



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:52 PM UTC

PDB ID : 9X7I / pdb_00009x7i
Title : Crystal of CCoV-HuPn-2018 3CL protease (3CLpro) in complex with compound 3
Authors : Nie, T.Q.; Su, H.X.; Li, M.J.; Xu, Y.C.
Deposited on : 2025-10-16
Resolution : 2.23 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:

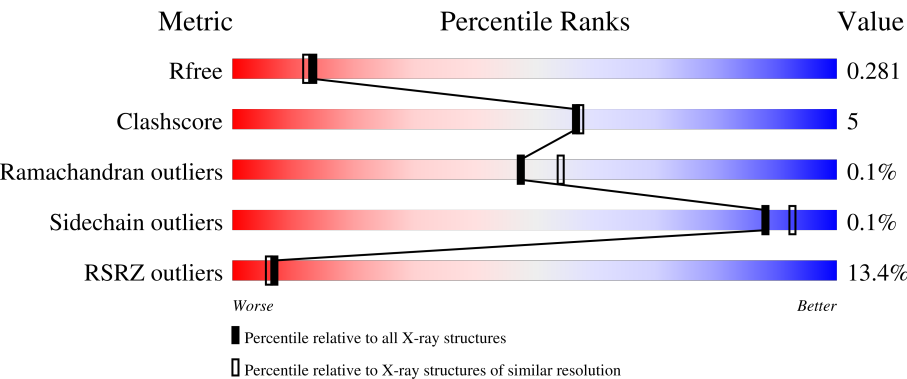
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.23 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.



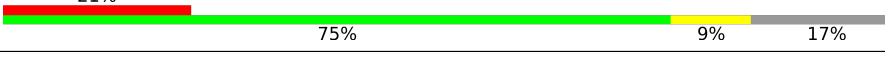
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	302	3% 92% 7%
1	B	302	3% 87% 11%
1	C	302	4% 88% 10%
1	D	302	6% 87% 12%
1	E	302	14% 87% 12%

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Mol	Chain	Length	Quality of chain
1	F	302	
1	G	302	
1	H	302	

2 Entry composition

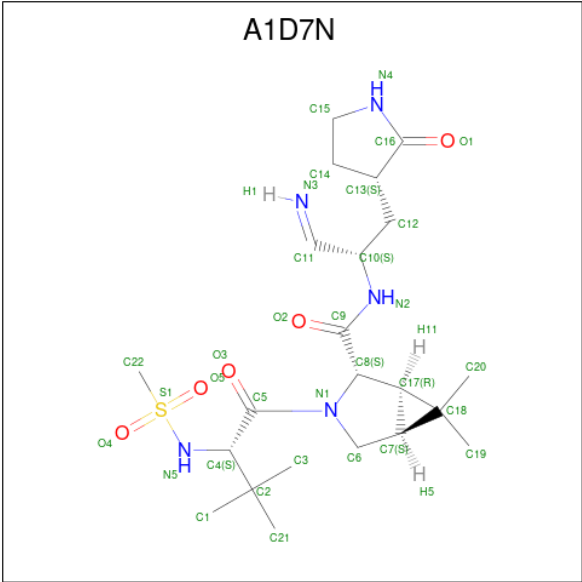
There are 3 unique types of molecules in this entry. The entry contains 17407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2257	1420	379	443	15			
1	B	298	Total	C	N	O	S	0	0	0
			2266	1427	382	442	15			
1	C	298	Total	C	N	O	S	0	0	0
			2255	1419	378	442	16			
1	D	299	Total	C	N	O	S	0	0	0
			2241	1412	377	436	16			
1	E	298	Total	C	N	O	S	0	0	0
			2217	1394	374	434	15			
1	F	284	Total	C	N	O	S	0	0	0
			2062	1288	350	409	15			
1	G	273	Total	C	N	O	S	0	0	0
			1882	1167	321	380	14			
1	H	251	Total	C	N	O	S	0	0	0
			1809	1131	302	362	14			

- Molecule 2 is (1 {R},2 {S},5 {S})- {N}-[(2 {S})-1-azanylidene-3-[(3 {S})-2-oxidanylidene-pyrrolidin-3-yl]propan-2-yl]-3-[(2 {S})-3,3-dimethyl-2-(methylsulfonylamino)butanoyl]-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide (CCD ID: A1D7N) (formula: C₂₂H₃₇N₅O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	B	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	C	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	D	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	E	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	F	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	G	1	Total	C	N	O	S	0	0
			33	22	5	5	1		
2	H	1	Total	C	N	O	S	0	0
			33	22	5	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	41	Total	O	0	0
			41	41		
3	C	21	Total	O	0	0
			21	21		
3	D	15	Total	O	0	0
			15	15		

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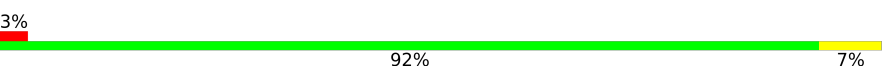
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	9	Total 9	O 9	0	0
3	F	23	Total 23	O 23	0	0
3	G	3	Total 3	O 3	0	0
3	H	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

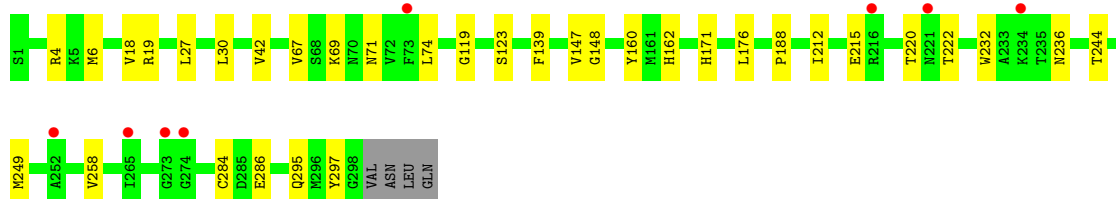
- Molecule 1: 3C-like protease

Chain A: 



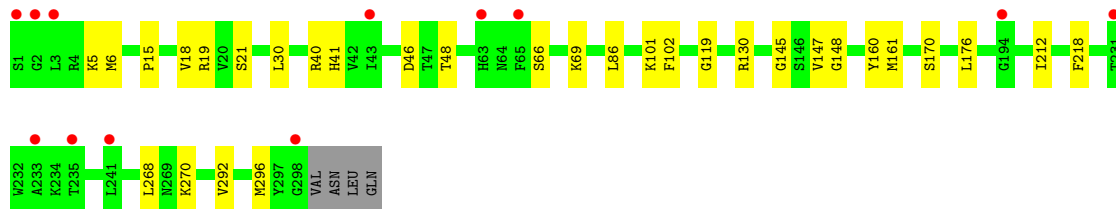
- Molecule 1: 3C-like protease

Chain B: 



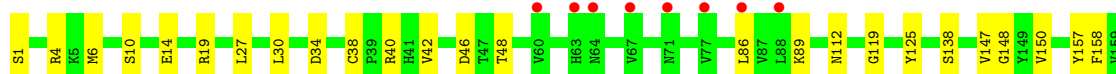
- Molecule 1: 3C-like protease

Chain C: 



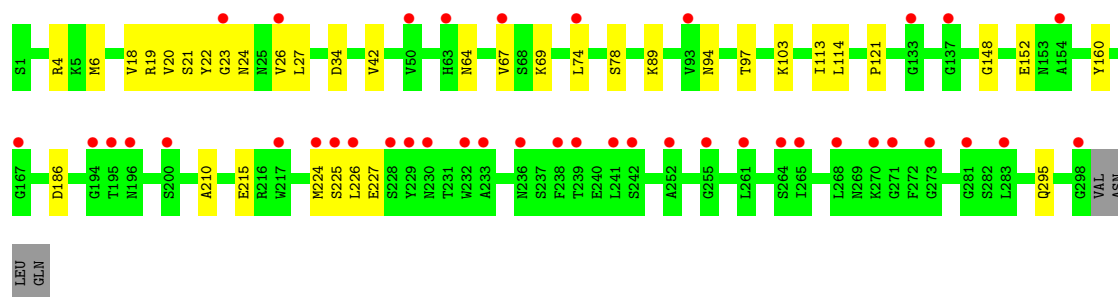
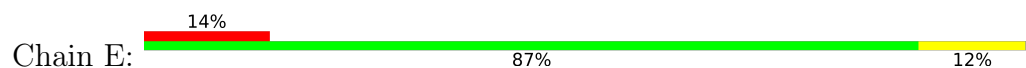
- Molecule 1: 3C-like protease

Chain D: 

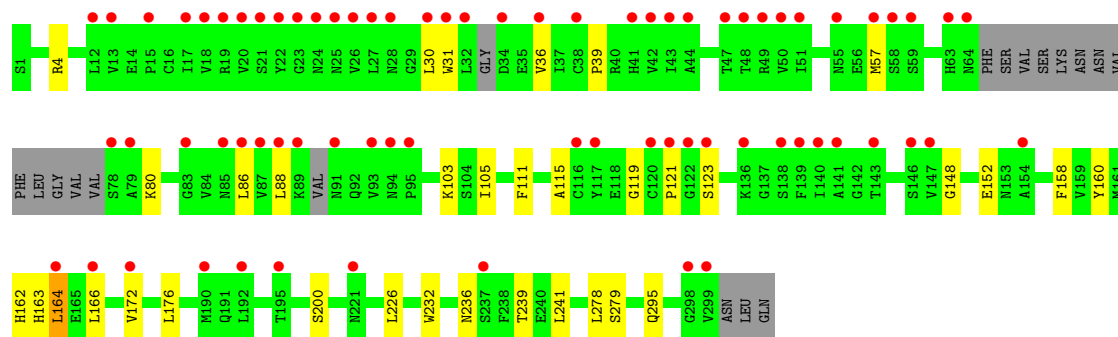
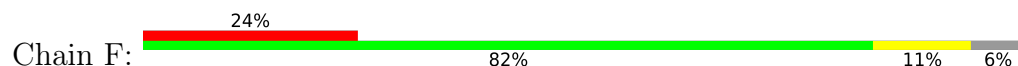




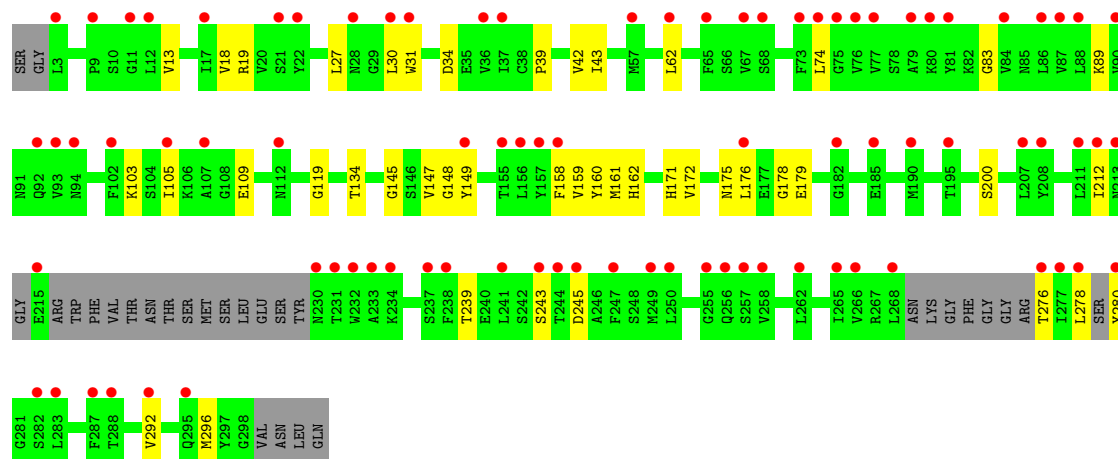
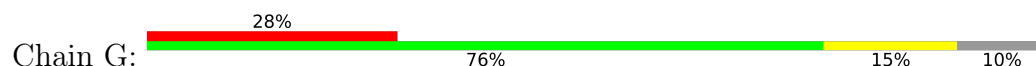
- Molecule 1: 3C-like protease



