



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 7D7L / pdb_00007d7l
Title : The crystal structure of SARS-CoV-2 papain-like protease in complex with YM155
Authors : Zhao, Y.; Sun, L.; Yang, H.T.; Rao, Z.H.
Deposited on : 2020-10-04
Resolution : 2.11 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

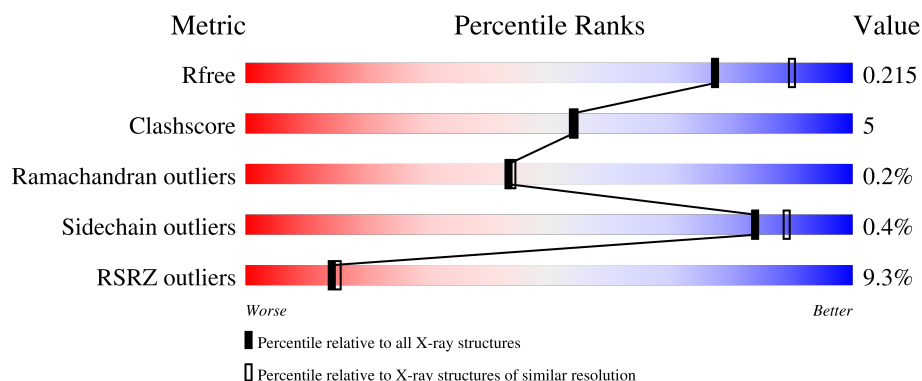
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	312	88% 12% .
1	B	312	17% 81% 17% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5544 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	A	312	Total	C	N	O	S	0	0	0
			2474	1576	407	473	18			
1	B	312	Total	C	N	O	S	0	0	0
			2429	1548	399	466	16			

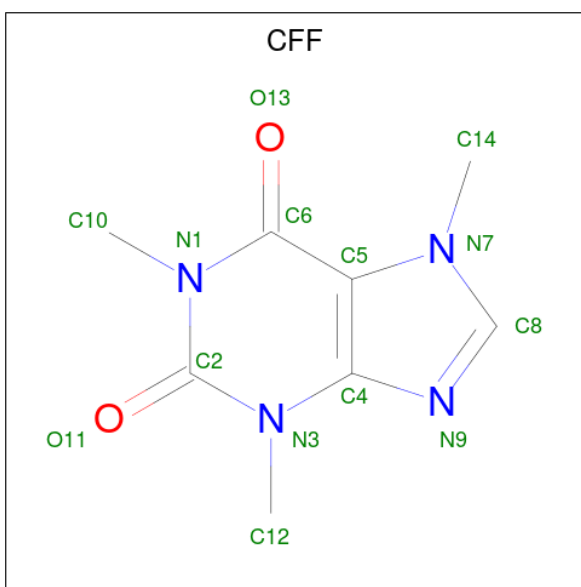
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	CYS	engineered mutation	UNP P0DTD1
B	111	SER	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

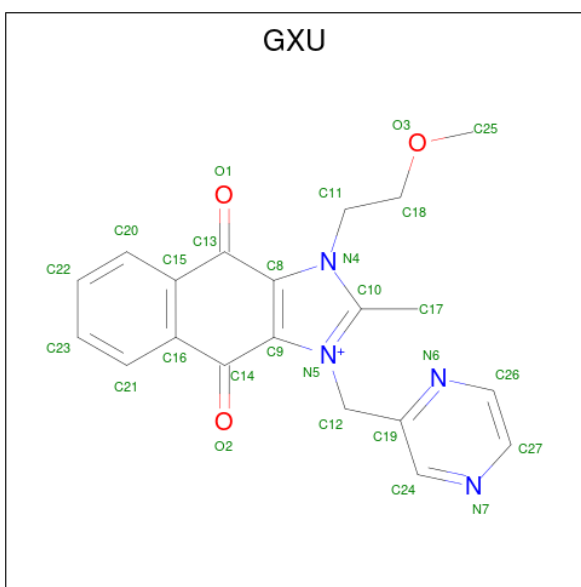
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	4	2		
3	B	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 4 is 1-(2-methoxyethyl)-2-methyl-3-(pyrazin-2-ylmethyl)benzo[f]benzimidazol-3-ium-4,9-dione (CCD ID: GXU) (formula: C₂₀H₁₉N₄O₃) (labeled as "Ligand of Interest" by depositor).



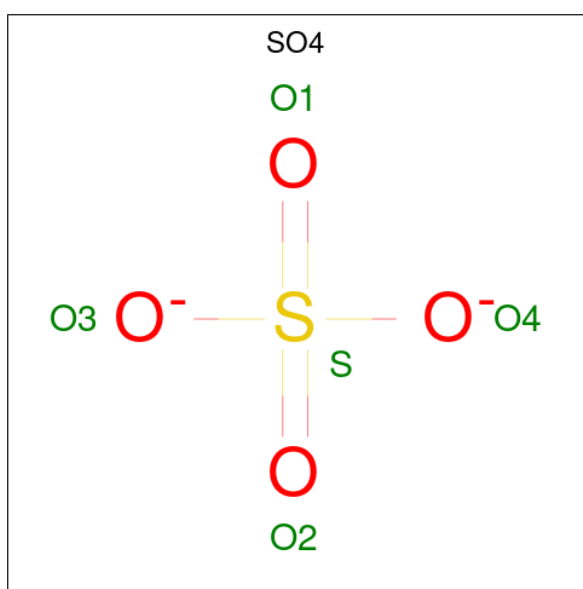
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	20	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	20	4	3		
4	B	1	Total	C	N	O	0	0
			27	20	4	3		
4	B	1	Total	C	N	O	0	0
			27	20	4	3		
4	B	1	Total	C	N	O	0	0
			27	20	4	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



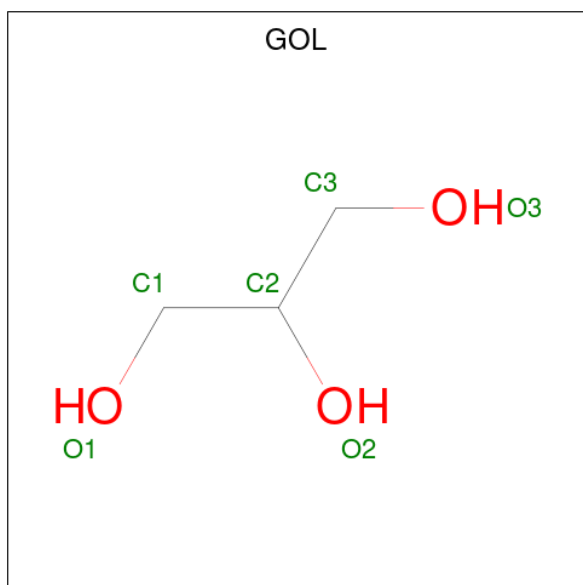
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

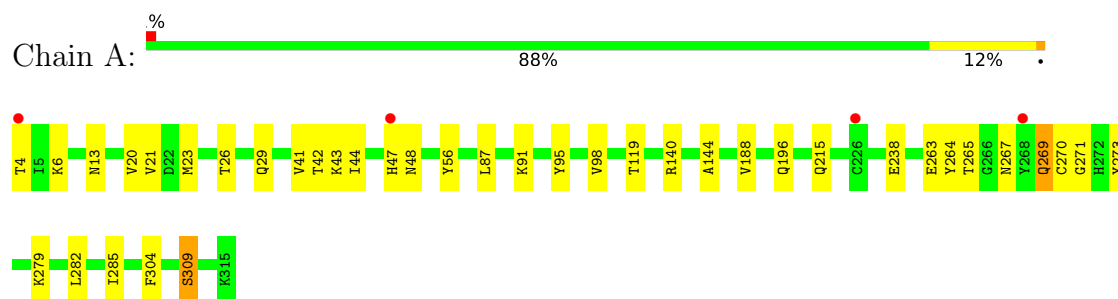
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	239	Total	O	0	0
			239	239		
7	B	180	Total	O	0	0
			180	180		

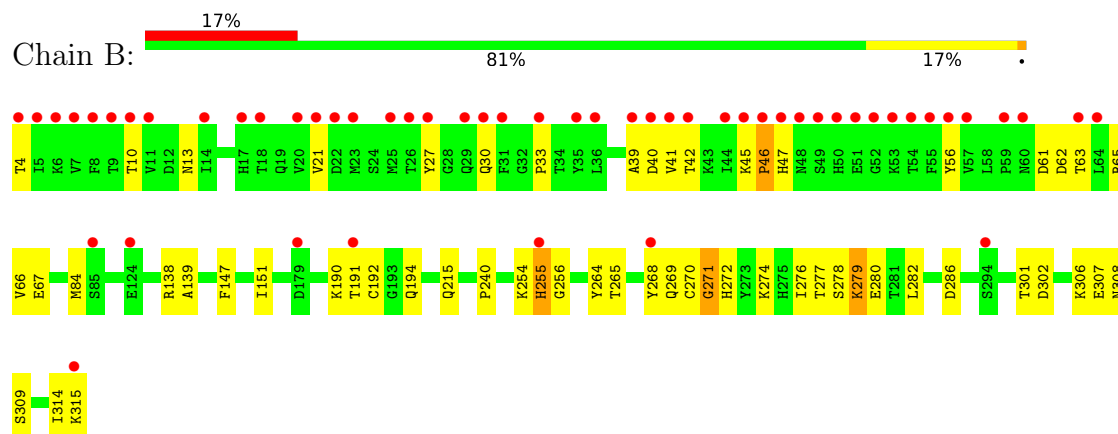
3 Residue-property plots

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	117.56Å 117.56Å 257.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.49 – 2.11 48.49 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.49-2.11) 100.0 (48.49-2.11)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.183 , 0.218 (Not available) , 0.215	Depositor DCC
R_{free} test set	2000 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: GOL, CFF, ZN, SO4, GXU

