



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:54 PM UTC

PDB ID : 7RVT / pdb_00007rvt
Title : Structure of the SARS-CoV-2 main protease in complex with inhibitor MPI20
Authors : Yang, K.; Sankaran, B.; Liu, W.
Deposited on : 2021-08-19
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

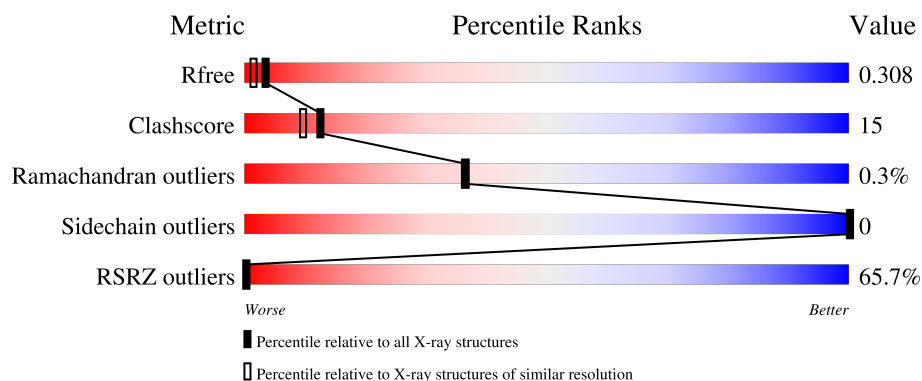
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	61% 66%31%..
1	B	306	67% 75%23%.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4852 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

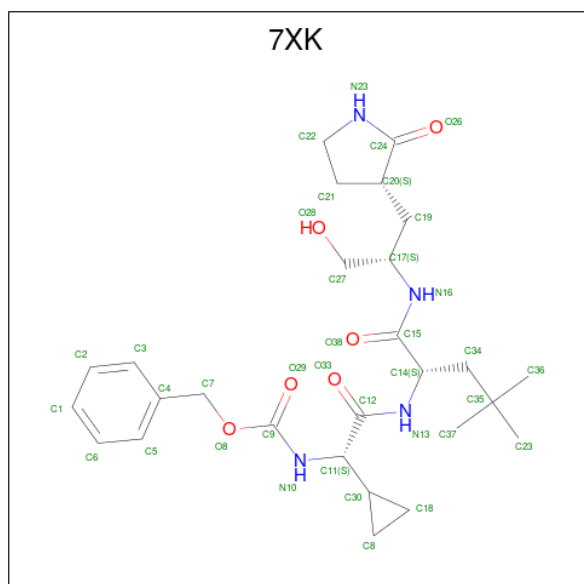
- Molecule 1 is a protein called 3C-like proteinase.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is N 2 -[(2S)-2-{[(benzyloxy)carbonyl]amino}-2-cyclopropylacetyl]-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-4-methyl-L-leucinamide (CCD ID: 7XK) (formula: C₂₇H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



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

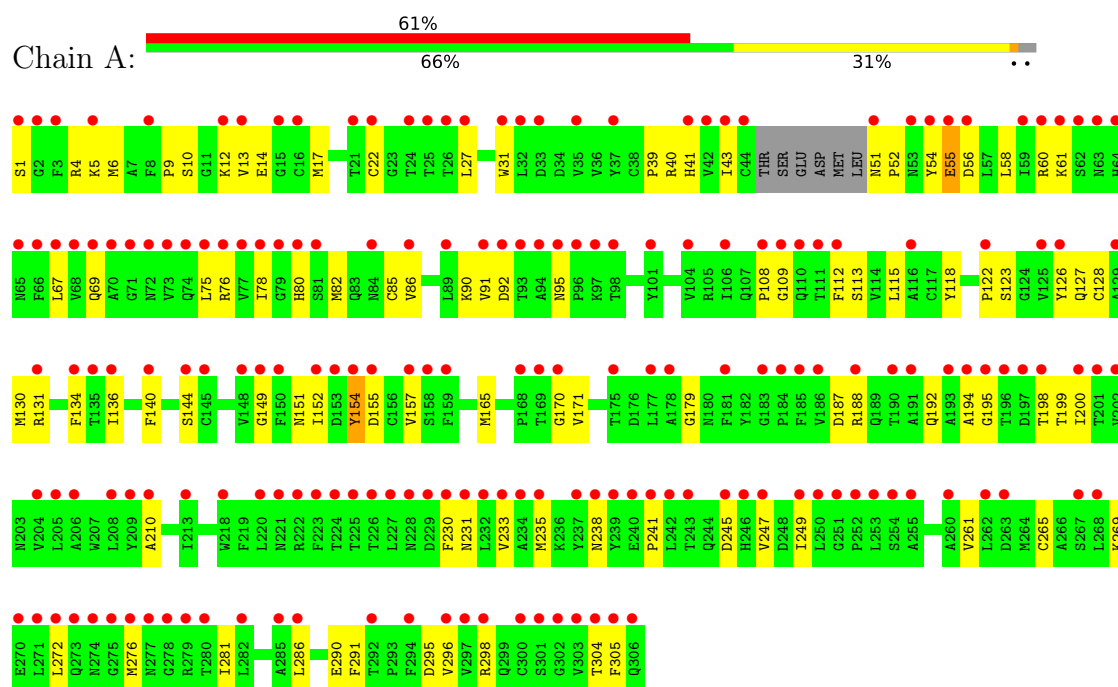
- Molecule 3 is water.

