Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:10 AM EDT

PDB ID	:	7RVT
Title	:	Structure of the SARS-CoV-2 main protease in complex with inhibitor MPI20
Authors	:	Yang, K.; Sankaran, B.; Liu, W.
Deposited on	:	2021-08-19
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 (i) 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 (i)) were used in the production of this report:

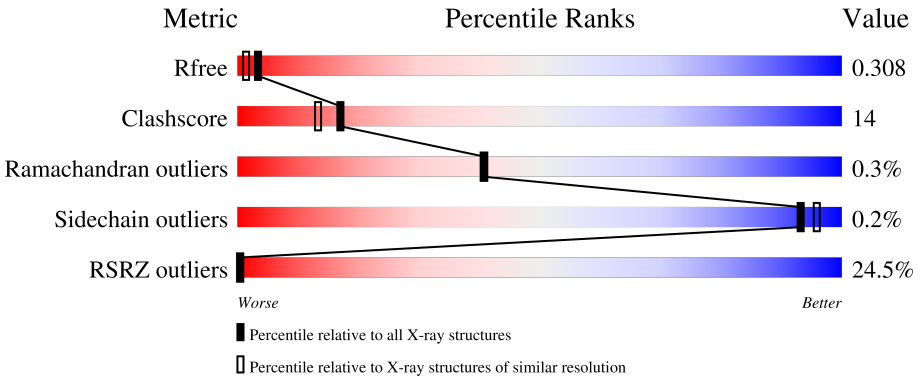
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	306	23% 68% 30%
1	B	306	25% 75% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4852 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.

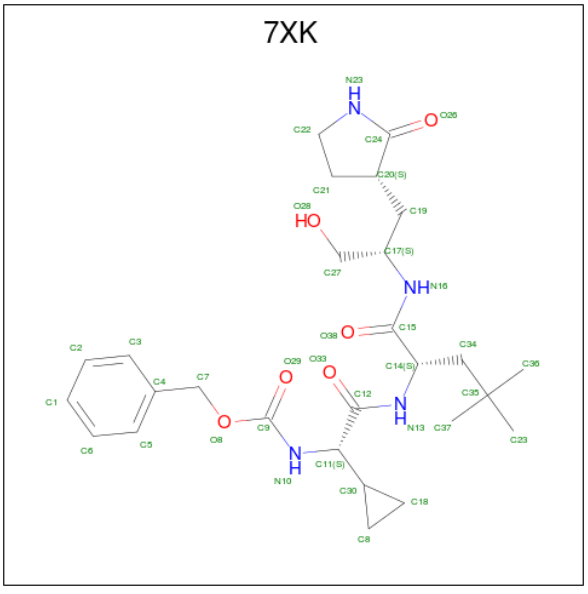
- Molecule 1 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2317	1470	396	430	21			
1	B	300	Total	C	N	O	S	0	0	0
			2317	1470	396	430	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	ALA	GLU	conflict	UNP P0DTD1
B	178	ALA	GLU	conflict	UNP P0DTD1

- Molecule 2 is N 2 -[(2S)-2-{[(benzyloxy)carbonyl]amino}-2-cyclopropylacetyl]-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-4-methyl-L-leucinamide (three-letter code: 7XK) (formula: $C_{27}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	27	4	6		
2	B	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 3 is water.

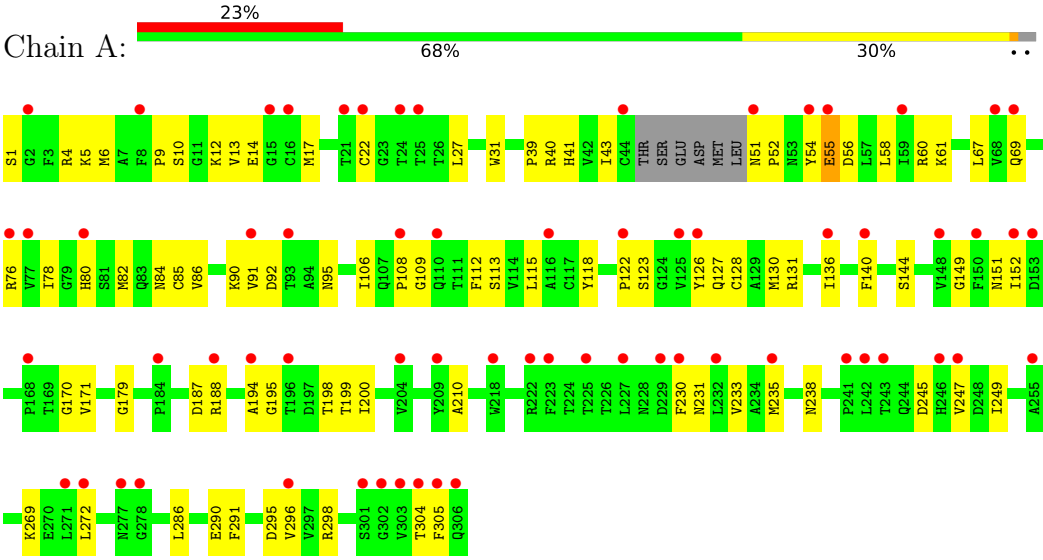
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	67	Total	O	0	0
			67	67		

