



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 9IR8 / pdb_00009ir8
Title : CCoV-HuPn-2018 3CL protease (3CLpro) in complex with compound 6
Authors : Nie, T.Q.; Su, H.X.; Li, M.J.; Xu, Y.C.
Deposited on : 2024-07-15
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

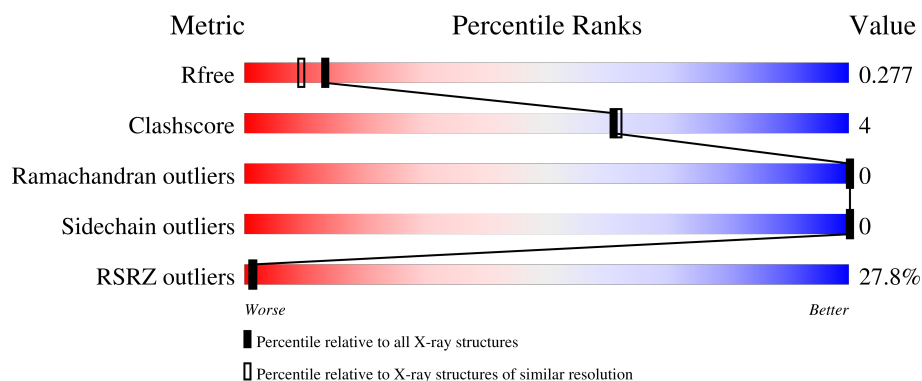
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	302	19% 92% 7% .
1	B	302	8% 91% 8% .
1	C	302	37% 84% 11% 5%
1	D	302	42% 77% 12% 10%

2 Entry composition [i](#)

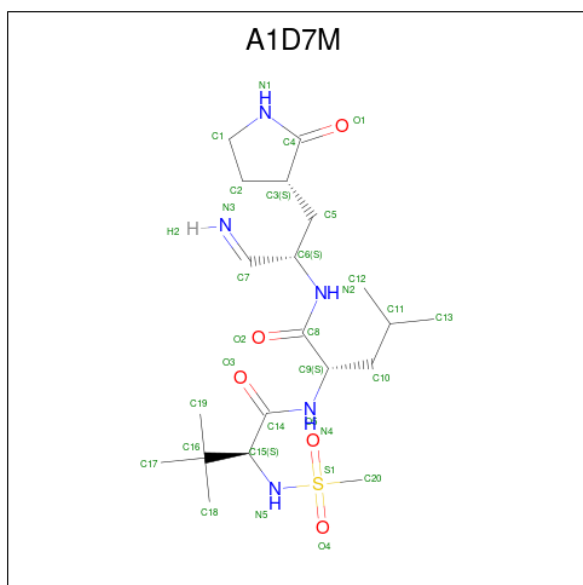
There are 3 unique types of molecules in this entry. The entry contains 8906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2272	1432	381	444	15			
1	B	299	Total	C	N	O	S	0	0	0
			2284	1438	385	445	16			
1	C	288	Total	C	N	O	S	0	0	0
			2110	1331	356	408	15			
1	D	271	Total	C	N	O	S	0	0	0
			1983	1242	343	384	14			

- Molecule 2 is (2 {S})- {N}-[(2 {S})-1-azanylidene-3-[(3 {S})-2-oxidanylidenepyrrolidin-3-yl]propan-2-yl]-2-[[(2 {S})-3,3-dimethyl-2-(methylsulfonylamino)butanoyl]amino]-4-methyl-pentanamide (CCD ID: A1D7M) (formula: C₂₀H₃₇N₅O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	20	5	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			31	20	5	5	1		
2	C	1	Total	C	N	O	S	0	0
			31	20	5	5	1		
2	D	1	Total	C	N	O	S	0	0
			31	20	5	5	1		

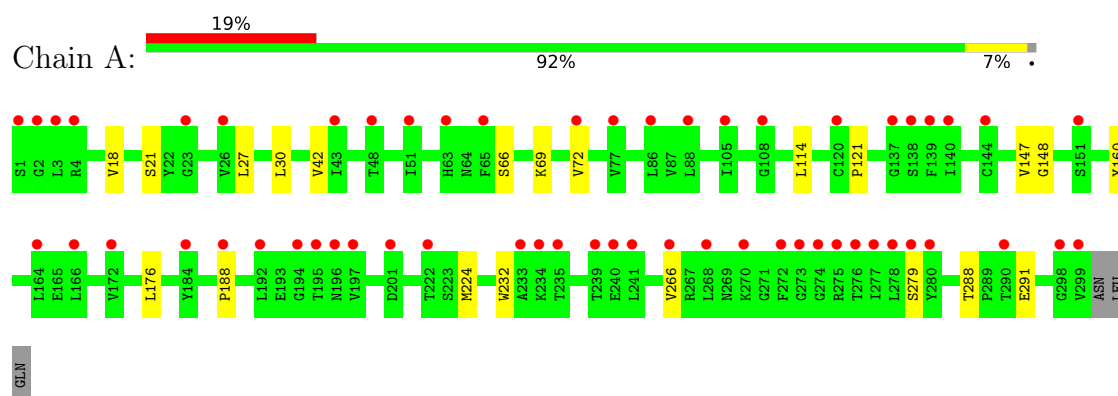
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	51	Total	O	0	0
			51	51		
3	C	26	Total	O	0	0
			26	26		
3	D	18	Total	O	0	0
			18	18		

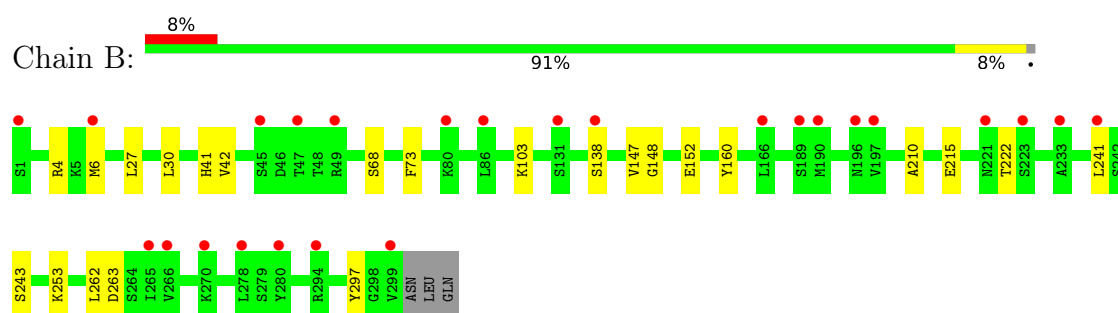
3 Residue-property plots [i](#)

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.

