



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2022 – 04:14 PM EDT

PDB ID : 7RVO
Title : Structure of the SARS-CoV-2 main protease in complex with inhibitor MPI13
Authors : Yang, K.; Sankaran, B.; Liu, W.
Deposited on : 2021-08-19
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

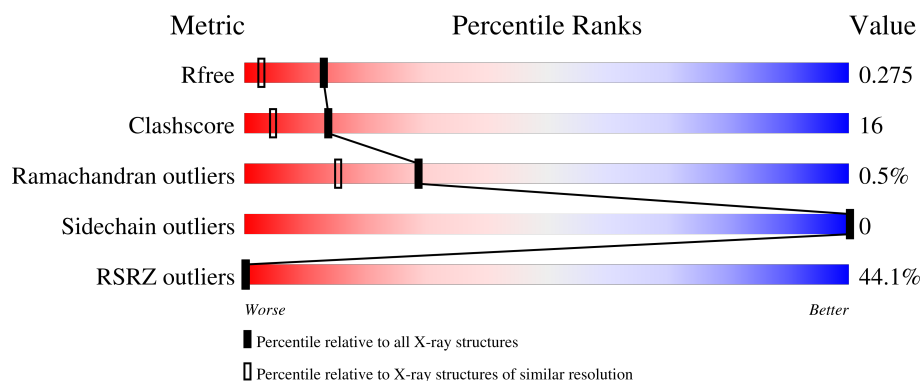
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	306	<div> <div>39%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>.</div> </div> </div>
1	B	306	<div> <div>49%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5044 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.

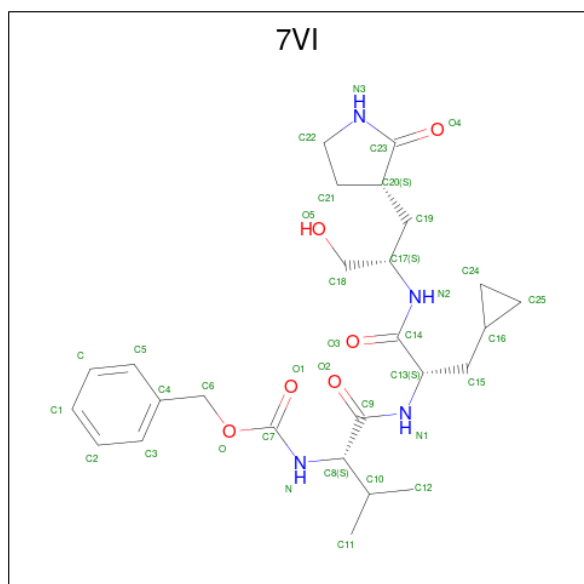
- Molecule 1 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2363	1497	402	442	22			
1	B	306	Total	C	N	O	S	0	0	0
			2363	1497	402	442	22			

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-[(benzyloxy)carbonyl]-L-valyl-3-cyclopropyl-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-alaninamide (three-letter code: 7VI) (formula: C₂₆H₃₈N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	26	4	6		
2	B	1	Total	C	N	O	0	0
			36	26	4	6		

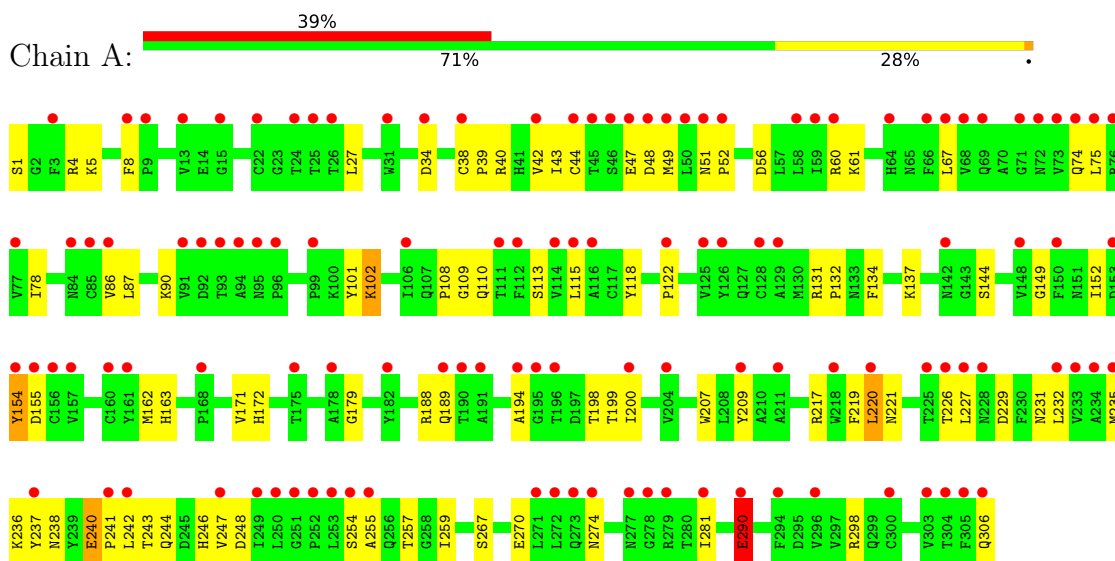
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	115	Total	O	0	0
			115	115		