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.

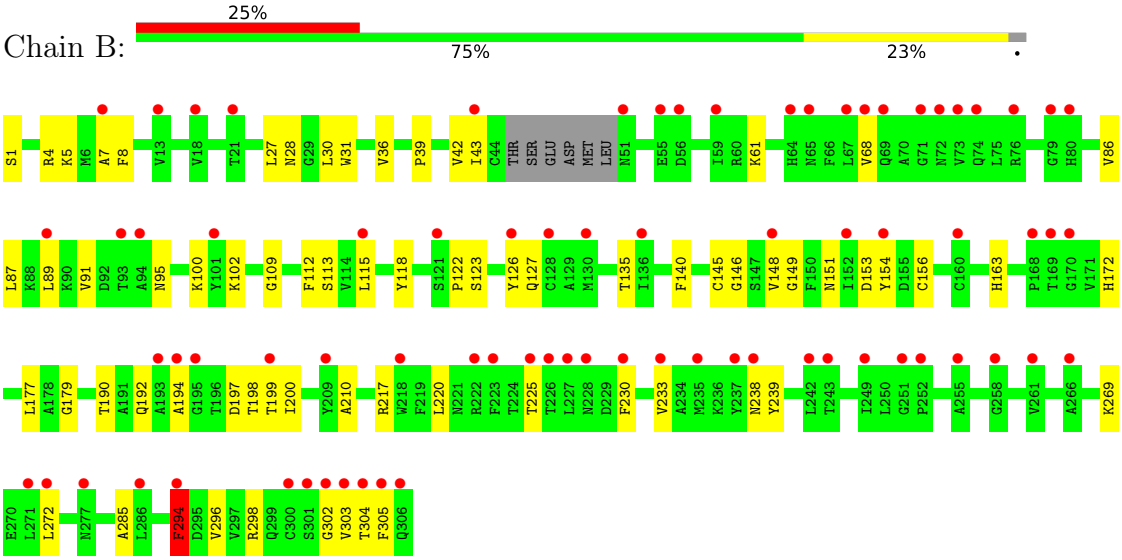
• Molecule 1: 3C-like proteinase

Chain A:



• Molecule 1: 3C-like proteinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.51Å 60.70Å 63.34Å 80.42° 68.42° 70.59°	Depositor
Resolution (Å)	32.85 – 2.10 32.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (32.85-2.10) 94.8 (32.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.270 , 0.308 0.270 , 0.308	Depositor DCC
R_{free} test set	2050 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.099 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4852	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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: 7XK

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	0.52	2/2369 (0.1%)	0.66	0/3219
1	B	0.46	0/2369	0.66	1/3219 (0.0%)
All	All	0.49	2/4738 (0.0%)	0.66	1/6438 (0.0%)

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	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CD-OE2	-8.68	1.16	1.25
1	A	106	ILE	C-N	-5.24	1.22	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	PHE	CB-CG-CD2	-5.58	116.89	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	GLU	Peptide
1	B	294	PHE	Sidechain

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	2317	0	2268	81	0
1	B	2317	0	2269	55	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
3	A	77	0	0	26	0
3	B	67	0	0	8	0
All	All	4852	0	4537	129	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 14.