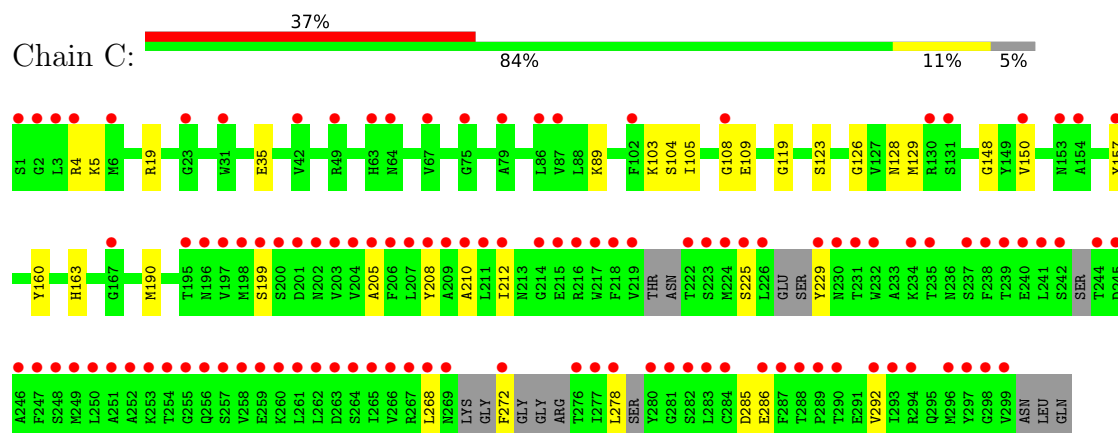
• Molecule 1: 3C-like protease



• Molecule 1: 3C-like protease

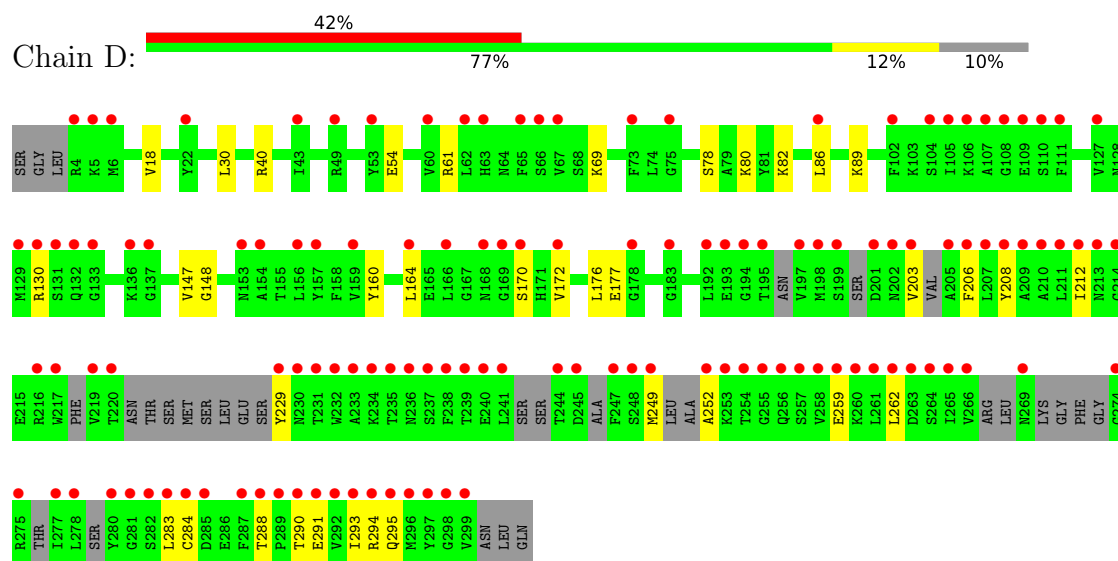


• Molecule 1: 3C-like protease



● Molecule 1: 3C-like protease

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.10Å 127.58Å 111.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.91 – 2.12 111.91 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.2 (111.91-2.12) 98.3 (111.91-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.242 , 0.273 (Not available) , 0.277	Depositor DCC
R_{free} test set	4341 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8906	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% 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: A1D7M

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	0.11	0/2317	0.30	0/3140
1	B	0.25	2/2329 (0.1%)	0.30	0/3154
1	C	0.30	4/2146 (0.2%)	0.31	0/2906
1	D	0.20	0/2010	0.40	0/2709
All	All	0.23	6/8802 (0.1%)	0.33	0/11909

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	HIS	CE1-NE2	-6.87	1.25	1.32
1	C	163	HIS	C-O	-6.42	1.14	1.23
1	B	41	HIS	C-O	-5.96	1.15	1.24
1	B	41	HIS	CE1-NE2	-5.80	1.26	1.32
1	C	163	HIS	CG-ND1	-5.38	1.32	1.38
1	C	163	HIS	CD2-NE2	-5.20	1.32	1.37

