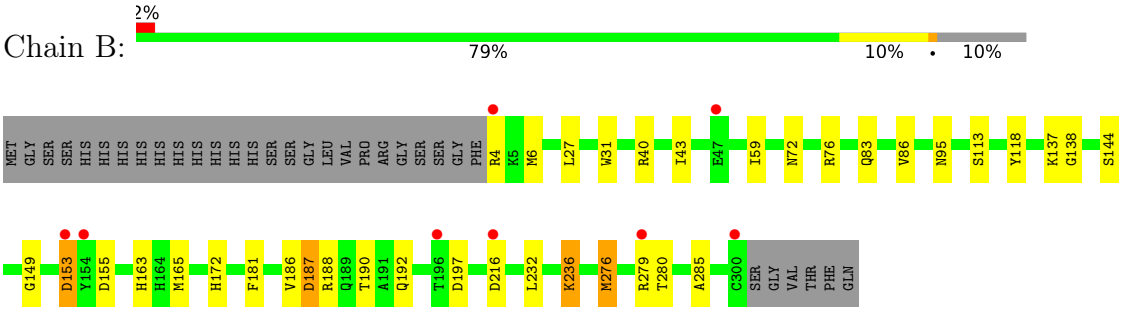
3 Residue-property plots (i)

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: 3C-like proteinase nsp5



• Molecule 1: 3C-like proteinase nsp5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.83Å 101.25Å 104.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.23 – 2.20 30.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.23-2.20) 99.2 (30.23-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.223 , 0.268 0.229 , 0.268	Depositor DCC
R_{free} test set	1765 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: EDO, A1L7P

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	0.58	0/2260	1.13	9/3081 (0.3%)
1	B	0.59	0/2322	1.11	4/3160 (0.1%)
All	All	0.59	0/4582	1.12	13/6241 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	CYS	CB-CA-C	-12.48	84.91	111.11
1	B	153	ASP	CB-CA-C	6.78	121.63	110.78
1	B	188	ARG	N-CA-CB	-6.29	99.75	111.13
1	A	196	THR	CA-CB-OG1	-6.07	100.49	109.60
1	A	263	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	26	THR	CA-CB-OG1	-5.80	100.89	109.60
1	A	92	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	187	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	103	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	187	ASP	CA-CB-CG	5.41	118.00	112.60
1	A	107	GLN	CB-CA-C	-5.11	100.80	108.61
1	A	217	ARG	CB-CA-C	-5.10	101.88	110.64
1	B	188	ARG	CB-CA-C	5.04	119.67	109.68