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

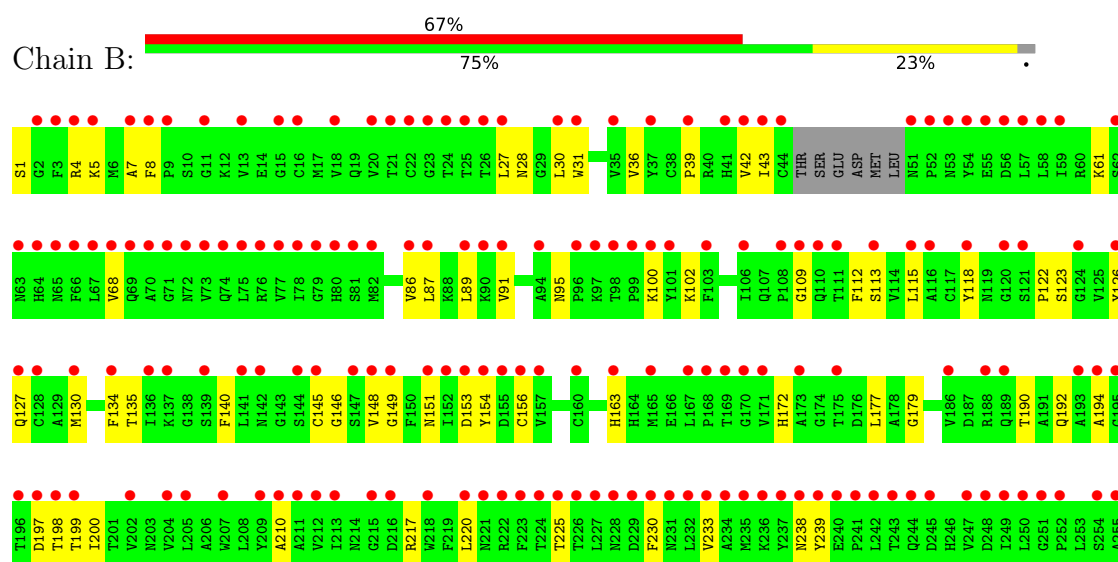
3 Residue-property plots

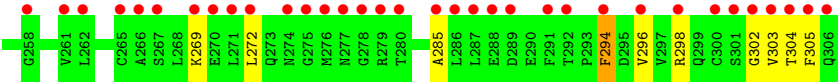
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 60.70Å 63.34Å 80.42° 68.42° 70.59°	Depositor
Resolution (Å)	32.85 – 2.10 32.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (32.85-2.10) 94.8 (32.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.270 , 0.308 0.271 , 0.308	Depositor DCC
R_{free} test set	2072 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.099 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4852	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 7XK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2369	0.63	3/3219 (0.1%)
1	B	0.38	0/2369	0.61	1/3219 (0.0%)
All	All	0.39	0/4738	0.62	4/6438 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	PHE	CB-CA-C	-6.07	101.27	110.92
1	A	55	GLU	N-CA-CB	-5.29	102.75	110.53
1	A	55	GLU	CA-CB-CG	5.08	124.26	114.10
1	A	55	GLU	CB-CA-C	5.01	118.40	109.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2317	0	2269	89	0
1	B	2317	0	2269	59	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
3	A	77	0	0	27	0
3	B	67	0	0	8	0
All	All	4852	0	4538	141	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 15.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:NZ	3:A:501:HOH:O	1.83	1.07
1:A:151:ASN:ND2	3:A:502:HOH:O	1.88	1.04
1:A:22:CYS:SG	1:A:61:LYS:NZ	2.38	0.95
1:A:151:ASN:O	3:A:503:HOH:O	1.90	0.89
1:B:197:ASP:OD2	3:B:501:HOH:O	1.93	0.86
1:A:152:ILE:HD13	3:A:503:HOH:O	1.77	0.84
1:B:5:LYS:HE3	1:B:127:GLN:HB2	1.62	0.81
1:B:113:SER:OG	1:B:127:GLN:OE1	1.97	0.81
1:A:233:VAL:HG21	1:A:269:LYS:HD3	1.65	0.78
1:A:131:ARG:O	3:A:504:HOH:O	2.01	0.78
1:B:27:LEU:HD13	1:B:39:PRO:HD2	1.64	0.78
1:B:233:VAL:HG21	1:B:269:LYS:HE3	1.66	0.76
1:B:177:LEU:O	3:B:503:HOH:O	2.04	0.75
1:B:5:LYS:HE3	1:B:127:GLN:CB	2.17	0.74
1:A:40:ARG:HH11	1:A:82:MET:CE	2.01	0.74
1:A:157:VAL:HA	3:A:503:HOH:O	1.87	0.73
1:B:8:PHE:HE2	1:B:151:ASN:HD22	1.36	0.72
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.71	0.72
1:A:1:SER:N	1:B:140:PHE:O	2.22	0.72
1:B:298:ARG:HG3	1:B:303:VAL:HB	1.72	0.71
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HD22	1:B:89:LEU:HG	1.73	0.70
1:B:30:LEU:HD22	1:B:148:VAL:HG11	1.73	0.69
1:B:130:MET:HE2	1:B:134:PHE:HA	1.76	0.68
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.58	0.68
1:B:135:THR:OG1	3:B:504:HOH:O	2.12	0.68
1:A:108:PRO:HB3	3:A:504:HOH:O	1.96	0.66
1:A:40:ARG:HH11	1:A:82:MET:HE3	1.61	0.65
1:A:298:ARG:NH2	3:A:517:HOH:O	2.29	0.64
1:B:153:ASP:OD2	3:B:502:HOH:O	2.14	0.64
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.80	0.64
1:A:52:PRO:HD2	1:A:188:ARG:HG3	1.78	0.64
1:A:130:MET:HE2	1:A:134:PHE:HA	1.81	0.62
1:B:298:ARG:NH2	3:B:510:HOH:O	2.33	0.61
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.35	0.61
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.83	0.60
1:B:194:ALA:O	3:B:505:HOH:O	2.16	0.60
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.84	0.60
1:A:304:THR:HG22	1:B:123:SER:HB2	1.81	0.60
1:A:10:SER:O	1:A:14:GLU:HG3	2.02	0.60
1:A:198:THR:HG22	1:A:238:ASN:OD1	2.03	0.59
1:A:91:VAL:O	3:A:506:HOH:O	2.17	0.59
1:A:245:ASP:O	1:A:249:ILE:HG13	2.03	0.59
1:A:5:LYS:HZ2	1:A:127:GLN:HG2	1.68	0.59
1:B:112:PHE:HA	1:B:151:ASN:HD21	1.68	0.59
1:B:91:VAL:O	3:B:506:HOH:O	2.17	0.58
1:A:195:GLY:N	3:A:513:HOH:O	2.22	0.58
1:B:130:MET:HE3	1:B:130:MET:HA	1.85	0.58
1:A:5:LYS:NZ	1:A:127:GLN:HG2	2.20	0.56
1:B:198:THR:HG22	1:B:238:ASN:OD1	2.06	0.56
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.88	0.55
1:A:247:VAL:HG22	1:A:261:VAL:HG11	1.89	0.55
1:A:4:ARG:HD2	1:B:126:TYR:CD1	2.41	0.54
1:A:199:THR:OG1	3:A:507:HOH:O	2.18	0.54
1:B:298:ARG:HD2	1:B:305:PHE:HZ	1.72	0.54
1:B:7:ALA:HA	1:B:127:GLN:OE1	2.08	0.53
1:A:233:VAL:HG21	1:A:269:LYS:CD	2.38	0.53
1:A:140:PHE:O	1:B:1:SER:N	2.43	0.52
1:A:170:GLY:O	3:A:508:HOH:O	2.19	0.52
1:A:230:PHE:CD1	1:A:265:CYS:HB3	2.45	0.51
1:A:130:MET:HE3	1:A:130:MET:HA	1.93	0.51
1:A:123:SER:HB2	1:B:304:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:MET:HE1	1:A:241:PRO:HA	1.93	0.51
1:A:290:GLU:OE1	3:A:510:HOH:O	2.20	0.50
1:B:39:PRO:HG2	1:B:145:CYS:HB3	1.92	0.50
1:A:56:ASP:O	1:A:60:ARG:HG3	2.11	0.50
1:B:190:THR:O	1:B:192:GLN:HG2	2.12	0.50
1:A:9:PRO:O	1:A:12:LYS:NZ	2.45	0.49
1:A:75:LEU:HD13	1:A:91:VAL:HG21	1.95	0.49
1:A:231:ASN:O	1:A:235:MET:HG2	2.13	0.49
1:B:102:LYS:HE2	1:B:156:CYS:SG	2.53	0.49