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	2272	0	2207	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2284	0	2229	15	0
1	C	2110	0	1960	21	0
1	D	1983	0	1827	25	0
2	A	31	0	0	1	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
3	A	38	0	0	0	0
3	B	51	0	0	0	0
3	C	26	0	0	0	0
3	D	18	0	0	0	0
All	All	8906	0	8223	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (71) 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:D:130:ARG:NH2	1:D:170:SER:OG	2.21	0.74
1:D:288:THR:HG23	1:D:291:GLU:H	1.54	0.73
1:D:290:THR:HG22	1:D:294:ARG:NH2	2.07	0.69
1:D:148:GLY:HA3	1:D:160:TYR:HB3	1.74	0.68
1:C:148:GLY:HA3	1:C:160:TYR:HB3	1.76	0.66
1:C:210:ALA:HB2	1:C:278:LEU:HD11	1.76	0.66
1:C:5:LYS:NZ	1:C:286:GLU:O	2.31	0.64
1:D:30:LEU:HD13	1:D:147:VAL:HG21	1.82	0.62
1:A:148:GLY:HA3	1:A:160:TYR:HB3	1.82	0.62
1:A:18:VAL:HG12	1:A:69:LYS:HB2	1.81	0.60
1:D:18:VAL:HG12	1:D:69:LYS:HB2	1.84	0.58
1:D:78:SER:OG	1:D:80:LYS:HE3	2.06	0.56
1:B:30:LEU:HD13	1:B:147:VAL:HG21	1.87	0.56
1:D:249:MET:O	1:D:252:ALA:N	2.40	0.55
1:C:225:SER:O	1:C:229:TYR:N	2.40	0.55
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.89	0.54
1:C:19:ARG:HB2	1:C:119:GLY:HA3	1.93	0.51
1:B:103:LYS:NZ	1:B:152:GLU:OE2	2.44	0.50
1:D:294:ARG:HH11	1:D:294:ARG:HG3	1.75	0.50
1:D:40:ARG:HA	1:D:86:LEU:HB2	1.94	0.50
1:A:232:TRP:CD2	1:A:266:VAL:HG22	2.47	0.49
1:C:205:ALA:HB1	1:C:292:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLY:HA3	1:B:160:TYR:HB3	1.94	0.49
1:B:4:ARG:HH22	1:C:5:LYS:HG2	1.78	0.48
1:B:253:LYS:HD3	1:B:297:TYR:CZ	2.49	0.48
1:B:138:SER:OG	1:C:4:ARG:HG3	2.13	0.48
1:A:232:TRP:CE2	1:A:266:VAL:HG22	2.49	0.48
1:A:21:SER:OG	1:A:66:SER:HB3	2.14	0.48
1:D:82:LYS:HE3	1:D:177:GLU:HA	1.95	0.47
1:B:222:THR:OG1	1:B:263:ASP:OD2	2.33	0.47
1:D:259:GLU:HA	1:D:262:LEU:HB2	1.97	0.47
1:A:188:PRO:HA	2:A:401:A1D7M:O4	2.15	0.47
1:C:35:GLU:HG2	1:C:89:LYS:HD2	1.97	0.46
1:C:199:SER:HB3	1:C:285:ASP:HB2	1.98	0.46
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.98	0.45
1:C:108:GLY:O	1:C:128:ASN:ND2	2.44	0.45
1:C:129:MET:HE2	1:C:129:MET:HB2	1.92	0.45
1:D:164:LEU:HG	1:D:172:VAL:HB	1.98	0.45
1:A:69:LYS:O	1:A:72:VAL:HG22	2.17	0.44
1:D:61:ARG:HD3	1:D:61:ARG:HA	1.73	0.44
1:D:259:GLU:HA	1:D:262:LEU:HD12	2.00	0.44
1:A:279:SER:O	1:A:279:SER:OG	2.30	0.44
1:A:288:THR:OG1	1:A:291:GLU:HB2	2.18	0.44
1:B:6:MET:HB3	1:C:123:SER:HB3	2.00	0.44
1:D:293:ILE:C	1:D:295:GLN:H	2.25	0.44
1:A:224:MET:HE1	1:A:266:VAL:HG21	2.00	0.44
1:C:268:LEU:HB3	1:C:272:PHE:CE1	2.53	0.43
1:D:54:GLU:H	1:D:54:GLU:CD	2.25	0.43
1:D:208:TYR:O	1:D:212:ILE:HG13	2.18	0.43
1:A:176:LEU:HD13	1:A:176:LEU:HA	1.89	0.43
1:B:68:SER:HB3	1:B:73:PHE:CD2	2.52	0.43
1:C:208:TYR:O	1:C:212:ILE:HG13	2.19	0.43
1:D:78:SER:HB3	1:D:89:LYS:HB2	2.01	0.43
1:D:176:LEU:HD13	1:D:176:LEU:HA	1.91	0.43
1:B:4:ARG:NH2	1:C:5:LYS:HG2	2.33	0.43
1:D:294:ARG:HG3	1:D:294:ARG:NH1	2.34	0.43
1:C:150:VAL:HG12	1:C:157:TYR:HB2	2.01	0.43
1:C:105:ILE:HG23	1:C:109:GLU:HB2	2.01	0.42
1:D:229:TYR:HB2	1:D:262:LEU:HD22	2.01	0.42
1:C:190:MET:HB2	1:C:190:MET:HE2	1.77	0.42
1:B:241:LEU:HD12	1:B:262:LEU:HD21	2.01	0.42
1:D:290:THR:CG2	1:D:294:ARG:NH2	2.80	0.42
1:A:114:LEU:HD11	1:A:121:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD13	1:A:147:VAL:HG21	2.02	0.42
1:A:224:MET:HE1	1:A:266:VAL:CG2	2.50	0.41
1:B:4:ARG:NH2	1:C:126:GLY:O	2.53	0.41
1:C:103:LYS:HG2	1:C:104:SER:N	2.34	0.41
1:B:241:LEU:HD22	1:B:243:SER:O	2.20	0.41
1:D:203:VAL:HG11	1:D:283:LEU:HD13	2.02	0.41
1:D:206:PHE:CG	1:D:284:CYS:HB3	2.55	0.41
1:B:210:ALA:HB1	1:B:215:GLU:HB2	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	297/302 (98%)	288 (97%)	9 (3%)	0	100	100
1	B	297/302 (98%)	287 (97%)	10 (3%)	0	100	100
1	C	275/302 (91%)	264 (96%)	11 (4%)	0	100	100
1	D	246/302 (82%)	233 (95%)	13 (5%)	0	100	100
All	All	1115/1208 (92%)	1072 (96%)	43 (4%)	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	251/258 (97%)	251 (100%)	0	100	100
1	B	254/258 (98%)	254 (100%)	0	100	100
1	C	217/258 (84%)	217 (100%)	0	100	100
1	D	203/258 (79%)	203 (100%)	0	100	100
All	All	925/1032 (90%)	925 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	HIS
1	C	196	ASN
1	C	236	ASN
1	D	41	HIS
1	D	236	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](#)

4 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	A1D7M	C	401	1	29,31,31	0.33	0	37,45,45	0.54	1 (2%)
2	A1D7M	D	401	1	29,31,31	0.39	0	37,45,45	0.95	1 (2%)
2	A1D7M	B	401	1	29,31,31	0.35	0	37,45,45	0.58	0
2	A1D7M	A	401	1	29,31,31	0.36	0	37,45,45	0.61	1 (2%)

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	A1D7M	C	401	1	-	0/35/47/47	0/1/1/1
2	A1D7M	D	401	1	-	8/35/47/47	0/1/1/1
2	A1D7M	B	401	1	-	0/35/47/47	0/1/1/1
2	A1D7M	A	401	1	-	3/35/47/47	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	A1D7M	C16-C15-C14	5.00	118.45	112.97
2	A	401	A1D7M	C16-C15-C14	2.24	115.42	112.97
2	C	401	A1D7M	C14-C15-N5	2.08	114.10	110.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1D7M	C15-N5-S1-O5
2	D	401	A1D7M	C15-N5-S1-O4
2	D	401	A1D7M	O2-C8-C9-N4
2	D	401	A1D7M	N2-C8-C9-N4
2	D	401	A1D7M	C5-C6-N2-C8
2	A	401	A1D7M	C15-N5-S1-C20
2	D	401	A1D7M	C15-N5-S1-C20
2	A	401	A1D7M	C15-N5-S1-O4
2	D	401	A1D7M	C7-C6-N2-C8