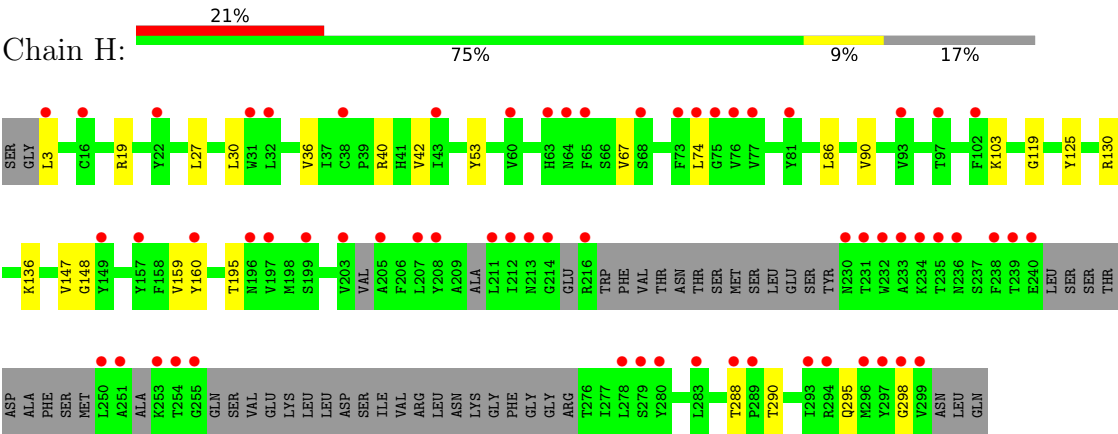
- Molecule 1: 3C-like protease



- Molecule 1: 3C-like protease



- Molecule 1: 3C-like protease



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.12Å 125.57Å 158.60Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	31.72 – 2.23 31.72 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.72-2.23) 99.2 (31.72-2.23)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.237 , 0.280 0.237 , 0.281	Depositor DCC
R_{free} test set	7468 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17407	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1D7N

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	0.19	0/2302	0.30	0/3124
1	B	0.17	0/2311	0.28	0/3132
1	C	0.18	0/2300	0.30	0/3120
1	D	0.16	0/2286	0.30	0/3104
1	E	0.15	0/2261	0.30	0/3070
1	F	0.27	0/2098	0.37	0/2843
1	G	0.17	0/1911	0.34	0/2604
1	H	0.21	0/1838	0.32	0/2490
All	All	0.19	0/17307	0.32	0/23487

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2257	0	2167	13	0
1	B	2266	0	2195	22	0
1	C	2255	0	2172	19	0
1	D	2241	0	2141	24	0
1	E	2217	0	2102	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2062	0	1901	20	0
1	G	1882	0	1620	25	0
1	H	1809	0	1630	15	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
2	E	33	0	0	0	0
2	F	33	0	0	1	0
2	G	33	0	0	0	0
2	H	33	0	0	0	0
3	A	36	0	0	0	0
3	B	41	0	0	0	0
3	C	21	0	0	0	0
3	D	15	0	0	0	0
3	E	9	0	0	0	0
3	F	23	0	0	0	0
3	G	3	0	0	1	0
3	H	6	0	0	0	0
All	All	17407	0	15928	152	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 (152) 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:H:30:LEU:HD13	1:H:147:VAL:HG21	1.62	0.80
1:D:200:SER:HB2	1:D:241:LEU:HD21	1.70	0.72
1:H:288:THR:HG22	1:H:290:THR:H	1.55	0.71
1:G:19:ARG:HB2	1:G:119:GLY:HA3	1.72	0.71
1:C:130:ARG:NH1	1:C:170:SER:OG	2.24	0.70
1:B:4:ARG:O	1:B:295:GLN:NE2	2.23	0.69
1:F:4:ARG:O	1:F:295:GLN:NE2	2.26	0.69
1:G:148:GLY:HA3	1:G:160:TYR:HB3	1.74	0.69
1:F:148:GLY:HA3	1:F:160:TYR:HB3	1.75	0.68
1:H:148:GLY:HA3	1:H:160:TYR:HB3	1.76	0.67
1:D:200:SER:HB2	1:D:241:LEU:CD2	2.26	0.66
1:H:74:LEU:HB3	1:H:90:VAL:HG11	1.79	0.64
1:D:148:GLY:HA3	1:D:160:TYR:HB3	1.79	0.63
1:A:69:LYS:O	1:A:72:VAL:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD13	1:C:147:VAL:HG21	1.81	0.62
1:B:148:GLY:HA3	1:B:160:TYR:HB3	1.81	0.62
1:G:162:HIS:HE1	1:G:171:HIS:HB3	1.65	0.61
1:C:148:GLY:HA3	1:C:160:TYR:HB3	1.82	0.61
1:A:148:GLY:HA3	1:A:160:TYR:HB3	1.82	0.61
1:D:30:LEU:HD13	1:D:147:VAL:HG21	1.83	0.61
1:G:30:LEU:HD13	1:G:147:VAL:HG21	1.83	0.60
1:H:27:LEU:HD21	1:H:42:VAL:HB	1.83	0.60
1:E:67:VAL:HG13	1:E:74:LEU:HB2	1.84	0.59
1:E:224:MET:C	1:F:57:MET:HE1	2.28	0.58
1:G:13:VAL:HG13	1:G:158:PHE:HE1	1.68	0.58
1:A:273:GLY:HA3	1:A:275:ARG:HH21	1.68	0.58
1:B:30:LEU:HD13	1:B:147:VAL:HG21	1.85	0.58
1:H:19:ARG:HB2	1:H:119:GLY:HA3	1.84	0.57
1:E:4:ARG:O	1:E:295:GLN:NE2	2.36	0.57
1:F:162:HIS:NE2	2:F:401:A1D7N:O1	2.30	0.57
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.85	0.57
1:E:19:ARG:O	1:E:67:VAL:HA	2.05	0.57
1:E:148:GLY:HA3	1:E:160:TYR:HB3	1.87	0.56
1:H:103:LYS:HB3	1:H:159:VAL:HG12	1.87	0.56
1:E:225:SER:O	1:E:227:GLU:N	2.34	0.55
1:G:62:LEU:H	1:G:62:LEU:HD12	1.70	0.55
1:H:67:VAL:HB	1:H:74:LEU:HB2	1.89	0.55
1:A:19:ARG:O	1:A:67:VAL:HA	2.08	0.54
1:C:40:ARG:HA	1:C:86:LEU:HB2	1.90	0.54
1:H:40:ARG:HD2	1:H:53:TYR:CD1	2.42	0.54
1:D:19:ARG:HB2	1:D:119:GLY:HA3	1.90	0.53
1:B:18:VAL:HG12	1:B:69:LYS:HB2	1.90	0.53
1:A:18:VAL:HG12	1:A:69:LYS:HB2	1.90	0.53
1:C:18:VAL:HG12	1:C:69:LYS:HB2	1.89	0.53
1:E:20:VAL:HG22	1:E:67:VAL:HG23	1.91	0.53
1:D:4:ARG:O	1:D:295:GLN:NE2	2.38	0.52
1:G:243:SER:HG	1:G:245:ASP:H	1.57	0.52
1:B:215:GLU:OE2	1:H:195:THR:HG23	2.09	0.52
1:F:226:LEU:HD11	1:F:241:LEU:HB3	1.92	0.52
1:B:232:TRP:O	1:B:236:ASN:ND2	2.35	0.52
1:E:34:ASP:CG	1:E:89:LYS:HE3	2.36	0.51
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.93	0.51
1:E:23:GLY:C	1:E:24:ASN:HD22	2.18	0.51
1:B:19:ARG:HB2	1:B:119:GLY:HA3	1.93	0.50
1:C:15:PRO:HA	1:C:69:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LEU:HD11	1:F:172:VAL:HG23	1.93	0.50
1:G:278:LEU:O	1:G:280:TYR:N	2.45	0.50
1:C:46:ASP:OD1	1:C:48:THR:OG1	2.24	0.50
1:C:212:ILE:HD13	1:C:296:MET:HG3	1.94	0.50
1:G:34:ASP:OD2	1:G:89:LYS:HE3	2.12	0.50
1:D:4:ARG:HB2	1:D:6:MET:HE3	1.93	0.49
1:E:18:VAL:HG12	1:E:69:LYS:HB2	1.95	0.49
1:F:103:LYS:NZ	1:F:152:GLU:OE2	2.46	0.49
1:G:83:GLY:HA3	1:G:178:GLY:HA3	1.94	0.48
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.94	0.48
1:F:36:VAL:HG22	1:F:88:LEU:HB2	1.96	0.48
1:E:34:ASP:OD2	1:E:89:LYS:HE3	2.13	0.48
1:A:188:PRO:HA	2:A:401:A1D7N:O5	2.14	0.47
1:G:27:LEU:HD13	1:G:39:PRO:HD2	1.96	0.47
1:A:34:ASP:HB3	1:A:93:VAL:HG22	1.96	0.47
1:G:13:VAL:HG21	1:G:149:TYR:CG	2.50	0.47
1:B:244:THR:HB	1:B:258:VAL:HG21	1.97	0.47
1:D:46:ASP:OD1	1:D:48:THR:HG22	2.15	0.47
1:G:105:ILE:HG23	1:G:109:GLU:HB2	1.96	0.47
1:B:67:VAL:HG12	1:B:74:LEU:HD12	1.96	0.47
1:D:34:ASP:OD2	1:D:89:LYS:HE2	2.15	0.47
1:G:200:SER:H	1:G:239:THR:HB	1.80	0.47
1:D:158:PHE:HB3	1:D:176:LEU:HD13	1.97	0.47
1:G:103:LYS:HB3	1:G:159:VAL:HG12	1.96	0.46
1:B:284:CYS:SG	1:B:286:GLU:HG2	2.55	0.46
1:G:276:THR:N	3:G:501:HOH:O	2.49	0.46
1:B:123:SER:HB3	1:D:6:MET:HB3	1.97	0.46
1:G:18:VAL:HG21	1:G:31:TRP:HB2	1.98	0.46
1:C:218:PHE:HB2	1:C:268:LEU:HD11	1.97	0.46
1:G:175:ASN:HD21	1:G:179:GLU:HB2	1.79	0.46
1:F:31:TRP:HA	1:F:36:VAL:HG12	1.97	0.46
1:G:145:GLY:HA2	1:G:161:MET:HG3	1.98	0.46
1:C:292:VAL:O	1:C:296:MET:HG2	2.15	0.46
1:D:10:SER:OG	1:D:14:GLU:OE2	2.33	0.45
1:H:3:LEU:HA	1:H:295:GLN:OE1	2.17	0.45
1:D:27:LEU:HD21	1:D:42:VAL:HB	1.98	0.45
1:D:40:ARG:HA	1:D:86:LEU:HB2	1.98	0.45
1:D:38:CYS:SG	1:D:86:LEU:HB3	2.57	0.45
1:A:94:ASN:HB3	1:A:97:THR:OG1	2.17	0.44
1:G:134:THR:HG22	1:G:172:VAL:HG22	1.98	0.44
1:G:31:TRP:CE2	1:G:74:LEU:HD21	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:VAL:HG13	1:G:43:ILE:HG23	1.99	0.44
1:B:139:PHE:O	1:D:1:SER:HB3	2.18	0.44
1:E:210:ALA:HB1	1:E:215:GLU:HB2	2.00	0.44
1:D:150:VAL:HG23	1:D:157:TYR:HB2	1.99	0.44
1:B:162:HIS:HE1	1:B:171:HIS:HB3	1.83	0.43
1:E:22:TYR:CE1	1:E:64:ASN:HB2	2.54	0.43
1:F:278:LEU:O	1:F:279:SER:HB3	2.18	0.43
1:B:188:PRO:HA	2:B:401:A1D7N:O5	2.18	0.43
1:F:158:PHE:CB	1:F:176:LEU:HD11	2.48	0.43
1:D:112:ASN:O	1:D:148:GLY:HA2	2.19	0.43
1:A:123:SER:HB2	1:C:6:MET:HB3	1.99	0.43
1:C:21:SER:HB3	1:C:66:SER:HB3	2.01	0.43
1:G:158:PHE:HB3	1:G:176:LEU:HD13	2.01	0.42
1:H:130:ARG:HD2	1:H:136:LYS:HG2	2.01	0.42
1:C:102:PHE:CE1	1:C:176:LEU:HD12	2.54	0.42
1:G:292:VAL:O	1:G:296:MET:HG2	2.19	0.42
1:B:212:ILE:HA	1:B:212:ILE:HD13	1.78	0.42
1:C:41:HIS:CD2	1:C:41:HIS:C	2.97	0.42
1:D:216:ARG:O	1:D:219:VAL:HG12	2.19	0.42
1:F:200:SER:H	1:F:239:THR:HG1	1.62	0.42
1:G:89:LYS:HB3	1:G:89:LYS:HE2	1.84	0.42
1:E:6:MET:HE2	1:H:125:TYR:CE1	2.55	0.42
1:B:71:ASN:OD1	1:B:71:ASN:N	2.53	0.41
1:C:145:GLY:HA2	1:C:161:MET:HG3	2.01	0.41
1:F:30:LEU:O	1:F:36:VAL:HA	2.20	0.41
1:D:232:TRP:CD2	1:D:266:VAL:HG12	2.56	0.41
1:E:94:ASN:HB3	1:E:97:THR:OG1	2.21	0.41
1:C:19:ARG:HB2	1:C:119:GLY:HA3	2.01	0.41
1:E:21:SER:HB2	1:E:26:VAL:HG12	2.02	0.41
1:D:241:LEU:HD12	1:D:262:LEU:HD21	2.02	0.41
1:F:105:ILE:HD13	1:F:111:PHE:HB3	2.02	0.41
1:F:232:TRP:O	1:F:236:ASN:ND2	2.39	0.41
1:B:6:MET:CE	1:D:138:SER:HB3	2.50	0.41
1:B:6:MET:HE2	1:D:125:TYR:CE1	2.56	0.41
1:D:162:HIS:HE1	1:D:171:HIS:HB3	1.85	0.41
1:E:103:LYS:NZ	1:E:152:GLU:OE1	2.53	0.41
1:F:115:ALA:HB3	1:F:123:SER:HB3	2.03	0.41
1:A:67:VAL:HG23	1:A:74:LEU:HB2	2.02	0.41
1:C:5:LYS:HA	1:C:5:LYS:HD2	1.82	0.41
1:C:101:LYS:HA	1:C:101:LYS:HD3	1.92	0.41
1:E:114:LEU:HD11	1:E:121:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PRO:HB3	1:F:163:HIS:CE1	2.56	0.41
1:A:105:ILE:HG12	1:A:159:VAL:HB	2.02	0.41
1:E:78:SER:HB3	1:E:89:LYS:HB3	2.02	0.41
1:C:270:LYS:HB3	1:C:270:LYS:HE3	1.85	0.40
1:F:163:HIS:HB3	1:F:164:LEU:HD23	2.03	0.40
1:A:211:LEU:HD11	1:A:261:LEU:HD21	2.04	0.40
1:B:176:LEU:HD13	1:B:176:LEU:HA	1.95	0.40
1:B:249:MET:HE1	1:B:297:TYR:CE2	2.56	0.40
1:B:220:THR:OG1	1:B:222:THR:OG1	2.40	0.40
1:F:80:LYS:O	1:F:86:LEU:HD12	2.21	0.40
1:F:119:GLY:O	1:F:121:PRO:HD3	2.21	0.40
1:E:113:ILE:HD13	1:E:113:ILE:HA	1.97	0.40
1:E:186:ASP:OD1	1:E:186:ASP:N	2.52	0.40
1:H:30:LEU:O	1:H:36:VAL:HA	2.21	0.40
1:H:40:ARG:HA	1:H:86:LEU:HB2	2.03	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	297/302 (98%)	286 (96%)	11 (4%)	0	100	100
1	B	296/302 (98%)	288 (97%)	8 (3%)	0	100	100
1	C	296/302 (98%)	289 (98%)	7 (2%)	0	100	100
1	D	297/302 (98%)	290 (98%)	7 (2%)	0	100	100
1	E	296/302 (98%)	277 (94%)	18 (6%)	1 (0%)	36	38
1	F	276/302 (91%)	260 (94%)	16 (6%)	0	100	100
1	G	264/302 (87%)	245 (93%)	18 (7%)	1 (0%)	30	30
1	H	236/302 (78%)	225 (95%)	10 (4%)	1 (0%)	30	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2258/2416 (94%)	2160 (96%)	95 (4%)	3 (0%)	48	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	212	ILE
1	E	226	LEU
1	H	298	GLY