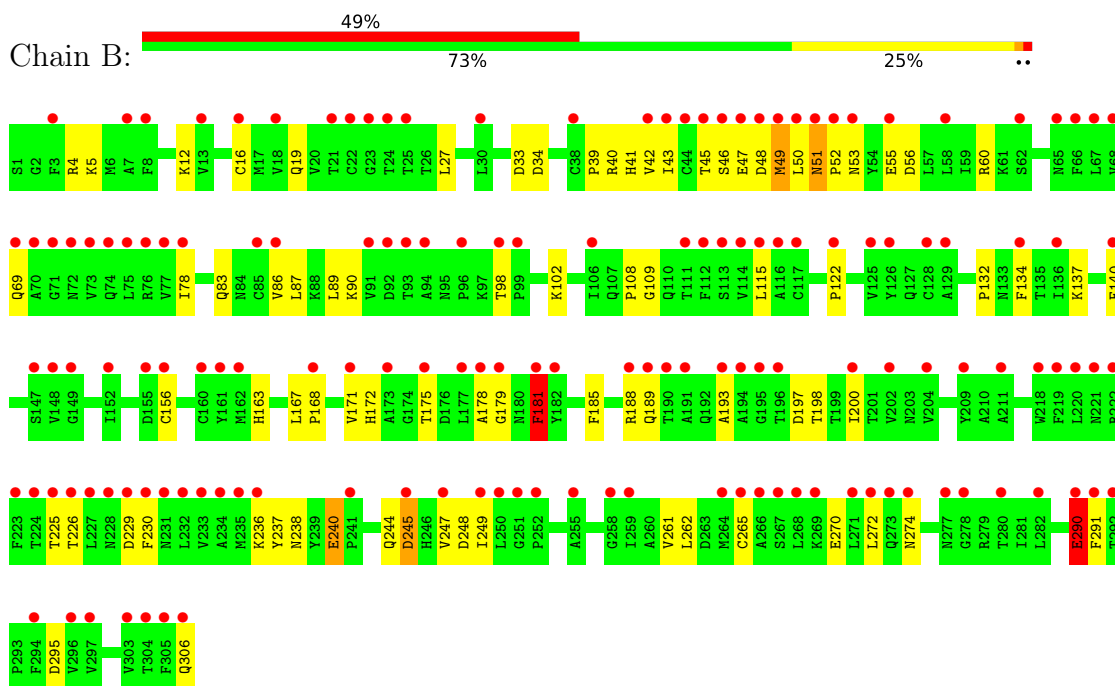
3 Residue-property plots [i](#)

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



- Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.51Å 60.54Å 63.15Å 79.98° 68.24° 70.25°	Depositor
Resolution (Å)	44.35 – 1.80 44.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.8 (44.35-1.80) 89.8 (44.35-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.244 , 0.275 0.244 , 0.275	Depositor DCC
R_{free} test set	2924 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.104 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5044	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7VI

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	0.51	0/2416	1.36	7/3284 (0.2%)
1	B	0.53	0/2416	1.81	19/3284 (0.6%)
All	All	0.52	0/4832	1.60	26/6568 (0.4%)

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	3
All	All	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ASP	CB-CG-OD1	43.72	157.64	118.30
1	A	240	GLU	OE1-CD-OE2	-41.93	72.98	123.30
1	B	245	ASP	CB-CG-OD2	-40.91	81.48	118.30
1	A	290	GLU	OE1-CD-OE2	-37.34	78.49	123.30
1	B	290	GLU	OE1-CD-OE2	-33.83	82.70	123.30
1	B	55	GLU	OE1-CD-OE2	-30.64	86.54	123.30
1	B	55	GLU	CG-CD-OE1	26.64	171.59	118.30
1	B	245	ASP	OD1-CG-OD2	-24.59	76.58	123.30
1	B	290	GLU	CG-CD-OE1	20.72	159.74	118.30
1	A	290	GLU	CG-CD-OE1	19.20	156.70	118.30
1	B	181	PHE	CB-CG-CD2	-18.86	107.60	120.80
1	A	240	GLU	CG-CD-OE1	18.09	154.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	GLU	CG-CD-OE2	-17.92	82.45	118.30
1	B	55	GLU	CG-CD-OE2	-16.42	85.46	118.30
1	B	290	GLU	CG-CD-OE2	-14.49	89.33	118.30
1	A	290	GLU	CG-CD-OE2	-12.45	93.40	118.30
1	B	51	ASN	CB-CA-C	-10.48	89.43	110.40
1	B	181	PHE	CB-CG-CD1	10.37	128.06	120.80
1	B	50	LEU	C-N-CA	-8.50	100.45	121.70
1	B	51	ASN	N-CA-CB	8.18	125.33	110.60
1	B	51	ASN	N-CA-C	-7.68	90.27	111.00
1	B	51	ASN	CB-CG-ND2	-6.65	100.75	116.70
1	B	181	PHE	N-CA-CB	6.18	121.72	110.60
1	A	102	LYS	CD-CE-NZ	5.95	125.38	111.70
1	B	55	GLU	CB-CG-CD	5.59	129.28	114.20
1	B	240	GLU	CA-CB-CG	5.52	125.53	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	GLU	Sidechain
1	B	181	PHE	Sidechain
1	B	290	GLU	Sidechain
1	B	51	ASN	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2363	0	2312	85	0
1	B	2363	0	2312	67	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
3	A	131	0	0	21	0
3	B	115	0	0	18	0
All	All	5044	0	4624	149	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 16.