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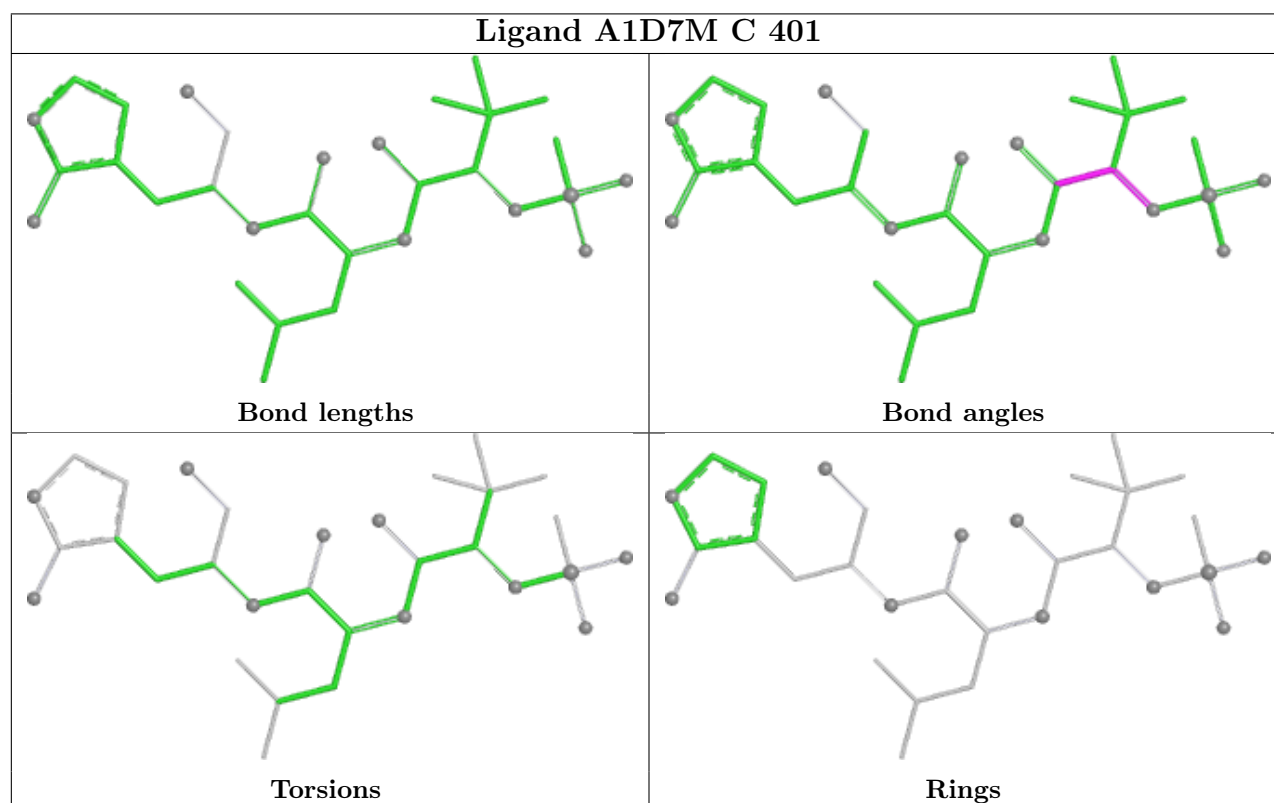
Mol	Chain	Res	Type	Atoms
2	D	401	A1D7M	O2-C8-C9-C10
2	D	401	A1D7M	N2-C8-C9-C10

There are no ring outliers.

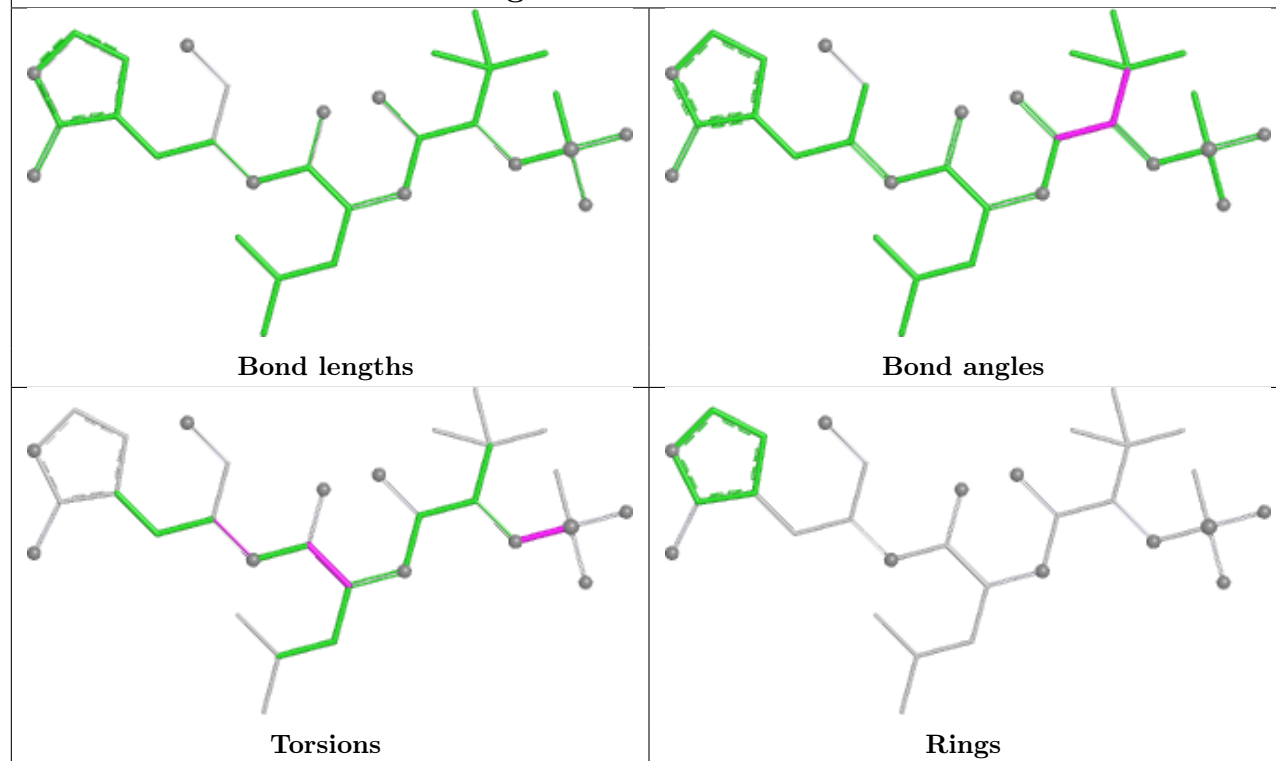
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	A1D7M	1	0