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	247/258 (96%)	247 (100%)	0	100	100
1	B	249/258 (96%)	249 (100%)	0	100	100
1	C	248/258 (96%)	248 (100%)	0	100	100
1	D	242/258 (94%)	242 (100%)	0	100	100
1	E	237/258 (92%)	237 (100%)	0	100	100
1	F	211/258 (82%)	210 (100%)	1 (0%)	81	86
1	G	177/258 (69%)	177 (100%)	0	100	100
1	H	185/258 (72%)	185 (100%)	0	100	100
All	All	1796/2064 (87%)	1795 (100%)	1 (0%)	88	92

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

Mol	Chain	Res	Type
1	F	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS

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Mol	Chain	Res	Type
1	B	41	HIS
1	B	63	HIS
1	B	269	ASN
1	C	41	HIS
1	C	92	GLN
1	C	132	GLN
1	C	196	ASN
1	C	269	ASN
1	D	64	ASN
1	D	269	ASN
1	E	24	ASN
1	E	41	HIS
1	E	70	ASN
1	E	171	HIS
1	F	196	ASN
1	F	269	ASN
1	G	24	ASN
1	G	41	HIS
1	G	128	ASN
1	H	41	HIS

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](#)

8 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	A1D7N	H	401	1	32,35,35	0.40	0	41,56,56	0.50	0
2	A1D7N	C	401	1	32,35,35	0.37	0	41,56,56	0.50	0
2	A1D7N	D	401	1	32,35,35	0.39	0	41,56,56	0.54	0
2	A1D7N	B	401	1	32,35,35	0.38	0	41,56,56	0.50	0
2	A1D7N	A	401	1	32,35,35	0.41	0	41,56,56	0.53	0
2	A1D7N	E	401	1	32,35,35	0.41	0	41,56,56	0.58	0
2	A1D7N	G	401	1	32,35,35	0.38	0	41,56,56	0.52	0
2	A1D7N	F	401	1	32,35,35	0.40	0	41,56,56	0.50	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	A1D7N	H	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	C	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	D	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	B	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	A	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	E	401	1	-	0/31/68/68	0/3/3/3
2	A1D7N	G	401	1	-	2/31/68/68	0/3/3/3
2	A1D7N	F	401	1	-	5/31/68/68	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1D7N	C4-N5-S1-O4
2	A	401	A1D7N	C4-N5-S1-C22
2	B	401	A1D7N	C4-N5-S1-O4
2	B	401	A1D7N	C4-N5-S1-C22
2	C	401	A1D7N	C4-N5-S1-O4

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Mol	Chain	Res	Type	Atoms
2	C	401	A1D7N	C4-N5-S1-C22
2	D	401	A1D7N	C4-N5-S1-O4
2	D	401	A1D7N	C4-N5-S1-C22
2	F	401	A1D7N	C2-C4-N5-S1
2	G	401	A1D7N	C4-N5-S1-O4
2	G	401	A1D7N	C4-N5-S1-C22
2	H	401	A1D7N	C4-N5-S1-O4
2	H	401	A1D7N	C4-N5-S1-C22
2	F	401	A1D7N	C4-N5-S1-O4
2	F	401	A1D7N	C4-N5-S1-O5
2	F	401	A1D7N	C5-C4-N5-S1
2	F	401	A1D7N	C4-N5-S1-C22

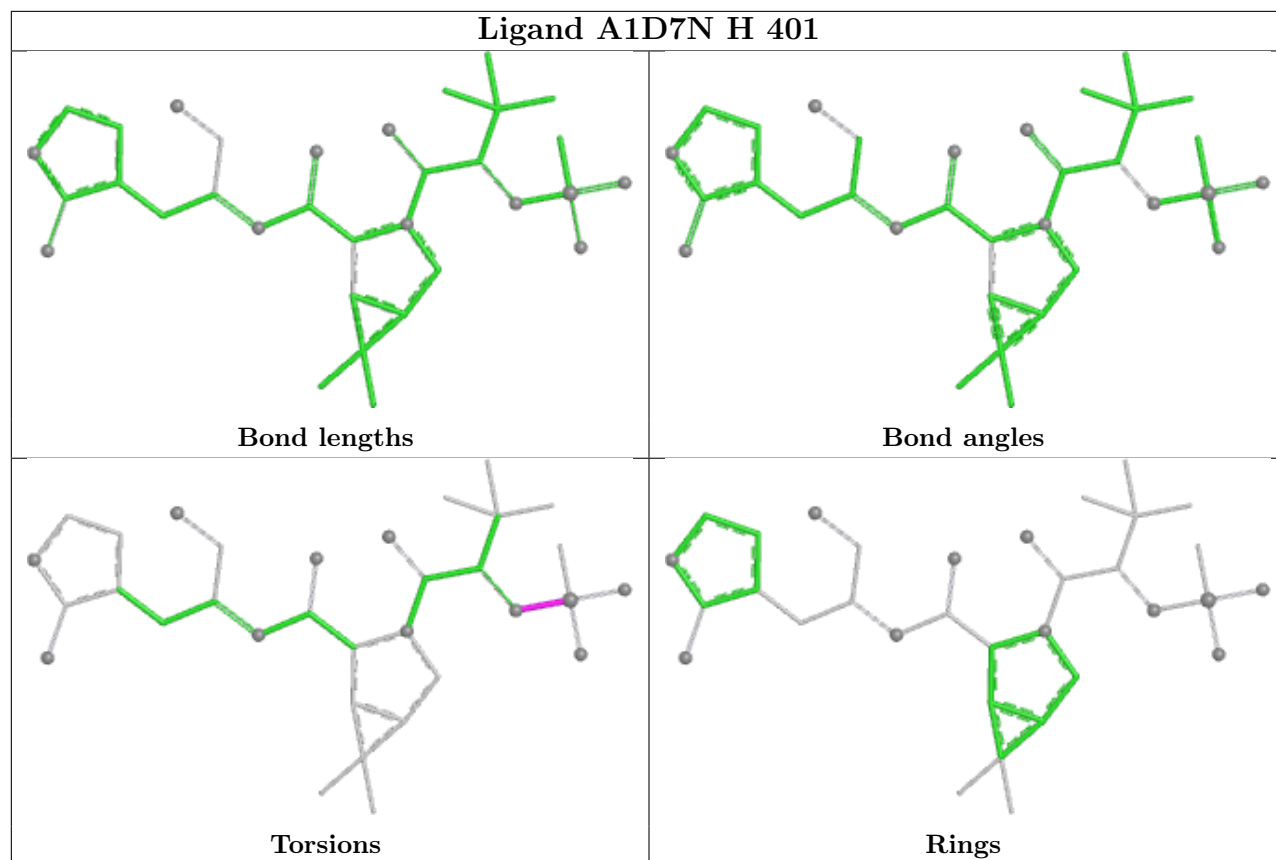
There are no ring outliers.