All (129) 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:5:LYS:NZ	3:A:501:HOH:O	1.83	1.07
1:A:151:ASN:ND2	3:A:502:HOH:O	1.88	1.04
1:A:22:CYS:SG	1:A:61:LYS:NZ	2.38	0.95
1:A:151:ASN:O	3:A:503:HOH:O	1.90	0.89
1:B:197:ASP:OD2	3:B:501:HOH:O	1.93	0.86
1:A:152:ILE:HD13	3:A:503:HOH:O	1.77	0.84
1:B:5:LYS:HE3	1:B:127:GLN:HB2	1.62	0.81
1:B:113:SER:OG	1:B:127:GLN:OE1	1.97	0.81
1:A:233:VAL:HG21	1:A:269:LYS:HD3	1.65	0.78
1:A:131:ARG:O	3:A:504:HOH:O	2.01	0.78
1:B:27:LEU:HD13	1:B:39:PRO:HD2	1.64	0.78
1:B:233:VAL:HG21	1:B:269:LYS:HE3	1.66	0.76
1:B:177:LEU:O	3:B:503:HOH:O	2.04	0.75
1:B:5:LYS:HE3	1:B:127:GLN:CB	2.17	0.74
1:A:40:ARG:HH11	1:A:82:MET:CE	2.01	0.74
1:A:157:VAL:HA	3:A:503:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HE2	1:B:151:ASN:HD22	1.36	0.72
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.71	0.72
1:A:1:SER:N	1:B:140:PHE:O	2.22	0.72
1:B:298:ARG:HG3	1:B:303:VAL:HB	1.72	0.71
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.73	0.71
1:B:87:LEU:HD22	1:B:89:LEU:HG	1.73	0.70
1:B:30:LEU:HD22	1:B:148:VAL:HG11	1.73	0.69
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.58	0.68
1:B:135:THR:OG1	3:B:504:HOH:O	2.12	0.68
1:A:108:PRO:HB3	3:A:504:HOH:O	1.96	0.66
1:A:298:ARG:NH2	3:A:517:HOH:O	2.29	0.64
1:B:153:ASP:OD2	3:B:502:HOH:O	2.14	0.64
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.80	0.64
1:A:52:PRO:HD2	1:A:188:ARG:HG3	1.78	0.64
1:B:298:ARG:NH2	3:B:510:HOH:O	2.33	0.61
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.35	0.61
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.83	0.60
1:B:194:ALA:O	3:B:505:HOH:O	2.16	0.60
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.84	0.60
1:A:304:THR:HG22	1:B:123:SER:HB2	1.81	0.60
1:A:10:SER:O	1:A:14:GLU:HG3	2.02	0.60
1:A:198:THR:HG22	1:A:238:ASN:OD1	2.03	0.59
1:A:91:VAL:O	3:A:506:HOH:O	2.17	0.59
1:A:40:ARG:HH11	1:A:82:MET:HE3	1.67	0.59
1:A:245:ASP:O	1:A:249:ILE:HG13	2.03	0.59
1:B:112:PHE:HA	1:B:151:ASN:HD21	1.68	0.59
1:B:91:VAL:O	3:B:506:HOH:O	2.17	0.58
1:A:195:GLY:N	3:A:513:HOH:O	2.22	0.58
1:A:5:LYS:NZ	1:A:127:GLN:HG2	2.20	0.56
1:B:198:THR:HG22	1:B:238:ASN:OD1	2.06	0.56
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.88	0.55
1:A:247:VAL:HG22	1:A:261:VAL:HG11	1.89	0.55
1:A:4:ARG:HD2	1:B:126:TYR:CD1	2.41	0.54
1:A:199:THR:OG1	3:A:507:HOH:O	2.18	0.54
1:B:298:ARG:HD2	1:B:305:PHE:HZ	1.72	0.54
1:B:7:ALA:HA	1:B:127:GLN:OE1	2.08	0.53
1:A:233:VAL:HG21	1:A:269:LYS:CD	2.38	0.53
1:A:170:GLY:O	3:A:508:HOH:O	2.19	0.52
1:A:230:PHE:CD1	1:A:265:CYS:HB3	2.45	0.51
1:A:123:SER:HB2	1:B:304:THR:HG22	1.92	0.51
1:A:290:GLU:OE1	3:A:510:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HG2	1:B:145:CYS:HB3	1.92	0.50
1:A:56:ASP:O	1:A:60:ARG:HG3	2.11	0.50
1:B:190:THR:O	1:B:192:GLN:HG2	2.12	0.50
1:A:75:LEU:HD13	1:A:91:VAL:HG21	1.95	0.49
1:A:231:ASN:O	1:A:235:MET:HG2	2.13	0.49
1:B:102:LYS:HE2	1:B:156:CYS:SG	2.53	0.49
1:B:28:ASN:O	1:B:146:GLY:HA3	2.11	0.49
1:B:199:THR:HG21	1:B:239:TYR:CZ	2.48	0.49
1:A:76:ARG:NH2	1:A:92:ASP:OD2	2.45	0.49