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	2211	0	2067	24	0
1	B	2269	0	2183	17	0
2	A	34	0	0	0	0
2	B	34	0	0	1	0
3	A	4	0	6	0	0
4	A	27	0	0	0	0
4	B	40	0	0	0	0
All	All	4619	0	4256	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (40) 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:21:THR:OG1	1:A:26:THR:HG22	1.69	0.93
1:A:231:ASN:HD21	1:A:242:LEU:H	1.31	0.78
1:A:256:GLN:HG2	1:A:256:GLN:O	1.87	0.74
1:A:62:SER:H	1:A:65:ASN:HD22	1.40	0.69
1:B:186:VAL:H	1:B:192:GLN:HE22	1.40	0.69
1:B:137:LYS:NZ	1:B:197:ASP:OD2	2.30	0.65
1:A:126:TYR:CD2	1:B:4:ARG:HD2	2.37	0.60
1:B:232:LEU:O	1:B:236:LYS:HD2	2.06	0.55
1:A:276:MET:O	1:A:279:ARG:HB3	2.08	0.54
1:A:114:VAL:HG11	1:A:140:PHE:CZ	2.43	0.53
1:B:165:MET:HE1	1:B:187:ASP:HA	1.91	0.52
1:B:276:MET:HE2	1:B:285:ALA:HA	1.91	0.51
1:A:169:THR:HG23	1:A:171:VAL:HG22	1.93	0.50
1:A:138:GLY:H	1:A:172:HIS:HD2	1.60	0.50
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.46	0.50
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.95	0.49
1:B:138:GLY:H	1:B:172:HIS:HD2	1.61	0.48
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.49	0.48
1:A:165:MET:CE	1:A:185:PHE:HB3	2.45	0.47
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.97	0.47
1:B:163:HIS:NE2	2:B:401:A1L7P:N06	2.63	0.47
1:B:113:SER:O	1:B:149:GLY:HA2	2.15	0.46
1:B:276:MET:O	1:B:279:ARG:HG2	2.15	0.46
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:O	1:B:86:VAL:HG12	2.16	0.46
1:A:22:CYS:HB3	1:A:42:VAL:O	2.17	0.45
1:B:40:ARG:O	1:B:43:ILE:HG12	2.17	0.45
1:A:113:SER:O	1:A:149:GLY:HA2	2.17	0.44
1:A:62:SER:H	1:A:65:ASN:ND2	2.12	0.43
1:B:27:LEU:C	1:B:27:LEU:HD12	2.44	0.43
1:A:161:TYR:CE1	1:A:174:GLY:HA3	2.54	0.42
1:A:138:GLY:H	1:A:172:HIS:CD2	2.37	0.42
1:A:256:GLN:O	1:A:256:GLN:CG	2.64	0.41
1:A:279:ARG:CG	1:A:280:THR:H	2.33	0.41
1:A:5:LYS:NZ	1:A:290:GLU:OE1	2.51	0.41
1:A:165:MET:HE1	1:A:185:PHE:HB3	2.02	0.41
1:A:254:SER:OG	1:A:260:ALA:HA	2.21	0.41
1:B:118:TYR:CE1	1:B:144:SER:HB3	2.56	0.41
1:A:108:PRO:HG3	1:A:134:PHE:CE1	2.57	0.40
1:B:165:MET:HE3	1:B:181:PHE:CZ	2.56	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	292/329 (89%)	285 (98%)	7 (2%)	0	100	100
1	B	296/329 (90%)	286 (97%)	10 (3%)	0	100	100
All	All	588/658 (89%)	571 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/283 (82%)	227 (98%)	5 (2%)	47 61
1	B	246/283 (87%)	235 (96%)	11 (4%)	23 30
All	All	478/566 (84%)	462 (97%)	16 (3%)	32 44

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	169	THR
1	A	225	THR
1	A	259	ILE
1	A	280	THR
1	B	6	MET
1	B	59	ILE
1	B	72	ASN
1	B	76	ARG
1	B	153	ASP
1	B	155	ASP
1	B	190	THR
1	B	216	ASP
1	B	236	LYS
1	B	276	MET
1	B	280	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	41	HIS
1	A	65	ASN
1	A	127	GLN
1	A	231	ASN
1	A	273	GLN

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Mol	Chain	Res	Type
1	B	19	GLN
1	B	64	HIS
1	B	72	ASN
1	B	107	GLN
1	B	119	ASN
1	B	164	HIS
1	B	172	HIS
1	B	192	GLN
1	B	228	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)