3 monomers are involved in 3 short contacts:

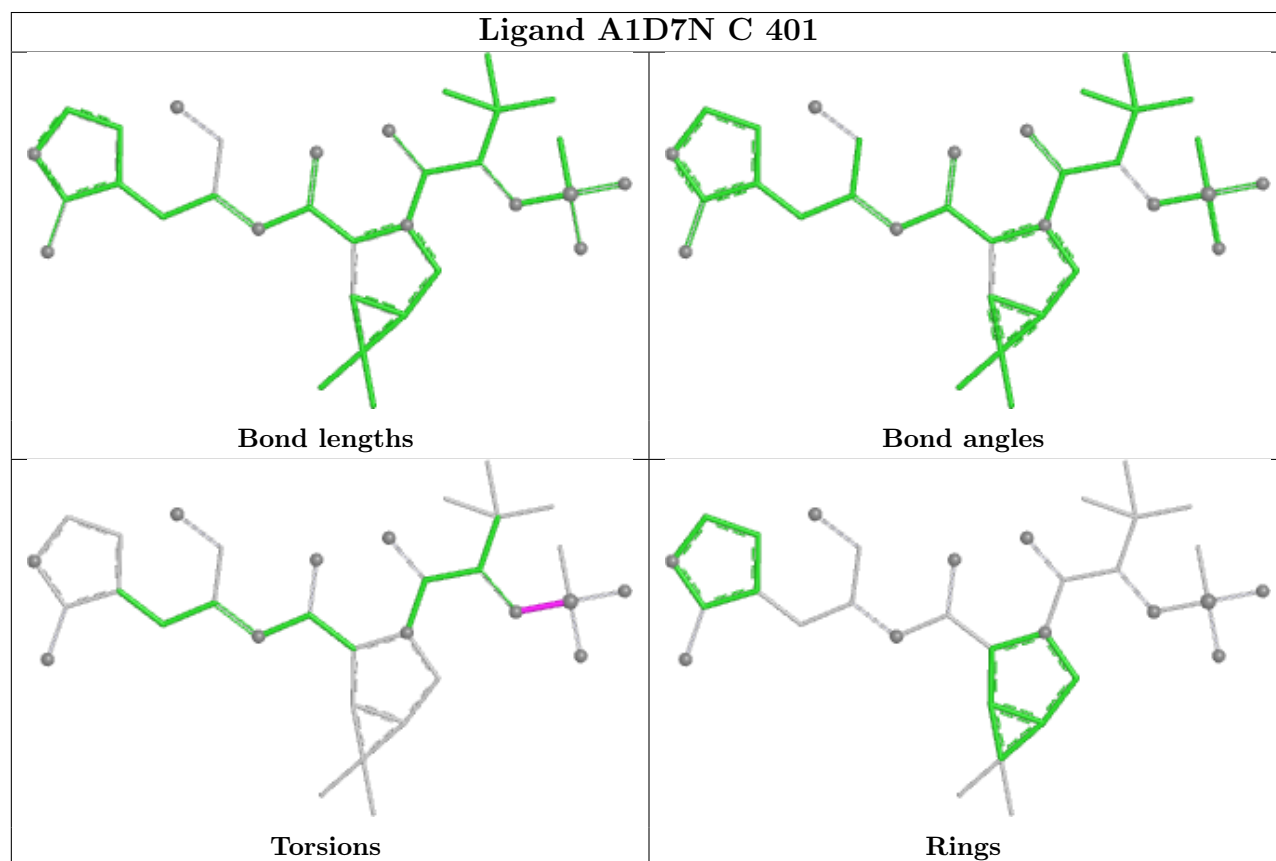
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A1D7N	1	0
2	A	401	A1D7N	1	0
2	F	401	A1D7N	1	0

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 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.