1:A:17:MET:HB2	3:A:553:HOH:O	2.13	0.49
1:A:41:HIS:HA	1:A:54:TYR:HE1	1.77	0.48
1:A:140:PHE:O	1:B:1:SER:N	2.43	0.48
1:A:40:ARG:NH2	1:A:187:ASP:OD1	2.39	0.47
1:B:8:PHE:HE2	1:B:151:ASN:ND2	2.07	0.47
1:B:112:PHE:HA	1:B:151:ASN:ND2	2.29	0.47
1:B:217:ARG:HB3	1:B:220:LEU:HD12	1.96	0.47
1:A:272:LEU:O	3:A:509:HOH:O	2.19	0.47
1:A:5:LYS:HD3	1:A:291:PHE:CZ	2.50	0.47
1:B:8:PHE:HE1	1:B:305:PHE:CZ	2.33	0.47
1:B:298:ARG:HD2	1:B:305:PHE:CZ	2.50	0.47
1:B:225:THR:HG21	1:B:230:PHE:HB2	1.97	0.46
1:B:233:VAL:HG11	1:B:269:LYS:HG3	1.97	0.46
1:A:140:PHE:CE1	3:A:505:HOH:O	2.56	0.46
1:A:171:VAL:HA	3:A:508:HOH:O	2.15	0.46
1:A:12:LYS:HE2	1:A:12:LYS:HB2	1.66	0.46
1:A:82:MET:HE3	1:A:84:ASN:O	2.16	0.46
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.97	0.46
1:A:304:THR:HG21	1:B:118:TYR:HB2	1.96	0.46
3:A:514:HOH:O	1:B:302:GLY:HA2	2.15	0.46
1:A:286:LEU:HD21	1:B:285:ALA:HB2	1.97	0.46
1:A:78:ILE:HG13	1:A:90:LYS:HG2	1.97	0.46
3:A:510:HOH:O	1:B:4:ARG:NH2	2.49	0.46
1:A:112:PHE:HZ	1:A:136:ILE:HG21	1.80	0.45
1:A:126:TYR:HE1	1:A:128:CYS:SG	2.39	0.45
1:A:233:VAL:HG11	1:A:269:LYS:HG3	1.98	0.45
1:A:5:LYS:HD2	1:A:5:LYS:HA	1.71	0.45
1:A:157:VAL:HG13	3:A:503:HOH:O	2.15	0.45
1:B:113:SER:O	1:B:149:GLY:HA2	2.17	0.45
1:A:13:VAL:HG12	1:A:115:LEU:HD23	1.99	0.45
1:A:155:ASP:OD1	1:A:155:ASP:N	2.46	0.45
1:A:67:LEU:HD23	1:A:69:GLN:HE21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:HD3	3:B:544:HOH:O	2.16	0.45
1:A:298:ARG:NH1	3:A:517:HOH:O	2.49	0.44
1:A:5:LYS:HZ1	1:A:127:GLN:HG2	1.80	0.44
1:A:298:ARG:CZ	3:A:517:HOH:O	2.66	0.44
1:A:9:PRO:C	1:A:12:LYS:HZ1	2.20	0.44
1:A:130:MET:HG3	3:A:504:HOH:O	2.17	0.44
1:A:27:LEU:HD13	1:A:39:PRO:HD2	2.00	0.43
1:A:113:SER:O	1:A:149:GLY:HA2	2.18	0.43
1:A:118:TYR:CE2	1:A:144:SER:HB3	2.53	0.43
1:A:171:VAL:HG11	3:A:570:HOH:O	2.18	0.43
1:A:231:ASN:O	1:A:235:MET:HE2	2.19	0.43
1:A:51:ASN:OD1	1:A:188:ARG:HD3	2.19	0.43
1:B:210:ALA:HB2	1:B:296:VAL:HG13	2.01	0.43
1:A:154:TYR:O	1:A:305:PHE:HB3	2.18	0.42
1:A:9:PRO:O	1:A:12:LYS:NZ	2.45	0.42
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.00	0.42
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.55	0.42
1:A:295:ASP:OD1	3:A:511:HOH:O	2.22	0.42
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.76	0.42
1:A:6:MET:HB3	1:A:298:ARG:HH21	1.84	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.75	0.41
1:A:31:TRP:CE2	1:A:75:LEU:HD11	2.56	0.41
1:A:58:LEU:HD11	1:A:80:HIS:CD2	2.56	0.41
1:A:194:ALA:N	3:A:513:HOH:O	2.53	0.41
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.56	0.41
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.86	0.41
1:A:210:ALA:HB2	1:A:296:VAL:HG13	2.01	0.41
1:B:36:VAL:HG21	1:B:68:VAL:HG11	2.03	0.41
1:A:40:ARG:O	1:A:43:ILE:HG12	2.22	0.40
1:A:78:ILE:N	1:A:90:LYS:O	2.49	0.40
1:B:43:ILE:HB	1:B:61:LYS:HE3	2.03	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	296/306 (97%)	291 (98%)	4 (1%)	1 (0%)	41	41
1	B	296/306 (97%)	284 (96%)	11 (4%)	1 (0%)	41	41
All	All	592/612 (97%)	575 (97%)	15 (2%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	TYR
1	A	154	TYR