1:B:28:ASN:O	1:B:146:GLY:HA3	2.11	0.49
1:B:199:THR:HG21	1:B:239:TYR:CZ	2.48	0.49
1:A:76:ARG:NH2	1:A:92:ASP:OD2	2.45	0.49
1:A:17:MET:HB2	3:A:553:HOH:O	2.13	0.49
1:A:126:TYR:OH	3:A:505:HOH:O	2.02	0.49
1:A:41:HIS:HA	1:A:54:TYR:HE1	1.77	0.48
1:A:235:MET:HE1	1:A:241:PRO:HB3	1.95	0.48
1:A:40:ARG:NH2	1:A:187:ASP:OD1	2.39	0.47
1:B:8:PHE:HE2	1:B:151:ASN:ND2	2.07	0.47
1:B:112:PHE:HA	1:B:151:ASN:ND2	2.29	0.47
1:B:217:ARG:HB3	1:B:220:LEU:HD12	1.96	0.47
1:A:272:LEU:O	3:A:509:HOH:O	2.19	0.47
1:A:5:LYS:HD3	1:A:291:PHE:CZ	2.50	0.47
1:B:8:PHE:HE1	1:B:305:PHE:CZ	2.33	0.47
1:B:298:ARG:HD2	1:B:305:PHE:CZ	2.50	0.47
1:B:225:THR:HG21	1:B:230:PHE:HB2	1.97	0.46
1:B:233:VAL:HG11	1:B:269:LYS:HG3	1.97	0.46
1:A:140:PHE:CE1	3:A:505:HOH:O	2.56	0.46
1:A:171:VAL:HA	3:A:508:HOH:O	2.15	0.46
1:A:12:LYS:HE2	1:A:12:LYS:HB2	1.66	0.46
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.97	0.46
1:A:304:THR:HG21	1:B:118:TYR:HB2	1.96	0.46
3:A:514:HOH:O	1:B:302:GLY:HA2	2.15	0.46
1:B:130:MET:HE2	1:B:134:PHE:C	2.40	0.46
1:A:286:LEU:HD21	1:B:285:ALA:HB2	1.97	0.46
1:A:78:ILE:HG13	1:A:90:LYS:HG2	1.97	0.46
3:A:510:HOH:O	1:B:4:ARG:NH2	2.49	0.46
1:A:112:PHE:HZ	1:A:136:ILE:HG21	1.80	0.45
1:A:126:TYR:HE1	1:A:128:CYS:SG	2.39	0.45
1:A:233:VAL:HG11	1:A:269:LYS:HG3	1.98	0.45
1:A:5:LYS:HD2	1:A:5:LYS:HA	1.71	0.45
1:A:40:ARG:CD	1:A:82:MET:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:MET:HE1	1:A:241:PRO:CA	2.47	0.45
1:A:157:VAL:HG13	3:A:503:HOH:O	2.15	0.45
1:B:113:SER:O	1:B:149:GLY:HA2	2.17	0.45
1:A:13:VAL:HG12	1:A:115:LEU:HD23	1.99	0.45
1:A:155:ASP:OD1	1:A:155:ASP:N	2.46	0.45
1:A:67:LEU:HD23	1:A:69:GLN:HE21	1.81	0.45
1:B:100:LYS:HD3	3:B:544:HOH:O	2.16	0.45
1:A:298:ARG:NH1	3:A:517:HOH:O	2.49	0.44
1:B:130:MET:HE2	1:B:134:PHE:CA	2.43	0.44
1:A:298:ARG:CZ	3:A:517:HOH:O	2.66	0.44
1:A:130:MET:HG3	3:A:504:HOH:O	2.17	0.44
1:A:27:LEU:HD13	1:A:39:PRO:HD2	2.00	0.43
1:A:113:SER:O	1:A:149:GLY:HA2	2.18	0.43
1:A:118:TYR:CE2	1:A:144:SER:HB3	2.53	0.43
1:A:171:VAL:HG11	3:A:570:HOH:O	2.18	0.43
1:A:130:MET:HE2	1:A:134:PHE:CA	2.48	0.43
1:A:51:ASN:OD1	1:A:188:ARG:HD3	2.19	0.43
1:A:130:MET:HE2	1:A:134:PHE:C	2.44	0.43
1:B:210:ALA:HB2	1:B:296:VAL:HG13	2.01	0.43
1:A:154:TYR:O	1:A:305:PHE:HB3	2.18	0.42
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.00	0.42
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.55	0.42
1:A:165:MET:HE1	1:A:192:GLN:NE2	2.35	0.42
1:A:295:ASP:OD1	3:A:511:HOH:O	2.22	0.42
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.76	0.42
1:A:6:MET:HB3	1:A:298:ARG:HH21	1.84	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.75	0.41
1:A:31:TRP:CE2	1:A:75:LEU:HD11	2.56	0.41
1:A:58:LEU:HD11	1:A:80:HIS:CD2	2.56	0.41
1:A:194:ALA:N	3:A:513:HOH:O	2.53	0.41
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.56	0.41
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.86	0.41
1:A:210:ALA:HB2	1:A:296:VAL:HG13	2.01	0.41
1:A:276:MET:HE3	1:A:281:ILE:HG13	2.02	0.41
1:B:36:VAL:HG21	1:B:68:VAL:HG11	2.03	0.41
1:A:40:ARG:O	1:A:43:ILE:HG12	2.22	0.40
1:A:78:ILE:N	1:A:90:LYS:O	2.49	0.40
1:B:43:ILE:HB	1:B:61:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	296/306 (97%)	291 (98%)	4 (1%)	1 (0%)	36	36
1	B	296/306 (97%)	284 (96%)	11 (4%)	1 (0%)	36	36
All	All	592/612 (97%)	575 (97%)	15 (2%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/262 (98%)	256 (100%)	0	100	100
1	B	256/262 (98%)	256 (100%)	0	100	100
All	All	512/524 (98%)	512 (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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	119	ASN
1	A	151	ASN
1	A	180	ASN
1	A	277	ASN
1	B	83	GLN
1	B	119	ASN
1	B	142	ASN
1	B	151	ASN
1	B	180	ASN
1	B	273	GLN
1	B	274	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	7XK	B	401	1	39,39,39	1.05	1 (2%)	46,54,54	0.96	2 (4%)
2	7XK	A	401	1	39,39,39	1.05	1 (2%)	46,54,54	1.14	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7XK	B	401	1	-	4/40/52/52	0/3/3/3
2	7XK	A	401	1	-	4/40/52/52	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7XK	O8-C9	5.37	1.45	1.35
2	A	401	7XK	O8-C9	5.04	1.45	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	7XK	C7-O8-C9	3.73	124.33	115.93
2	B	401	7XK	O8-C9-N10	3.12	117.13	110.45
2	A	401	7XK	O26-C24-C20	-2.80	122.98	126.21
2	A	401	7XK	C19-C20-C24	-2.78	106.80	112.81
2	A	401	7XK	O8-C7-C4	2.73	116.02	109.40
2	B	401	7XK	O8-C9-O29	-2.43	119.59	124.26
2	A	401	7XK	O8-C9-N10	2.20	115.17	110.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