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	0.71	7/2533 (0.3%)	0.66	0/3437
1	B	0.85	19/2486 (0.8%)	0.68	1/3379 (0.0%)
All	All	0.78	26/5019 (0.5%)	0.67	1/6816 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	279	LYS	C-O	-9.25	1.16	1.23
1	B	272	HIS	C-O	-7.59	1.15	1.23
1	A	265	THR	C-O	-6.74	1.16	1.24
1	B	282	LEU	C-O	-6.60	1.16	1.24
1	B	276	ILE	C-O	-6.52	1.17	1.24
1	B	278	SER	C-O	-6.50	1.16	1.24
1	A	269	GLN	C-O	-6.37	1.16	1.24
1	A	279	LYS	C-O	-6.21	1.18	1.23
1	B	190	LYS	C-O	-6.14	1.16	1.24
1	B	255	HIS	C-O	-6.14	1.16	1.23
1	B	254	LYS	C-O	-5.87	1.17	1.24
1	A	188	VAL	C-O	-5.83	1.17	1.24
1	B	306	LYS	C-O	-5.74	1.16	1.23
1	B	270	CYS	C-O	-5.67	1.17	1.23
1	B	280	GLU	C-O	-5.55	1.17	1.24
1	A	309	SER	C-O	-5.45	1.17	1.23
1	A	270	CYS	C-O	-5.34	1.18	1.23
1	A	282	LEU	C-O	-5.33	1.17	1.23
1	B	139	ALA	C-O	-5.30	1.17	1.24
1	B	308	ASN	C-O	-5.30	1.17	1.24
1	B	265	THR	C-O	-5.29	1.17	1.24
1	B	192	CYS	C-O	-5.20	1.17	1.24
1	B	277	THR	C-O	-5.19	1.17	1.23
1	B	309	SER	C-O	-5.19	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	GLY	C-O	-5.16	1.18	1.23
1	B	256	GLY	C-O	-5.00	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	TYR	N-CA-C	6.13	120.03	112.54

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	2474	0	2416	21	0
1	B	2429	0	2333	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	10	0	0
3	B	14	0	10	0	0
4	A	54	0	0	0	0
4	B	81	0	0	0	0
5	A	25	0	0	1	0
5	B	20	0	0	0	0
6	A	12	0	16	1	0
7	A	239	0	0	3	0
7	B	180	0	0	1	0
All	All	5544	0	4785	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (49) 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:41:VAL:HA	1:A:44:ILE:HD12	1.65	0.78
1:B:215:GLN:HG2	7:B:634:HOH:O	1.83	0.77
1:B:63:THR:O	1:B:67:GLU:HG3	1.87	0.74
1:A:87:LEU:HG	1:A:91:LYS:HE2	1.71	0.71
1:A:48:ASN:ND2	7:A:501:HOH:O	2.24	0.71
1:B:194:GLN:HE22	1:B:315:LYS:HE2	1.57	0.69
1:A:47:HIS:HB3	5:A:408:SO4:O1	1.98	0.63
1:B:40:ASP:OD1	1:B:42:THR:HG22	1.98	0.62
1:B:61:ASP:OD1	1:B:62:ASP:N	2.35	0.60
1:B:13:ASN:HB2	1:B:56:TYR:OH	2.04	0.58
1:B:194:GLN:NE2	1:B:315:LYS:HE2	2.21	0.55
1:B:45:LYS:O	1:B:47:HIS:N	2.42	0.53
1:A:238:GLU:OE2	1:A:309:SER:OG	2.24	0.53
1:B:240:PRO:HA	1:B:307:GLU:O	2.09	0.52
1:A:4:THR:HA	1:A:21:VAL:O	2.11	0.51
1:A:4:THR:HG23	1:A:20:VAL:HG13	1.93	0.50
1:A:196:GLN:HG3	7:A:641:HOH:O	2.12	0.50
1:B:314:ILE:HG22	1:B:315:LYS:HG3	1.94	0.50
1:A:140:ARG:HH22	6:A:410:GOL:H32	1.78	0.49
1:B:4:THR:HA	1:B:21:VAL:O	2.13	0.48
1:B:33:PRO:HA	1:B:42:THR:HB	1.95	0.48
1:B:147:PHE:CE2	1:B:151:ILE:HD11	2.49	0.48
1:B:61:ASP:O	1:B:65:ARG:HG3	2.14	0.48
1:B:63:THR:HA	1:B:66:VAL:HG12	1.96	0.47
1:A:98:VAL:HG11	1:A:285:ILE:HG23	1.96	0.46
1:B:65:ARG:HG3	1:B:65:ARG:HH11	1.80	0.45
1:A:264:TYR:OH	1:A:271:GLY:HA3	2.16	0.45
1:B:274:LYS:HE2	1:B:286:ASP:OD2	2.16	0.45
1:B:27:TYR:HA	1:B:30:GLN:NE2	2.32	0.45
1:A:42:THR:HB	1:A:43:LYS:HD3	1.99	0.45
1:B:65:ARG:HG3	1:B:65:ARG:NH1	2.32	0.45
1:B:301:THR:HG23	1:B:302:ASP:OD1	2.18	0.44
1:B:56:TYR:CD2	1:B:84:MET:HE3	2.52	0.44
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.82	0.44
1:A:95:TYR:CD1	1:A:144:ALA:HB3	2.53	0.44
1:B:10:THR:HG21	1:B:13:ASN:HA	2.00	0.43
1:A:263:GLU:O	1:A:273:TYR:HA	2.17	0.43
1:A:215:GLN:HG2	7:A:630:HOH:O	2.18	0.43
1:B:63:THR:O	1:B:66:VAL:HG12	2.18	0.42
1:A:13:ASN:HB2	1:A:56:TYR:OH	2.19	0.42
1:B:27:TYR:CE2	1:B:46:PRO:HA	2.55	0.42
1:A:26:THR:OG1	1:A:29:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:N	1:A:23:MET:HG2	2.35	0.41
1:A:119:THR:HG21	1:A:304:PHE:CZ	2.56	0.41
1:A:267:ASN:OD1	1:A:269:GLN:N	2.54	0.41
1:B:264:TYR:OH	1:B:271:GLY:HA3	2.20	0.41
1:B:39:ALA:O	1:B:41:VAL:HG23	2.21	0.40
1:B:255:HIS:NE2	1:B:279:LYS:O	2.44	0.40
1:A:6:LYS:HB2	1:A:6:LYS:HE3	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/312 (99%)	302 (97%)	8 (3%)	0	100	100
1	B	310/312 (99%)	300 (97%)	9 (3%)	1 (0%)	36	36
All	All	620/624 (99%)	602 (97%)	17 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	PRO