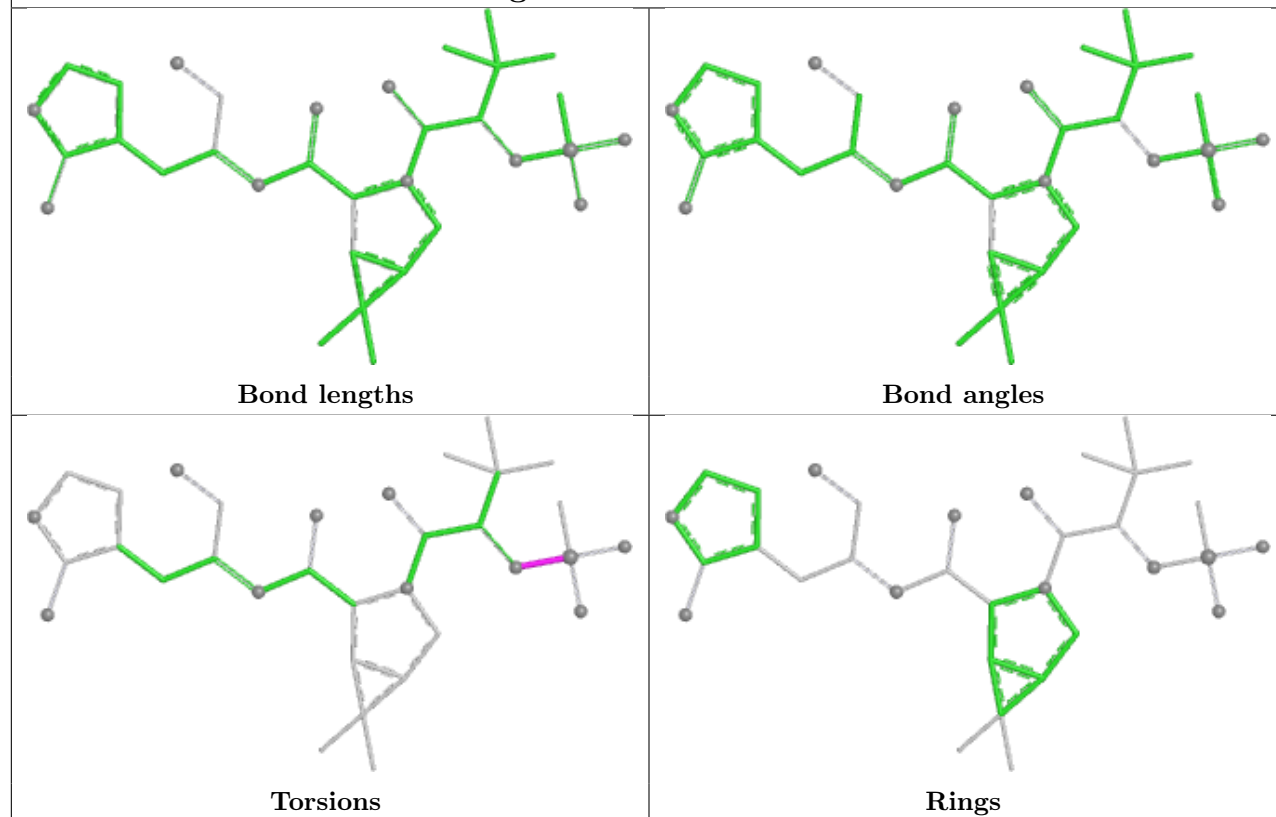
Ligand A1D7N H 401



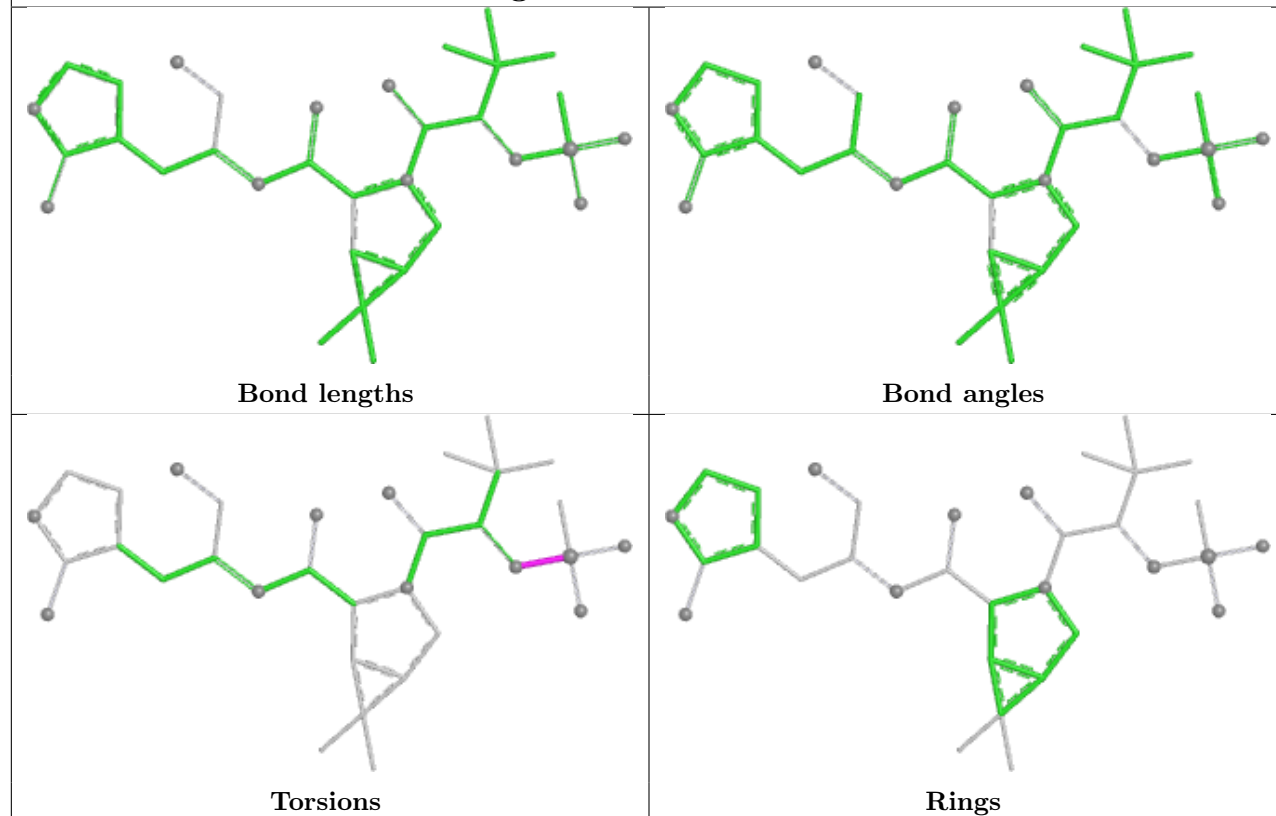
Ligand A1D7N C 401



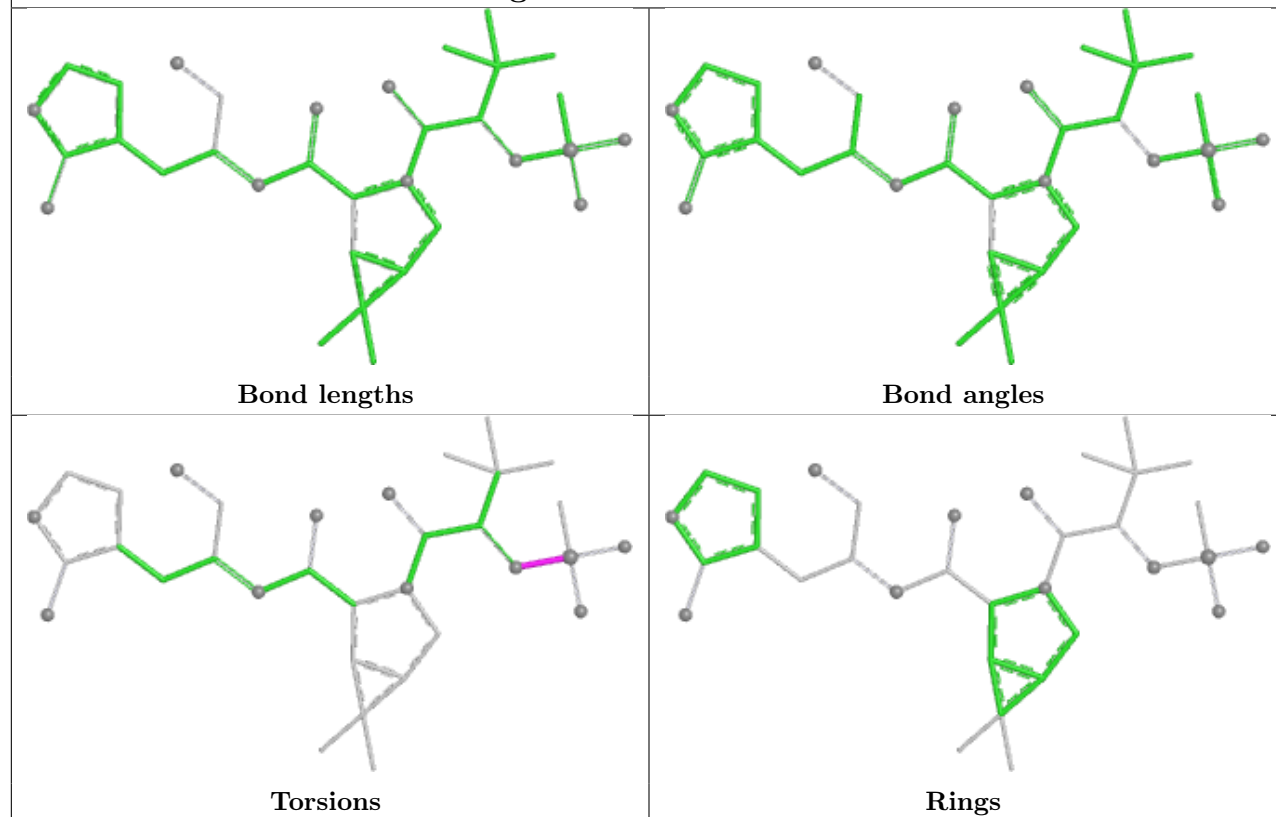
Ligand A1D7N D 401



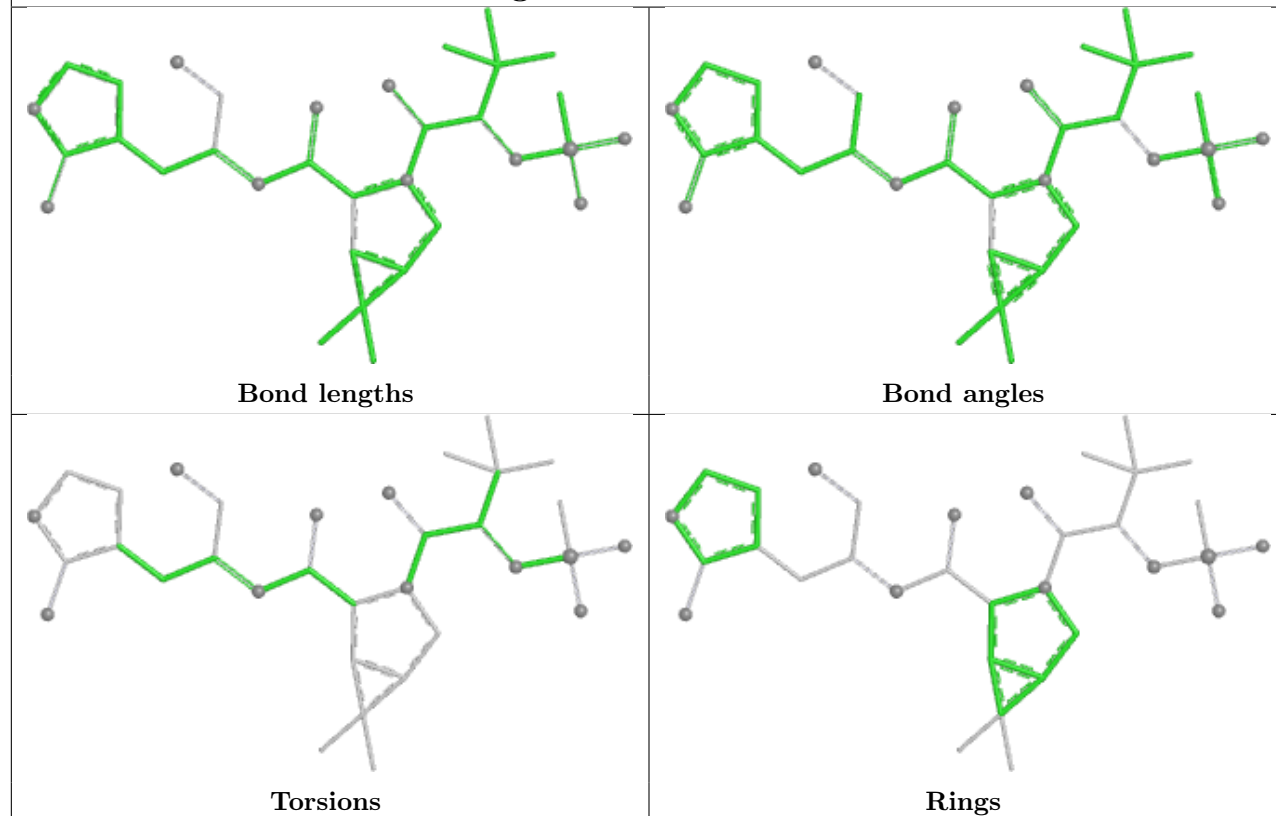
Ligand A1D7N B 401



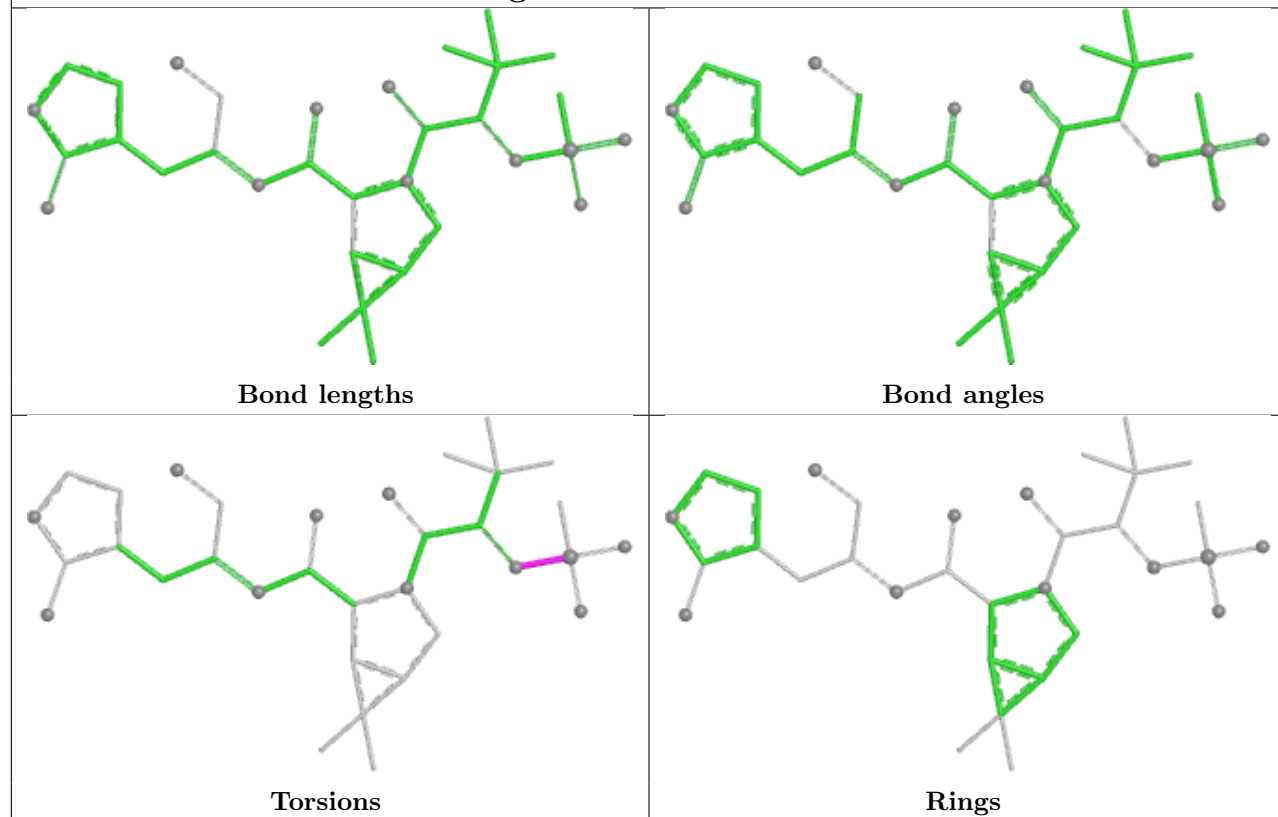
Ligand A1D7N A 401



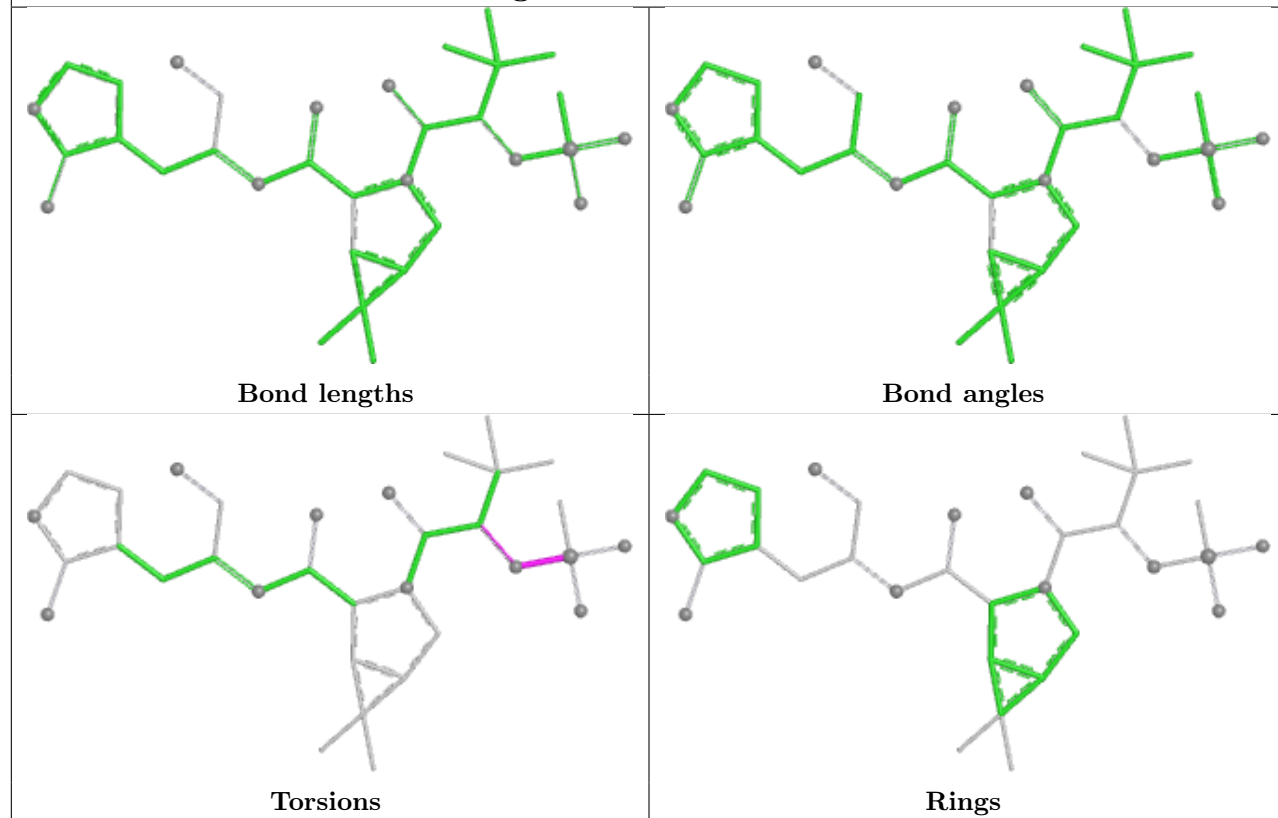
Ligand A1D7N E 401



Ligand A1D7N G 401



Ligand A1D7N F 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, 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	299/302 (99%)	0.54	8 (2%) 56 57	28, 41, 60, 74	0
1	B	298/302 (98%)	0.59	8 (2%) 56 57	28, 42, 61, 71	0
1	C	298/302 (98%)	0.82	12 (4%) 42 41	30, 48, 66, 79	0
1	D	299/302 (99%)	0.97	19 (6%) 25 24	30, 52, 72, 83	0
1	E	298/302 (98%)	1.12	41 (13%) 6 6	31, 52, 75, 88	0
1	F	284/302 (94%)	1.29	73 (25%) 1 1	31, 51, 77, 88	0
1	G	273/302 (90%)	1.69	85 (31%) 1 1	36, 67, 99, 109	0
1	H	251/302 (83%)	1.51	63 (25%) 1 1	38, 61, 93, 105	0
All	All	2300/2416 (95%)	1.05	309 (13%) 7 6	28, 50, 83, 109	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	ALA	7.0
1	E	229	TYR	6.6
1	F	93	VAL	5.3
1	G	233	ALA	5.0
1	F	43	ILE	4.9
1	G	208	TYR	4.8
1	E	233	ALA	4.8
1	G	283	LEU	4.8
1	F	79	ALA	4.8
1	F	25	ASN	4.7
1	H	230	ASN	4.7
1	H	255	GLY	4.7
1	H	208	TYR	4.6
1	G	232	TRP	4.5
1	E	236	ASN	4.4
1	G	231	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	58	SER	4.2
1	E	232	TRP	4.1
1	H	212	ILE	4.1
1	F	20	VAL	4.1
1	G	257	SER	4.1
1	F	42	VAL	4.1
1	F	22	TYR	3.9
1	F	26	VAL	3.9
1	F	27	LEU	3.9
1	G	75	GLY	3.9
1	G	21	SER	3.9
1	F	63	HIS	3.9
1	H	68	SER	3.8
1	F	299	VAL	3.8
1	C	194	GLY	3.8
1	D	63	HIS	3.7
1	F	140	ILE	3.7
1	D	241	LEU	3.6
1	H	207	LEU	3.6
1	H	299	VAL	3.6
1	F	48	THR	3.6
1	G	265	ILE	3.6
1	G	62	LEU	3.6
1	G	86	LEU	3.6
1	G	244	THR	3.6
1	C	1	SER	3.6
1	F	122	GLY	3.6
1	G	158	PHE	3.6
1	G	211	LEU	3.6
1	G	258	VAL	3.6
1	F	190	MET	3.5
1	G	278	LEU	3.5
1	F	172	VAL	3.5
1	F	78	SER	3.5
1	H	231	THR	3.5
1	F	116	CYS	3.5
1	F	94	ASN	3.5
1	F	44	ALA	3.5
1	F	298	GLY	3.5
1	E	225	SER	3.4
1	C	298	GLY	3.4
1	H	205	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	216	ARG	3.4
1	F	31	TRP	3.4
1	F	36	VAL	3.4
1	D	88	LEU	3.4
1	F	23	GLY	3.4
1	H	297	TYR	3.3
1	F	88	LEU	3.3
1	H	102	PHE	3.3
1	E	264	SER	3.3
1	F	28	ASN	3.3
1	H	213	ASN	3.3
1	G	262	LEU	3.3
1	F	50	VAL	3.3
1	G	268	LEU	3.2
1	G	157	TYR	3.2
1	H	250	LEU	3.2
1	D	244	THR	3.2
1	F	47	THR	3.2
1	H	65	PHE	3.2
1	G	266	VAL	3.2
1	C	63	HIS	3.2
1	H	43	ILE	3.2
1	D	64	ASN	3.1
1	G	87	VAL	3.1
1	G	74	LEU	3.1
1	H	73	PHE	3.1
1	F	64	ASN	3.1
1	E	268	LEU	3.1
1	E	224	MET	3.1
1	C	233	ALA	3.1
1	E	67	VAL	3.1
1	C	3	LEU	3.1
1	F	30	LEU	3.1
1	G	212	ILE	3.0
1	E	242	SER	3.0
1	D	190	MET	3.0
1	G	67	VAL	3.0
1	G	93	VAL	3.0
1	G	80	LYS	3.0
1	F	21	SER	3.0
1	E	196	ASN	3.0
1	G	230	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	287	PHE	3.0
1	F	141	ALA	3.0
1	G	241	LEU	3.0
1	H	293	ILE	3.0
1	C	235	THR	3.0
1	H	196	ASN	3.0
1	E	238	PHE	2.9
1	G	73	PHE	2.9
1	G	247	PHE	2.9
1	E	241	LEU	2.9
1	F	166	LEU	2.9
1	G	156	LEU	2.9
1	D	299	VAL	2.9
1	F	117	TYR	2.9
1	H	283	LEU	2.9
1	G	277	ILE	2.9
1	F	57	MET	2.9
1	H	214	GLY	2.9
1	G	282	SER	2.9
1	E	137	GLY	2.9
1	G	81	TYR	2.9
1	F	95	PRO	2.9
1	H	253	LYS	2.9
1	E	226	LEU	2.9
