



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 7E35 / pdb_00007e35
Title : Crystal structure of the SARS-CoV-2 papain-like protease (PLPro) C112S mutant bound to compound S43
Authors : Liu, J.; Wang, Y.; Xu, X.; Pan, L.
Deposited on : 2021-02-08
Resolution : 2.40 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

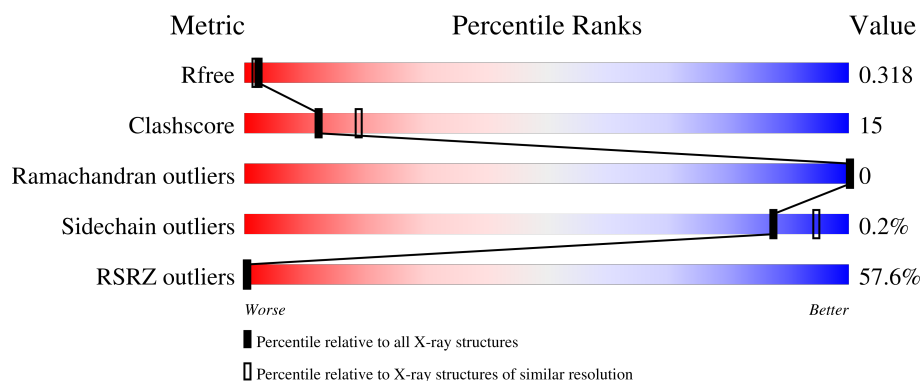
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	315	34% 72% 27% .
1	B	315	77% 65% 26% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4472 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	287	Total	C	N	O	S	0	0	0
			2017	1285	337	381	14			
1	A	315	Total	C	N	O	S	0	0	0
			2389	1537	392	442	18			

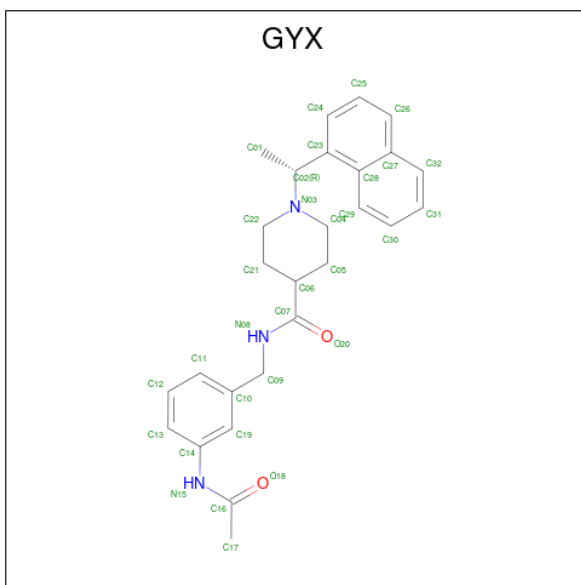
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	SER	CYS	engineered mutation	UNP P0DTD1
A	112	SER	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-[(3-acetamidophenyl)methyl]-1-[(1R)-1-naphthalen-1-ylethyl]piperidine-4-carboxamide (CCD ID: GYX) (formula: C₂₇H₃₁N₃O₂) (labeled as "Ligand of Interest" by depositor).

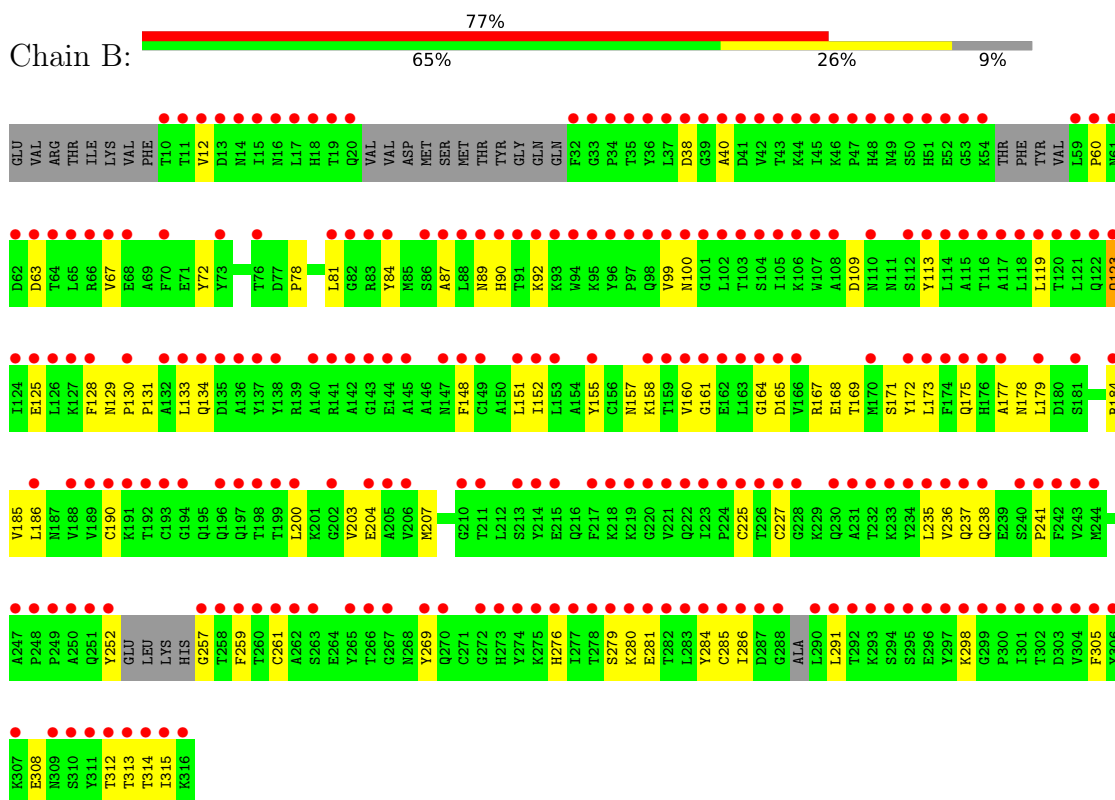


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 32	C 27	N 3	O 2	0	0
3	A	1	Total 32	C 27	N 3	O 2	0	0