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	272/272 (100%)	272 (100%)	0	100	100
1	B	259/272 (95%)	257 (99%)	2 (1%)	73	80
All	All	531/544 (98%)	529 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	THR
1	B	269	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	122	GLN
1	A	215	GLN
1	B	17	HIS
1	B	30	GLN
1	B	174	GLN
1	B	186	ASN
1	B	194	GLN
1	B	250	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z > 2$
5	SO4	B	408	-	4,4,4	0.26	0	6,6,6	0.25	0
5	SO4	A	406	-	4,4,4	0.30	0	6,6,6	0.33	0
5	SO4	A	405	-	4,4,4	0.29	0	6,6,6	0.25	0
5	SO4	A	407	-	4,4,4	0.24	0	6,6,6	0.30	0
5	SO4	B	406	-	4,4,4	0.28	0	6,6,6	0.32	0
5	SO4	A	408	-	4,4,4	0.23	0	6,6,6	0.26	0
4	GXU	A	403	-	29,30,30	5.14	20 (68%)	34,43,43	1.43	6 (17%)
3	CFF	A	402	-	15,15,15	2.52	5 (33%)	23,23,23	2.04	7 (30%)
5	SO4	A	409	-	4,4,4	0.23	0	6,6,6	0.25	0
5	SO4	B	407	-	4,4,4	0.33	0	6,6,6	0.18	0
6	GOL	A	411	-	5,5,5	1.22	0	5,5,5	0.97	0
4	GXU	B	405	-	29,30,30	5.19	20 (68%)	34,43,43	1.47	6 (17%)
5	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.14	0
4	GXU	A	404	-	29,30,30	5.04	18 (62%)	34,43,43	2.64	10 (29%)
3	CFF	B	402	-	15,15,15	2.42	4 (26%)	23,23,23	2.08	9 (39%)
4	GXU	B	404	-	29,30,30	5.15	19 (65%)	34,43,43	1.42	8 (23%)
4	GXU	B	403	-	29,30,30	5.06	19 (65%)	34,43,43	1.42	8 (23%)
6	GOL	A	410	-	5,5,5	1.33	1 (20%)	5,5,5	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GXU	A	403	-	-	0/8/24/24	0/4/4/4
3	CFF	A	402	-	-	-	0/2/2/2
6	GOL	A	411	-	-	2/4/4/4	-
4	GXU	B	405	-	-	2/8/24/24	0/4/4/4
4	GXU	A	404	-	-	4/8/24/24	0/4/4/4
3	CFF	B	402	-	-	-	0/2/2/2
4	GXU	B	404	-	-	5/8/24/24	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GXU	B	403	-	-	4/8/24/24	0/4/4/4
6	GOL	A	410	-	-	2/4/4/4	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	GXU	C20-C15	11.14	1.56	1.39
4	B	403	GXU	C20-C15	10.97	1.56	1.39
4	A	403	GXU	C20-C15	10.96	1.56	1.39
4	B	405	GXU	C20-C15	10.96	1.56	1.39
4	B	405	GXU	C21-C16	10.96	1.56	1.39
4	B	404	GXU	C21-C16	10.80	1.56	1.39
4	A	403	GXU	C21-C16	10.61	1.56	1.39
4	B	403	GXU	C21-C16	10.52	1.55	1.39
4	A	404	GXU	C20-C15	10.49	1.55	1.39
4	A	404	GXU	C21-C16	10.26	1.55	1.39
4	B	404	GXU	C23-C21	8.63	1.53	1.38
4	B	405	GXU	C24-C19	8.56	1.54	1.39
4	A	403	GXU	C22-C20	8.47	1.53	1.38
4	B	405	GXU	C22-C20	8.42	1.53	1.38
4	B	403	GXU	C23-C21	8.34	1.53	1.38
4	A	404	GXU	C24-C19	8.34	1.54	1.39
4	A	403	GXU	C23-C21	8.33	1.53	1.38
4	B	403	GXU	C22-C20	8.30	1.53	1.38
4	B	405	GXU	C23-C21	8.27	1.53	1.38
4	B	404	GXU	C24-C19	8.25	1.53	1.39
4	B	404	GXU	C22-C20	8.11	1.52	1.38
4	A	404	GXU	C23-C21	8.02	1.52	1.38
4	A	403	GXU	C24-C19	8.02	1.53	1.39
4	B	403	GXU	C24-C19	7.94	1.53	1.39
4	A	404	GXU	C22-C20	7.59	1.51	1.38
4	A	404	GXU	C9-C14	7.22	1.61	1.44
4	A	403	GXU	C9-C14	6.83	1.60	1.44
3	A	402	CFF	C4-N3	6.83	1.49	1.38
4	B	403	GXU	C9-C14	6.81	1.60	1.44
4	B	405	GXU	C23-C22	6.77	1.53	1.38
4	B	404	GXU	C9-C14	6.75	1.59	1.44
4	B	404	GXU	C23-C22	6.67	1.52	1.38
4	A	403	GXU	C23-C22	6.58	1.52	1.38
4	A	404	GXU	C23-C22	6.57	1.52	1.38
4	B	405	GXU	C9-C14	6.44	1.59	1.44
3	B	402	CFF	C4-N3	6.39	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	GXU	C23-C22	6.37	1.52	1.38
4	A	404	GXU	C27-C26	5.79	1.53	1.38
4	A	403	GXU	C19-N6	5.78	1.46	1.34
4	B	405	GXU	C24-N7	5.76	1.46	1.34
4	A	404	GXU	C24-N7	5.75	1.46	1.34
4	A	403	GXU	C27-C26	5.64	1.53	1.38
4	B	405	GXU	C27-C26	5.61	1.53	1.38
4	A	404	GXU	C26-N6	5.60	1.46	1.34
4	B	404	GXU	C27-C26	5.60	1.53	1.38
4	A	404	GXU	C19-N6	5.59	1.46	1.34
4	A	403	GXU	C24-N7	5.56	1.46	1.34
4	B	405	GXU	C19-N6	5.55	1.46	1.34
4	B	404	GXU	C19-N6	5.54	1.46	1.34
4	B	405	GXU	C26-N6	5.52	1.46	1.34
4	B	403	GXU	C27-C26	5.48	1.53	1.38
4	B	404	GXU	C26-N6	5.48	1.46	1.34
4	A	404	GXU	C8-C13	5.47	1.61	1.46
4	A	403	GXU	C26-N6	5.44	1.46	1.34
4	B	404	GXU	C24-N7	5.42	1.45	1.34
4	A	403	GXU	C8-C13	5.38	1.60	1.46
4	B	403	GXU	C26-N6	5.37	1.45	1.34
4	B	403	GXU	C24-N7	5.33	1.45	1.34
4	B	403	GXU	C19-N6	5.32	1.45	1.34
4	B	404	GXU	C8-C13	5.25	1.60	1.46
4	B	403	GXU	C8-C13	5.06	1.60	1.46
4	B	405	GXU	C8-C13	4.76	1.59	1.46
4	B	404	GXU	C27-N7	4.45	1.46	1.33
4	A	404	GXU	C27-N7	4.42	1.46	1.33
4	B	405	GXU	C27-N7	4.37	1.46	1.33
4	A	403	GXU	C27-N7	4.29	1.45	1.33
4	B	403	GXU	C27-N7	4.29	1.45	1.33
4	B	405	GXU	C9-N5	-4.18	1.34	1.39
3	B	402	CFF	C5-C6	4.04	1.53	1.43
3	A	402	CFF	C2-N3	3.95	1.46	1.39
4	B	403	GXU	C9-N5	-3.92	1.34	1.39
4	B	405	GXU	C16-C15	3.86	1.47	1.40
4	A	403	GXU	C16-C15	3.69	1.46	1.40
3	A	402	CFF	C5-C6	3.63	1.52	1.43
4	A	403	GXU	C9-N5	-3.60	1.34	1.39
4	B	403	GXU	C16-C15	3.59	1.46	1.40
4	A	404	GXU	C16-C15	3.53	1.46	1.40
3	B	402	CFF	C2-N3	3.51	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	GXU	C9-N5	-3.47	1.35	1.39
4	B	404	GXU	C16-C15	3.40	1.46	1.40
4	B	404	GXU	C16-C14	2.96	1.53	1.48
3	B	402	CFF	C2-N1	2.91	1.44	1.39
4	B	405	GXU	C8-N4	-2.89	1.33	1.39
4	A	403	GXU	C15-C13	2.86	1.53	1.48
4	A	404	GXU	C16-C14	2.82	1.53	1.48
3	A	402	CFF	C2-N1	2.79	1.44	1.39
4	B	403	GXU	C15-C13	2.65	1.53	1.48
4	A	404	GXU	C8-N4	-2.57	1.34	1.39
4	B	405	GXU	C15-C13	2.47	1.52	1.48
4	B	405	GXU	C16-C14	2.45	1.52	1.48
4	B	403	GXU	C8-N4	-2.43	1.34	1.39
4	A	404	GXU	C17-C10	2.42	1.53	1.48
4	A	404	GXU	C9-N5	-2.41	1.36	1.39
4	B	404	GXU	C15-C13	2.39	1.52	1.48
4	B	404	GXU	C17-C10	2.36	1.53	1.48
4	B	404	GXU	C8-N4	-2.36	1.34	1.39
4	B	403	GXU	C16-C14	2.34	1.52	1.48
3	A	402	CFF	O11-C2	-2.27	1.18	1.22
4	B	403	GXU	C17-C10	2.25	1.53	1.48
4	A	403	GXU	C17-C10	2.24	1.53	1.48
4	A	403	GXU	C8-N4	-2.23	1.34	1.39
4	A	403	GXU	C16-C14	2.22	1.52	1.48
6	A	410	GOL	C3-C2	2.20	1.60	1.51
4	B	405	GXU	O2-C14	-2.18	1.18	1.23
4	B	405	GXU	O1-C13	-2.14	1.18	1.23
4	A	403	GXU	C12-C19	2.14	1.54	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	GXU	C19-C12-N5	10.31	126.66	112.37
4	A	404	GXU	C12-N5-C10	-6.27	118.91	126.18
3	A	402	CFF	C5-C6-N1	4.56	120.41	112.06
3	B	402	CFF	C5-C6-N1	4.48	120.27	112.06
3	B	402	CFF	N3-C4-N9	4.16	132.81	126.27
4	A	404	GXU	C18-C11-N4	-4.02	105.61	112.26
3	A	402	CFF	N3-C4-N9	3.97	132.51	126.27
4	B	405	GXU	C19-C12-N5	-3.94	106.91	112.37
4	A	404	GXU	C12-C19-N6	3.90	122.46	116.08
4	B	405	GXU	C18-C11-N4	-3.48	106.51	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	CFF	C6-N1-C2	-3.41	120.11	125.66
3	A	402	CFF	C6-N1-C2	-3.19	120.48	125.66
4	B	403	GXU	C19-C12-N5	-3.15	108.00	112.37
4	A	403	GXU	C12-C19-N6	3.07	121.11	116.08
3	A	402	CFF	C10-N1-C2	2.98	122.53	117.33
4	B	404	GXU	C19-C24-N7	-2.93	119.14	122.72
3	B	402	CFF	C6-C5-C4	-2.92	119.25	122.92
4	B	404	GXU	O2-C14-C9	-2.90	118.64	122.64
4	A	403	GXU	C19-C12-N5	-2.88	108.38	112.37
4	B	403	GXU	C19-C24-N7	-2.70	119.41	122.72
4	A	404	GXU	C20-C15-C16	2.69	122.28	119.26
3	B	402	CFF	C5-C4-N9	-2.66	106.83	112.10
4	A	404	GXU	O1-C13-C15	-2.64	117.35	121.57
4	A	403	GXU	C26-N6-C19	2.62	121.09	117.41
4	B	404	GXU	C15-C13-C8	2.54	120.67	115.54
4	B	403	GXU	C18-C11-N4	-2.49	108.14	112.26
3	A	402	CFF	C6-C5-C4	-2.46	119.82	122.92
3	B	402	CFF	N7-C8-N9	-2.45	109.04	113.48
4	B	405	GXU	C12-C19-N6	2.44	120.08	116.08
3	B	402	CFF	C8-N9-C4	2.36	108.63	102.98
4	A	403	GXU	C13-C8-N4	2.29	132.73	128.87
4	B	403	GXU	C12-C19-N6	2.28	119.81	116.08
4	A	404	GXU	C11-N4-C10	2.23	126.81	124.82
4	B	405	GXU	O1-C13-C8	-2.22	119.53	122.95
4	B	403	GXU	C26-N6-C19	2.21	120.51	117.41
3	A	402	CFF	C5-C4-N9	-2.17	107.79	112.10
4	B	404	GXU	C13-C8-N4	2.17	132.51	128.87
4	B	403	GXU	C27-N7-C24	2.16	120.64	116.85
4	B	404	GXU	O1-C13-C15	-2.16	118.12	121.57
4	B	404	GXU	C27-N7-C24	2.15	120.62	116.85
4	B	404	GXU	C26-N6-C19	2.13	120.40	117.41
4	A	403	GXU	C27-N7-C24	2.13	120.58	116.85
3	B	402	CFF	O13-C6-C5	-2.12	122.03	126.38
4	B	405	GXU	C15-C13-C8	2.12	119.82	115.54
4	A	404	GXU	C26-N6-C19	2.09	120.35	117.41
4	B	403	GXU	C15-C13-C8	2.08	119.73	115.54
3	B	402	CFF	N3-C2-N1	2.04	119.69	117.14
4	A	404	GXU	C15-C13-C8	2.04	119.65	115.54
4	A	403	GXU	C19-C24-N7	-2.03	120.24	122.72
3	A	402	CFF	O13-C6-C5	-2.02	122.24	126.38
4	B	404	GXU	C27-C26-N6	-2.02	119.35	122.19
4	B	405	GXU	C19-C24-N7	-2.01	120.27	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	GXU	O2-C14-C16	-2.00	118.37	121.57
4	B	403	GXU	C13-C8-N4	2.00	132.24	128.87