All (149) 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:38:CYS:SG	3:A:510:HOH:O	2.25	0.92
1:A:34:ASP:OD2	1:A:90:LYS:NZ	2.02	0.92
1:B:52:PRO:HD2	1:B:188:ARG:HG2	1.51	0.92
1:B:16:CYS:SG	3:B:502:HOH:O	2.24	0.86
1:A:131:ARG:HG3	1:A:137:LYS:HE2	1.55	0.86
1:B:69:GLN:OE1	3:B:501:HOH:O	1.93	0.85
1:B:12:LYS:O	3:B:502:HOH:O	1.93	0.85
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.58	0.84
1:A:226:THR:HG23	1:A:229:ASP:H	1.43	0.84
1:B:193:ALA:O	3:B:503:HOH:O	1.96	0.82
1:B:5:LYS:NZ	1:B:290:GLU:HG3	1.97	0.80
1:A:194:ALA:O	3:A:501:HOH:O	1.99	0.79
1:B:46:SER:HA	1:B:49:MET:SD	2.22	0.78
1:A:61:LYS:NZ	3:A:507:HOH:O	2.16	0.78
1:A:257:THR:OG1	3:A:502:HOH:O	2.02	0.78
1:A:75:LEU:O	3:A:503:HOH:O	2.04	0.75
1:B:226:THR:HG23	1:B:229:ASP:H	1.51	0.75
1:B:69:GLN:NE2	3:B:504:HOH:O	2.14	0.72
1:A:8:PHE:HB3	1:A:152:ILE:HD13	1.72	0.71
1:A:274:ASN:ND2	3:A:504:HOH:O	2.05	0.71
1:B:132:PRO:HB3	1:B:240:GLU:OE2	1.91	0.70
1:A:306:GLN:NE2	3:A:509:HOH:O	2.24	0.70
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.76	0.68
1:A:51:ASN:HA	1:A:188:ARG:HD3	1.75	0.66
1:A:110:GLN:HG2	3:A:617:HOH:O	1.95	0.66
1:A:259:ILE:O	3:A:502:HOH:O	2.15	0.64
1:B:295:ASP:OD1	3:B:506:HOH:O	2.15	0.64
1:B:5:LYS:HG2	1:B:291:PHE:CZ	2.32	0.64
1:B:290:GLU:OE2	3:B:505:HOH:O	2.15	0.64
1:B:5:LYS:HZ2	1:B:290:GLU:HG3	1.63	0.63
1:B:137:LYS:HD2	1:B:171:VAL:HG12	1.81	0.63
1:B:60:ARG:CZ	3:B:512:HOH:O	2.47	0.62
1:B:52:PRO:HD2	1:B:188:ARG:CG	2.29	0.62
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.82	0.61
1:B:19:GLN:HB2	3:B:574:HOH:O	2.00	0.61
1:A:102:LYS:HD3	3:A:573:HOH:O	1.99	0.61
1:B:69:GLN:NE2	3:B:501:HOH:O	2.33	0.61
1:A:270:GLU:OE1	3:A:505:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HZ1	1:B:290:GLU:HG3	1.66	0.60
1:B:87:LEU:O	3:B:507:HOH:O	2.16	0.60
1:A:209:TYR:HE1	3:A:502:HOH:O	1.84	0.60
1:A:227:LEU:HD11	1:A:242:LEU:HD22	1.84	0.59
1:A:254:SER:HA	3:A:502:HOH:O	2.02	0.59
1:B:60:ARG:NH2	3:B:512:HOH:O	2.34	0.59
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.85	0.59
1:A:27:LEU:HD11	3:A:510:HOH:O	2.04	0.57
1:A:86:VAL:HG13	1:A:179:GLY:CA	2.33	0.57
1:B:245:ASP:O	1:B:249:ILE:HG13	2.05	0.56
1:B:69:GLN:HB2	3:B:504:HOH:O	2.05	0.56
1:B:49:MET:HB3	1:B:189:GLN:HG3	1.87	0.56
1:A:231:ASN:O	1:A:235:MET:HG3	2.06	0.56
1:A:78:ILE:HG13	1:A:90:LYS:HG3	1.87	0.55
1:A:242:LEU:HD21	1:A:247:VAL:HG23	1.87	0.55
1:B:27:LEU:HD13	1:B:39:PRO:HD2	1.89	0.55
1:A:40:ARG:HA	1:A:87:LEU:HG	1.87	0.55
1:A:137:LYS:HZ3	1:A:171:VAL:HG11	1.71	0.55
1:B:270:GLU:HG3	1:B:274:ASN:ND2	2.22	0.55
1:A:227:LEU:CD1	1:A:242:LEU:HD22	2.37	0.54
1:B:47:GLU:N	1:B:47:GLU:OE1	2.40	0.54
1:B:69:GLN:CD	3:B:501:HOH:O	2.37	0.53
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.43	0.53
1:A:219:PHE:O	1:A:220:LEU:O	2.27	0.53
1:A:217:ARG:NH2	3:A:511:HOH:O	2.27	0.52
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.89	0.52
1:A:220:LEU:O	1:A:221:ASN:HB3	2.09	0.52
1:A:78:ILE:HD11	1:A:90:LYS:HE3	1.90	0.52
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.92	0.51
1:B:78:ILE:HG13	1:B:90:LYS:HG3	1.92	0.51
1:A:4:ARG:NH1	1:B:290:GLU:OE1	2.42	0.51
1:A:40:ARG:O	1:A:43:ILE:HG12	2.10	0.51
1:A:101:TYR:O	1:A:102:LYS:HE2	2.11	0.51
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.93	0.51
1:B:274:ASN:ND2	3:B:515:HOH:O	2.43	0.51
1:A:44:CYS:HB3	1:A:49:MET:SD	2.51	0.51
1:B:41:HIS:ND1	3:B:509:HOH:O	2.26	0.51
1:B:175:THR:HG22	1:B:181:PHE:CD1	2.46	0.51
1:A:244:GLN:NE2	1:A:248:ASP:OD1	2.44	0.50
1:A:199:THR:O	1:A:240:GLU:HG2	2.12	0.50
1:B:244:GLN:NE2	1:B:248:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:O	1:A:102:LYS:CE	2.60	0.49
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.47	0.49