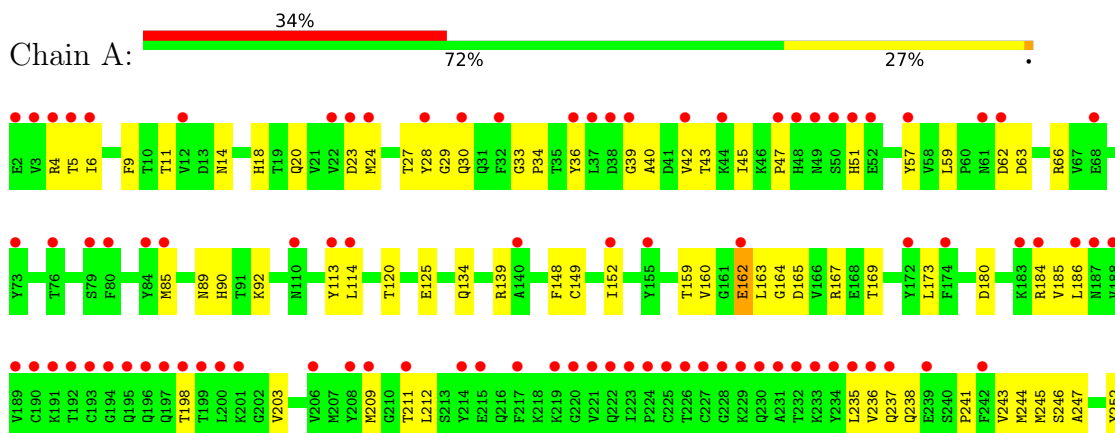
3 Residue-property plots

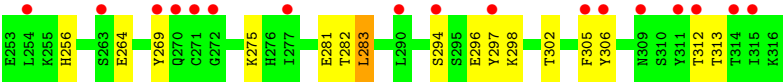
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Non-structural protein 3



• Molecule 1: Non-structural protein 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.82Å 99.82Å 298.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.45 – 2.40 86.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	48.2 (86.45-2.40) 48.4 (86.45-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.281 , 0.317 0.285 , 0.318	Depositor DCC
R_{free} test set	871 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: GYX, ZN

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	0.68	0/2447	1.11	5/3332 (0.2%)
1	B	0.50	0/2061	1.02	3/2819 (0.1%)
All	All	0.60	0/4508	1.07	8/6151 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	GLN	CA-CB-CG	10.46	135.02	114.10
1	A	209	MET	CB-CG-SD	8.98	139.65	112.70
1	B	123	GLN	N-CA-CB	-6.83	100.63	110.80
1	B	123	GLN	CB-CG-CD	-6.42	101.69	112.60
1	A	209	MET	CG-SD-CE	-6.22	87.21	100.90
1	A	162	GLU	CA-CB-CG	5.57	125.24	114.10
1	A	20	GLN	N-CA-CB	5.49	121.10	111.55
1	A	283	LEU	N-CA-C	5.25	117.30	108.96