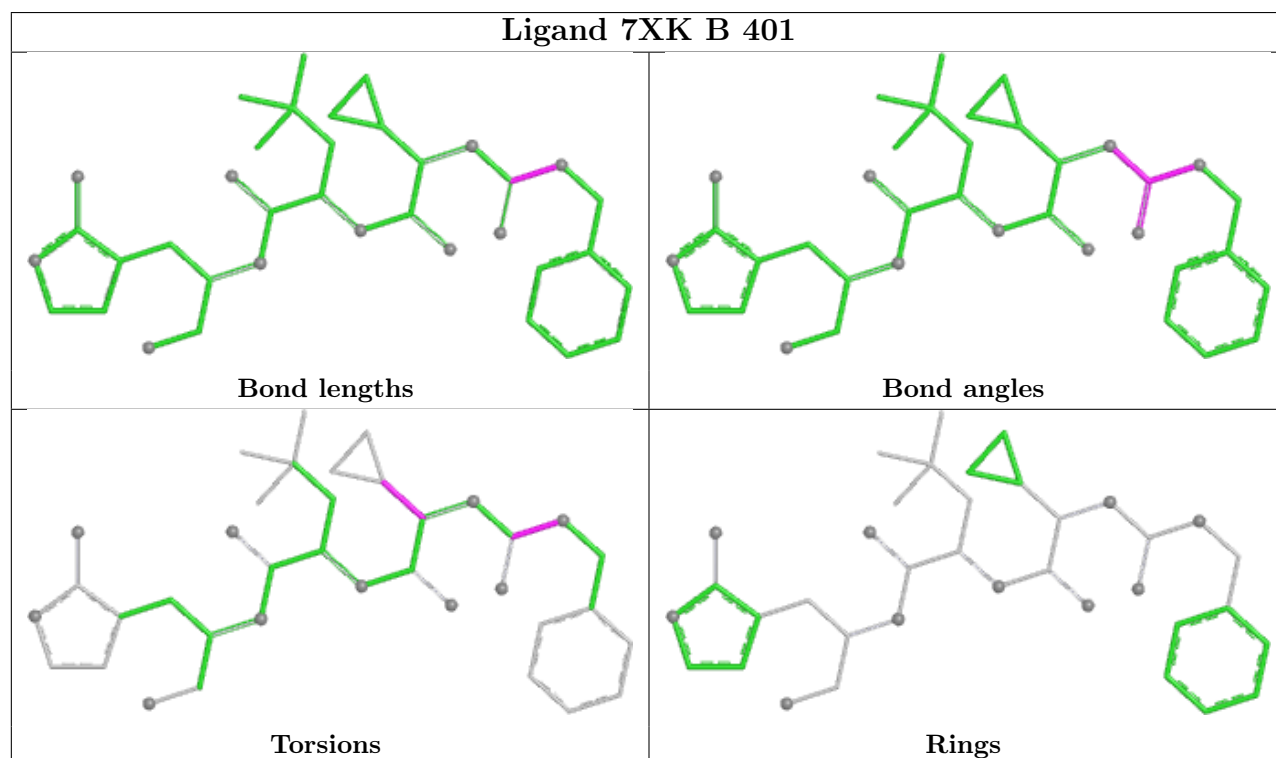
Mol	Chain	Res	Type	Atoms
2	A	401	7XK	C12-C11-C30-C18
2	A	401	7XK	C4-C7-O8-C9
2	B	401	7XK	C12-C11-C30-C18
2	B	401	7XK	O29-C9-O8-C7
2	B	401	7XK	N10-C9-O8-C7
2	A	401	7XK	N10-C9-O8-C7
2	A	401	7XK	O29-C9-O8-C7
2	B	401	7XK	N10-C11-C30-C18