1:A:198:THR:HG22	1:A:238:ASN:OD1	2.13	0.49
1:A:47:GLU:OE1	1:A:47:GLU:N	2.45	0.49
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.78	0.49
1:A:27:LEU:HD13	1:A:39:PRO:HD2	1.94	0.48
1:B:56:ASP:O	1:B:60:ARG:HD3	2.13	0.48
1:A:86:VAL:HG12	1:A:162:MET:CE	2.43	0.48
1:B:225:THR:O	1:B:262:LEU:HD13	2.14	0.48
1:A:200:ILE:HA	1:A:240:GLU:CD	2.34	0.48
1:A:242:LEU:HD23	1:A:243:THR:O	2.13	0.48
1:A:5:LYS:HE2	1:A:290:GLU:CG	2.44	0.47
1:A:137:LYS:HD2	1:A:171:VAL:HG12	1.96	0.47
1:B:247:VAL:HG22	1:B:261:VAL:HG11	1.96	0.47
1:A:255:ALA:HB3	3:A:515:HOH:O	2.14	0.47
1:B:198:THR:HG22	1:B:238:ASN:OD1	2.14	0.47
1:B:53:ASN:OD1	1:B:56:ASP:N	2.31	0.47
1:B:12:LYS:NZ	1:B:306:GLN:O	2.48	0.47
1:B:56:ASP:HB3	1:B:60:ARG:NH1	2.30	0.47
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.80	0.46
1:A:132:PRO:HG3	1:A:240:GLU:OE1	2.16	0.46
1:B:83:GLN:HG2	1:B:178:ALA:O	2.16	0.46
1:A:242:LEU:CD2	1:A:247:VAL:HG23	2.45	0.45
1:B:34:ASP:OD2	1:B:90:LYS:NZ	2.39	0.45
1:A:56:ASP:O	1:A:60:ARG:HG2	2.16	0.45
1:A:108:PRO:HG3	1:A:134:PHE:CE1	2.51	0.45
1:A:226:THR:CG2	1:A:229:ASP:H	2.23	0.45
1:A:232:LEU:HD13	1:A:235:MET:SD	2.57	0.45
1:B:40:ARG:HA	1:B:87:LEU:HG	1.99	0.44
1:A:267:SER:OG	3:A:508:HOH:O	2.21	0.44
1:B:40:ARG:O	1:B:43:ILE:HG12	2.18	0.44
1:A:74:GLN:HG2	3:A:503:HOH:O	2.18	0.43
1:B:108:PRO:HG3	1:B:134:PHE:CE1	2.53	0.43
1:A:49:MET:HB3	1:A:189:GLN:CG	2.47	0.43
1:A:113:SER:O	1:A:149:GLY:HA2	2.19	0.43
1:A:207:TRP:CH2	1:A:281:ILE:HB	2.53	0.43
1:A:220:LEU:O	1:A:221:ASN:CB	2.67	0.43
1:A:236:LYS:HD3	1:A:236:LYS:C	2.39	0.42
1:B:102:LYS:HE2	1:B:156:CYS:SG	2.59	0.42
1:A:240:GLU:HA	1:A:241:PRO:HD3	1.85	0.42
1:A:86:VAL:HG12	1:A:162:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASP:O	1:B:238:ASN:ND2	2.46	0.42
1:B:33:ASP:OD1	1:B:98:THR:HG21	2.19	0.42
1:B:236:LYS:HD2	1:B:237:TYR:CE2	2.54	0.42
1:A:137:LYS:HZ3	1:A:171:VAL:CG1	2.33	0.42
1:A:290:GLU:OE1	1:B:4:ARG:NH1	2.53	0.42
1:A:154:TYR:CE1	1:A:306:GLN:HB2	2.55	0.42
1:B:181:PHE:CD2	1:B:185:PHE:HB2	2.55	0.42
1:A:243:THR:HG21	3:A:544:HOH:O	2.19	0.41
1:B:230:PHE:CD1	1:B:265:CYS:HB3	2.56	0.41
1:A:137:LYS:NZ	1:A:171:VAL:HG11	2.35	0.41
1:A:48:ASP:O	1:A:52:PRO:HB3	2.21	0.41
1:A:220:LEU:HA	1:A:220:LEU:HD23	1.88	0.41
1:A:236:LYS:HD2	1:A:237:TYR:CE2	2.55	0.41
1:A:1:SER:HA	3:A:602:HOH:O	2.20	0.41
1:A:27:LEU:HD21	1:A:42:VAL:HB	2.03	0.41
1:B:167:LEU:HB3	1:B:168:PRO:HD3	2.02	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.86	0.41
1:A:118:TYR:CE2	1:A:144:SER:HB3	2.55	0.41
1:B:16:CYS:N	3:B:502:HOH:O	2.53	0.41
1:B:175:THR:HG22	1:B:181:PHE:HD1	1.85	0.41
1:A:243:THR:O	1:A:246:HIS:HB2	2.20	0.41
1:B:45:THR:OG1	1:B:48:ASP:OD2	2.36	0.41
1:A:298:ARG:NH2	3:A:519:HOH:O	2.46	0.41
1:A:1:SER:N	1:B:140:PHE:O	2.48	0.40
1:A:155:ASP:OD1	1:A:155:ASP:N	2.53	0.40
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.93	0.40
1:A:236:LYS:HD2	1:A:237:TYR:CZ	2.56	0.40
1:A:78:ILE:CG1	1:A:90:LYS:HG3	2.51	0.40
1:B:89:LEU:HG	3:B:507:HOH:O	2.21	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	304/306 (99%)	292 (96%)	10 (3%)	2 (1%)	22	10
1	B	304/306 (99%)	294 (97%)	9 (3%)	1 (0%)	41	27
All	All	608/612 (99%)	586 (96%)	19 (3%)	3 (0%)	29	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	B	49	MET
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	262/262 (100%)	262 (100%)	0	100	100
1	B	262/262 (100%)	262 (100%)	0	100	100
All	All	524/524 (100%)	524 (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	A	69	GLN
1	A	214	ASN
1	B	41	HIS
1	B	189	GLN
1	B	273	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	7VI	B	401	1	38,38,38	1.02	1 (2%)	47,51,51	1.23	5 (10%)
2	7VI	A	401	1	38,38,38	1.04	1 (2%)	47,51,51	1.15	4 (8%)