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	2389	0	2244	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2017	0	1743	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	0	2	0
3	B	32	0	0	0	0
All	All	4472	0	3987	131	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 (131) 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:4:ARG:HB3	1:A:24:MET:HE3	1.42	1.01
1:B:261:CYS:HG	1:B:305:PHE:HD1	1.14	0.95
1:A:34:PRO:HB2	1:A:59:LEU:HD21	1.58	0.86
1:B:184:ARG:HE	1:B:238:GLN:NE2	1.74	0.86
1:B:284:TYR:HB3	1:B:291:LEU:HD11	1.59	0.85
1:B:128:PHE:H	1:B:134:GLN:HE21	1.28	0.80
1:B:186:LEU:HD22	1:B:235:LEU:HA	1.62	0.79
1:A:237:GLN:HG2	1:A:312:THR:HG22	1.62	0.79
1:B:200:LEU:HD23	1:B:204:GLU:HB3	1.68	0.75
1:B:148:PHE:O	1:B:152:ILE:HD12	1.86	0.75
1:B:123:GLN:OE1	1:B:276:HIS:NE2	2.21	0.74
1:A:252:TYR:O	1:A:298:LYS:HA	1.89	0.72
1:B:128:PHE:H	1:B:134:GLN:NE2	1.87	0.72
1:B:257:GLY:N	1:B:279:SER:HG	1.86	0.72
1:B:158:LYS:HZ3	1:B:164:GLY:HA2	1.55	0.70
1:A:59:LEU:HD22	1:A:59:LEU:N	2.07	0.69
1:B:40:ALA:HA	1:B:89:ASN:ND2	2.09	0.68
1:B:286:ILE:HG13	1:B:291:LEU:HD13	1.77	0.66
1:B:72:TYR:HA	1:B:131:PRO:HG2	1.77	0.66
1:B:158:LYS:NZ	1:B:164:GLY:HA2	2.11	0.66
1:B:171:SER:HA	1:B:207:MET:HE1	1.79	0.65
1:B:184:ARG:HE	1:B:238:GLN:HE21	1.46	0.64
1:A:5:THR:HG22	1:A:23:ASP:HA	1.80	0.64
1:B:128:PHE:HB2	1:B:134:GLN:HG2	1.80	0.63
1:A:163:LEU:HB3	3:A:402:GYX:C09	2.28	0.63
1:B:148:PHE:CD2	1:B:152:ILE:HD11	2.34	0.62
1:B:60:PRO:HD3	1:B:81:LEU:HD22	1.82	0.61
1:A:90:HIS:HB2	1:A:160:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ALA:HA	1:B:89:ASN:HD22	1.66	0.61
1:A:29:GLY:HA2	1:A:33:GLY:O	2.01	0.61
1:B:148:PHE:CE2	1:B:152:ILE:HD11	2.36	0.59
1:B:129:ASN:OD1	1:B:178:ASN:HB2	2.03	0.59
1:B:184:ARG:NE	1:B:238:GLN:NE2	2.49	0.58
1:A:159:THR:N	1:A:162:GLU:OE1	2.30	0.58
1:A:34:PRO:CB	1:A:59:LEU:HD21	2.32	0.58
1:B:128:PHE:N	1:B:134:GLN:HE21	2.00	0.58
1:B:237:GLN:HG2	1:B:312:THR:HG22	1.83	0.58
1:A:63:ASP:HA	1:A:66:ARG:HH21	1.68	0.58
1:A:134:GLN:HA	1:A:134:GLN:OE1	2.04	0.57
1:B:203:VAL:HG13	1:B:207:MET:HE3	1.86	0.57
1:B:172:TYR:O	1:B:175:GLN:HB2	2.03	0.57
1:B:285:CYS:O	1:B:291:LEU:HD12	2.04	0.57
1:B:269:TYR:HE1	1:A:269:TYR:HE1	1.54	0.56
1:B:12:VAL:HG11	1:B:60:PRO:HG3	1.87	0.56
1:B:38:ASP:O	1:B:92:LYS:NZ	2.32	0.56
1:A:211:THR:O	1:A:245:MET:HB3	2.05	0.56
1:B:313:THR:CG2	1:B:315:ILE:HD12	2.36	0.55
1:A:9:PHE:HA	1:A:18:HIS:O	2.06	0.55
1:B:313:THR:HG22	1:B:315:ILE:H	1.71	0.55
1:A:28:TYR:OH	1:A:51:HIS:ND1	2.37	0.54
1:A:236:VAL:HG23	1:A:313:THR:HG22	1.90	0.54
1:B:259:PHE:O	1:B:279:SER:HB3	2.07	0.54
1:A:256:HIS:HB2	1:A:283:LEU:HD11	1.91	0.53
1:B:133:LEU:HD11	1:B:155:TYR:CE2	2.44	0.52
1:B:87:ALA:HA	1:B:160:VAL:CG2	2.40	0.51
1:B:109:ASP:O	1:B:161:GLY:HA2	2.11	0.51
1:B:113:TYR:CG	1:B:164:GLY:HA3	2.46	0.51
1:A:212:LEU:O	1:A:306:TYR:OH	2.28	0.51
1:B:84:TYR:HE1	1:B:151:LEU:HG	1.75	0.51
1:A:235:LEU:HD21	1:A:238:GLN:HB2	1.91	0.50
1:A:212:LEU:HD11	1:A:247:ALA:HB3	1.93	0.50
1:B:119:LEU:O	1:B:123:GLN:NE2	2.45	0.50
1:B:90:HIS:CB	1:B:160:VAL:HG11	2.42	0.50
1:A:34:PRO:HA	1:A:43:THR:OG1	2.11	0.50
1:B:78:PRO:HG2	1:A:180:ASP:OD2	2.12	0.49
1:A:27:THR:HG22	1:A:30:GLN:CD	2.37	0.49
1:B:130:PRO:HG2	1:B:133:LEU:HD13	1.93	0.49
1:B:190:CYS:SG	1:B:225:CYS:SG	3.11	0.49
1:B:99:VAL:HG21	1:B:286:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLY:HA2	1:A:85:MET:HE3	1.95	0.49
1:A:185:VAL:HG12	1:A:236:VAL:CG1	2.43	0.49
1:A:281:GLU:HG2	1:A:282:THR:N	2.28	0.49
1:B:113:TYR:CD2	1:B:164:GLY:HA3	2.48	0.48
1:B:152:ILE:HG23	1:B:173:LEU:HD11	1.94	0.48
1:B:269:TYR:CD2	1:B:269:TYR:O	2.66	0.48
1:A:281:GLU:HG2	1:A:282:THR:HG23	1.96	0.48
1:A:256:HIS:HB2	1:A:283:LEU:CD1	2.44	0.47
1:B:177:ALA:HB3	1:B:179:LEU:HD21	1.96	0.47
1:A:139:ARG:HG3	1:A:139:ARG:HH21	1.77	0.47
1:B:165:ASP:O	1:B:169:THR:HG22	2.14	0.47
1:A:152:ILE:HG22	1:A:173:LEU:HD21	1.96	0.47
1:A:125:GLU:HB3	1:A:241:PRO:HB2	1.97	0.47
1:A:186:LEU:HB2	1:A:198:THR:HG23	1.96	0.47
1:A:165:ASP:OD1	1:A:167:ARG:HG2	2.15	0.47
1:B:167:ARG:HH21	1:B:168:GLU:HG3	1.80	0.46
1:B:125:GLU:HB3	1:B:241:PRO:HB2	1.97	0.46
1:B:157:ASN:OD1	1:A:203:VAL:HG12	2.16	0.46
1:B:186:LEU:CD2	1:B:235:LEU:HA	2.39	0.46
1:A:36:TYR:CB	1:A:85:MET:HE2	2.46	0.46
1:A:114:LEU:HD22	1:A:152:ILE:HD12	1.98	0.46
1:B:184:ARG:HB2	1:B:238:GLN:HE22	1.80	0.46
1:B:185:VAL:O	1:B:186:LEU:HD23	2.16	0.46
1:B:241:PRO:HA	1:B:308:GLU:O	2.15	0.45
1:A:62:ASP:C	1:A:66:ARG:NH2	2.75	0.45
1:A:283:LEU:HD12	1:A:283:LEU:N	2.31	0.45
1:B:171:SER:CA	1:B:207:MET:HE1	2.44	0.45
1:A:264:GLU:CD	1:A:297:TYR:OH	2.60	0.45
1:A:269:TYR:O	1:A:269:TYR:CD2	2.70	0.45
1:B:84:TYR:CE1	1:B:151:LEU:HG	2.52	0.45
1:A:148:PHE:O	1:A:152:ILE:HG12	2.16	0.45
1:B:99:VAL:HG21	1:B:286:ILE:CG2	2.47	0.44
1:B:90:HIS:HB3	1:B:160:VAL:HG11	2.00	0.43
1:A:36:TYR:HA	1:A:40:ALA:O	2.18	0.43
1:A:302:THR:HG21	3:A:402:GYX:C01	2.49	0.43
1:B:63:ASP:O	1:B:67:VAL:HG12	2.19	0.43
1:B:225:CYS:SG	1:B:227:CYS:SG	3.04	0.43
1:A:11:THR:O	1:A:57:TYR:HA	2.18	0.43
1:A:59:LEU:N	1:A:59:LEU:CD2	2.80	0.43
1:B:281:GLU:H	1:B:281:GLU:CD	2.27	0.43
1:B:185:VAL:O	1:B:236:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HG3	1:A:139:ARG:NH2	2.34	0.42
1:A:113:TYR:CD2	1:A:164:GLY:HA3	2.54	0.42
1:B:313:THR:CG2	1:B:314:THR:N	2.83	0.42
1:B:167:ARG:HH21	1:B:168:GLU:CG	2.32	0.42
1:A:42:VAL:HB	1:A:45:ILE:CG2	2.50	0.42
1:B:123:GLN:HE21	1:B:123:GLN:HB2	1.24	0.42
1:A:14:ASN:HB2	1:A:57:TYR:OH	2.20	0.42
1:A:89:ASN:HA	1:A:92:LYS:HE2	2.02	0.41
1:A:264:GLU:CD	1:A:275:LYS:HE3	2.44	0.41
1:A:294:SER:OG	1:A:296:GLU:O	2.29	0.41
1:B:252:TYR:O	1:B:298:LYS:HA	2.21	0.41
1:A:244:MET:HE2	1:A:246:SER:OG	2.20	0.41
1:A:114:LEU:HD22	1:A:152:ILE:CD1	2.50	0.41
1:B:276:HIS:O	1:B:285:CYS:HA	2.21	0.41
1:A:184:ARG:HH22	1:A:243:VAL:HG13	1.86	0.41
1:A:149:CYS:O	1:A:152:ILE:HG13	2.20	0.41
1:B:100:ASN:ND2	1:B:284:TYR:CG	2.90	0.40
1:B:280:LYS:HB2	1:B:281:GLU:H	1.69	0.40
1:B:99:VAL:HG23	1:B:99:VAL:O	2.22	0.40
1:A:6:ILE:HD11	1:A:47:PRO:HB3	2.03	0.40
1:A:120:THR:HG21	1:A:305:PHE:CZ	2.57	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	313/315 (99%)	303 (97%)	10 (3%)	0	100	100
1	B	277/315 (88%)	269 (97%)	8 (3%)	0	100	100
All	All	590/630 (94%)	572 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	235/275 (86%)	234 (100%)	1 (0%)	84	92
1	B	175/275 (64%)	175 (100%)	0	100	100
All	All	410/550 (74%)	409 (100%)	1 (0%)	87	94