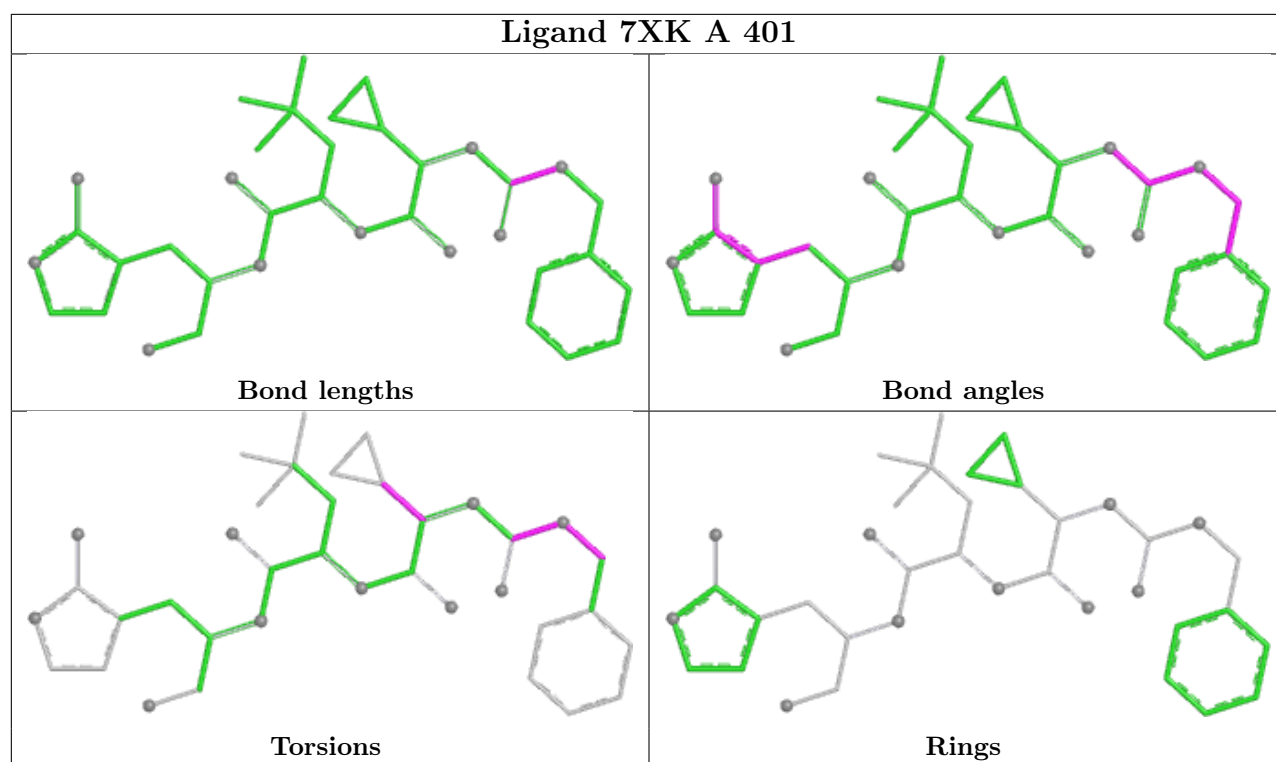
There are no ring outliers.

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	300/306 (98%)	2.45	188 (62%) 0 0	16, 30, 49, 72	0
1	B	300/306 (98%)	2.65	206 (68%) 0 0	16, 30, 50, 67	0
All	All	600/612 (98%)	2.55	394 (65%) 0 0	16, 30, 50, 72	0