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	7VI	B	401	1	-	0/39/51/51	0/3/3/3
2	7VI	A	401	1	-	0/39/51/51	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	7VI	O-C7	5.23	1.45	1.35
2	A	401	7VI	O-C7	5.22	1.45	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7VI	C16-C15-C13	-5.80	106.72	114.52
2	A	401	7VI	C16-C15-C13	-4.71	108.18	114.52
2	B	401	7VI	O-C7-N	2.81	116.22	110.50
2	B	401	7VI	O-C7-O1	-2.38	119.69	124.25
2	A	401	7VI	O-C7-N	2.31	115.21	110.50
2	A	401	7VI	O-C7-O1	-2.29	119.85	124.25
2	B	401	7VI	O4-C23-C20	-2.25	123.59	126.23
2	A	401	7VI	C19-C20-C21	-2.09	109.62	117.31
2	B	401	7VI	C19-C17-C18	-2.04	108.82	111.65

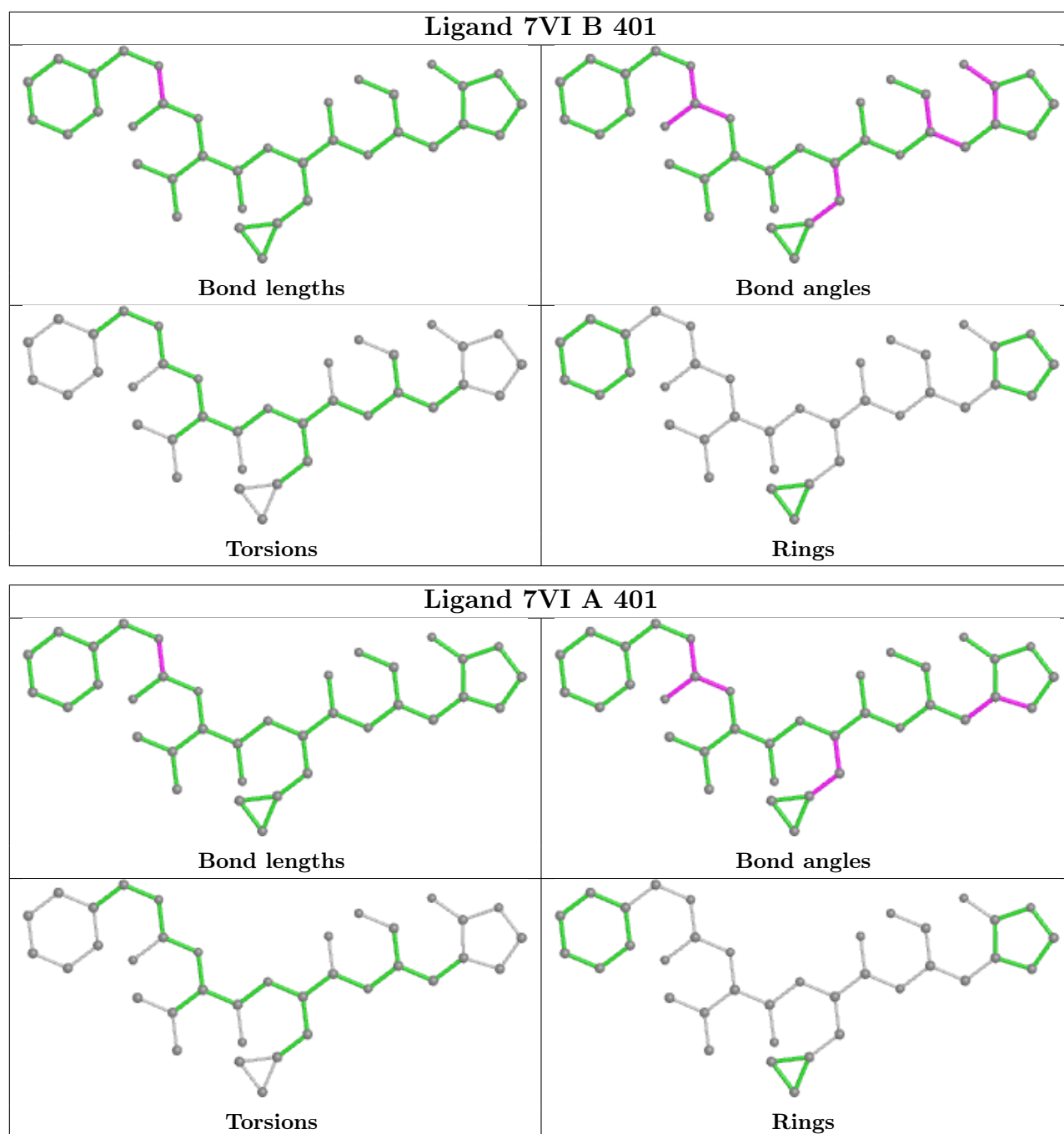
There are no chirality outliers.