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

Mol	Chain	Res	Type
1	A	169	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	176	HIS
1	B	238	GLN
1	B	270	GLN
1	A	14	ASN
1	A	123	GLN
1	A	251	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
3	GYX	B	402	-	35,35,35	2.80	12 (34%)	45,48,48	2.37	12 (26%)
3	GYX	A	402	-	35,35,35	2.70	11 (31%)	45,48,48	1.85	6 (13%)

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
3	GYX	B	402	-	-	7/21/31/31	0/4/4/4
3	GYX	A	402	-	-	2/21/31/31	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	GYX	C02-N03	-8.38	1.28	1.48
3	A	402	GYX	C02-N03	-8.07	1.29	1.48
3	A	402	GYX	C23-C02	6.97	1.60	1.52
3	B	402	GYX	C23-C02	6.56	1.60	1.52
3	B	402	GYX	C16-N15	6.38	1.48	1.36
3	A	402	GYX	C16-N15	5.08	1.45	1.36
3	A	402	GYX	C07-N08	4.84	1.45	1.33
3	B	402	GYX	C07-N08	4.72	1.44	1.33
3	A	402	GYX	C01-C02	4.14	1.61	1.52
3	A	402	GYX	C21-C06	-3.96	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	GYX	C01-C02	3.87	1.61	1.52
3	B	402	GYX	C14-N15	3.55	1.48	1.41
3	B	402	GYX	C05-C06	-3.48	1.44	1.53
3	B	402	GYX	C21-C06	-3.41	1.44	1.53
3	A	402	GYX	C05-C06	-3.15	1.45	1.53
3	B	402	GYX	C28-C27	-3.03	1.37	1.43
3	A	402	GYX	C14-N15	2.76	1.47	1.41
3	A	402	GYX	C28-C27	-2.42	1.38	1.43
3	B	402	GYX	C22-N03	-2.35	1.42	1.47
3	B	402	GYX	O20-C07	-2.26	1.19	1.23
3	B	402	GYX	C04-N03	-2.26	1.43	1.47
3	A	402	GYX	C04-N03	-2.04	1.43	1.47
3	A	402	GYX	O20-C07	-2.03	1.19	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	GYX	C09-N08-C07	-6.76	113.01	122.29
3	B	402	GYX	C09-N08-C07	-6.53	113.32	122.29
3	A	402	GYX	C05-C06-C21	5.38	121.35	110.00
3	B	402	GYX	C04-C05-C06	5.35	119.02	110.54
3	B	402	GYX	C06-C07-N08	5.22	122.66	115.99
3	A	402	GYX	C04-C05-C06	4.69	117.97	110.54
3	B	402	GYX	C05-C06-C07	-4.46	101.39	110.79
3	B	402	GYX	C21-C06-C07	-4.39	101.53	110.79
3	B	402	GYX	C01-C02-C23	-4.31	104.95	114.02
3	B	402	GYX	C05-C06-C21	4.19	118.84	110.00
3	B	402	GYX	C22-C21-C06	4.03	116.92	110.54
3	B	402	GYX	C17-C16-N15	3.10	119.62	114.95
3	A	402	GYX	C06-C07-N08	2.87	119.66	115.99
3	A	402	GYX	C10-C09-N08	-2.33	108.17	113.07
3	A	402	GYX	C24-C23-C02	-2.33	118.00	120.90
3	B	402	GYX	O20-C07-N08	-2.20	118.32	122.98
3	B	402	GYX	C11-C10-C19	2.12	121.48	118.55
3	B	402	GYX	O20-C07-C06	-2.08	118.98	122.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GYX	C01-C02-C23-C24
3	B	402	GYX	C01-C02-C23-C28