All (394) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	PHE	8.9
1	B	154	TYR	8.2
1	B	222	ARG	7.1
1	A	222	ARG	7.0
1	B	303	VAL	6.9
1	B	306	GLN	6.9
1	B	305	PHE	6.7
1	A	305	PHE	6.5
1	B	121	SER	6.3
1	B	72	ASN	6.1
1	B	43	ILE	6.0
1	B	251	GLY	5.9
1	B	168	PRO	5.8
1	A	247	VAL	5.8
1	A	54	TYR	5.8
1	B	223	PHE	5.6
1	A	110	GLN	5.5
1	A	306	GLN	5.5
1	A	154	TYR	5.4
1	A	2	GLY	5.4
1	B	73	VAL	5.2
1	B	74	GLN	5.2
1	B	304	THR	5.2
1	B	245	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	5.0
1	B	170	GLY	5.0
1	B	59	ILE	4.8
1	B	65	ASN	4.8
1	B	233	VAL	4.8
1	A	190	THR	4.8
1	B	237	TYR	4.7
1	B	226	THR	4.7
1	B	109	GLY	4.7
1	B	215	GLY	4.7
1	B	67	LEU	4.6
1	A	69	GLN	4.6
1	B	272	LEU	4.6
1	B	225	THR	4.5
1	B	160	CYS	4.5
1	A	223	PHE	4.5
1	B	68	VAL	4.5
1	A	108	PRO	4.5
1	A	77	VAL	4.5
1	A	72	ASN	4.4
1	B	56	ASP	4.4
1	A	24	THR	4.4
1	A	155	ASP	4.4
1	B	169	THR	4.3
1	A	55	GLU	4.3
1	B	22	CYS	4.3
1	B	64	HIS	4.3
1	B	302	GLY	4.3
1	B	101	TYR	4.3
1	B	224	THR	4.3
1	A	25	THR	4.2
1	A	56	ASP	4.2
1	B	87	LEU	4.2
1	A	51	ASN	4.1
1	A	227	LEU	4.1
1	A	157	VAL	4.1
1	A	196	THR	4.1
1	B	90	LYS	4.1
1	A	254	SER	4.1
1	B	70	ALA	4.0
1	A	278	GLY	4.0
1	A	271	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	GLY	4.0
1	A	230	PHE	4.0
1	B	235	MET	4.0
1	A	272	LEU	3.9
1	B	21	THR	3.9
1	A	78	ILE	3.9
1	B	275	GLY	3.9
1	B	89	LEU	3.9
1	A	304	THR	3.9
1	A	245	ASP	3.9
1	A	241	PRO	3.9
1	A	66	PHE	3.8
1	A	302	GLY	3.8
1	A	243	THR	3.8
1	B	55	GLU	3.8
1	B	266	ALA	3.8
1	A	96	PRO	3.8
1	A	233	VAL	3.8
1	A	21	THR	3.8
1	A	122	PRO	3.8
1	B	261	VAL	3.8
1	A	59	ILE	3.7
1	A	235	MET	3.8
1	A	16	CYS	3.7
1	A	93	THR	3.7
1	B	242	LEU	3.7
1	A	22	CYS	3.7
1	A	301	SER	3.7
1	A	286	LEU	3.7
1	B	120	GLY	3.7
1	B	51	ASN	3.7
1	B	66	PHE	3.7
1	B	301	SER	3.6
1	A	202	VAL	3.6
1	A	153	ASP	3.6
1	B	234	ALA	3.6
1	B	108	PRO	3.6
1	A	152	ILE	3.6
1	B	7	ALA	3.6
1	B	52	PRO	3.6
1	B	27	LEU	3.6
1	B	300	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	218	TRP	3.5
1	A	73	VAL	3.5
1	B	78	ILE	3.5
1	B	230	PHE	3.5
1	A	15	GLY	3.5
1	B	69	GLN	3.5
1	A	232	LEU	3.5
1	A	81	SER	3.5
1	B	243	THR	3.5
1	A	43	ILE	3.5
1	A	76	ARG	3.5
1	A	240	GLU	3.5
1	A	296	VAL	3.5
1	B	136	ILE	3.4
1	B	227	LEU	3.4
1	A	225	THR	3.4
1	A	70	ALA	3.4
1	A	197	ASP	3.4
1	A	188	ARG	3.4
1	A	229	ASP	3.4
1	B	75	LEU	3.4
1	A	221	ASN	3.3
1	A	71	GLY	3.3
1	A	94	ALA	3.3
1	A	260	ALA	3.3
1	B	94	ALA	3.3
1	B	271	LEU	3.3
1	A	8	PHE	3.3
1	B	247	VAL	3.3
1	A	294	PHE	3.3
1	B	31	TRP	3.2
1	B	130	MET	3.2
1	A	74	GLN	3.2
1	B	195	GLY	3.2
1	A	204	VAL	3.2
1	A	97	LYS	3.2
1	B	221	ASN	3.2
1	B	134	PHE	3.2
1	B	258	GLY	3.2
1	A	91	VAL	3.1
1	A	27	LEU	3.1
1	A	169	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	3.1
1	B	153	ASP	3.1
1	B	210	ALA	3.1
1	B	298	ARG	3.1
1	B	58	LEU	3.1
1	A	79	GLY	3.1
1	B	199	THR	3.1
1	B	110	GLN	3.1
1	B	220	LEU	3.1
1	A	170	GLY	3.1
1	B	151	ASN	3.1
1	B	277	ASN	3.1
1	B	76	ARG	3.1
1	B	240	GLU	3.1
1	A	80	HIS	3.1
1	A	205	LEU	3.1
1	A	237	TYR	3.0
1	A	206	ALA	3.0
1	B	250	LEU	3.0
1	B	254	SER	3.0
1	B	2	GLY	3.0
1	B	96	PRO	3.0
1	B	252	PRO	3.0
1	A	282	LEU	3.0
1	A	53	ASN	3.0
1	B	80	HIS	3.0
1	A	262	LEU	3.0
1	B	18	VAL	3.0
1	B	238	ASN	3.0
1	A	198	THR	3.0
1	B	229	ASP	3.0
1	A	136	ILE	2.9
1	A	292	THR	2.9
1	B	216	ASP	2.9
1	A	116	ALA	2.9
1	B	57	LEU	2.9
1	A	95	ASN	2.9
1	A	285	ALA	2.9
1	A	246	HIS	2.9
1	A	263	ASP	2.8
1	A	249	ILE	2.8
1	B	39	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	2.8
1	A	298	ARG	2.8
1	B	71	GLY	2.8
1	B	197	ASP	2.8
1	B	248	ASP	2.8
1	B	285	ALA	2.8
1	A	177	LEU	2.8
1	B	26	THR	2.8
1	B	98	THR	2.8
1	B	241	PRO	2.8
1	A	276	MET	2.8
1	A	201	THR	2.8
1	B	13	VAL	2.8
1	B	99	PRO	2.8
1	A	63	ASN	2.8
1	B	244	GLN	2.8
1	A	104	VAL	2.8
1	A	303	VAL	2.8
1	B	79	GLY	2.7
1	A	178	ALA	2.7
1	A	220	LEU	2.7
1	A	242	LEU	2.7
1	A	224	THR	2.7
1	B	42	VAL	2.7
1	B	249	ILE	2.7
1	A	267	SER	2.7
1	A	98	THR	2.7
1	A	226	THR	2.7
1	B	25	THR	2.7
1	A	84	ASN	2.7
1	B	228	ASN	2.7
1	B	91	VAL	2.7
1	A	213	ILE	2.7
1	A	75	LEU	2.7
1	A	253	LEU	2.7
1	A	184	PRO	2.7
1	B	288	GLU	2.7
1	A	239	TYR	2.7
1	B	231	ASN	2.6
1	A	1	SER	2.6
1	A	62	SER	2.6
1	A	101	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	128	CYS	2.6
1	A	275	GLY	2.6
1	A	181	PHE	2.6
1	A	279	ARG	2.6
1	B	188	ARG	2.6
1	B	152	ILE	2.6
1	B	15	GLY	2.6
1	A	129	ALA	2.6
1	B	100	LYS	2.6
1	B	236	LYS	2.6
1	B	35	VAL	2.6
1	B	77	VAL	2.6
1	B	148	VAL	2.6
1	B	171	VAL	2.6
1	B	209	TYR	2.6
1	A	194	ALA	2.6
1	A	158	SER	2.6
1	B	141	LEU	2.6
1	B	103	PHE	2.5
1	A	200	ILE	2.5
1	B	54	TYR	2.5
1	A	61	LYS	2.5
1	B	5	LYS	2.5
1	B	286	LEU	2.5
1	A	149	GLY	2.5
1	B	296	VAL	2.5
1	A	44	CYS	2.5
1	A	92	ASP	2.5
1	A	111	THR	2.5
1	B	194	ALA	2.5
1	A	140	PHE	2.5
1	A	185	PHE	2.5
1	A	31	TRP	2.5
1	B	41	HIS	2.5
1	A	125	VAL	2.5
1	B	157	VAL	2.5
1	B	142	ASN	2.5
1	B	82	MET	2.5
1	A	183	GLY	2.5
1	A	35	VAL	2.4
1	B	213	ILE	2.5
1	B	16	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	44	CYS	2.4
1	B	62	SER	2.4
1	A	250	LEU	2.4
1	B	115	LEU	2.4
1	A	41	HIS	2.4
1	A	131	ARG	2.4
1	A	238	ASN	2.4
1	B	20	VAL	2.4
1	B	204	VAL	2.4
1	A	193	ALA	2.4
1	B	167	LEU	2.4
1	B	205	LEU	2.4
1	B	262	LEU	2.4
1	B	189	GLN	2.4
1	B	270	GLU	2.4
1	A	13	VAL	2.4
1	A	145	CYS	2.4
1	B	24	THR	2.4
1	B	280	THR	2.4
1	A	3	PHE	2.4
1	A	159	PHE	2.4
1	A	186	VAL	2.4
1	B	139	SER	2.4
1	B	9	PRO	2.4
1	A	209	TYR	2.3
1	A	191	ALA	2.3
1	A	210	ALA	2.3
1	B	255	ALA	2.3
1	A	32	LEU	2.3
1	A	277	ASN	2.3
1	A	297	VAL	2.3
1	B	147	SER	2.3
1	A	64	HIS	2.3
1	A	126	TYR	2.3
1	A	234	ALA	2.3
1	A	67	LEU	2.3
1	A	195	GLY	2.3
1	B	278	GLY	2.3
1	B	81	SER	2.3
1	A	65	ASN	2.3
1	B	287	LEU	2.3
1	B	269	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	113	SER	2.3
1	B	3	PHE	2.3
1	A	106	ILE	2.3
1	B	86	VAL	2.3
1	A	252	PRO	2.3
1	A	5	LYS	2.3
1	B	11	GLY	2.3
1	B	97	LYS	2.3
1	B	267	SER	2.2
1	A	135	THR	2.2
1	A	168	PRO	2.2
1	A	251	GLY	2.2
1	B	116	ALA	2.2
1	A	268	LEU	2.2
1	A	60	ARG	2.2
1	A	112	PHE	2.2
1	B	279	ARG	2.2
1	A	26	THR	2.2
1	B	292	THR	2.2
1	B	155	ASP	2.2
1	B	289	ASP	2.2
1	B	124	GLY	2.2
1	B	30	LEU	2.2
1	A	37	TYR	2.2
1	B	37	TYR	2.2
1	B	239	TYR	2.2
1	B	144	SER	2.2
1	A	228	ASN	2.2
1	A	42	VAL	2.2
1	B	127	GLN	2.2
1	B	193	ALA	2.2
1	B	211	ALA	2.2
1	B	118	TYR	2.2
1	B	137	LYS	2.2
1	B	63	ASN	2.2
1	A	218	TRP	2.2
1	B	165	MET	2.2
1	B	207	TRP	2.2
1	A	175	THR	2.2
1	B	111	THR	2.2
1	B	175	THR	2.2
1	B	291	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	2.1
1	B	202	VAL	2.1
1	B	163	HIS	2.1
1	B	265	CYS	2.1
1	A	231	ASN	2.1
1	B	276	MET	2.1
1	B	106	ILE	2.1
1	B	186	VAL	2.1
1	B	212	VAL	2.1
1	B	53	ASN	2.1
1	A	33	ASP	2.1
1	A	280	THR	2.1
1	B	23	GLY	2.1
1	B	149	GLY	2.1
1	A	150	PHE	2.1
1	B	173	ALA	2.1
1	A	89	LEU	2.1
1	B	232	LEU	2.1
1	A	270	GLU	2.1
1	B	274	ASN	2.1
1	B	126	TYR	2.1
1	B	8	PHE	2.1
1	A	208	LEU	2.0
1	A	274	ASN	2.0
1	A	273	GLN	2.0
1	A	300	CYS	2.0
1	B	145	CYS	2.0
1	B	4	ARG	2.0
1	B	198	THR	2.0
1	A	12	LYS	2.0
1	A	148	VAL	2.0
1	A	144	SER	2.0
1	B	156	CYS	2.0
1	B	196	THR	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](#)