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	GXU	C19-C12-N5-C10
4	A	404	GXU	C19-C12-N5-C9
4	B	403	GXU	N5-C12-C19-C24
4	B	403	GXU	N5-C12-C19-N6
6	A	410	GOL	C1-C2-C3-O3
6	A	411	GOL	C1-C2-C3-O3
6	A	411	GOL	O2-C2-C3-O3
4	A	404	GXU	N4-C11-C18-O3
4	B	403	GXU	C11-C18-O3-C25
4	B	404	GXU	N4-C11-C18-O3
4	A	404	GXU	C11-C18-O3-C25
4	B	403	GXU	N4-C11-C18-O3
4	B	404	GXU	N5-C12-C19-C24
4	B	404	GXU	N5-C12-C19-N6
6	A	410	GOL	O2-C2-C3-O3
4	B	404	GXU	C11-C18-O3-C25
4	B	404	GXU	C18-C11-N4-C10
4	B	405	GXU	N5-C12-C19-C24
4	B	405	GXU	N5-C12-C19-N6

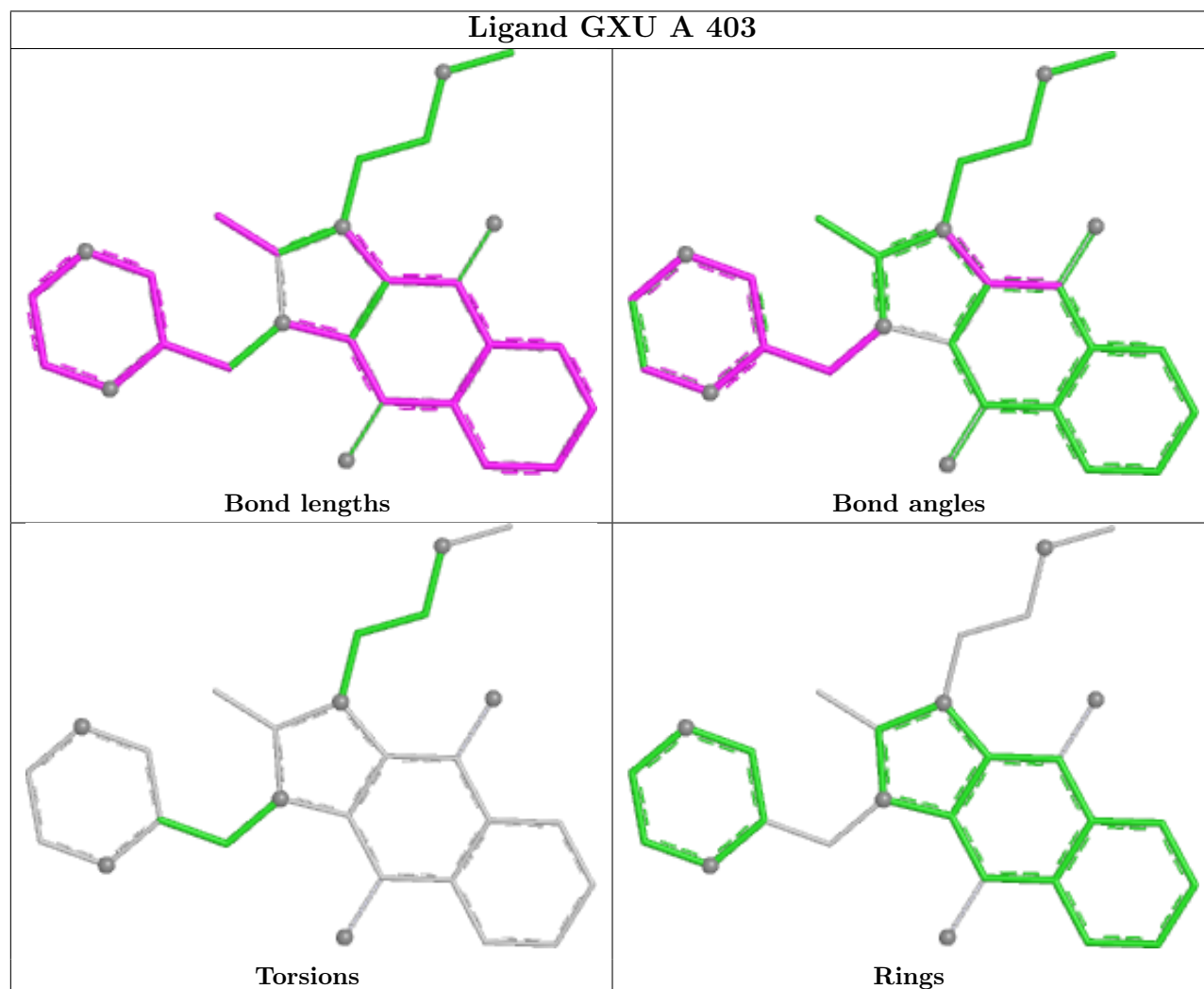
There are no ring outliers.

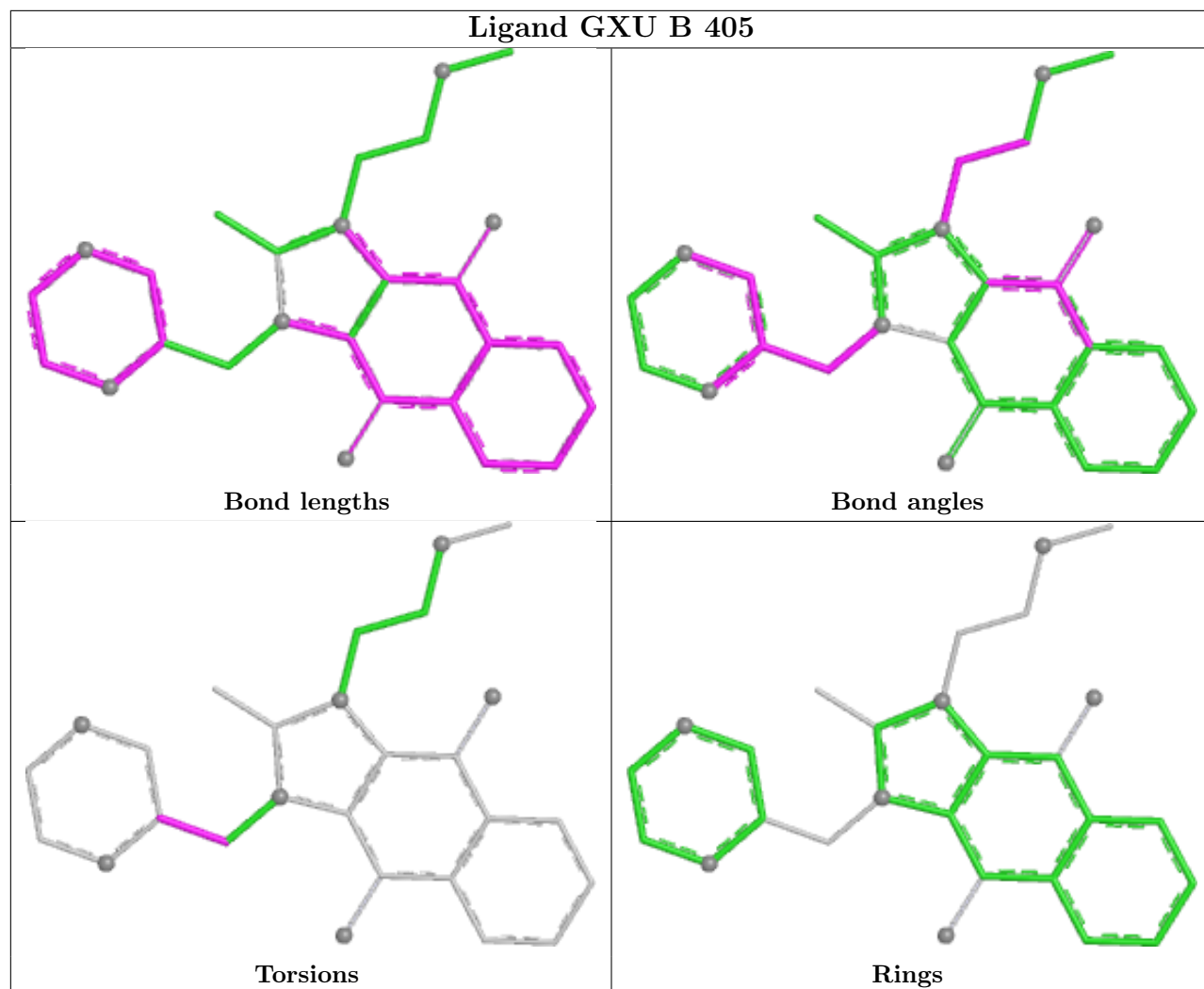
2 monomers are involved in 2 short contacts:

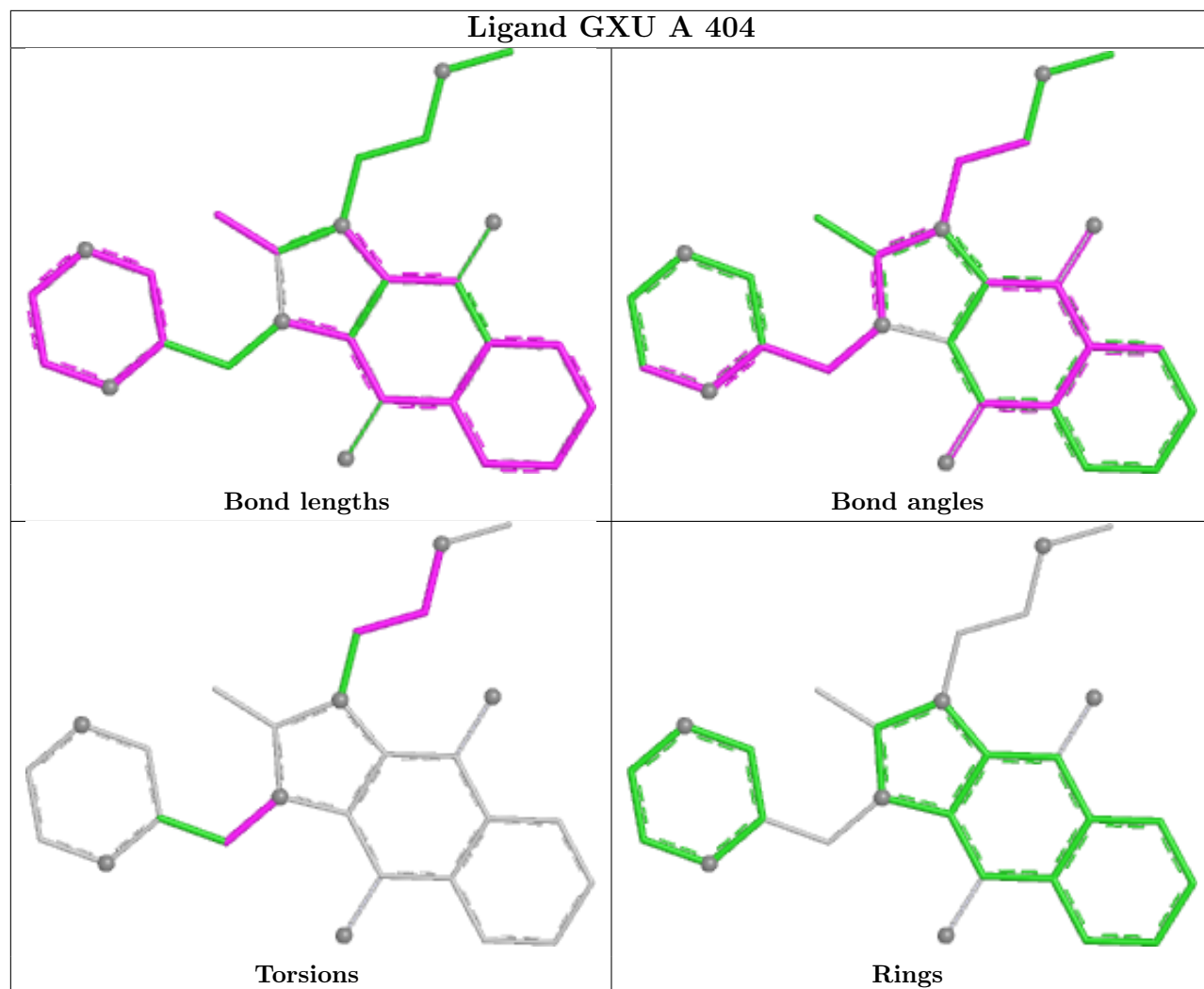
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	SO4	1	0
6	A	410	GOL	1	0

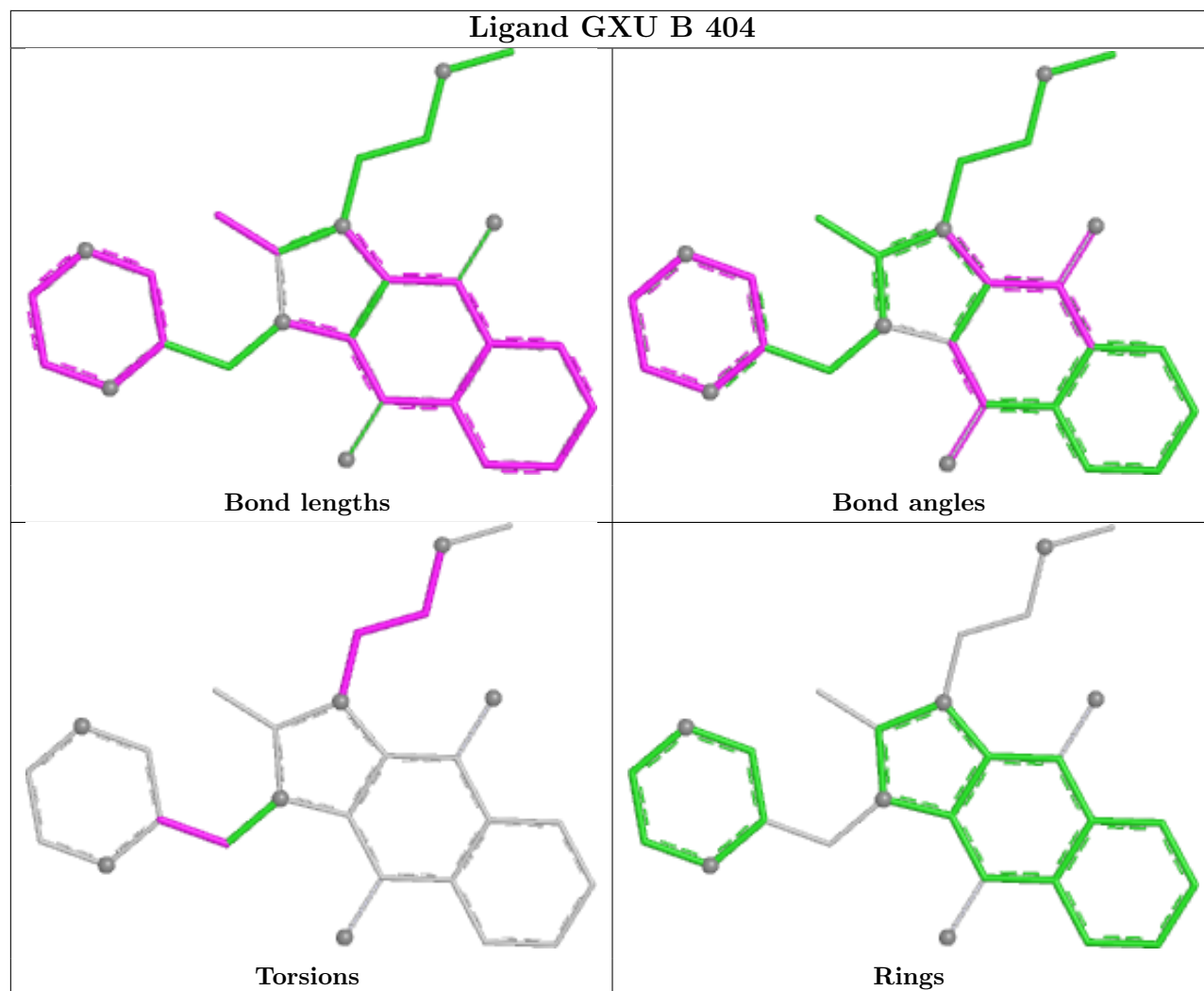
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