3 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	A1L7P	B	401	-	38,38,38	2.75	16 (42%)	46,56,56	3.39	13 (28%)
2	A1L7P	A	501	-	38,38,38	2.87	19 (50%)	46,56,56	3.64	14 (30%)
3	EDO	A	502	-	3,3,3	0.49	0	2,2,2	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1L7P	B	401	-	-	0/12/20/20	0/5/5/5
2	A1L7P	A	501	-	-	0/12/20/20	0/5/5/5
3	EDO	A	502	-	-	0/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1L7P	C12-N22	7.79	1.54	1.37
2	A	501	A1L7P	C12-N22	7.05	1.52	1.37
2	B	401	A1L7P	C14-N13	6.98	1.57	1.46
2	B	401	A1L7P	C21-C20	6.21	1.58	1.50
2	A	501	A1L7P	C09-N08	6.11	1.51	1.42
2	A	501	A1L7P	C33-N22	5.96	1.49	1.38
2	A	501	A1L7P	C21-C20	4.68	1.56	1.50
2	A	501	A1L7P	C14-C15	4.24	1.55	1.50
2	A	501	A1L7P	C09-N11	4.16	1.44	1.36
2	A	501	A1L7P	C14-N13	4.04	1.53	1.46
2	B	401	A1L7P	F31-C30	-3.63	1.26	1.35
2	B	401	A1L7P	C07-N06	3.59	1.42	1.34
2	A	501	A1L7P	C23-C24	-3.45	1.45	1.51
2	A	501	A1L7P	F29-C28	-3.45	1.29	1.35
2	B	401	A1L7P	C03-C02	3.41	1.44	1.39
2	B	401	A1L7P	F27-C26	-3.38	1.26	1.35
2	B	401	A1L7P	C23-N22	3.37	1.52	1.47
2	A	501	A1L7P	C21-N13	3.07	1.51	1.46
2	A	501	A1L7P	C07-C02	3.06	1.45	1.38
2	B	401	A1L7P	C12-N11	-3.00	1.27	1.31
2	A	501	A1L7P	C26-C28	2.87	1.43	1.37
2	B	401	A1L7P	C03-C04	2.78	1.44	1.39
2	A	501	A1L7P	C30-C28	2.77	1.43	1.37
2	B	401	A1L7P	F29-C28	-2.71	1.30	1.35
2	B	401	A1L7P	C05-C04	2.57	1.43	1.38
2	B	401	A1L7P	C30-C28	2.41	1.42	1.37
2	A	501	A1L7P	C03-C04	2.39	1.43	1.39
2	A	501	A1L7P	C12-N13	2.30	1.44	1.37
2	A	501	A1L7P	C32-C30	2.23	1.41	1.37
2	B	401	A1L7P	C07-C02	2.22	1.43	1.38
2	B	401	A1L7P	C26-C28	2.18	1.42	1.37
2	A	501	A1L7P	C03-C02	2.17	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1L7P	C12-N13	2.09	1.43	1.37
2	A	501	A1L7P	C33-N08	2.03	1.44	1.40
2	A	501	A1L7P	C05-N06	2.00	1.38	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	A1L7P	C15-C14-N13	14.26	109.20	102.46
2	A	501	A1L7P	C15-C14-N13	13.83	109.00	102.46
2	A	501	A1L7P	C20-C21-N13	12.65	108.44	102.46
2	A	501	A1L7P	C24-C23-N22	11.13	130.47	113.15
2	B	401	A1L7P	C20-C21-N13	9.20	106.81	102.46
2	B	401	A1L7P	C24-C23-N22	7.97	125.55	113.15
2	B	401	A1L7P	C05-C04-N08	6.61	127.58	119.57
2	A	501	A1L7P	C33-N08-C09	-5.15	118.12	124.86
2	B	401	A1L7P	C33-N08-C09	-4.67	118.74	124.86
2	B	401	A1L7P	C14-C15-C20	-4.62	106.87	110.53
2	A	501	A1L7P	C05-C04-N08	3.79	124.16	119.57
2	A	501	A1L7P	C04-N08-C33	3.22	121.21	117.11
2	B	401	A1L7P	C03-C04-C05	-3.12	117.01	119.48
2	A	501	A1L7P	C03-C04-C05	-3.01	117.09	119.48
2	B	401	A1L7P	C03-C04-N08	-2.99	115.41	119.12
2	A	501	A1L7P	C14-C15-C20	-2.98	108.17	110.53
2	A	501	A1L7P	C23-C24-C25	-2.94	114.57	120.25
2	B	401	A1L7P	C04-N08-C33	2.91	120.81	117.11
2	B	401	A1L7P	C21-C20-C15	-2.85	108.27	110.53
2	B	401	A1L7P	C23-C24-C32	-2.65	115.13	120.25
2	A	501	A1L7P	C07-N06-C05	2.36	120.70	117.48
2	A	501	A1L7P	C23-N22-C33	-2.33	113.61	116.97
2	B	401	A1L7P	C23-N22-C33	-2.30	113.66	116.97
2	A	501	A1L7P	C24-C25-C26	2.18	120.78	119.37
2	B	401	A1L7P	C21-C20-C19	2.05	132.88	128.85
2	A	501	A1L7P	C32-C24-C25	2.04	121.78	118.98
2	A	501	A1L7P	C25-C26-C28	-2.00	118.80	121.68

There are no chirality outliers.

There are no torsion outliers.