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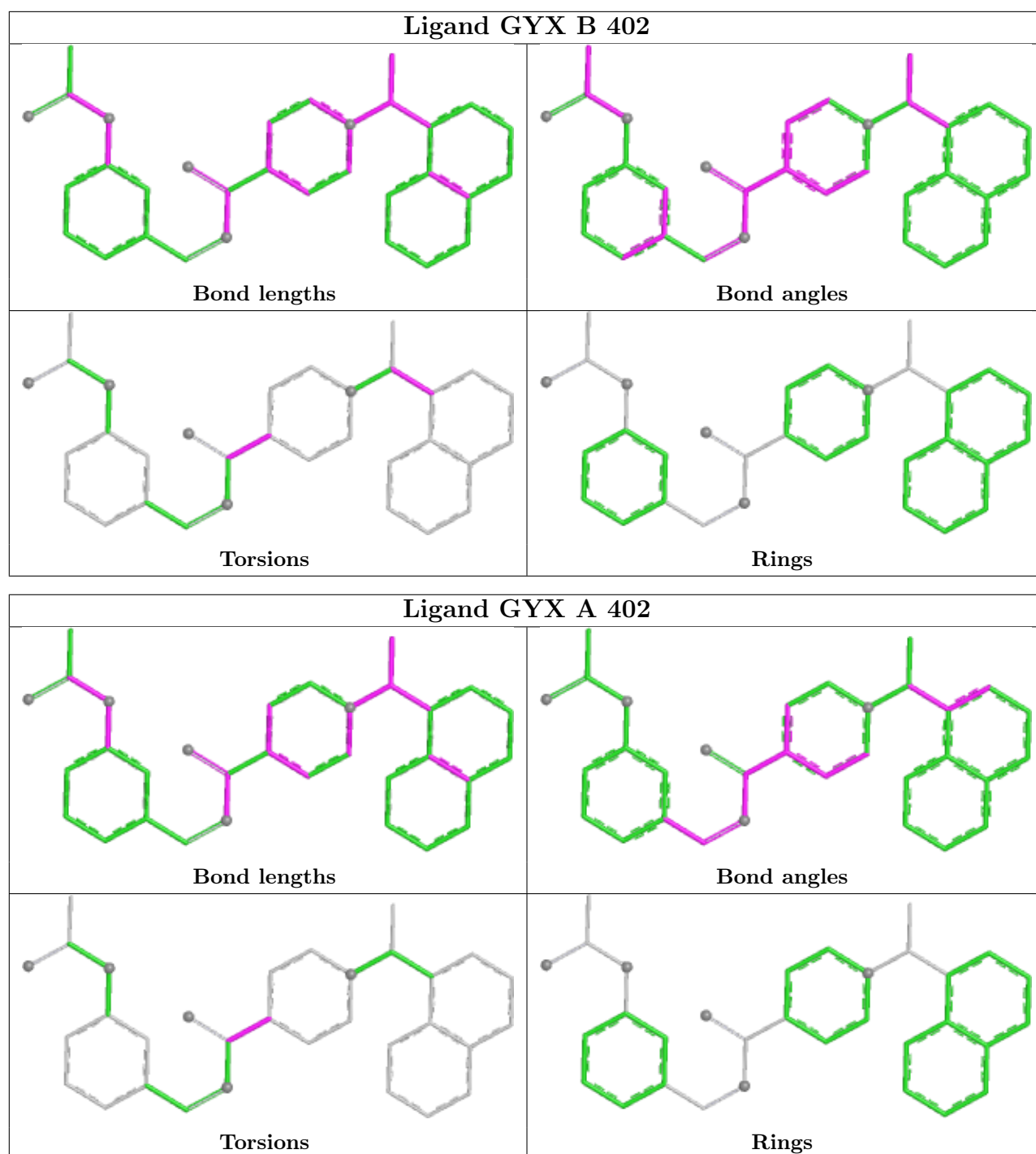
Mol	Chain	Res	Type	Atoms
3	B	402	GYX	N03-C02-C23-C24
3	B	402	GYX	N03-C02-C23-C28
3	A	402	GYX	C21-C06-C07-O20
3	B	402	GYX	C05-C06-C07-N08
3	A	402	GYX	C21-C06-C07-N08
3	B	402	GYX	C05-C06-C07-O20
3	B	402	GYX	C21-C06-C07-O20

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GYX	2	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.