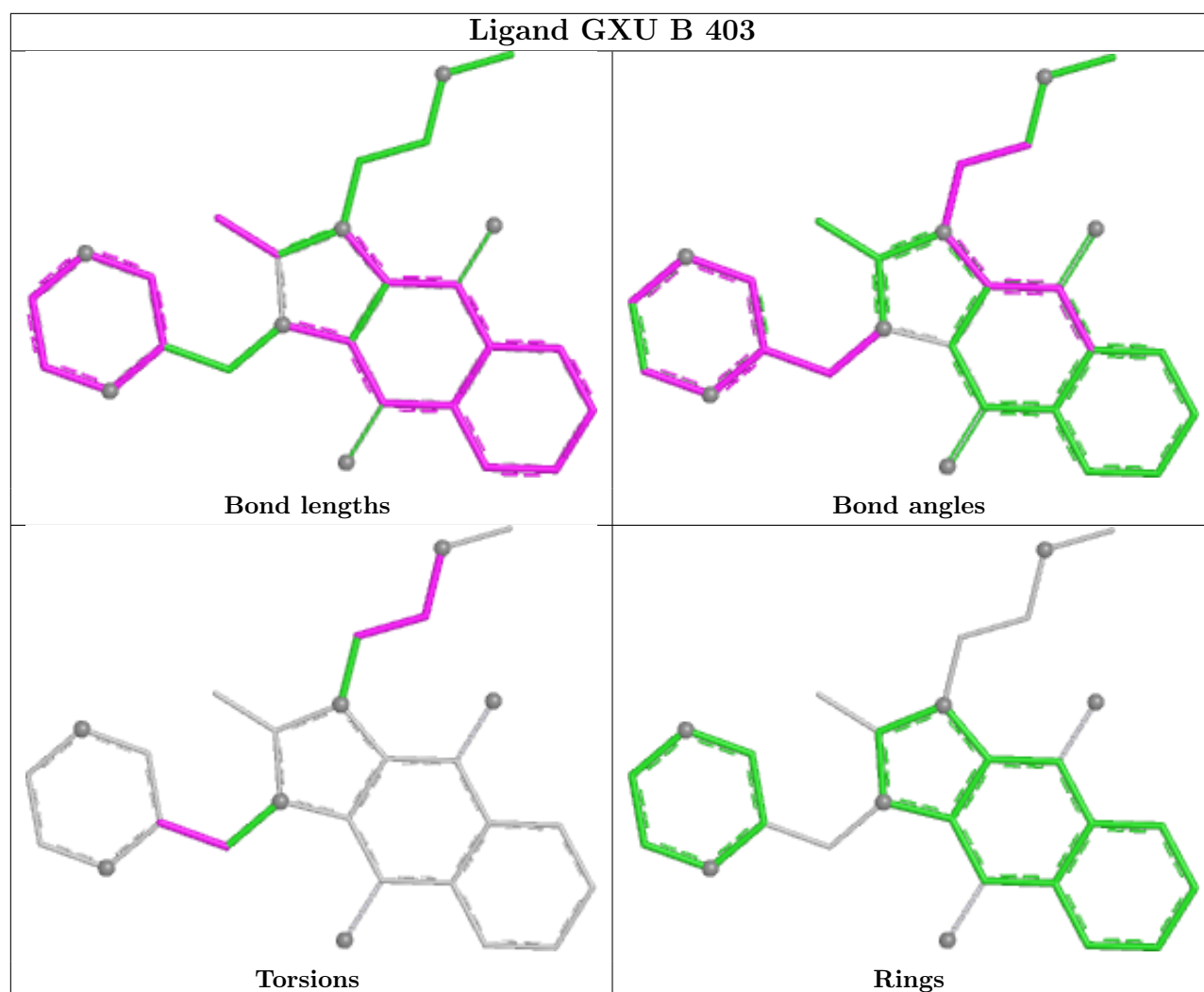
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	312/312 (100%)	0.41	4 (1%) 75 77	28, 42, 75, 91	0
1	B	312/312 (100%)	0.86	54 (17%) 4 4	31, 45, 118, 138	0
All	All	624/624 (100%)	0.63	58 (9%) 14 15	28, 44, 104, 138	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	VAL	5.9
1	B	268	TYR	5.7
1	B	21	VAL	5.6
1	B	5	ILE	4.8
1	B	22	ASP	4.7
1	B	33	PRO	4.5
1	A	268	TYR	4.2
1	B	27	TYR	3.7
1	B	8	PHE	3.6
1	B	4	THR	3.6
1	B	25	MET	3.5
1	B	9	THR	3.5
1	B	44	ILE	3.3
1	B	23	MET	3.2
1	B	55	PHE	3.2
1	B	46	PRO	3.2
1	B	42	THR	3.0
1	B	50	HIS	3.0
1	B	57	VAL	3.0
1	B	255	HIS	3.0
1	B	64	LEU	2.9
1	B	47	HIS	2.9
1	B	56	TYR	2.9
1	B	52	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	48	ASN	2.9
1	B	26	THR	2.8
1	B	191	THR	2.8
1	B	31	PHE	2.8
1	B	41	VAL	2.8
1	B	29	GLN	2.7
1	B	59	PRO	2.7
1	A	47	HIS	2.6
1	B	7	VAL	2.6
1	B	315	LYS	2.5
1	B	18	THR	2.5
1	B	36	LEU	2.5
1	B	39	ALA	2.4
1	B	6	LYS	2.4
1	B	35	TYR	2.3
1	B	11	VAL	2.3
1	B	63	THR	2.3
1	B	53	LYS	2.3
1	B	17	HIS	2.2
1	B	49	SER	2.2
1	B	14	ILE	2.2
1	B	54	THR	2.2
1	B	51	GLU	2.2
1	B	85	SER	2.2
1	B	124	GLU	2.2
1	B	294	SER	2.2
1	A	226	CYS	2.1
1	B	45	LYS	2.1
1	B	60	ASN	2.1
1	B	40	ASP	2.1
1	B	10	THR	2.1
1	B	30	GLN	2.1
1	B	179	ASP	2.0
1	A	4	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](#)

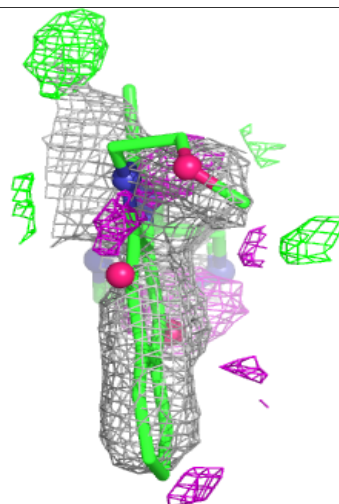
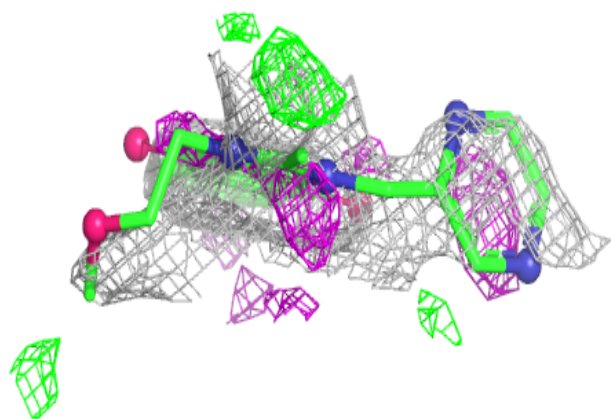
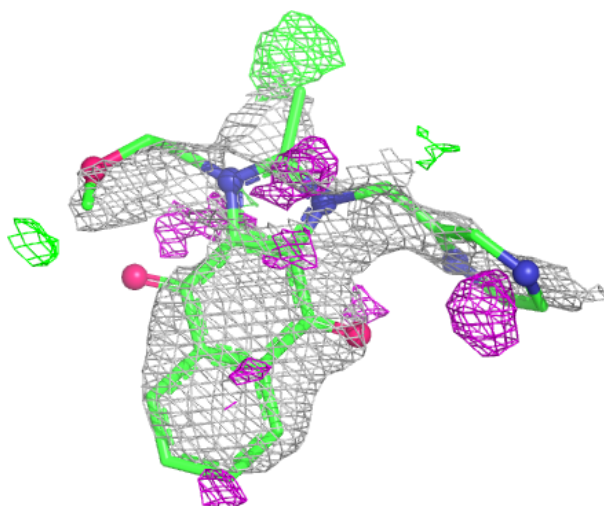
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	408	5/5	0.52	0.10	108,110,124,142	0
5	SO4	B	408	5/5	0.55	0.13	86,86,111,126	0
4	GXU	A	404	27/27	0.56	0.24	64,91,112,117	0
6	GOL	A	410	6/6	0.66	0.22	56,78,80,81	0
5	SO4	A	406	5/5	0.68	0.10	81,92,111,119	0
5	SO4	B	409	5/5	0.70	0.09	107,110,139,150	0
4	GXU	B	404	27/27	0.70	0.20	60,92,105,114	0
5	SO4	B	407	5/5	0.71	0.12	88,94,104,131	0
5	SO4	A	409	5/5	0.73	0.14	94,102,117,130	0
4	GXU	A	403	27/27	0.76	0.21	63,87,105,108	0
4	GXU	B	403	27/27	0.76	0.20	67,89,104,106	0
5	SO4	A	405	5/5	0.82	0.11	71,80,106,112	0
4	GXU	B	405	27/27	0.82	0.15	53,74,85,87	0
5	SO4	A	407	5/5	0.87	0.10	54,70,82,88	0
6	GOL	A	411	6/6	0.89	0.15	49,56,65,70	0
5	SO4	B	406	5/5	0.91	0.09	58,62,67,74	0
3	CFF	B	402	14/14	0.91	0.12	32,41,43,45	14
3	CFF	A	402	14/14	0.96	0.08	28,30,36,36	14
2	ZN	A	401	1/1	0.97	0.05	83,83,83,83	0
2	ZN	B	401	1/1	0.98	0.06	49,49,49,49	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.