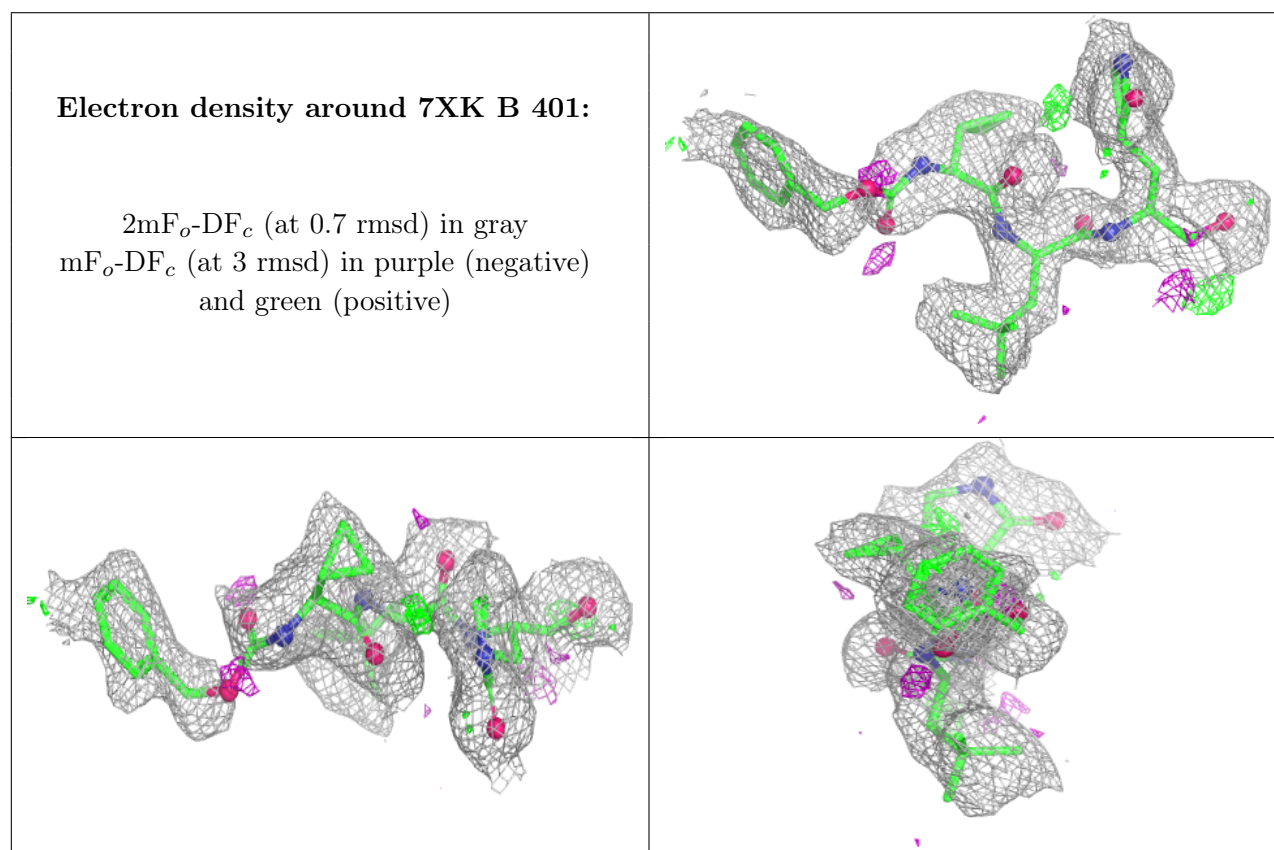
There are no oligosaccharides in this entry.