1	F	18	VAL	2.9
1	D	243	SER	2.8
1	G	11	GLY	2.8
1	F	41	HIS	2.8
1	G	79	ALA	2.8
1	F	59	SER	2.8
1	F	121	PRO	2.8
1	G	76	VAL	2.8
1	F	51	ILE	2.8
1	H	279	SER	2.8
1	A	74	LEU	2.8
1	G	36	VAL	2.8
1	G	28	ASN	2.8
1	H	238	PHE	2.8
1	H	232	TRP	2.7
1	G	215	GLU	2.7
1	H	22	TYR	2.7
1	H	149	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	280	TYR	2.7
1	A	299	VAL	2.7
1	D	60	VAL	2.7
1	E	217	TRP	2.7
1	G	250	LEU	2.7
1	E	26	VAL	2.7
1	D	71	ASN	2.7
1	D	183	GLY	2.7
1	G	65	PHE	2.7
1	F	34	ASP	2.7
1	E	281	GLY	2.7
1	E	228	SER	2.7
1	F	138	SER	2.7
1	F	86	LEU	2.7
1	A	73	PHE	2.6
1	H	197	VAL	2.6
1	H	296	MET	2.6
1	F	32	LEU	2.6
1	H	235	THR	2.6
1	E	74	LEU	2.6
1	G	107	ALA	2.6
1	F	24	ASN	2.6
1	F	91	ASN	2.6
1	A	75	GLY	2.6
1	H	239	THR	2.6
1	G	213	ASN	2.6
1	F	164	LEU	2.5
1	D	196	ASN	2.5
1	E	230	ASN	2.5
1	G	182	GLY	2.5
1	F	87	VAL	2.5
1	G	90	VAL	2.5
1	G	149	TYR	2.5
1	F	85	ASN	2.5
1	E	265	ILE	2.5
1	F	17	ILE	2.5
1	G	207	LEU	2.5
1	C	65	PHE	2.5
1	G	237	SER	2.5
1	A	63	HIS	2.5
1	E	23	GLY	2.5
1	E	167	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	255	GLY	2.5
1	F	147	VAL	2.4
1	G	12	LEU	2.4
1	C	2	GLY	2.4
1	E	133	GLY	2.4
1	G	185	GLU	2.4
1	H	16	CYS	2.4
1	D	67	VAL	2.4
1	G	238	PHE	2.4
1	G	31	TRP	2.4
1	G	57	MET	2.4
1	D	226	LEU	2.4
1	H	278	LEU	2.4
1	B	221	ASN	2.4
1	F	221	ASN	2.4
1	G	256	GLN	2.4
1	A	137	GLY	2.4
1	E	154	ALA	2.4
1	G	243	SER	2.4
1	C	43	ILE	2.4
1	F	192	LEU	2.4
1	F	136	LYS	2.4
1	G	37	ILE	2.4
1	H	60	VAL	2.4
1	H	77	VAL	2.4
1	E	255	GLY	2.3
1	H	75	GLY	2.3
1	E	195	THR	2.3
1	E	239	THR	2.3
1	H	254	THR	2.3
1	G	295	GLN	2.3
1	D	229	TYR	2.3
1	H	234	LYS	2.3
1	H	233	ALA	2.3
1	H	288	THR	2.3
1	H	93	VAL	2.3
1	G	88	LEU	2.3
1	A	70	ASN	2.3
1	H	236	ASN	2.3
1	F	15	PRO	2.3
1	H	157	TYR	2.3
1	C	231	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	195	THR	2.3
1	F	49	ARG	2.3
1	F	146	SER	2.3
1	H	76	VAL	2.3
1	F	120	CYS	2.3
1	H	160	TYR	2.3
1	G	276	THR	2.3
1	F	12	LEU	2.2
1	F	13	VAL	2.3
1	G	176	LEU	2.2
1	H	3	LEU	2.2
1	H	203	VAL	2.3
1	H	211	LEU	2.2
1	E	194	GLY	2.2
1	H	294	ARG	2.2
1	F	195	THR	2.2
1	F	123	SER	2.2
1	G	105	ILE	2.2
1	C	241	LEU	2.2
1	E	283	LEU	2.2
1	B	73	PHE	2.2
1	E	93	VAL	2.2
1	D	230	ASN	2.2
1	H	64	ASN	2.2
1	G	9	PRO	2.2
1	E	271	GLY	2.2
1	G	92	GLN	2.2
1	E	252	ALA	2.2
1	H	74	LEU	2.2
1	D	77	VAL	2.2
1	G	84	VAL	2.2
1	H	240	GLU	2.2
1	G	155	THR	2.2
1	G	22	TYR	2.2
1	H	81	TYR	2.2
1	H	31	TRP	2.2
1	E	261	LEU	2.2
1	F	55	ASN	2.2
1	G	102	PHE	2.2
1	G	245	ASP	2.2
1	H	289	PRO	2.2
1	H	63	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	195	THR	2.2
1	E	200	SER	2.2
1	B	216	ARG	2.1
1	G	280	TYR	2.1
1	G	292	VAL	2.1
1	F	19	ARG	2.1
1	B	234	LYS	2.1
1	B	265	ILE	2.1
1	E	270	LYS	2.1
1	H	32	LEU	2.1
1	G	77	VAL	2.1
1	B	273	GLY	2.1
1	E	63	HIS	2.1
1	H	97	THR	2.1
1	H	199	SER	2.1
1	F	154	ALA	2.1
1	D	86	LEU	2.1
1	G	112	ASN	2.1
1	A	42	VAL	2.1
1	E	50	VAL	2.1
1	B	274	GLY	2.1
1	E	298	GLY	2.1
1	F	139	PHE	2.1
1	F	89	LYS	2.0
1	F	237	SER	2.0
1	G	190	MET	2.0
1	G	249	MET	2.0
1	F	38	CYS	2.0
1	H	38	CYS	2.0
1	G	94	ASN	2.0
1	E	273	GLY	2.0
1	F	83	GLY	2.0
1	H	298	GLY	2.0
1	F	143	THR	2.0
1	G	68	SER	2.0
1	G	288	THR	2.0
1	B	252	ALA	2.0
1	G	3	LEU	2.0
1	G	30	LEU	2.0
1	G	17	ILE	2.0
1	G	234	LYS	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](#)