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	315/315 (100%)	1.67	106 (33%)  	14, 44, 109, 171	0
1	B	287/315 (91%)	3.77	241 (83%)  	50, 99, 151, 190	0
All	All	602/630 (95%)	2.67	347 (57%)  	14, 71, 143, 190	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	LEU	10.1
1	B	117	ALA	9.3
1	B	277	ILE	9.0
1	B	278	THR	8.5
1	B	147	ASN	8.4
1	B	10	THR	7.7
1	B	64	THR	7.1
1	B	304	VAL	6.8
1	A	224	PRO	6.8
1	B	290	LEU	6.7
1	A	217	PHE	6.6
1	B	105	ILE	6.5
1	B	126	LEU	6.3
1	B	17	LEU	6.3
1	B	297	TYR	6.3
1	B	16	ASN	6.3
1	B	36	TYR	6.3
1	B	282	THR	6.3
1	B	133	LEU	6.2
1	B	258	THR	6.2
1	B	20	GLN	6.1
1	B	12	VAL	6.1
1	B	39	GLY	6.1
1	B	115	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	37	LEU	6.0
1	B	272	GLY	6.0
1	A	186	LEU	6.0
1	B	275	LYS	5.9
1	B	163	LEU	5.9
1	B	46	LYS	5.9
1	B	138	TYR	5.9
1	B	214	TYR	5.9
1	B	19	THR	5.9
1	B	284	TYR	5.8
1	B	47	PRO	5.8
1	B	303	ASP	5.8
1	B	51	HIS	5.7
1	B	148	PHE	5.7
1	B	288	GLY	5.7
1	B	99	VAL	5.7
1	B	242	PHE	5.7
1	A	189	VAL	5.7
1	B	309	ASN	5.7
1	B	84	TYR	5.7
1	B	40	ALA	5.7
1	B	119	LEU	5.6
1	B	259	PHE	5.6
1	B	38	ASP	5.6
1	B	62	ASP	5.6
1	B	63	ASP	5.6
1	B	15	ILE	5.5
1	B	34	PRO	5.5
1	B	43	THR	5.5
1	A	208	TYR	5.4
1	B	73	TYR	5.4
1	B	296	GLU	5.4
1	B	315	ILE	5.4
1	B	281	GLU	5.3
1	B	220	GLY	5.3
1	B	257	GLY	5.3
1	B	66	ARG	5.3
1	B	153	LEU	5.3
1	B	224	PRO	5.2
1	B	128	PHE	5.2
1	B	155	TYR	5.2
1	B	116	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	94	TRP	5.1
1	B	164	GLY	5.1
1	B	263	SER	5.1
1	B	260	THR	5.1
1	A	233	LYS	5.1
1	B	252	TYR	5.1
1	B	251	GLN	5.1
1	B	285	CYS	5.1
1	B	311	TYR	5.1
1	B	18	HIS	5.1
1	B	121	LEU	5.1
1	B	276	HIS	5.0
1	B	151	LEU	5.0
1	B	250	ALA	5.0
1	A	191	LYS	5.0
1	B	286	ILE	4.9
1	B	221	VAL	4.9
1	B	232	THR	4.9
1	A	36	TYR	4.9
1	B	283	LEU	4.9
1	B	262	ALA	4.8
1	B	86	SER	4.8
1	A	50	SER	4.8
1	B	61	ASN	4.8
1	B	41	ASP	4.8
1	B	188	VAL	4.8
1	B	174	PHE	4.8
1	B	222	GLN	4.8
1	A	227	CYS	4.8
1	B	101	GLY	4.7
1	B	265	TYR	4.7
1	A	230	GLN	4.7
1	A	194	GLY	4.6
1	A	231	ALA	4.6
1	B	42	VAL	4.6
1	B	59	LEU	4.6
1	B	107	TRP	4.6
1	B	144	GLU	4.5
1	B	54	LYS	4.5
1	B	160	VAL	4.5
1	B	243	VAL	4.5
1	A	114	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	4.5
1	B	305	PHE	4.5
1	B	162	GLU	4.5
1	B	90	HIS	4.4
1	A	223	ILE	4.4
1	B	32	PHE	4.4
1	B	48	HIS	4.4
1	B	295	SER	4.4
1	B	50	SER	4.3
1	B	44	LYS	4.3
1	A	190	CYS	4.3
1	B	53	GLY	4.3
1	B	189	VAL	4.2
1	B	102	LEU	4.2
1	B	45	ILE	4.2
1	B	293	LYS	4.2
1	B	306	TYR	4.2
1	B	149	CYS	4.2
1	B	67	VAL	4.2
1	B	14	ASN	4.2
1	B	49	ASN	4.2
1	B	52	GLU	4.1
1	B	142	ALA	4.1
1	B	186	LEU	4.1
1	B	191	LYS	4.0
1	A	188	VAL	4.0
1	B	218	LYS	4.0
1	A	187	ASN	4.0
1	B	88	LEU	4.0
1	B	123	GLN	4.0
1	B	65	LEU	3.9
1	B	35	THR	3.9
1	A	209	MET	3.9
1	B	190	CYS	3.9
1	B	33	GLY	3.9
1	B	223	ILE	3.9
1	B	98	GLN	3.9
1	B	202	GLY	3.8
1	B	235	LEU	3.8
1	B	291	LEU	3.8
1	B	159	THR	3.8
1	A	232	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	82	GLY	3.8
1	B	307	LYS	3.8
1	B	122	GLN	3.8
1	A	197	GLN	3.8
1	B	313	THR	3.7
1	B	13	ASP	3.7
1	B	266	THR	3.7
1	A	198	THR	3.7
1	A	226	THR	3.7
1	B	118	LEU	3.7
1	B	113	TYR	3.7
1	B	274	TYR	3.7
1	A	37	LEU	3.6
1	B	217	PHE	3.6
1	B	97	PRO	3.6
1	B	11	THR	3.6
1	B	226	THR	3.6
1	B	312	THR	3.6
1	B	213	SER	3.6
1	B	145	ALA	3.6
1	B	68	GLU	3.5
1	B	125	GLU	3.5
1	A	76	THR	3.5
1	A	221	VAL	3.5
1	B	196	GLN	3.5
1	B	60	PRO	3.5
1	A	193	CYS	3.5
1	A	229	LYS	3.5
1	B	228	GLY	3.4
1	B	172	TYR	3.4
1	A	113	TYR	3.4
1	B	161	GLY	3.4
1	B	124	ILE	3.4
1	B	81	LEU	3.4
1	B	280	LYS	3.4
1	B	298	LYS	3.4
1	A	211	THR	3.4
1	B	299	GLY	3.4
1	A	270	GLN	3.4
1	B	234	TYR	3.3
1	A	315	ILE	3.3
1	A	235	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	192	THR	3.3
1	A	236	VAL	3.3
1	B	96	TYR	3.3
1	B	270	GLN	3.3
1	B	120	THR	3.3
1	B	237	GLN	3.2
1	B	316	LYS	3.2
1	B	302	THR	3.2
1	B	301	ILE	3.2
1	B	87	ALA	3.2
1	B	110	ASN	3.2
1	B	236	VAL	3.2
1	B	227	CYS	3.2
1	A	225	CYS	3.2
1	A	195	GLN	3.1
1	B	279	SER	3.1
1	B	206	VAL	3.1
1	A	311	TYR	3.1
1	B	198	THR	3.1
1	B	108	ALA	3.1
1	A	312	THR	3.1
1	B	92	LYS	3.1
1	B	106	LYS	3.1
1	B	135	ASP	3.1
1	A	3	VAL	3.1
1	B	76	THR	3.1
1	B	233	LYS	3.1
1	B	267	GLY	3.1
1	B	136	ALA	3.0
1	B	287	ASP	3.0
1	B	294	SER	3.0
1	A	272	GLY	3.0
1	B	247	ALA	3.0
1	B	314	THR	3.0
1	A	214	TYR	3.0
1	B	141	ARG	3.0
1	B	181	SER	3.0
1	B	215	GLU	3.0
1	A	44	LYS	3.0
1	B	152	ILE	2.9
1	A	24	MET	2.9
1	A	162	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	292	THR	2.9
1	B	231	ALA	2.9
1	B	137	TYR	2.9
1	A	152	ILE	2.9
1	B	100	ASN	2.9
1	A	314	THR	2.9
1	A	234	TYR	2.9
1	A	309	ASN	2.9
1	B	269	TYR	2.9
1	B	95	LYS	2.8
1	B	127	LYS	2.8
1	B	219	LYS	2.8
1	A	220	GLY	2.8
1	B	238	GLN	2.8
1	B	70	PHE	2.8
1	A	48	HIS	2.8
1	B	140	ALA	2.8
1	A	201	LYS	2.8
1	A	39	GLY	2.8
1	B	173	LEU	2.8
1	A	85	MET	2.8
1	A	51	HIS	2.8
1	B	112	SER	2.7
1	B	240	SER	2.7
1	A	23	ASP	2.7
1	A	228	GLY	2.7
1	B	158	LYS	2.6
1	B	248	PRO	2.6
1	A	290	LEU	2.6
1	B	132	ALA	2.6
1	B	134	GLN	2.6
1	A	174	PHE	2.6
1	A	68	GLU	2.6
1	A	215	GLU	2.6
1	B	104	SER	2.6
1	B	197	GLN	2.6
1	B	230	GLN	2.6
1	A	222	GLN	2.6
1	A	12	VAL	2.5
1	B	225	CYS	2.5
1	B	199	THR	2.5
1	A	277	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLU	2.5
1	A	305	PHE	2.5
1	B	273	HIS	2.5
1	B	241	PRO	2.5
1	B	143	GLY	2.5
1	B	200	LEU	2.5
1	A	199	THR	2.5
1	B	93	LYS	2.5
1	B	166	VAL	2.5
1	B	192	THR	2.5
1	B	211	THR	2.5
1	B	193	CYS	2.4
1	A	38	ASP	2.4
1	B	179	LEU	2.4
1	A	42	VAL	2.4
1	A	219	LYS	2.4
1	A	62	ASP	2.4
1	B	83	ARG	2.4
1	A	30	GLN	2.4
1	A	297	TYR	2.4
1	A	47	PRO	2.4
1	A	271	CYS	2.4
1	B	205	ALA	2.4
1	B	310	SER	2.3
1	B	177	ALA	2.3
1	B	103	THR	2.3
1	A	5	THR	2.3
1	B	194	GLY	2.3
1	A	2	GLU	2.3
1	B	204	GLU	2.3
1	A	84	TYR	2.3
1	A	155	TYR	2.3
1	B	300	PRO	2.3
1	B	184	ARG	2.3
1	B	91	THR	2.2
1	A	294	SER	2.2
1	A	32	PHE	2.2
1	A	206	VAL	2.2
1	B	244	MET	2.2
1	A	254	LEU	2.2
1	A	184	ARG	2.2
1	B	89	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	GLN	2.2
1	A	269	TYR	2.2
1	B	261	CYS	2.2
1	A	200	LEU	2.2
1	A	263	SER	2.2
1	B	130	PRO	2.2
1	A	183	LYS	2.2
1	A	110	ASN	2.1
1	A	28	TYR	2.1
1	A	4	ARG	2.1
1	A	196	GLN	2.1
1	A	306	TYR	2.1
1	B	249	PRO	2.1
1	A	242	PHE	2.1
1	A	237	GLN	2.1
1	A	140	ALA	2.1
1	A	57	TYR	2.1
1	A	172	TYR	2.1
1	B	170	MET	2.1
1	B	176	HIS	2.1
1	A	22	VAL	2.1
1	A	49	ASN	2.1
1	A	52	GLU	2.1
1	A	6	ILE	2.1
1	A	73	TYR	2.1
1	A	80	PHE	2.0
1	A	79	SER	2.0
1	A	61	ASN	2.0
1	B	165	ASP	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](#)