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	256/262 (98%)	256 (100%)	0	100	100
1	B	256/262 (98%)	255 (100%)	1 (0%)	91	94
All	All	512/524 (98%)	511 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	294	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	84	ASN
1	A	151	ASN
1	A	189	GLN
1	B	151	ASN

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Mol	Chain	Res	Type
1	B	273	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	7XK	B	401	1	39,39,39	1.08	1 (2%)	50,54,54	1.24	5 (10%)
2	7XK	A	401	1	39,39,39	1.10	1 (2%)	50,54,54	1.44	8 (16%)

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	7XK	B	401	1	-	3/40/52/52	0/3/3/3
2	7XK	A	401	1	-	4/40/52/52	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7XK	O8-C9	5.58	1.45	1.35
2	A	401	7XK	O8-C9	5.25	1.45	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	7XK	C8-C30-C11	-4.99	109.46	119.59
2	B	401	7XK	C8-C30-C11	-4.64	110.17	119.59
2	A	401	7XK	C7-O8-C9	3.76	124.33	115.93
2	B	401	7XK	O8-C9-N10	3.26	117.13	110.50
2	A	401	7XK	C18-C30-C11	-2.80	113.90	119.59
2	A	401	7XK	O26-C24-C20	-2.77	122.98	126.23
2	A	401	7XK	C19-C20-C24	-2.77	106.80	112.89
2	A	401	7XK	O8-C7-C4	2.76	116.02	109.39
2	B	401	7XK	O8-C9-O29	-2.43	119.59	124.25
2	A	401	7XK	C19-C17-C27	-2.35	108.39	111.65
2	A	401	7XK	O8-C9-N10	2.30	115.17	110.50
2	B	401	7XK	C18-C30-C11	-2.20	115.12	119.59
2	B	401	7XK	C19-C20-C21	-2.19	109.27	117.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	7XK	C12-C11-C30-C18
2	A	401	7XK	C4-C7-O8-C9
2	B	401	7XK	C12-C11-C30-C18
2	B	401	7XK	O29-C9-O8-C7
2	B	401	7XK	N10-C9-O8-C7
2	A	401	7XK	N10-C9-O8-C7
2	A	401	7XK	O29-C9-O8-C7

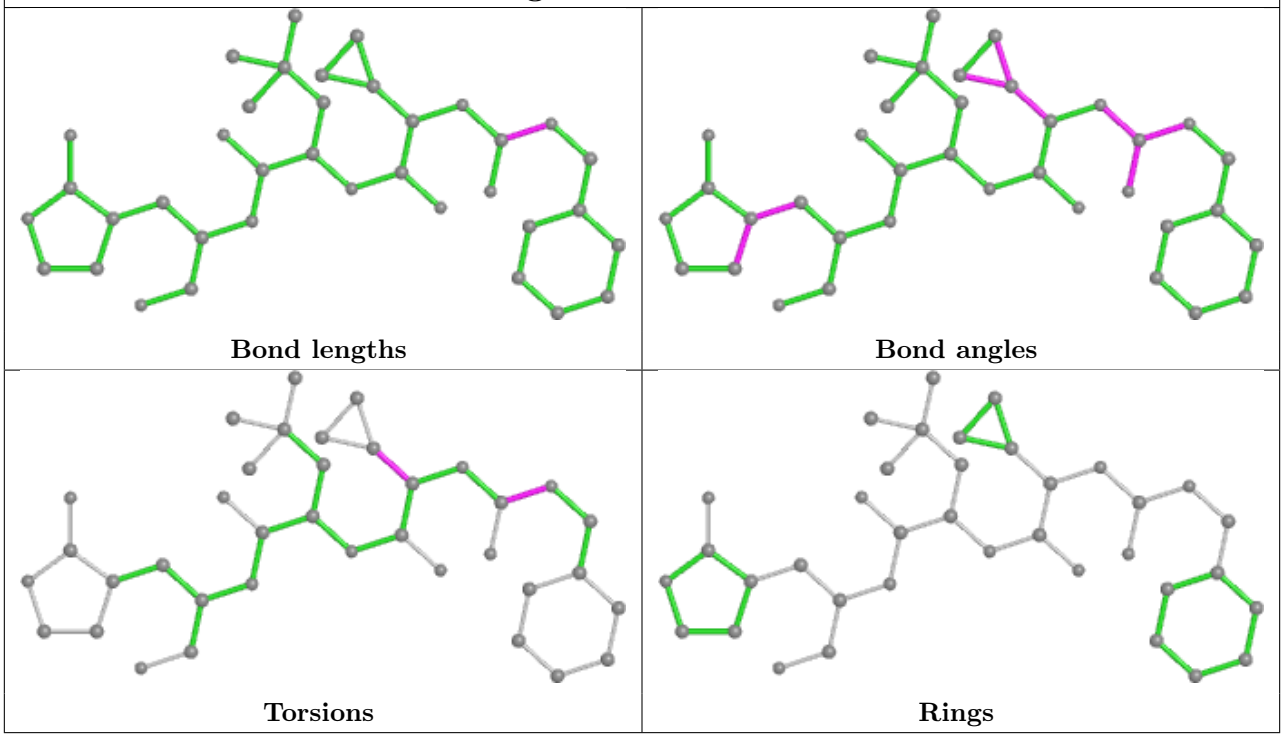
There are no ring outliers.