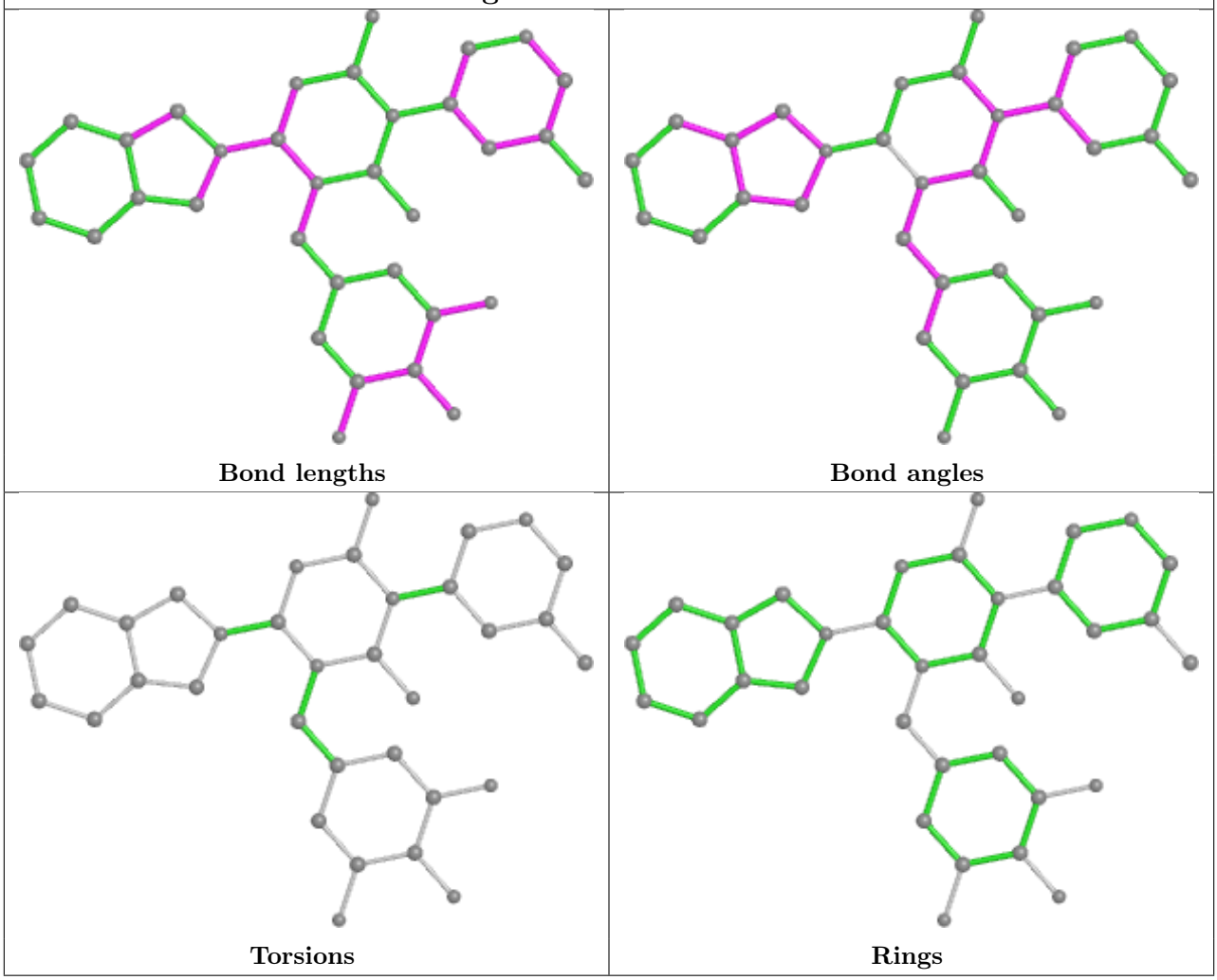
There are no ring outliers.

1 monomer is involved in 1 short contact:

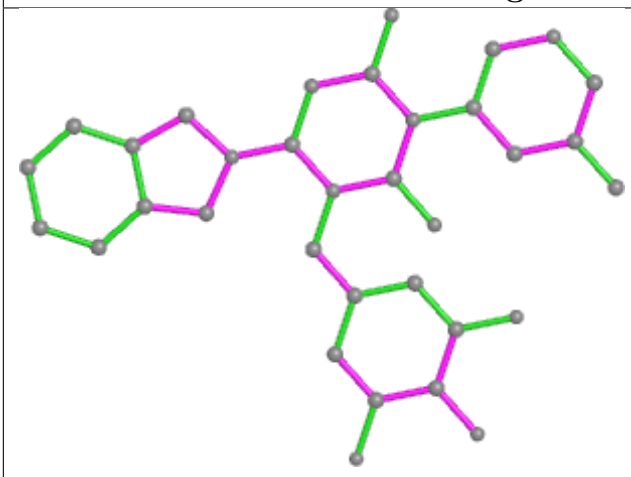
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A1L7P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