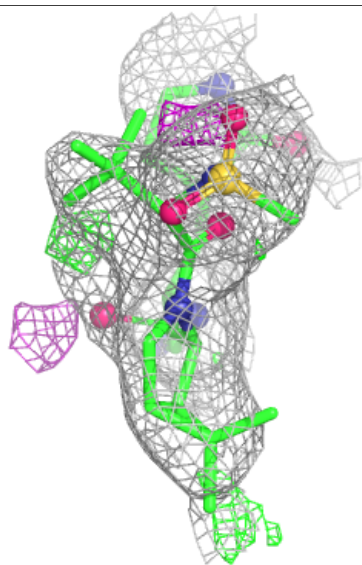
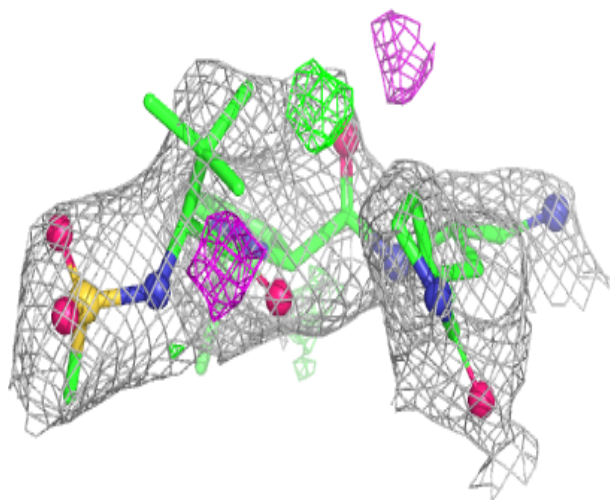
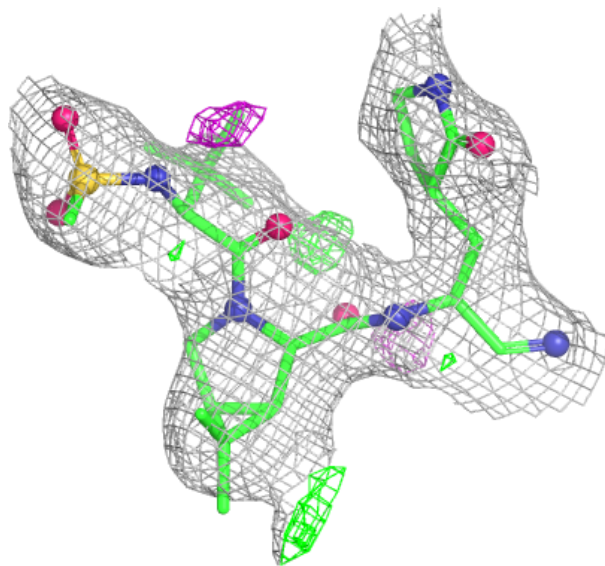
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1D7N	F	401	33/33	0.81	0.18	59,76,89,97	0
2	A1D7N	A	401	33/33	0.90	0.14	29,47,57,71	0
2	A1D7N	E	401	33/33	0.92	0.12	43,63,73,77	0
2	A1D7N	D	401	33/33	0.92	0.10	32,41,58,63	0
2	A1D7N	G	401	33/33	0.92	0.10	29,39,56,73	0
2	A1D7N	H	401	33/33	0.92	0.11	37,46,53,56	0
2	A1D7N	C	401	33/33	0.93	0.10	31,41,51,56	0
2	A1D7N	B	401	33/33	0.93	0.11	37,43,58,59	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.

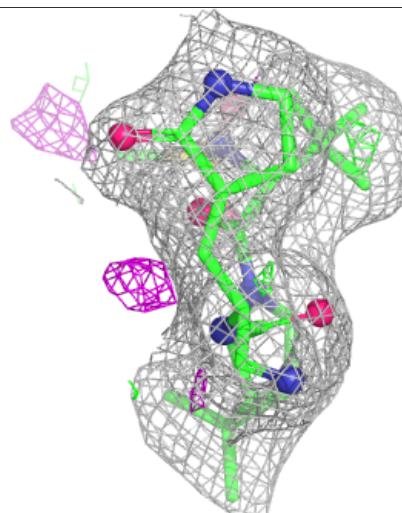
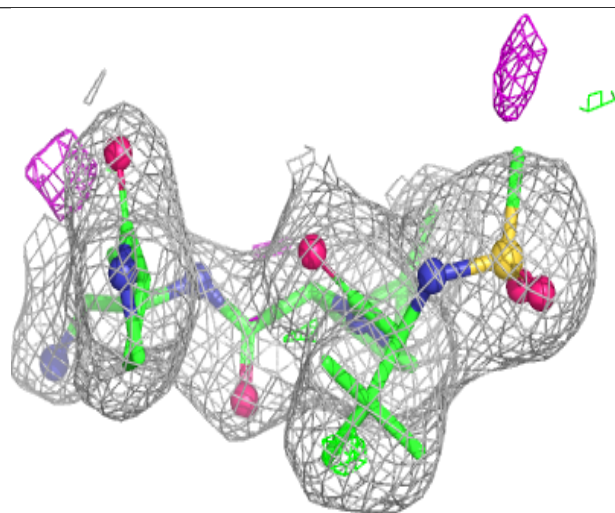
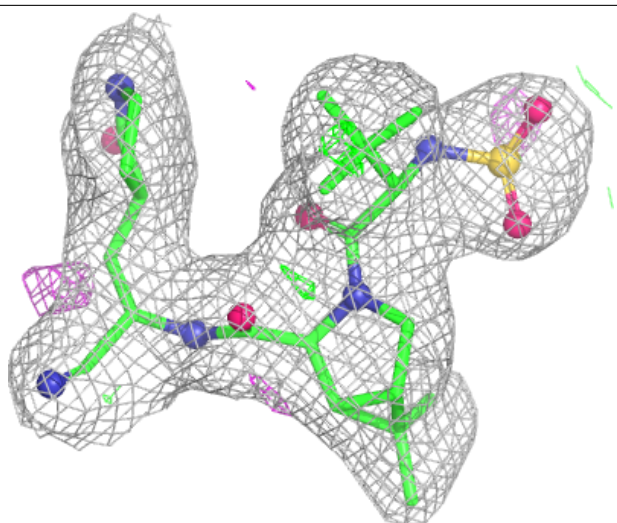
Electron density around A1D7N F 401:

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



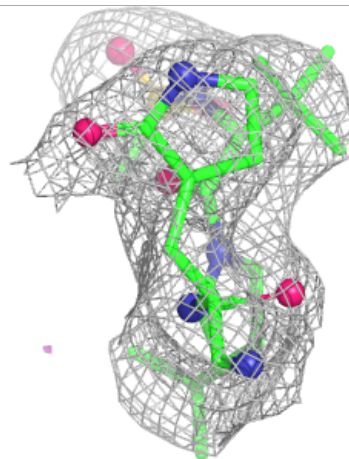
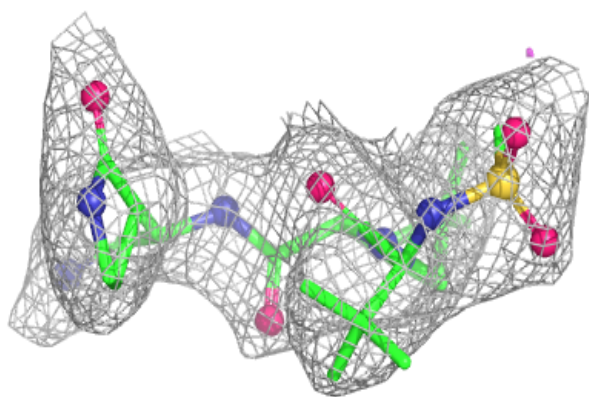
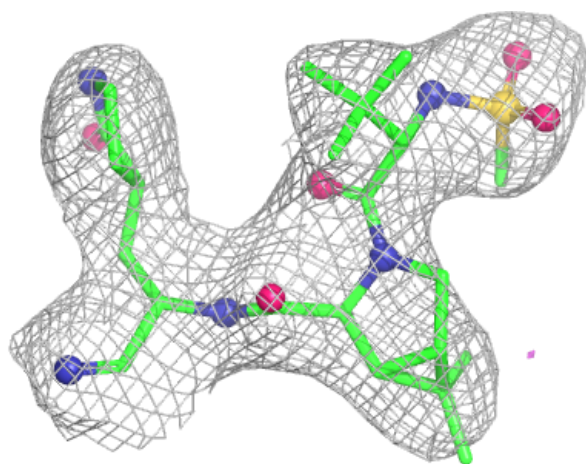
Electron density around A1D7N A 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