There are no torsion outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/306 (100%)	1.96	119 (38%) 0 0	15, 30, 48, 65	0
1	B	306/306 (100%)	2.21	151 (49%) 0 0	15, 31, 50, 67	0
All	All	612/612 (100%)	2.08	270 (44%) 0 0	15, 30, 50, 67	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ASN	7.0
1	A	72	ASN	6.7
1	B	24	THR	6.6
1	A	154	TYR	6.6
1	B	46	SER	6.5
1	A	46	SER	6.4
1	B	50	LEU	6.4
1	B	49	MET	6.2
1	B	278	GLY	6.1
1	B	303	VAL	5.9
1	B	255	ALA	5.7
1	A	45	THR	5.6
1	A	47	GLU	5.6
1	B	47	GLU	5.6
1	B	235	MET	5.5
1	B	51	ASN	5.4
1	B	223	PHE	5.3
1	A	75	LEU	5.3
1	B	234	ALA	5.2
1	A	92	ASP	5.2
1	B	72	ASN	5.2
1	B	306	GLN	5.1
1	A	233	VAL	5.0
1	A	24	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	4.7
1	B	45	THR	4.7
1	A	303	VAL	4.6
1	B	224	THR	4.6
1	A	306	GLN	4.5
1	B	232	LEU	4.4
1	B	277	ASN	4.4
1	A	49	MET	4.4
1	A	235	MET	4.3
1	B	93	THR	4.3
1	A	50	LEU	4.3
1	B	181	PHE	4.3
1	A	67	LEU	4.2
1	A	93	THR	4.2
1	B	200	ILE	4.2
1	B	233	VAL	4.2
1	B	128	CYS	4.1
1	B	226	THR	4.1
1	B	194	ALA	4.1
1	B	52	PRO	4.0
1	B	305	PHE	4.0
1	A	94	ALA	3.9
1	B	92	ASP	3.9
1	A	196	THR	3.9
1	B	115	LEU	3.8
1	A	44	CYS	3.8
1	A	191	ALA	3.8
1	A	74	GLN	3.8
1	A	59	ILE	3.7
1	B	114	VAL	3.7
1	A	125	VAL	3.7
1	B	148	VAL	3.7
1	B	258	GLY	3.7
1	A	153	ASP	3.7
1	A	51	ASN	3.7
1	B	112	PHE	3.7
1	B	76	ARG	3.7
1	A	247	VAL	3.6
1	B	222	ARG	3.6
1	B	191	ALA	3.5
1	A	60	ARG	3.5
1	B	228	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	73	VAL	3.5
1	B	125	VAL	3.5
1	A	68	VAL	3.5
1	B	190	THR	3.5
1	B	225	THR	3.4
1	A	128	CYS	3.4
1	B	22	CYS	3.4
1	B	77	VAL	3.4
1	A	71	GLY	3.4
1	A	114	VAL	3.4
1	B	188	ARG	3.3
1	A	220	LEU	3.3
1	B	67	LEU	3.3
1	B	241	PRO	3.3
1	B	193	ALA	3.3
1	A	294	PHE	3.3
1	B	155	ASP	3.3
1	A	77	VAL	3.3
1	A	200	ILE	3.3
1	A	91	VAL	3.3
1	B	196	THR	3.3
1	B	296	VAL	3.2
1	B	7	ALA	3.2
1	B	160	CYS	3.2
1	A	227	LEU	3.2
1	B	126	TYR	3.2
1	B	227	LEU	3.2
1	A	76	ARG	3.1
1	A	48	ASP	3.1
1	A	278	GLY	3.1
1	B	91	VAL	3.1
1	B	136	ILE	3.1
1	B	304	THR	3.1
1	A	22	CYS	3.1
1	B	129	ALA	3.1
1	B	48	ASP	3.0
1	B	177	LEU	3.0
1	A	69	GLN	3.0
1	B	53	ASN	3.0
1	B	231	ASN	3.0
1	A	237	TYR	3.0
1	A	52	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	232	LEU	3.0
1	A	106	ILE	3.0
1	A	115	LEU	2.9
1	B	55	GLU	2.9
1	B	21	THR	2.9
1	B	25	THR	2.9
1	B	106	ILE	2.9
1	B	259	ILE	2.9
1	B	122	PRO	2.9
1	A	155	ASP	2.9
1	B	202	VAL	2.9
1	A	189	GLN	2.9
1	B	189	GLN	2.9
1	B	75	LEU	2.9
1	B	161	TYR	2.8
1	B	218	TRP	2.8
1	B	62	SER	2.8
1	B	269	LYS	2.8
1	B	13	VAL	2.8
1	B	68	VAL	2.8
1	A	249	ILE	2.8
1	A	168	PRO	2.8
1	A	241	PRO	2.8
1	A	73	VAL	2.8
1	A	255	ALA	2.8
1	B	265	CYS	2.8
1	B	152	ILE	2.8
1	B	182	TYR	2.8
1	B	111	THR	2.7
1	B	16	CYS	2.7
1	B	44	CYS	2.7
1	B	85	CYS	2.7
1	A	279	ARG	2.7
1	B	71	GLY	2.7
1	A	157	VAL	2.7
1	A	160	CYS	2.7
1	A	228	ASN	2.7
1	A	86	VAL	2.7
1	B	236	LYS	2.7
1	A	234	ALA	2.6
1	A	142	ASN	2.6
1	B	230	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	VAL	2.6
1	B	274	ASN	2.6
1	B	8	PHE	2.6
1	A	58	LEU	2.6
1	A	116	ALA	2.6
1	A	252	PRO	2.6
1	A	296	VAL	2.6
1	A	34	ASP	2.5
1	B	42	VAL	2.5
1	B	245	ASP	2.5
1	B	96	PRO	2.5
1	B	168	PRO	2.5
1	A	190	THR	2.5
1	A	218	TRP	2.5
1	B	267	SER	2.5
1	A	96	PRO	2.5
1	B	116	ALA	2.5
1	B	58	LEU	2.5
1	B	220	LEU	2.5
1	B	292	THR	2.5
1	B	99	PRO	2.5
1	B	178	ALA	2.5
1	A	204	VAL	2.5
1	B	282	LEU	2.5
1	A	42	VAL	2.4
1	B	221	ASN	2.4
1	A	175	THR	2.4
1	A	225	THR	2.4
1	A	161	TYR	2.4
1	B	117	CYS	2.4
1	B	149	GLY	2.4
1	B	18	VAL	2.4
1	B	134	PHE	2.4
1	A	84	ASN	2.4
1	B	249	ILE	2.4
1	B	66	PHE	2.4
1	B	70	ALA	2.4
1	B	23	GLY	2.4
1	A	182	TYR	2.4
1	A	211	ALA	2.4
1	B	266	ALA	2.4
1	B	30	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	2.3
1	B	65	ASN	2.3
1	B	175	THR	2.3
1	A	99	PRO	2.3
1	A	148	VAL	2.3
1	A	126	TYR	2.3
1	A	304	THR	2.3
1	A	150	PHE	2.3
1	A	254	SER	2.3
1	A	271	LEU	2.3
1	B	229	ASP	2.3
1	A	112	PHE	2.3
1	A	273	GLN	2.3
1	A	274	ASN	2.3
1	B	69	GLN	2.3
1	A	281	ILE	2.3
1	B	195	GLY	2.3
1	A	38	CYS	2.3
1	B	98	THR	2.3
1	B	156	CYS	2.3
1	A	8	PHE	2.3
1	A	251	GLY	2.3
1	B	264	MET	2.3
1	A	250	LEU	2.3
1	B	38	CYS	2.3
1	A	129	ALA	2.2
1	A	226	THR	2.2
1	B	78	ILE	2.2
1	B	140	PHE	2.2
1	B	113	SER	2.2
1	B	204	VAL	2.2
1	A	195	GLY	2.2
1	B	268	LEU	2.2
1	B	179	GLY	2.2
1	A	272	LEU	2.2
1	B	251	GLY	2.2
1	B	291	PHE	2.2
1	B	250	LEU	2.1
1	B	271	LEU	2.1
1	A	3	PHE	2.1
1	A	66	PHE	2.1
1	A	13	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	64	HIS	2.1
1	B	290	GLU	2.1
1	B	297	VAL	2.1
1	A	242	LEU	2.1
1	B	86	VAL	2.1
1	B	171	VAL	2.1
1	A	85	CYS	2.1
1	A	156	CYS	2.1
1	B	280	THR	2.1
1	B	43	ILE	2.1
1	B	272	LEU	2.1
1	B	147	SER	2.1
1	A	9	PRO	2.1
1	B	209	TYR	2.1
1	A	290	GLU	2.1
1	A	305	PHE	2.1
1	B	211	ALA	2.1
1	A	95	ASN	2.1
1	B	162	MET	2.1
1	B	3	PHE	2.1
1	B	74	GLN	2.1
1	A	209	TYR	2.0
1	B	219	PHE	2.0
1	A	31	TRP	2.0
1	B	173	ALA	2.0
1	A	122	PRO	2.0
1	B	252	PRO	2.0
1	A	253	LEU	2.0
1	A	25	THR	2.0
1	B	273	GLN	2.0
1	A	15	GLY	2.0
1	B	94	ALA	2.0
1	B	294	PHE	2.0
1	A	26	THR	2.0
1	A	111	THR	2.0
1	A	300	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