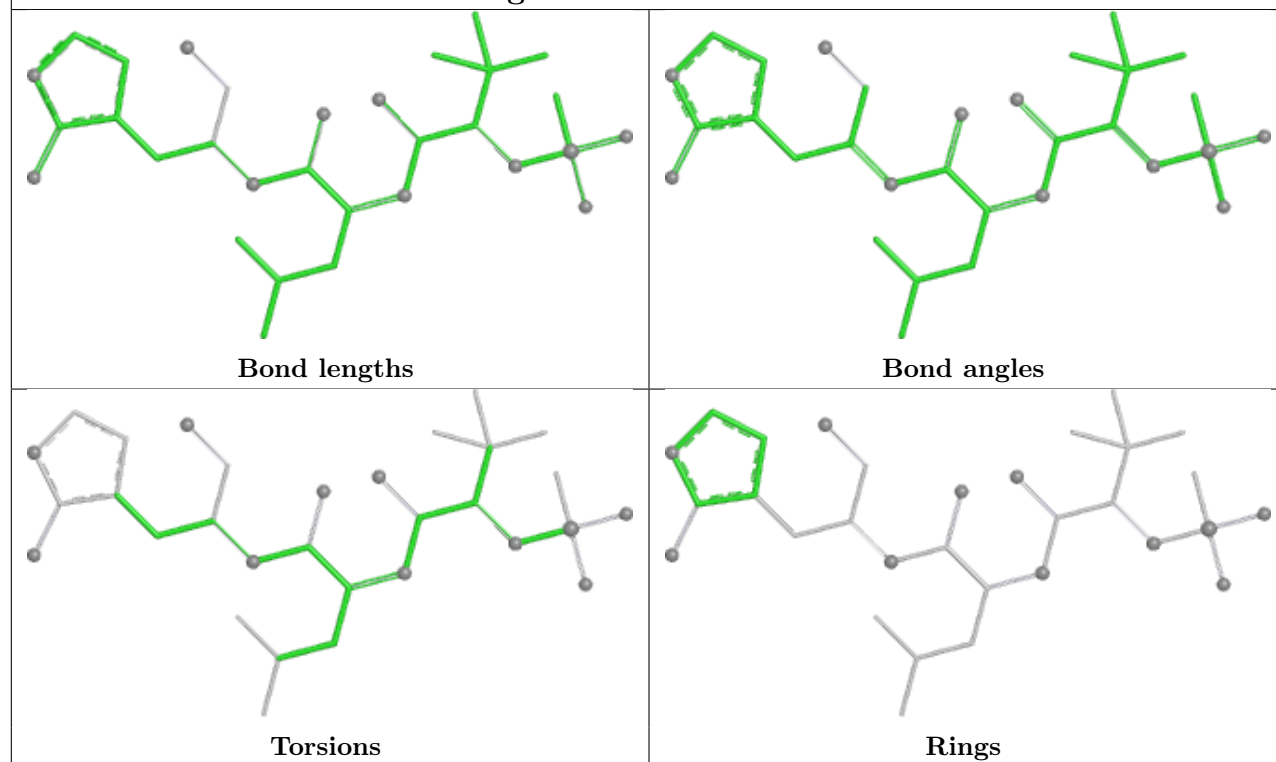
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