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.

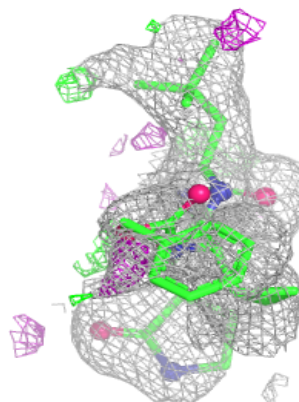
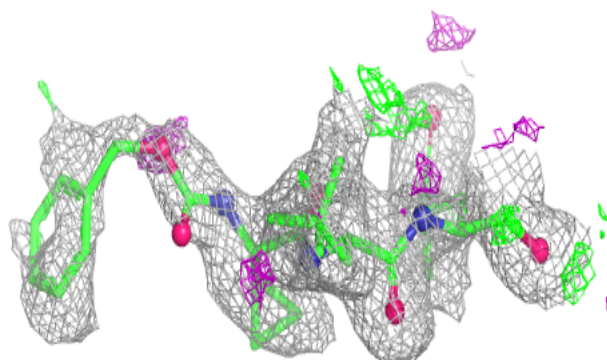
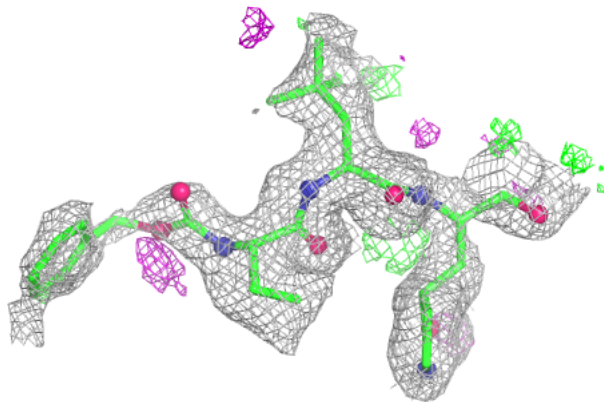
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7XK	B	401	37/37	0.80	0.17	19,28,43,43	0
2	7XK	A	401	37/37	0.82	0.17	21,26,41,44	0

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



Electron density around 7XK 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.