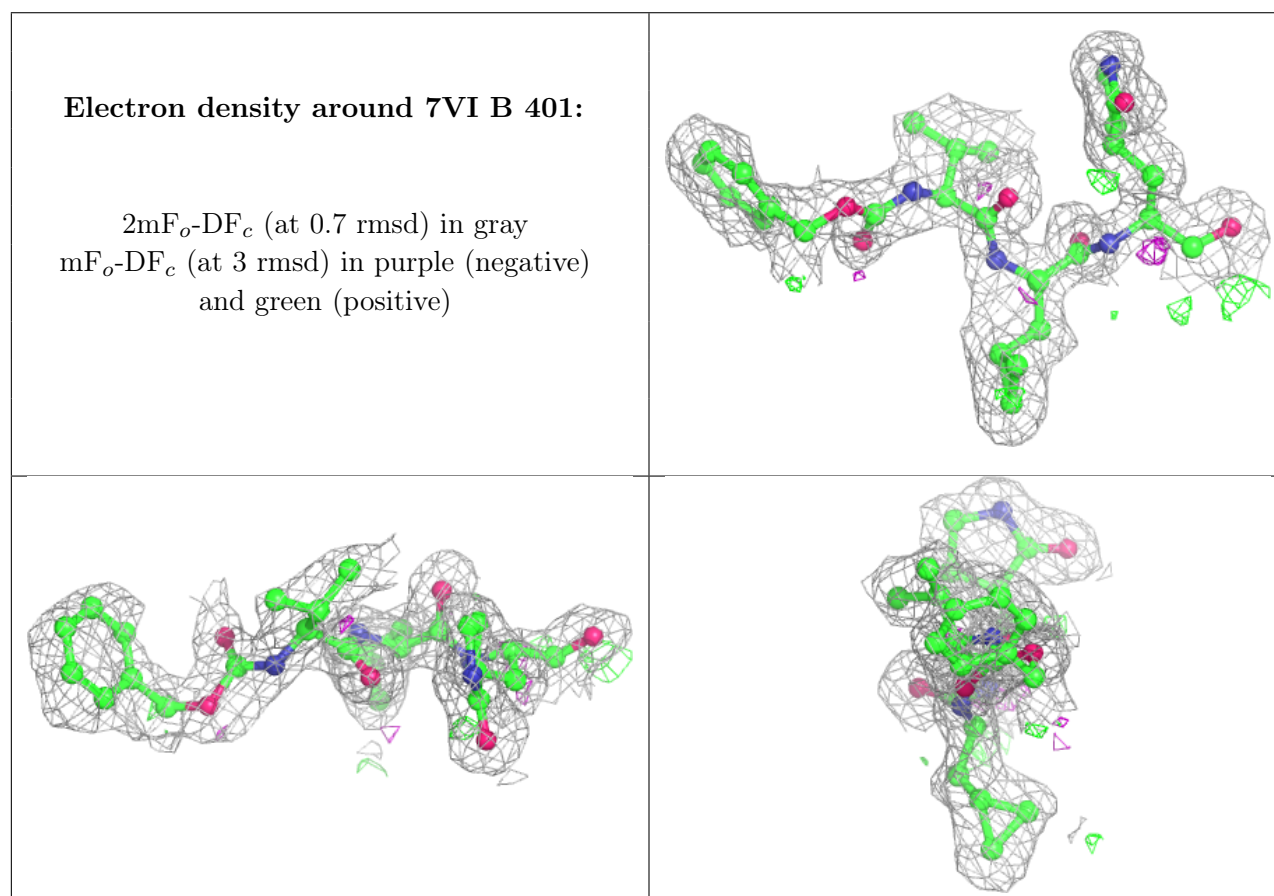
There are no monosaccharides in this entry.