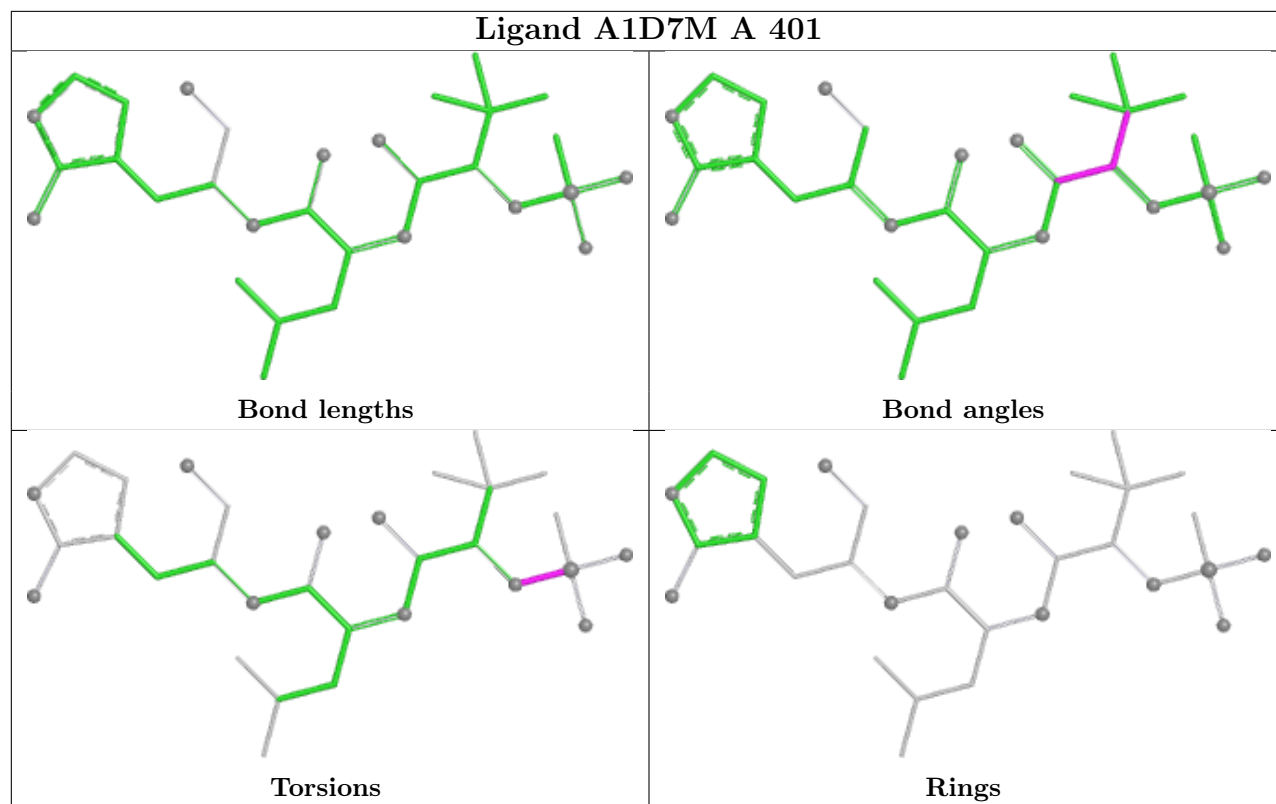


Ligand A1D7M D 401



Ligand A1D7M B 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%)	1.27	57 (19%) 3 3	34, 48, 67, 86	0
1	B	299/302 (99%)	0.89	25 (8%) 17 18	32, 44, 61, 80	0
1	C	288/302 (95%)	2.06	113 (39%) 1 1	35, 54, 94, 103	0
1	D	271/302 (89%)	2.25	127 (46%) 0 0	33, 58, 97, 103	0
All	All	1157/1208 (95%)	1.60	322 (27%) 1 1	32, 49, 91, 103	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	292	VAL	9.5
1	D	208	TYR	7.9
1	C	229	TYR	7.6
1	C	244	THR	7.2
1	C	241	LEU	7.2
1	C	226	LEU	7.1
1	D	277	ILE	7.0
1	C	250	LEU	6.6
1	D	207	LEU	6.6
1	C	262	LEU	6.5
1	D	299	VAL	6.5
1	D	203	VAL	6.5
1	C	222	THR	6.4
1	D	195	THR	6.4
1	A	273	GLY	6.4
1	D	241	LEU	6.3
1	D	297	TYR	6.3
1	C	254	THR	6.3
1	D	194	GLY	6.2
1	D	206	PHE	6.2
1	C	230	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	283	LEU	6.0
1	D	239	THR	6.0
1	C	277	ILE	6.0
1	D	205	ALA	5.9
1	D	212	ILE	5.9
1	C	272	PHE	5.8
1	C	278	LEU	5.7
1	D	229	TYR	5.7
1	D	247	PHE	5.6
1	C	245	ASP	5.6
1	B	299	VAL	5.5
1	D	232	TRP	5.5
1	C	212	ILE	5.4
1	C	204	VAL	5.4
1	C	280	TYR	5.4
1	C	1	SER	5.4
1	D	219	VAL	5.3
1	C	258	VAL	5.2
1	D	287	PHE	5.2
1	C	207	LEU	5.2
1	C	256	GLN	5.2
1	C	219	VAL	5.2
1	D	265	ILE	5.1
1	D	244	THR	5.1
1	C	299	VAL	5.1
1	D	262	LEU	5.1
1	D	108	GLY	5.1
1	D	278	LEU	5.0
1	D	288	THR	5.0
1	D	266	VAL	5.0
1	D	284	CYS	5.0
1	D	209	ALA	5.0
1	C	206	PHE	5.0
1	C	223	SER	4.9
1	C	208	TYR	4.9
1	D	291	GLU	4.8
1	D	261	LEU	4.8
1	D	258	VAL	4.8
1	C	225	SER	4.8
1	D	249	MET	4.8
1	D	275	ARG	4.7
1	C	203	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	4.7
1	D	252	ALA	4.6
1	C	3	LEU	4.6
1	C	261	LEU	4.6
1	D	217	TRP	4.6
1	D	197	VAL	4.6
1	A	299	VAL	4.6
1	D	199	SER	4.6
1	C	239	THR	4.5
1	D	231	THR	4.5
1	C	249	MET	4.4
1	C	246	ALA	4.4
1	C	257	SER	4.4
1	D	281	GLY	4.4
1	D	210	ALA	4.4
1	A	274	GLY	4.3
1	D	289	PRO	4.3
1	C	251	ALA	4.3
1	D	131	SER	4.3
1	C	255	GLY	4.3
1	C	283	LEU	4.3
1	C	289	PRO	4.2
1	A	138	SER	4.2
1	C	153	ASN	4.2
1	B	190	MET	4.2
1	A	197	VAL	4.2
1	C	64	ASN	4.1
1	C	2	GLY	4.1
1	D	240	GLU	4.1
1	A	192	LEU	4.1
1	C	297	TYR	4.1
1	C	217	TRP	4.0
1	A	195	THR	4.0
1	D	213	ASN	4.0
1	C	240	GLU	4.0
1	C	247	PHE	3.9
1	D	236	ASN	3.9
1	D	238	PHE	3.9
1	D	201	ASP	3.9
1	D	269	ASN	3.9
1	C	298	GLY	3.8
1	D	282	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	231	THR	3.8
1	D	137	GLY	3.8
1	C	238	PHE	3.8
1	D	280	TYR	3.8
1	D	234	LYS	3.8
1	B	1	SER	3.7
1	C	131	SER	3.7
1	C	210	ALA	3.7
1	C	197	VAL	3.7
1	D	293	ILE	3.6
1	D	132	GLN	3.6
1	A	72	VAL	3.6
1	C	287	PHE	3.6
1	C	290	THR	3.5
1	C	242	SER	3.5
1	C	216	ARG	3.5
1	A	1	SER	3.5
1	C	199	SER	3.5
1	D	257	SER	3.5
1	C	252	ALA	3.5
1	C	268	LEU	3.4
1	D	264	SER	3.4
1	C	4	ARG	3.4
1	C	232	TRP	3.4
1	D	237	SER	3.4
1	D	211	LEU	3.4
1	C	234	LYS	3.4
1	D	107	ALA	3.4
1	D	127	VAL	3.4
1	D	298	GLY	3.4
1	C	293	ILE	3.4
1	D	296	MET	3.3
1	C	266	VAL	3.3
1	D	170	SER	3.3
1	C	218	PHE	3.3
1	D	260	LYS	3.3
1	C	150	VAL	3.3
1	D	105	ILE	3.3
1	D	4	ARG	3.3
1	D	109	GLU	3.3
1	A	279	SER	3.2
1	D	220	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	290	THR	3.2
1	C	281	GLY	3.2
1	D	60	VAL	3.2
1	B	47	THR	3.2
1	C	267	ARG	3.2
1	C	205	ALA	3.2
1	C	260	LYS	3.2
1	D	245	ASP	3.2
1	D	263	ASP	3.2
1	C	211	LEU	3.2
1	D	294	ARG	3.2
1	C	195	THR	3.2
1	A	275	ARG	3.1
1	D	102	PHE	3.1
1	A	276	THR	3.1
1	C	276	THR	3.1
1	C	200	SER	3.1
1	C	196	ASN	3.1
1	D	192	LEU	3.1
1	A	2	GLY	3.0
1	C	157	TYR	3.0
1	C	202	ASN	3.0
1	C	102	PHE	3.0
1	D	233	ALA	3.0
1	D	254	THR	3.0
1	A	272	PHE	3.0
1	A	88	LEU	3.0
1	A	278	LEU	3.0
1	C	215	GLU	3.0
1	C	235	THR	3.0
1	D	285	ASP	3.0
1	C	294	ARG	2.9
1	C	214	GLY	2.9
1	C	263	ASP	2.9
1	A	188	PRO	2.9
1	A	298	GLY	2.9
1	C	23	GLY	2.9
1	D	256	GLN	2.9
1	D	216	ARG	2.9
1	D	274	GLY	2.9
1	B	6	MET	2.8
1	C	284	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	2.8
1	D	111	PHE	2.8
1	A	184	TYR	2.8
1	D	157	TYR	2.8
1	D	255	GLY	2.8
1	A	233	ALA	2.8
1	D	154	ALA	2.8
1	B	197	VAL	2.8
1	C	248	SER	2.7
1	D	248	SER	2.7
1	D	235	THR	2.7
1	A	86	LEU	2.7
1	C	63	HIS	2.7
1	C	154	ALA	2.7
1	B	196	ASN	2.7
1	D	193	GLU	2.7
1	C	201	ASP	2.7
1	D	178	GLY	2.7
1	C	282	SER	2.6
1	C	265	ILE	2.6
1	D	230	ASN	2.6
1	A	290	THR	2.6
1	C	86	LEU	2.6
1	A	51	ILE	2.6
1	A	280	TYR	2.6
1	C	292	VAL	2.6
1	C	259	GLU	2.6
1	A	194	GLY	2.6
1	C	296	MET	2.6
1	D	130	ARG	2.6
1	A	77	VAL	2.5
1	D	133	GLY	2.5
1	C	224	MET	2.5
1	B	189	SER	2.5
1	A	137	GLY	2.5
1	A	270	LYS	2.5
1	D	183	GLY	2.5
1	A	266	VAL	2.5
1	D	295	GLN	2.5
1	D	198	MET	2.5
1	A	108	GLY	2.5
1	C	237	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	136	LYS	2.4
1	D	63	HIS	2.4
1	D	259	GLU	2.4
1	B	233	ALA	2.4
1	C	49	ARG	2.4
1	A	241	LEU	2.4
1	D	86	LEU	2.4
1	D	214	GLY	2.4
1	A	140	ILE	2.4
1	A	172	VAL	2.4
1	B	266	VAL	2.4
1	C	31	TRP	2.4
1	D	164	LEU	2.4
1	D	168	ASN	2.4
1	D	73	PHE	2.4
1	C	6	MET	2.4
1	D	104	SER	2.4
1	D	202	ASN	2.3
1	C	198	MET	2.3
1	A	43	ILE	2.3
1	B	265	ILE	2.3
1	D	43	ILE	2.3
1	C	75	GLY	2.3
1	B	294	ARG	2.3
1	A	63	HIS	2.3
1	A	48	THR	2.3
1	A	240	GLU	2.3
1	D	110	SER	2.3
1	D	159	VAL	2.3
1	A	235	THR	2.3
1	D	153	ASN	2.3
1	A	120	CYS	2.3
1	C	79	ALA	2.3
1	D	75	GLY	2.3
1	D	106	LYS	2.3
1	D	169	GLY	2.3
1	A	268	LEU	2.2
1	D	22	TYR	2.2
1	C	264	SER	2.2
1	A	139	PHE	2.2
1	B	49	ARG	2.2
1	A	105	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	THR	2.2
1	A	23	GLY	2.2
1	A	164	LEU	2.2
1	B	45	SER	2.2
1	A	234	LYS	2.2
1	D	5	LYS	2.2
1	A	239	THR	2.2
1	C	108	GLY	2.2
1	B	166	LEU	2.2
1	A	4	ARG	2.2
1	B	80	LYS	2.2
1	C	269	ASN	2.2
1	D	129	MET	2.2
1	C	288	THR	2.2
1	D	172	VAL	2.1
1	A	144	CYS	2.1
1	D	253	LYS	2.1
1	A	26	VAL	2.1
1	C	87	VAL	2.1
1	D	49	ARG	2.1
1	A	166	LEU	2.1
1	B	270	LYS	2.1
1	B	138	SER	2.1
1	D	62	LEU	2.1
1	D	66	SER	2.1
1	D	166	LEU	2.1
1	A	196	ASN	2.1
1	A	201	ASP	2.1
1	B	280	TYR	2.1
1	A	65	PHE	2.1
1	C	67	VAL	2.1
1	A	3	LEU	2.1
1	B	241	LEU	2.1
1	B	278	LEU	2.1
1	B	221	ASN	2.1
1	C	130	ARG	2.1
1	C	253	LYS	2.1
1	D	65	PHE	2.1
1	D	67	VAL	2.1
1	A	151	SER	2.1
1	B	223	SER	2.1
1	C	286	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	2.0
1	D	53	TYR	2.0
1	C	42	VAL	2.0
1	B	131	SER	2.0
1	D	6	MET	2.0
1	D	156	LEU	2.0
1	C	167	GLY	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](#)