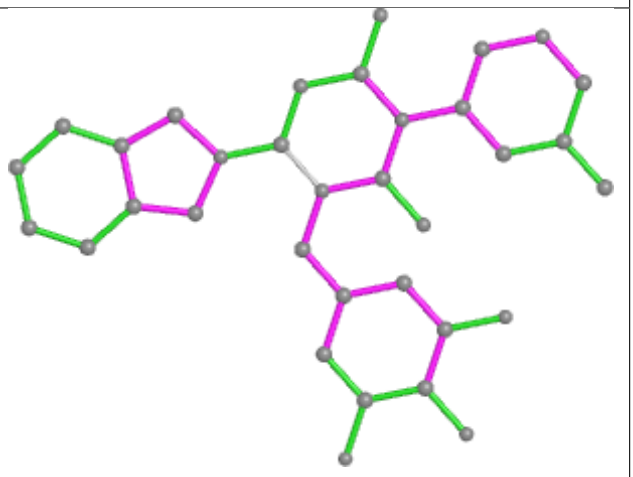
Ligand A1L7P B 401



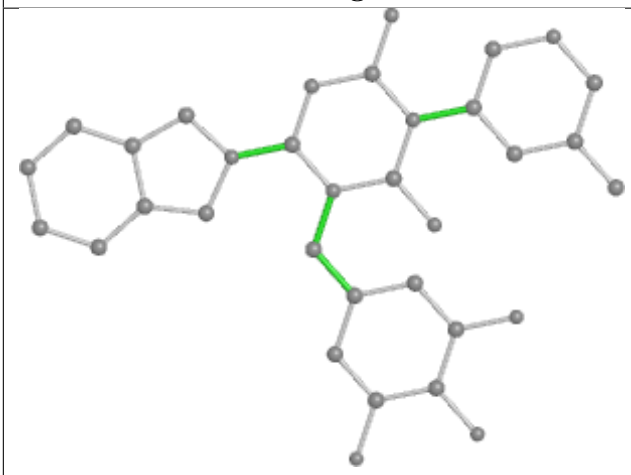
Ligand A1L7P A 501



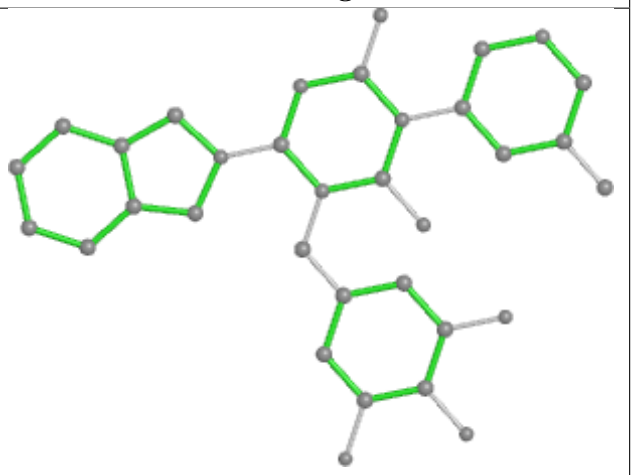
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/329 (89%)	0.44	28 (9%)	15	13	11, 29, 49, 63	0
1	B	297/329 (90%)	-0.01	8 (2%)	56	53	10, 21, 41, 54	1 (0%)
All	All	593/658 (90%)	0.22	36 (6%)	28	25	10, 24, 47, 63	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	PHE	4.0
1	A	225	THR	3.9
1	A	228	ASN	3.7
1	A	279	ARG	3.6
1	B	300	CYS	3.5
1	A	139	SER	2.9
1	B	4	ARG	2.9
1	A	229	ASP	2.9
1	A	233	VAL	2.8
1	A	3	PHE	2.8
1	A	255	ALA	2.8
1	A	262	LEU	2.8
1	B	47	GLU	2.6
1	A	73	VAL	2.6
1	A	260	ALA	2.5
1	A	138	GLY	2.5
1	A	276	MET	2.4
1	B	196	THR	2.4
1	A	259	ILE	2.4
1	A	59	ILE	2.4
1	A	50	LEU	2.4
1	A	24	THR	2.3
1	B	153	ASP	2.3
1	A	235	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	169	THR	2.2
1	A	258	GLY	2.2
1	B	154	TYR	2.2
1	A	283	GLY	2.2
1	B	216	ASP	2.1
1	A	191	ALA	2.1
1	A	226	THR	2.1
1	A	155	ASP	2.1
1	B	279	ARG	2.1
1	A	237	TYR	2.1
1	A	227	LEU	2.1
1	A	261	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