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, 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.

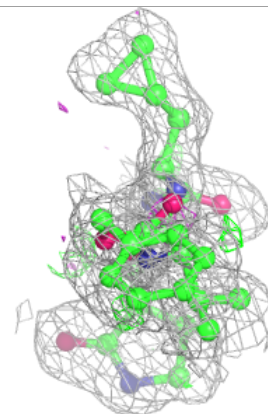
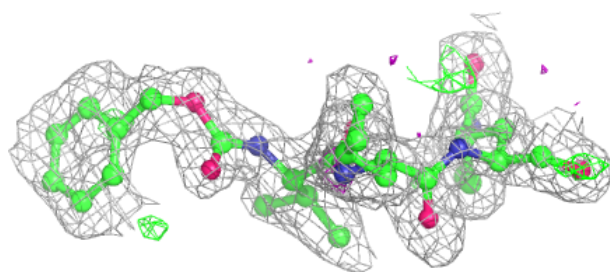
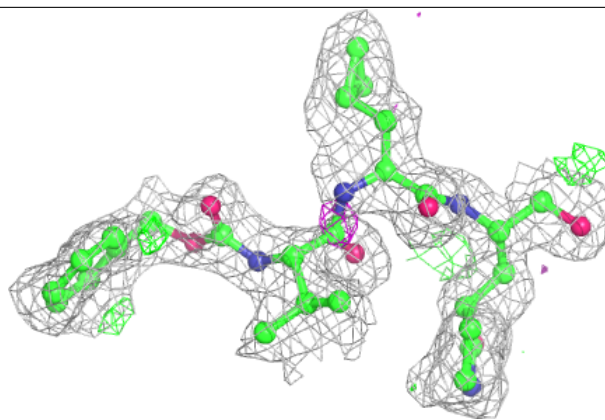
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	7VI	B	401	36/36	0.72	0.21	22,32,46,47	0
2	7VI	A	401	36/36	0.78	0.17	24,30,41,42	0

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 7VI 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.