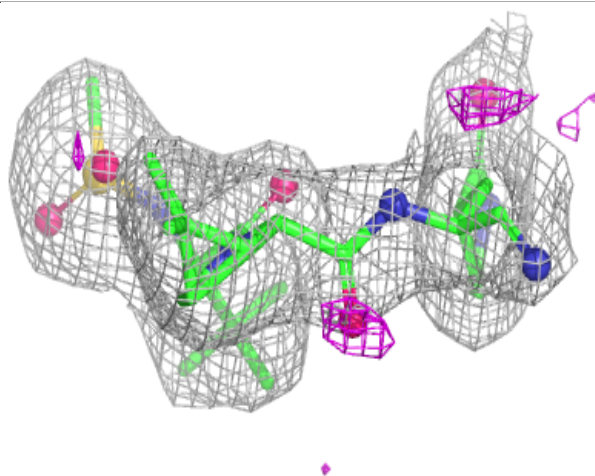
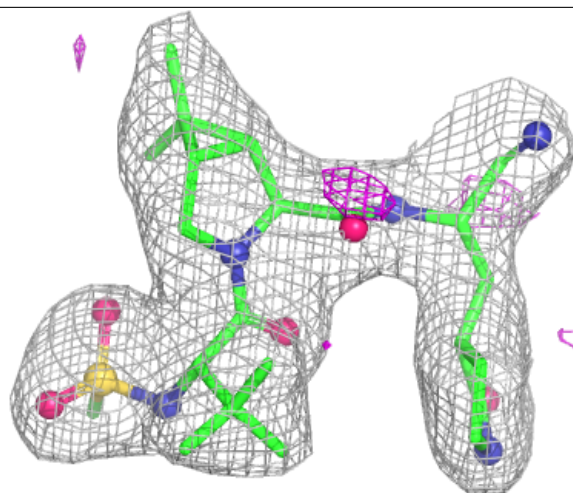
Electron density around A1D7N E 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



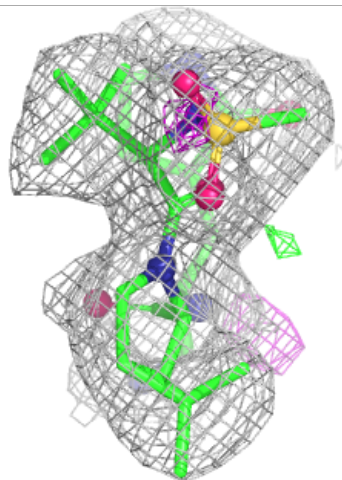
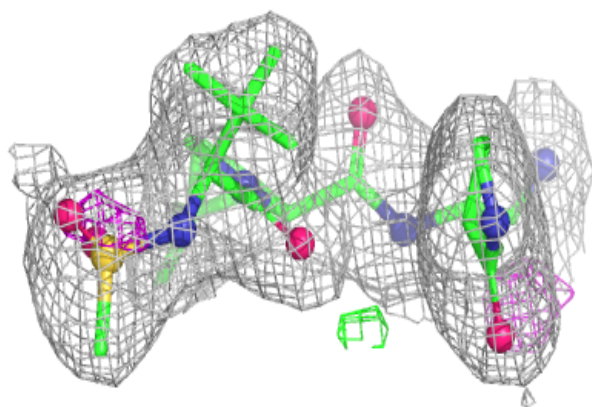
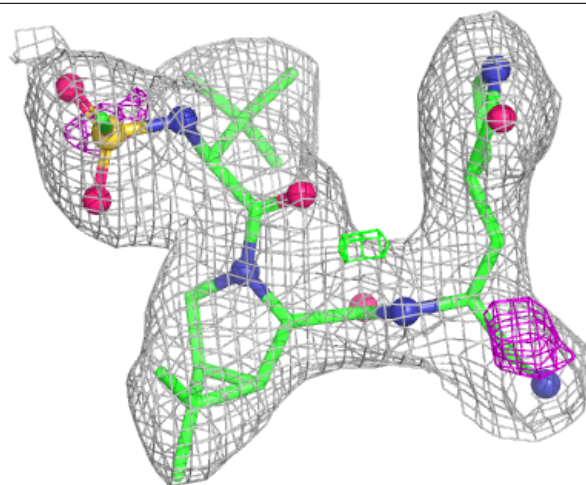
Electron density around A1D7N D 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



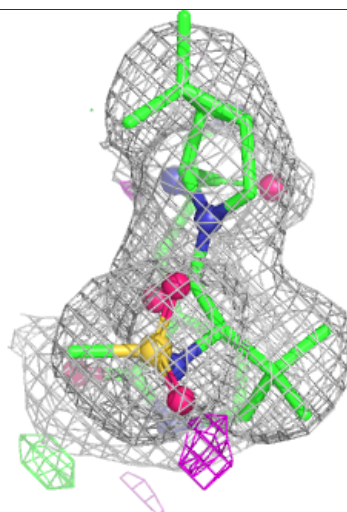
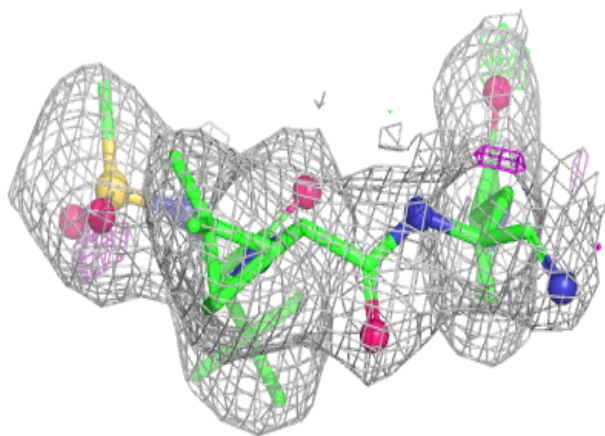
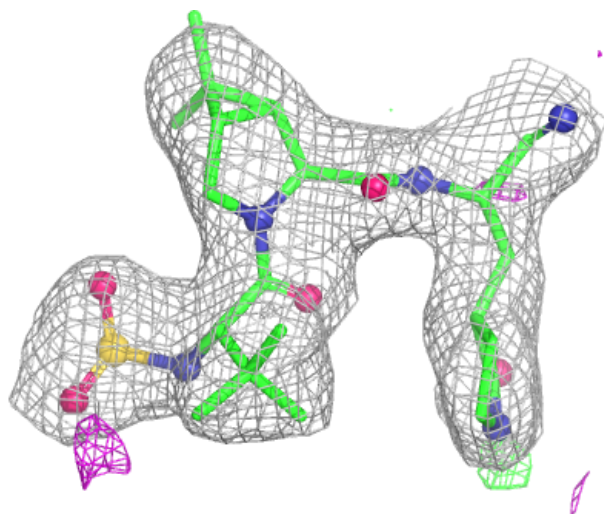
Electron density around A1D7N G 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



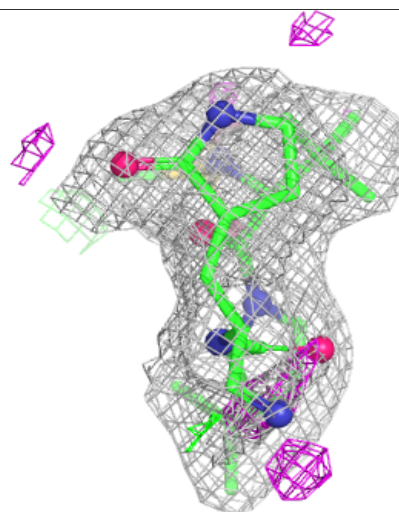
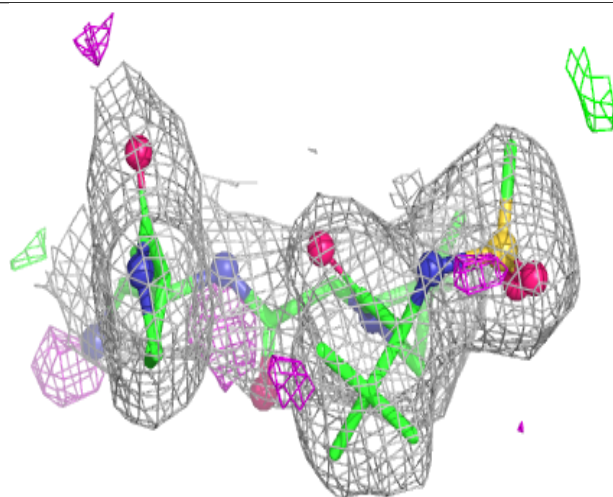
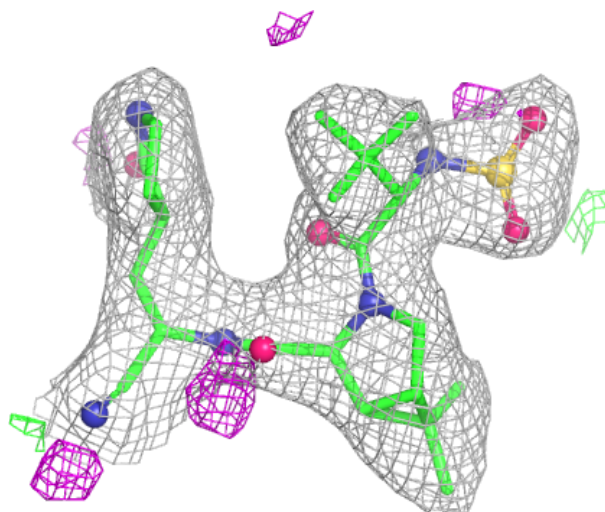
Electron density around A1D7N H 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



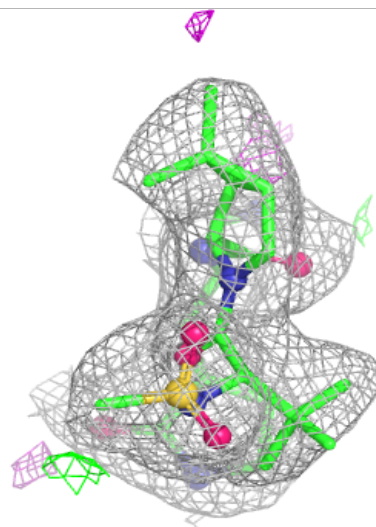
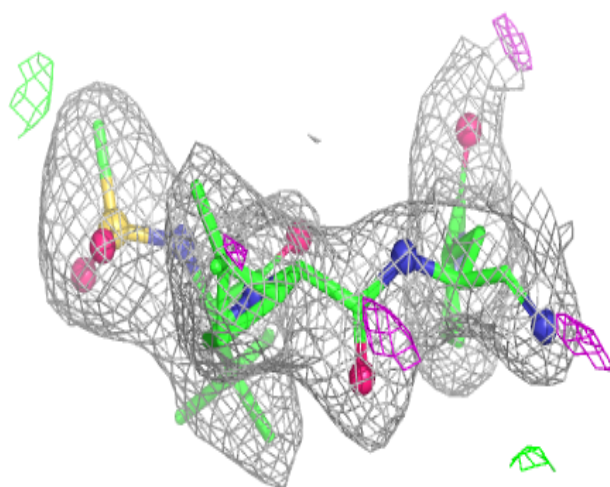
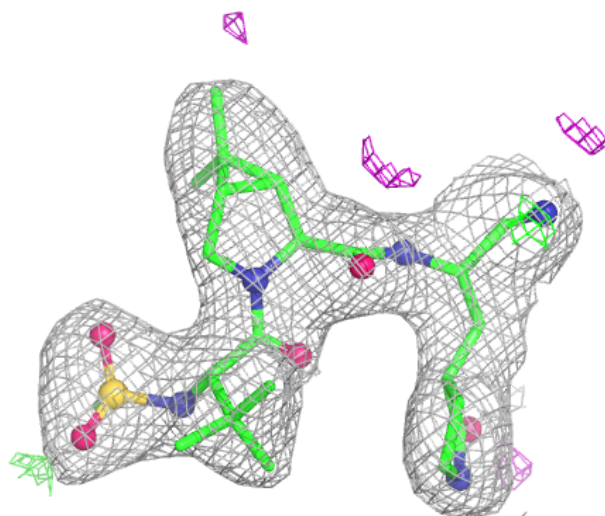
Electron density around A1D7N C 401:

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



Electron density around A1D7N 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.