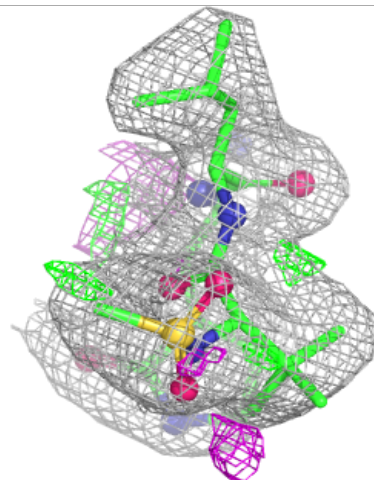
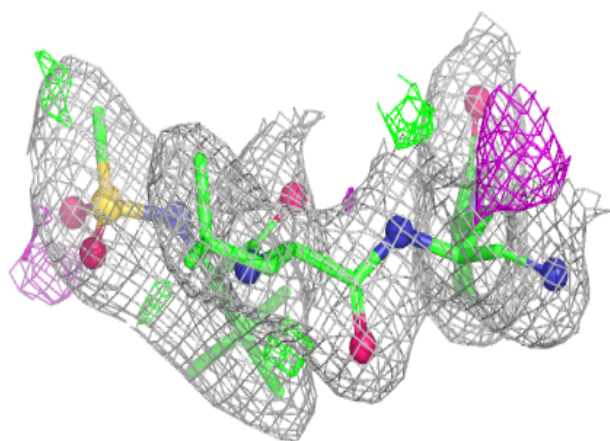
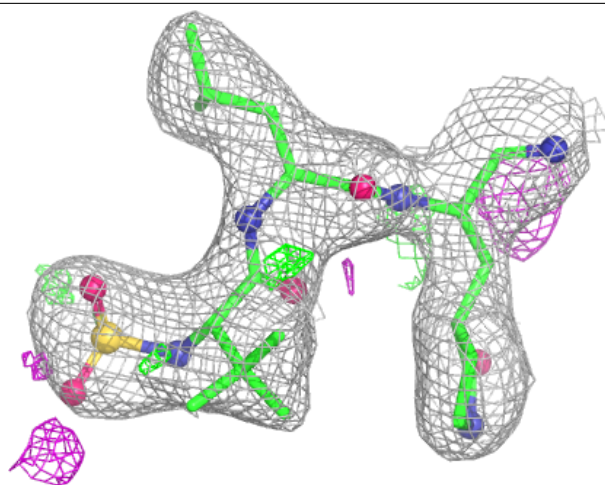
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1D7M	A	401	31/31	0.87	0.15	37,51,63,74	0
2	A1D7M	D	401	31/31	0.91	0.14	33,50,60,68	0
2	A1D7M	B	401	31/31	0.92	0.12	41,51,59,65	0
2	A1D7M	C	401	31/31	0.95	0.11	32,42,50,58	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.