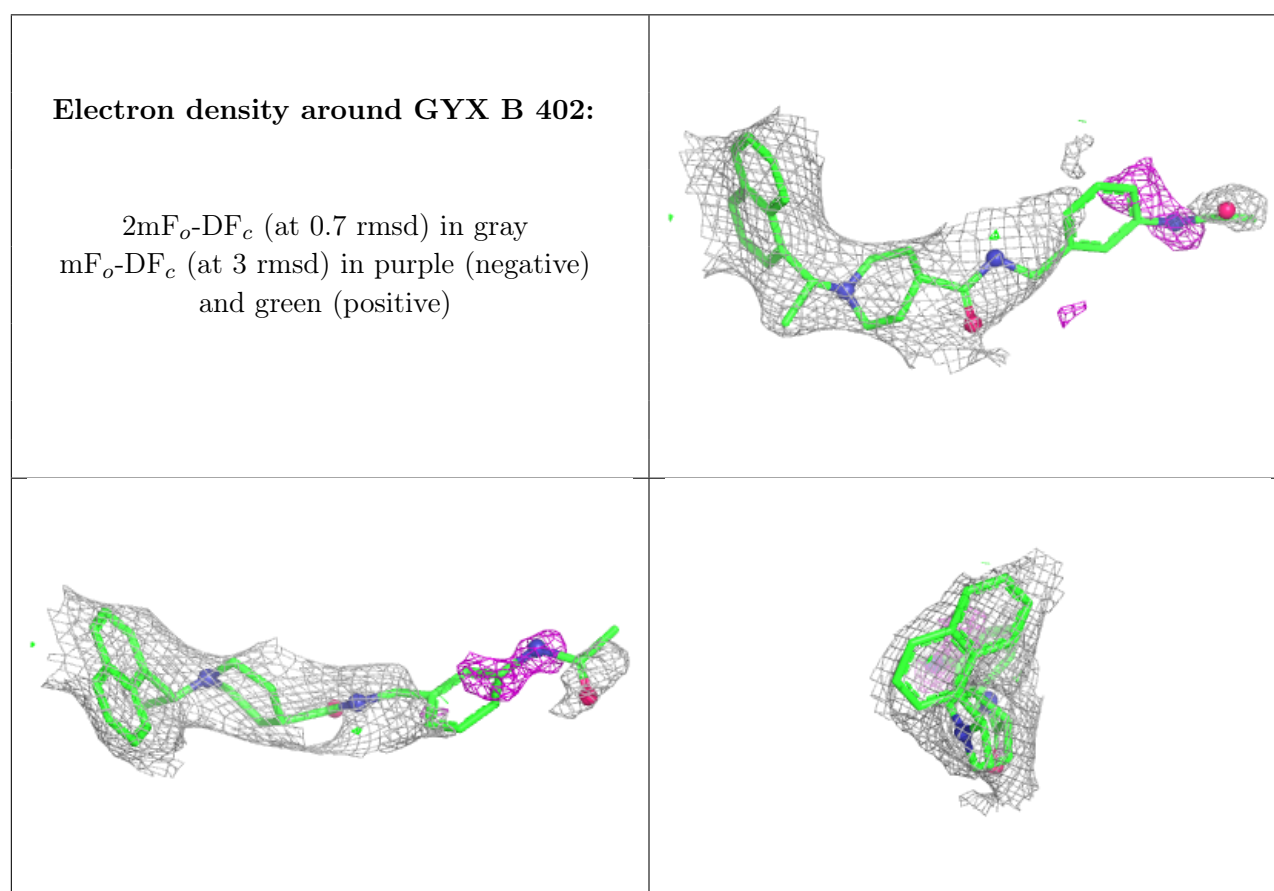
There are no oligosaccharides in this entry.