No monomer is involved in short contacts.

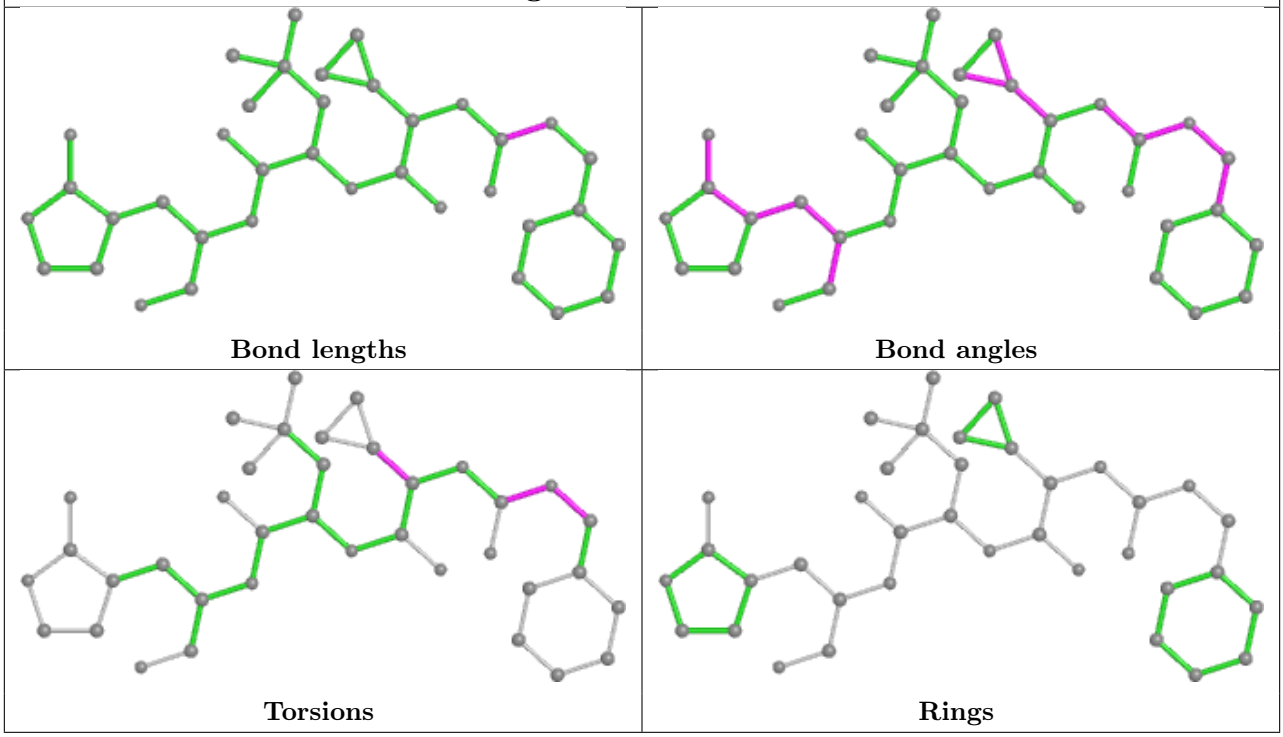
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 7XK B 401