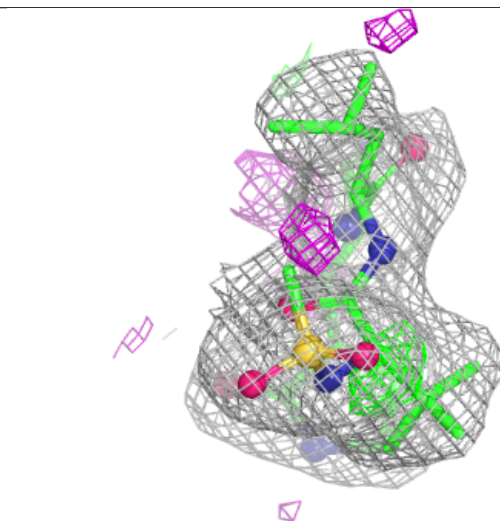
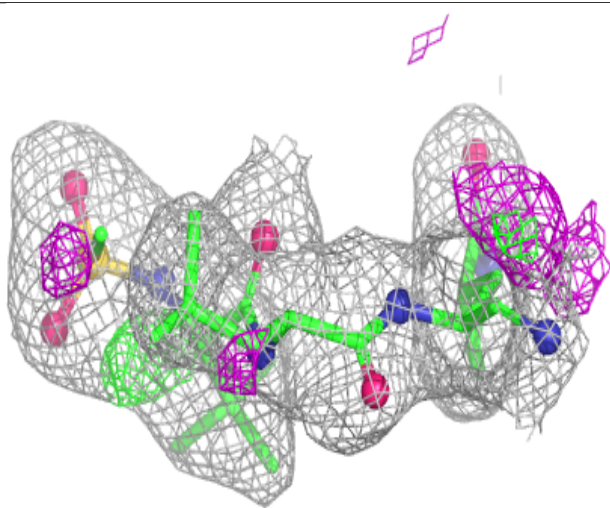
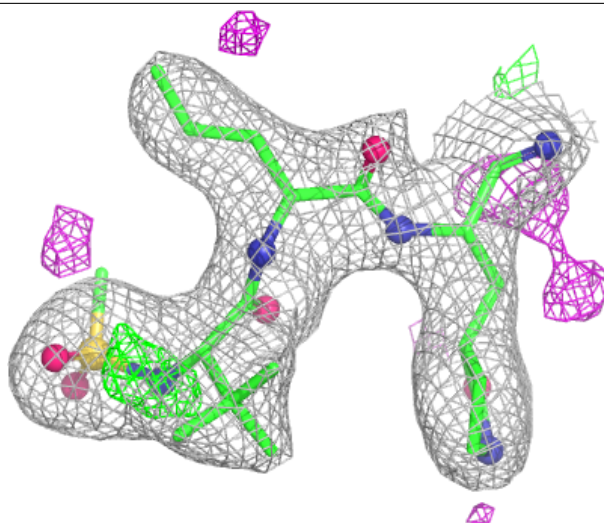
Electron density around A1D7M A 401:

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



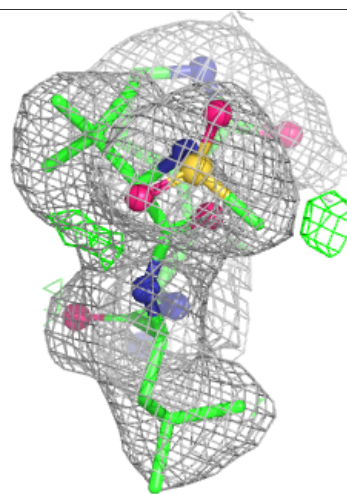
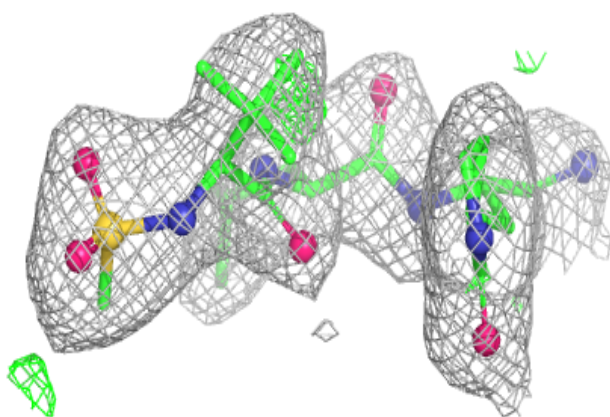
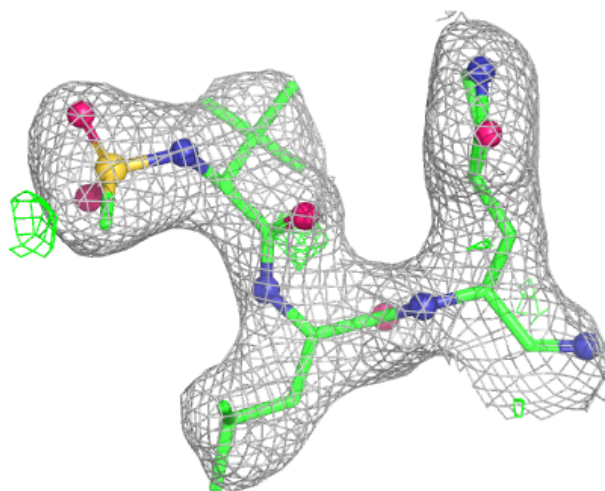
Electron density around A1D7M D 401:

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



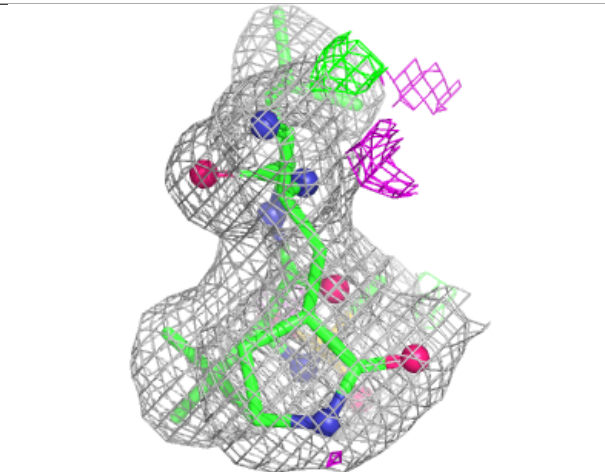
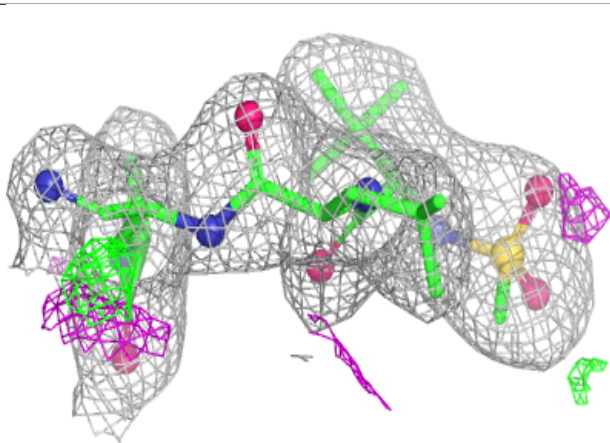
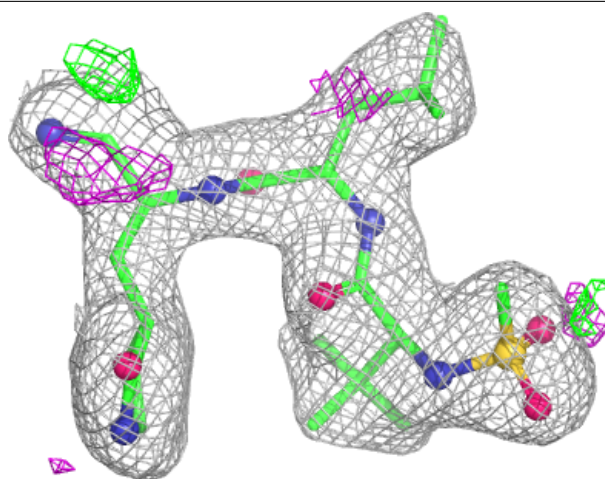
Electron density around A1D7M B 401:

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



Electron density around A1D7M 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.