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.

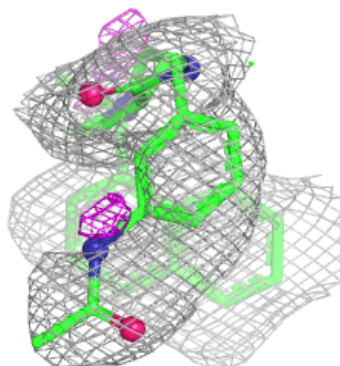
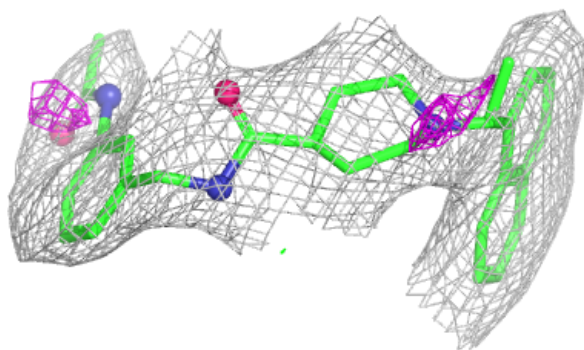
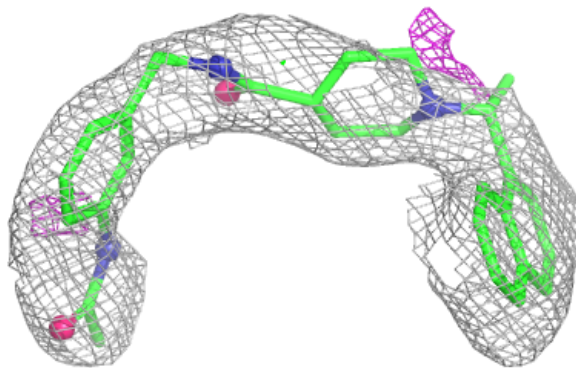
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GYX	B	402	32/32	0.73	0.24	68,79,98,102	0
3	GYX	A	402	32/32	0.80	0.17	47,57,70,73	0
2	ZN	A	401	1/1	0.90	0.13	191,191,191,191	0
2	ZN	B	401	1/1	0.96	0.06	127,127,127,127	0

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 GYX A 402:

$2mF_o-DF_c$ (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.