Ligand 7XK A 401



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	300/306 (98%)	1.49	71 (23%)	0	0	16, 30, 49, 72	0
1	B	300/306 (98%)	1.65	76 (25%)	0	0	16, 30, 50, 67	0
All	All	600/612 (98%)	1.57	147 (24%)	0	0	16, 30, 50, 72	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	GLN	7.1
1	B	294	PHE	6.9
1	B	154	TYR	6.8
1	B	222	ARG	6.6
1	B	306	GLN	6.0
1	B	72	ASN	6.0
1	B	303	VAL	5.8
1	A	222	ARG	5.7
1	B	305	PHE	5.5
1	B	304	THR	5.2
1	A	305	PHE	5.2
1	B	226	THR	5.2
1	A	154	TYR	4.7
1	A	72	ASN	4.7
1	B	74	GLN	4.5
1	B	233	VAL	4.4
1	B	168	PRO	4.4
1	A	235	MET	4.4
1	A	247	VAL	4.1
1	A	51	ASN	4.0
1	B	225	THR	4.0
1	B	235	MET	3.9
1	A	278	GLY	3.9
1	B	101	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	3.7
1	A	76	ARG	3.6
1	A	196	THR	3.6
1	A	74	GLN	3.6
1	A	54	TYR	3.6
1	B	237	TYR	3.6
1	A	77	VAL	3.6
1	A	255	ALA	3.5
1	B	272	LEU	3.5
1	A	93	THR	3.5
1	A	2	GLY	3.4
1	A	25	THR	3.3
1	A	110	GLN	3.2
1	B	169	THR	3.2
1	B	223	PHE	3.2
1	B	258	GLY	3.1
1	B	7	ALA	3.1
1	B	251	GLY	3.1
1	B	121	SER	3.1
1	B	79	GLY	3.1
1	A	232	LEU	3.0
1	B	193	ALA	3.0
1	A	155	ASP	2.9
1	A	243	THR	2.9
1	A	302	GLY	2.9
1	B	160	CYS	2.9
1	A	230	PHE	2.9
1	B	64	HIS	2.9
1	B	59	ILE	2.9
1	A	15	GLY	2.9
1	B	238	ASN	2.9
1	A	223	PHE	2.8
1	A	168	PRO	2.8
1	A	241	PRO	2.8
1	B	93	THR	2.8
1	A	227	LEU	2.8
1	B	94	ALA	2.8
1	B	300	CYS	2.8
1	B	148	VAL	2.7
1	B	218	TRP	2.7
1	A	157	VAL	2.7
1	B	170	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	252	PRO	2.7
1	A	8	PHE	2.7
1	B	76	ARG	2.7
1	A	303	VAL	2.6
1	A	125	VAL	2.6
1	B	128	CYS	2.6
1	B	243	THR	2.6
1	A	271	LEU	2.6
1	B	199	THR	2.6
1	B	89	LEU	2.6
1	B	228	ASN	2.6
1	A	21	THR	2.6
1	A	301	SER	2.6
1	B	136	ILE	2.6
1	A	277	ASN	2.6
1	A	55	GLU	2.5
1	B	261	VAL	2.5
1	B	277	ASN	2.5
1	A	272	LEU	2.5
1	B	13	VAL	2.5
1	A	80	HIS	2.5
1	A	153	ASP	2.5
1	B	266	ALA	2.5
1	B	227	LEU	2.4
1	A	68	VAL	2.4
1	A	91	VAL	2.4
1	A	148	VAL	2.4
1	B	242	LEU	2.4
1	B	51	ASN	2.4
1	B	130	MET	2.4
1	A	296	VAL	2.4
1	A	16	CYS	2.4
1	B	301	SER	2.4
1	B	302	GLY	2.4
1	A	136	ILE	2.4
1	B	43	ILE	2.4
1	A	184	PRO	2.3
1	B	18	VAL	2.3
1	B	230	PHE	2.3
1	A	122	PRO	2.3
1	B	80	HIS	2.3
1	A	152	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	ARG	2.3
1	A	150	PHE	2.3
1	A	304	THR	2.3
1	A	69	GLN	2.3
1	A	24	THR	2.2
1	A	140	PHE	2.2
1	A	22	CYS	2.2
1	A	44	CYS	2.2
1	A	108	PRO	2.2
1	A	242	LEU	2.2
1	B	55	GLU	2.2
1	B	21	THR	2.2
1	B	249	ILE	2.2
1	B	71	GLY	2.2
1	B	115	LEU	2.2
1	A	126	TYR	2.2
1	A	209	TYR	2.2
1	B	286	LEU	2.2
1	B	73	VAL	2.1
1	B	56	ASP	2.1
1	A	116	ALA	2.1
1	A	75	LEU	2.1
1	B	68	VAL	2.1
1	B	69	GLN	2.1
1	A	204	VAL	2.1
1	B	194	ALA	2.1
1	B	255	ALA	2.1
1	B	152	ILE	2.1
1	A	229	ASP	2.1
1	A	225	THR	2.1
1	B	209	TYR	2.1
1	A	59	ILE	2.0
1	B	65	ASN	2.0
1	B	271	LEU	2.0
1	B	126	TYR	2.0
1	B	195	GLY	2.0
1	A	218	TRP	2.0
1	A	246	HIS	2.0
1	A	194	ALA	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)