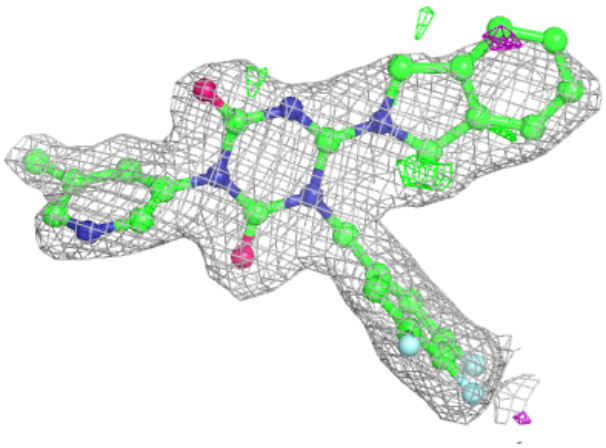
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

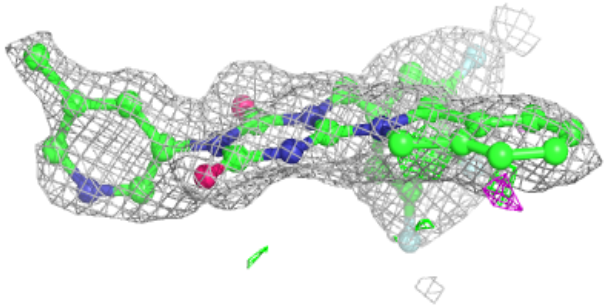
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1L7P	A	501	34/34	0.82	0.16	36,46,71,75	0
3	EDO	A	502	4/4	0.83	0.13	26,27,27,30	0
2	A1L7P	B	401	34/34	0.92	0.09	18,24,38,40	0

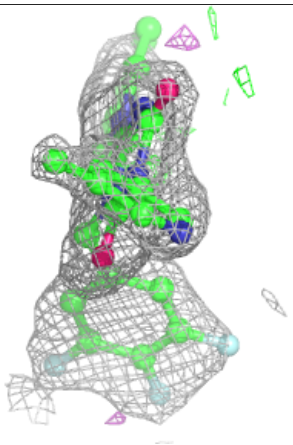
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1L7P A 501:

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

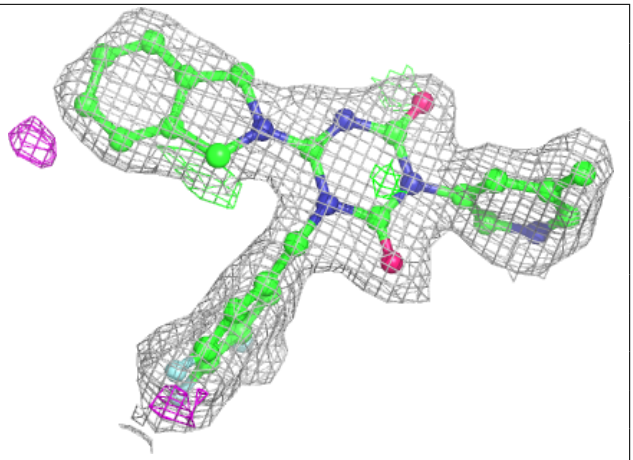


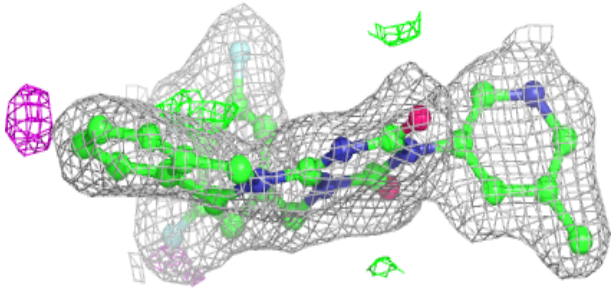


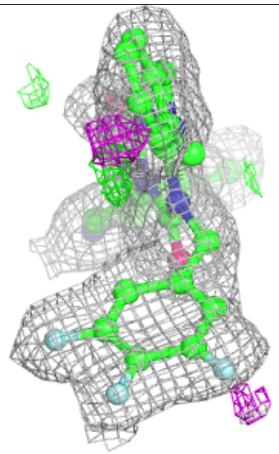


Electron density around A1L7P B 401:

$2mF_o$-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

There are no such residues in this entry.