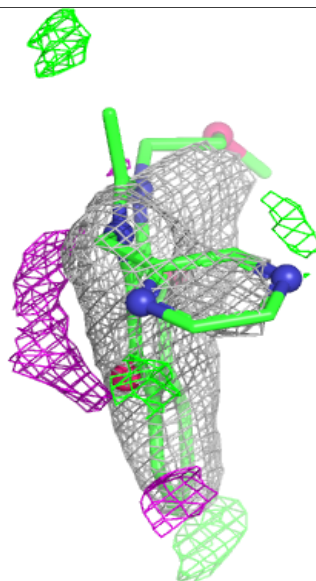
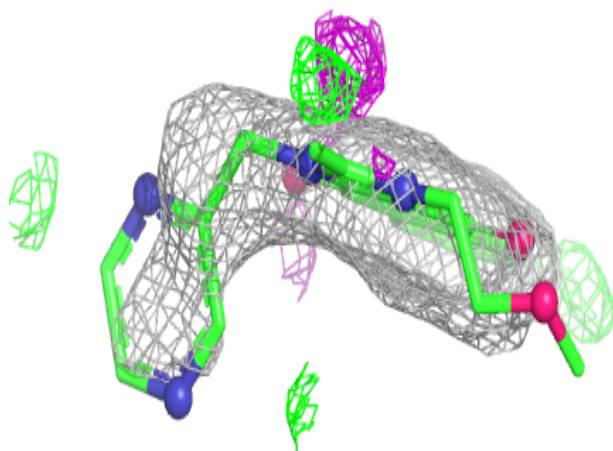
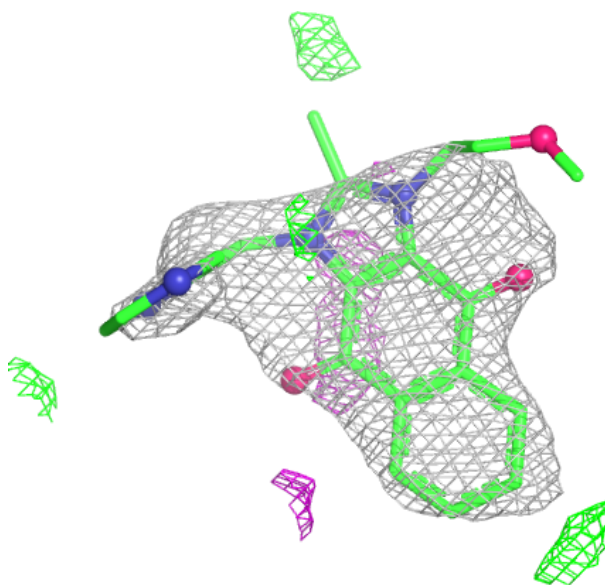
Electron density around GXU A 404:

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



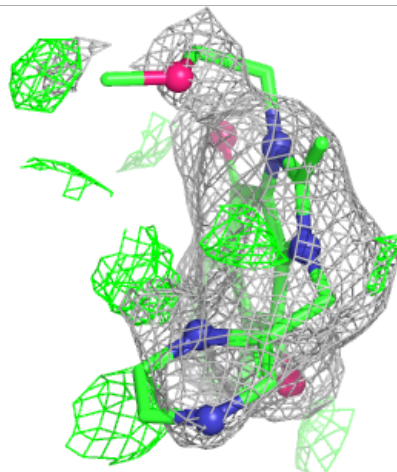
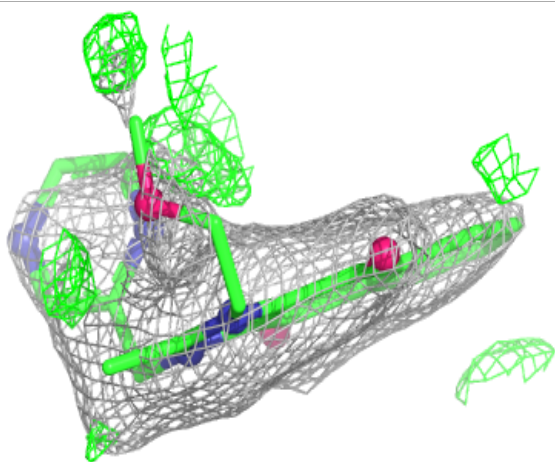
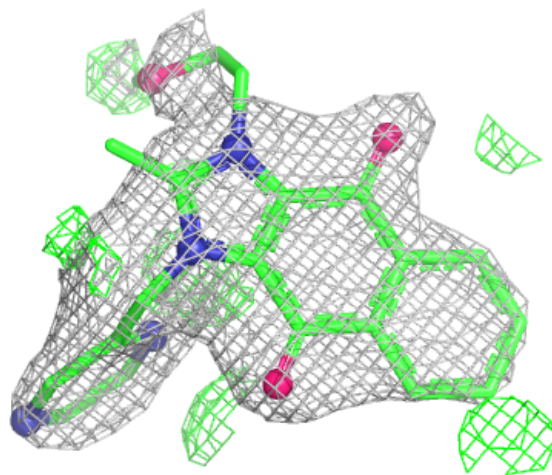
Electron density around GXU B 404:

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



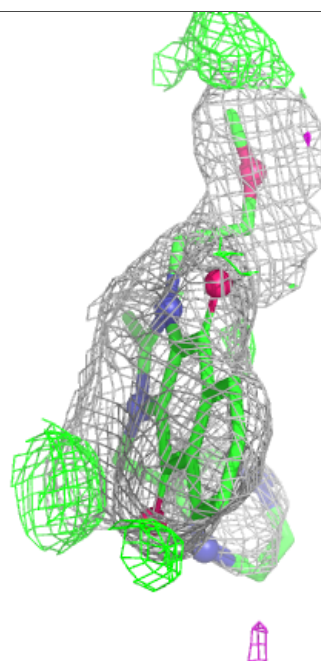
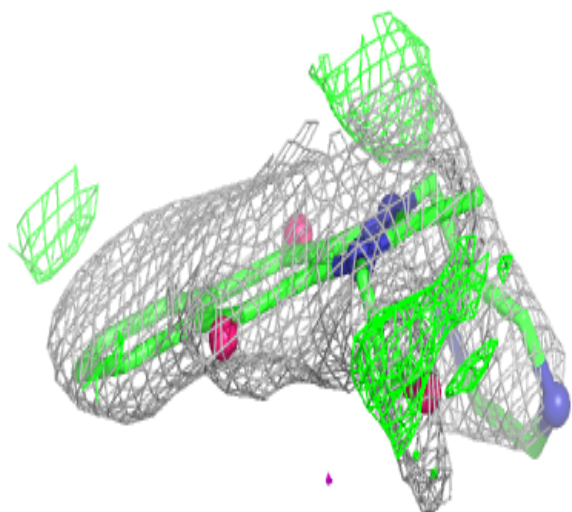
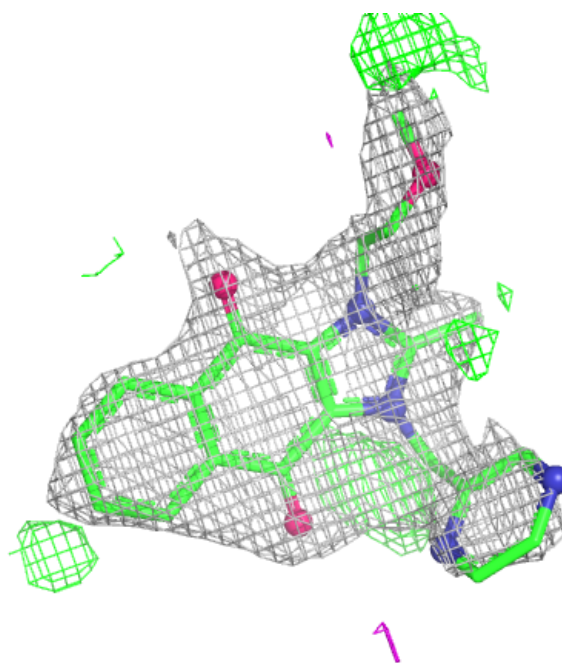
Electron density around GXU A 403:

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



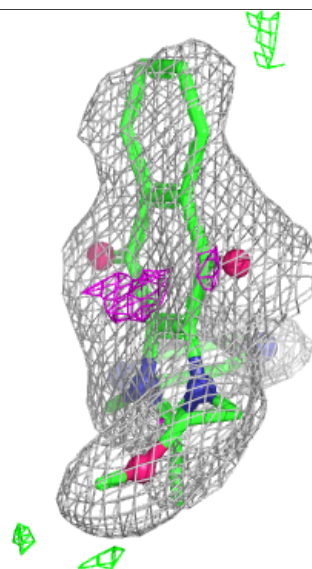
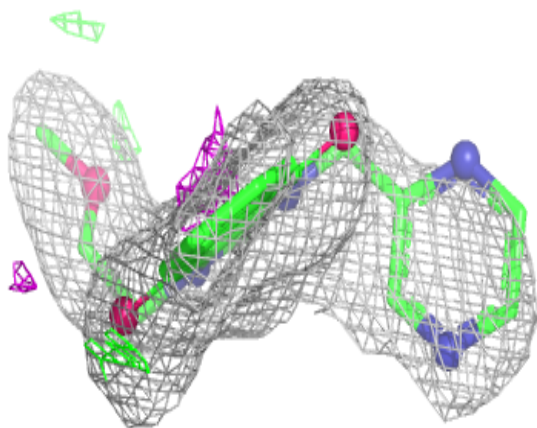
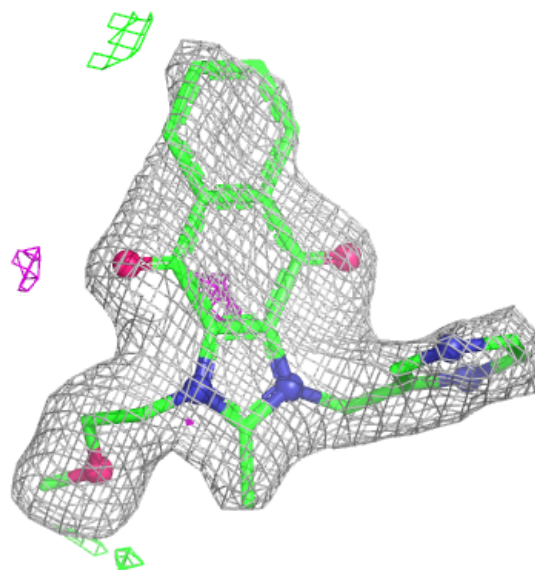
Electron density around GXU B 403:

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



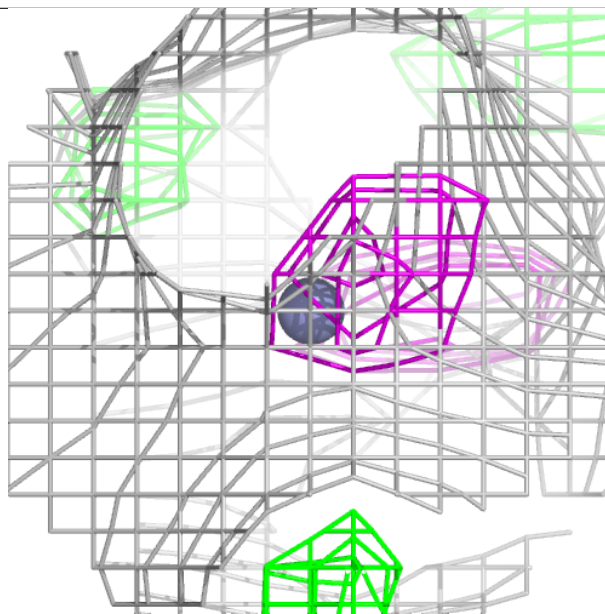
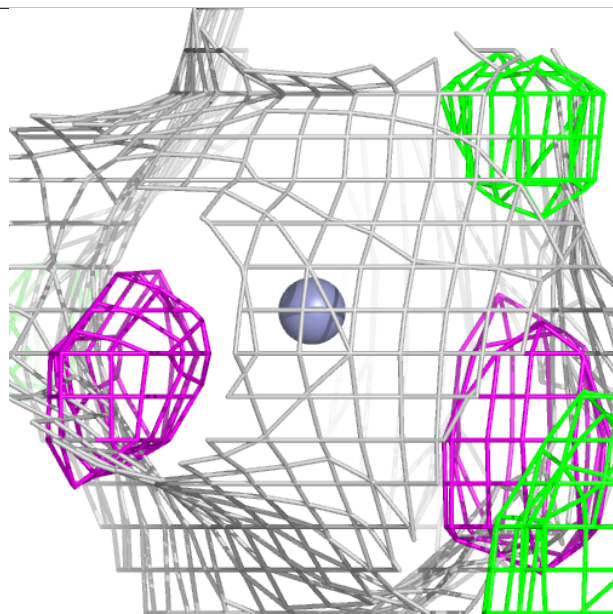
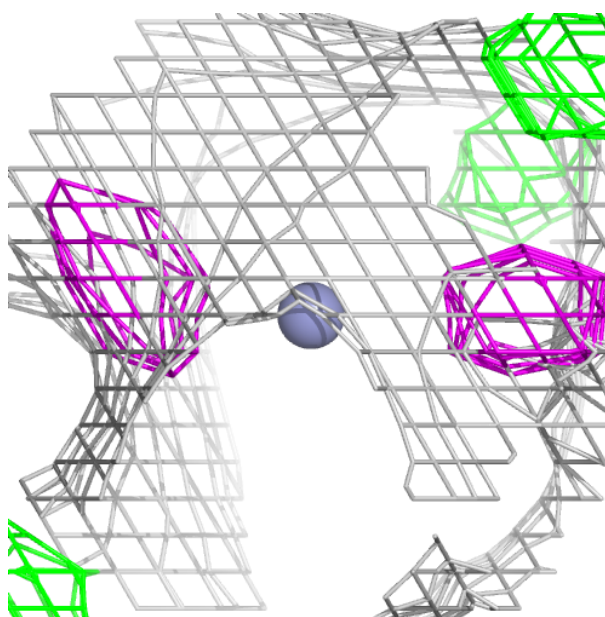
Electron density around GXU B 405:

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



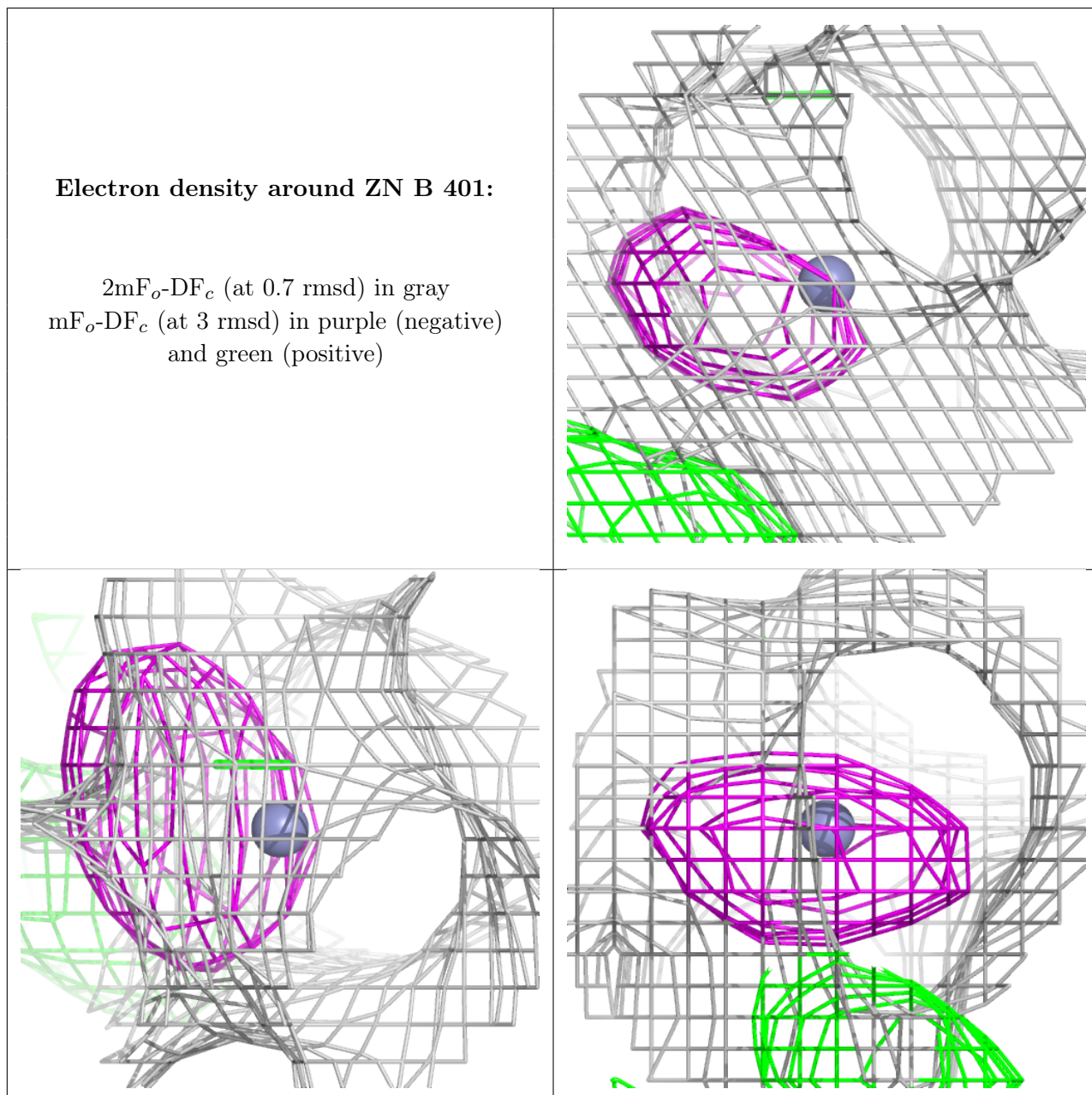
Electron density around ZN A 401:

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



Electron density around ZN B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.