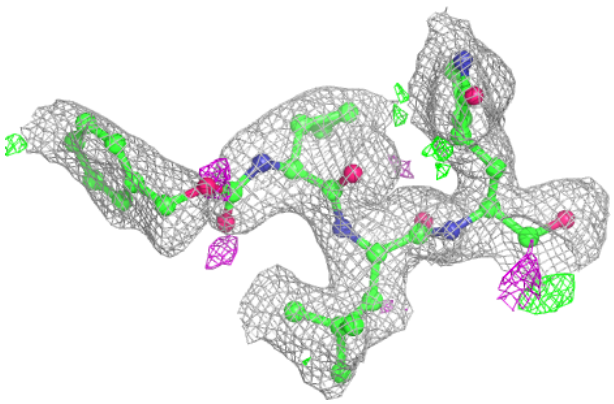
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

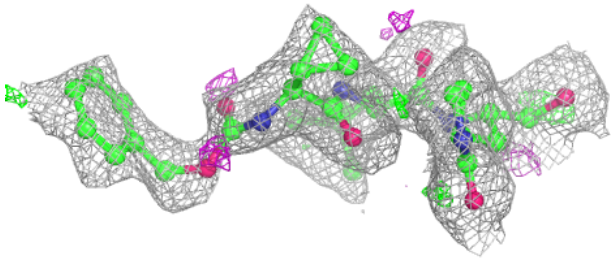
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7XK	B	401	37/37	0.78	0.23	19,28,43,43	0
2	7XK	A	401	37/37	0.83	0.24	21,26,41,44	0

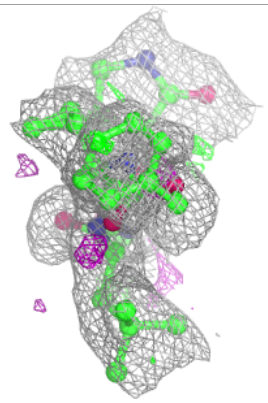
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7XK 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)

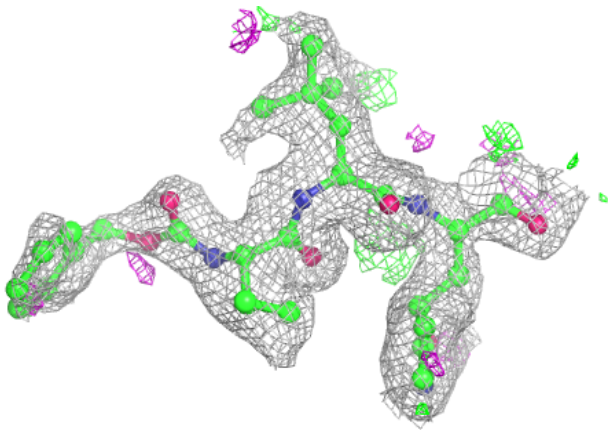


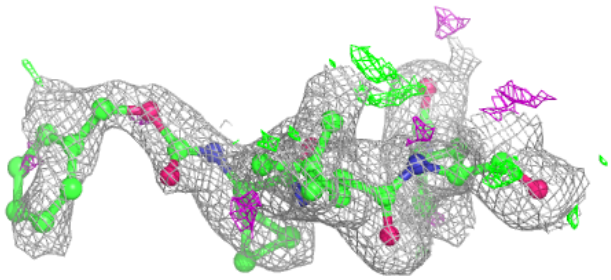


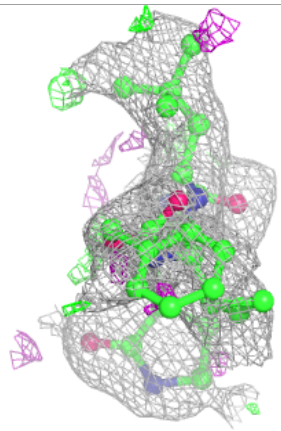


Electron density around 7XK A 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.